On coalescence equations and related models

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1 Introduction

Coalescence is a widespread phenomenon in nature and is one of the mechanisms by which particles (clusters) grow, the underlying process being successive mergers. In particular, coalescence phenomena are met and play an important role in various fields of physics (aerosol and raindrops formation, smoke, sprays, ...), chemistry (polymer, ...), astrophysics (formation of galaxies) and biology (hematology, animal grouping, ...) and take place at different scales [33]. At the level of particles, *coalescence* (or *coagulation* or *aggregation*) refers to mechanisms by which two (mother) particles encounter and merge into a single (daughter) particle. In the simple situation where each particle is fully identified by its mass (or size) $y \in Y$ (where $Y = \mathbb{N} \setminus \{0\}$ or $Y = \mathbb{R}_+ := (0, +\infty)$) and is denoted by $\{y\}$, the coalescence mechanism can be represented in a schematic way as

$$\{y\} + \{y'\} \stackrel{a(y,y')}{\longrightarrow} \{y + y'\}\,, \tag{1}$$

where a stands for the probability (or rate) of occurrence of such an event. Let us observe right now that, during each coalescence event (1), the total mass is conserved, while the number of particles decreases and the mean size of the particles increases (from $(y + y')/2$ to $y + y'$).

From the modelling point of view, there are basically three levels of description of a system of a large number of particles undergoing coalescence events.

- The microscopic level: we consider a system of N particles, $N \gg 1$, which evolves according to the coalescence mechanism (1), the coagulation events occurring in a random way. Such a description is mainly stochastic as was originally proposed by Smoluchowski [97, 98]. Among the stochastic models of coalescence, we mention the Markus-Lushnikov process [77, 82] which has been extensively studied recently [2, 55, 89]. Stochastic models of coalescence are currently an active field of research in probability theory and we refer to the survey by Aldous [2] and to [10, 27, 36, 37, 55, 56] (and the references therein) for a more detailed account.
- The mesoscopic level: when we are not interested in the description of each identified particle in the system but rather in statistical properties of the system, a less accurate (mean-field) description is meaningful. We then introduce the statistical distribution $f(t, y) \geq 0$ of particles of mass $y \in Y$ at time $t \geq 0$ and mainly consider the time evolution of f. The most commonly used mean-field equation for f is the celebrated Smoluchowski coagulation equation on which we will focus in this survey. We will discuss at length its main properties below, as well as some related models.
- The macroscopic level: the physically observable quantities are often averages of f with respect to y and a coarser description of the system can be reduced to the evolution of these quantities. However, the derivation of macroscopic equations for coalescence mechanisms is not yet clear and requires further investigations.

Still, there are links between these different levels and, in particular, the relationship between the microscopic and the mesoscopic levels is now well understood, and convergence proofs are available as well: convergence of the Marcus-Lushnikov process to the Smoluchowski equation [55, 89], Boltzmann-Grad limit of Smoluchowski's description [60]. As for connections between the mesoscopic and the macroscopic levels, we are only aware of the recent work [39].

The aim of this survey is to present an overview of the mathematical analysis of coalescence equations and related models, and focus on the statistical description at the mesoscopic level. We point out some of the main mathematical problems and results with physical interest, as well as some mathematical tools and strategies that we think of efficiency to investigate further these models. We also provide a (non-exhaustive) list of recent contributions and stress here that we mainly consider the deterministic approach to study coalescence models.

From now on, we thus restrict ourselves to the statistical description at the mesoscopic level and first consider the case where the distribution function $f = f(t, y)$ depends only on the time and mass variables (t, y), that is, each particle is fully identified by its mass at the microscopic level. In order to understand the time evolution of f, the main issue is to figure out how exchange of mass takes place in the system. In fact, a central feature of the models considered herein is that mass "can be lost" during the time evolution. More precisely, the total mass of particles in the system $Y_1(t)$ at time t given by

$$Y_1(t) := \int_Y f(t, y)\, y\, dy$$

might not remain constant through time evolution, though mass is conserved in each coalescence event at the microscopic level. A physical explanation for this phenomenon is the occurrence of a phase transition, the loss of mass accounting for the particles being transfered to the newly created phase. From a mathematical viewpoint, the underlying mechanism is that mass escapes as $y \to +\infty$ which may be interpretated as the formation of particles with infinite mass. Since the statistical description does not take explicitly into account particles with infinite mass ($y = +\infty$), their possible appearance is represented by a loss of mass. Let us mention here that, from the modelling point of view, a statistical description of a system of particles undergoing coalescence events and including particles with infinite mass, is still lacking, besides some attempts in [41, 113]. Depending on the model, this loss of mass may occur

- either in finite time: this is the *gelation* phenomenon,
- or in the large time asymptotics : this is the *saturation* phenomenon.

Though the understanding of these two phenomena is still far from being complete, several relevant mathematical results are now available. Our aim is thus to present what can be said on these two phenomena from a mathematical point of view, along with conjectures proposed by physicists. The main question we will discuss below is then: when and how does the gelation/saturation phenomenon occur?

1.1 The Smoluchowski coagulation equation

In this subsection, we restrict ourselves to the statistical description of a system of particles, each of them being fully identified by its mass, and the evolution of the system is assumed to be governed by the sole coalescence process (1). The most widely used mean-field equation in that situation is the Smoluchowski coagulation equation which was originally derived by Smoluchowski in [97, 98] in a discrete setting ($Y = \mathbb{N}\backslash\{0\}$) and subsequently extended to the continuous case $Y = \mathbb{R}_+$ by Müller [87] (see also [33] for further information on that issue). We mainly consider the latter to simplify the presentation.

The dynamics of the density $f = f(t,y) \geq 0$ of particles with mass $y \in \mathbb{R}_+$ at time $t \geq 0$ is governed by the Smoluchowski equation

$$\partial_t f = Q_c(f) := Q_1(f) - Q_2(f)\,, \qquad (t,y) \in (0,+\infty) \times Y\,, \tag{2}$$

$$f(0) = f^{in}, \qquad y \in Y\,. \tag{3}$$

The reaction term $Q_c(f)$ describing the effect of coalescence on the evolution of f is given by

$$Q_1(f)(y) = \frac{1}{2} \int_0^y a(y', y-y')\ f(y')\ f(y-y')\ dy'\,,$$

$$Q_2(f)(y) = \int_0^\infty a(y,y')\ f(y)\ f(y')\ dy'\,,$$

for $y \in \mathbb{R}_+$. The meaning of these terms is the following: $Q_1(f)(y)$ accounts for the formation of particles $\{y\}$ by coalescence of smaller ones, i.e. by the reaction

$$\{y'\} + \{y-y'\} \ \stackrel{a(y-y',y')}{\longrightarrow}\ \{y\}\,, \qquad y' \in (0,y)\,,$$

while $Q_2(f)(y)$ describes the depletion of particles $\{y\}$ by merging with other particles, i.e. by the reaction

$$\{y\} + \{y'\} \ \stackrel{a(y,y')}{\longrightarrow}\ \{y+y'\}\,, \qquad y' \in \mathbb{R}_+\,.$$

The coalescence coefficient (kernel, rate) a depends on the precise physical mechanism by which pairs of particles do stick. It thus depends on the physical context. In his original model for colloidal particles, Smoluchowski derives the following expression for a:

$$a(y,y') = (y^\alpha + (y')^\alpha)^\beta\ (y^{-\gamma} + (y')^{-\gamma}) \tag{4}$$

with $\alpha = \gamma = 1/3$, $\beta = 1$ [97], and the more general case with $\alpha, \beta, \gamma \geq 0$ may also be considered under the restriction $\alpha\,\beta \leq 1$. Other commonly used kernels a involve products of powers such as

$$a(y,y') = y^\alpha\ (y')^\beta + (y')^\alpha\ y^\beta\,, \quad \alpha, \beta \in [0,1], \tag{5}$$

and includes Golovin's kernel $(\alpha,\beta) = (0,1)$ [48] and Stockmayer's kernel $\alpha=\beta=1$ [105]. Also of interest is the ballistic kernel

$$a(y,y') = (y^\alpha + (y')^\alpha)^\beta\, |y^\gamma - (y')^\gamma| \,, \tag{6}$$

with $\alpha,\beta,\gamma \geq 0$ and $\alpha\,\beta+\gamma \leq 1$. We refer to [33] for more information on the coagulation coefficient a.

Observe that, under the indicated restrictions on the exponents α,β,γ, all the above kernels satisfy the symmetry condition

$$0 < a(y,y') = a(y',y) \qquad \text{for a.e.} \quad y,y' \in Y \times Y\,, \tag{7}$$

the growth condition

$$a(y,y') \leq C_\delta\, y\, y' \qquad \text{for} \quad (y,y') \in (\delta,+\infty) \times (\delta,+\infty) \tag{8}$$

for every $\delta > 0$, as well as the additional structure condition

$$a(y,y') \leq a(y,y+y') + a(y',y+y') \qquad \text{for} \quad (y,y') \in Y \times Y\,. \tag{9}$$

Throughout the paper we will always assume that the coagulation coefficient a satisfies (7) and (8). At some places, we will also require in addition the structure assumption (5) or (9) to be fulfilled.

The starting point of the qualitative analysis of the Smoluchowski coagulation equation (2) is the following fundamental (and formal) identity: for any $\phi\ : Y \to \mathbb{R}$ there holds

$$\int_Y Q_c(f)\ \phi\ dy = \frac{1}{2}\int_Y \int_Y a(y,y')\ f\ f'\ \left(\phi'' - \phi - \phi'\right)\ dy'dy. \tag{10}$$

Here and below, we put $g = g(y)$, $g' = g(y')$ and $g'' = g(y+y')$ to shorten notations. This identity is obtained after a change of variables and applying (without justification) the Fubini theorem to $Q_1(f)$. Suitable choices of functions ϕ in (10) lead to several qualitative (but formal) information on the reaction term $Q_c(f)$, and on the solution f as well. We list some of them now.

- For $k \in \mathbb{R}$ and $\phi(y) = y^k$, we have sign $(\phi''-\phi-\phi') =$ sign $(k-1)$ and it readily follows from (10) that

$$t \longmapsto Y_k(t) := \int_Y y\, f(t,y)\, dy \quad \text{is} \quad \begin{cases} \text{decreasing if } k < 1\,, \\ \text{constant if } k = 1\,, \\ \text{increasing if } k > 1\,. \end{cases} \tag{11}$$

Roughly speaking, (11) reflects the fact that small particles aggregate to create larger ones while preserving the total mass. Let us stress here again that the computations leading to (11) are formal and, in particular, that the last two assertions of (11) only hold true on a finite time interval in general.

- Under the structure assumption (9), another interesting piece of information is obtained with the choice $\phi(y) = p\, f(t,y)^{p-1}$, from which one deduces that

$$t \mapsto \|f(t)\|_{L^p} \quad \text{is non-increasing for any} \quad p \geq 1\,, \tag{12}$$

together with some information on $Q_c(f)$ as well (see Lemma 3 in Section 4.1 below). A straightforward consequence of (12) is that the aggregation process takes place without concentration at a fixed mass.

Actually, both (11) and (12) express some monotonicity of the coalescence evolution (as well as irreversibility).

After this general discussion, let us come back to the question of total mass conservation which has attracted the attention of physicists in the eighties. At first, it is easily seen from (2) that Y_1 is a non-increasing function of time. Indeed, for $R > 0$, the choice $\phi(y) = \min\{y, R\}$ in (10) entails that

$$t \longmapsto \int_Y \min\{y, R\}\, f(t,y)\, dy$$

is non-increasing, and the claimed monotonicity of Y_1 then readily follows by the Fatou lemma after letting $R \to +\infty$. Next, it turns out that an elementary but fundamental argument shows that the conservation of mass

$$Y_1(t) = Y_1(0)\,, \qquad t \geq 0\,, \tag{13}$$

cannot be true for the multiplicative coalescence kernel $a(y,y') = y\,y'$ [73]. Indeed, taking $\phi(y) = 1$ in (10) implies that a solution to (2) satisfies

$$Y_0(T) + \frac{1}{2}\int_0^T Y_1^2(s)\, ds = Y_0(0) \qquad \text{for every} \quad T > 0\,.$$

In particular, since $Y_0 \geq 0$, we realize that $Y_1 \in L^2(\mathbb{R}_+)$, which contradicts (13). Consequently, the total mass conservation breaks down in finite time, a phenomenon known as the *occurrence of gelation*: more precisely, there exists a time $T_g \geq 0$ such that $Y_1(t) = Y_1(0)$ for each $t \in [0, T_g)$ and $Y_1(t) < Y_1(0)$ for each $t > T_g$. The gelation time T_g is then defined by

$$T_g := \inf\{t \geq 0\,,\ Y_1(t) < Y_1(0)\}\,. \tag{14}$$

More generally, for the coalescence coefficient (5) with $\lambda := \alpha + \beta \in (1,2]$, it is shown in [42] that

$$Y_k \in L^2(\mathbb{R}_+) \quad \text{if} \quad k \in (\lambda/2, (1+\lambda)/2). \tag{15}$$

In particular, $Y_1 \in L^2(\mathbb{R}_+)$ since $\lambda > 1$, which implies that gelation occurs in that case. We will sketch the proof of (15) in Section 3. The occurrence of gelation for the coefficient (5) with $\lambda \in (1,2)$ had been previously proved by Jeon

[55] with probabilistic arguments, and (15) actually provides an alternative and simpler proof (as well as a more accurate statement).

On the other hand, it was proved by White [108] and Ball & Carr [6] that the conservation of mass (13) holds true under the condition $a(y,y') \leq A\,(1+y+y')$ (for the coalescence coefficient (5), this case corresponds to the range of parameters (α,β) for which $\lambda = \alpha+\beta \leq 1$).

In addition, the total number of particles Y_0 decays to zero as time goes to infinity:

$$Y_0(t) \;\to\; 0 \quad \text{when} \quad t \to +\infty\,. \tag{16}$$

Such a property is heuristically clear as a consequence of the coalescence mechanism (1) and can be rigorously proved in several situations. For instance, the convergence (16) holds true when $a > 0$ on the set $\{(y,y') \in Y^2,\; y \neq y'\}$ (further additional assumptions have to be made in the discrete case $Y = \mathbb{N}^*$), see [68], and when $a > 0$ a.e. on Y^2 and a satisfies (9), see [85]. The assertion (16) actually means that all the particles with a given and finite mass $y > 0$ have merged in the large time limit. Therefore, when the conservation of mass (13) holds true, the loss of mass does not take place in finite time but in infinite time. We then put

$$T_* = \begin{cases} +\infty & \text{if (13) holds true}\,, \\ T_g & \text{if gelation occurs}\,. \end{cases} \tag{17}$$

The next step is to understand when and how the loss of mass occurs. The answer to the first question being obvious in the absence of gelation since $T_* = +\infty$, we assume that we are in a situation where gelation occurs at the finite time T_g and look for information on T_g. It turns out that, for the multiplicative kernel $a = y\,y'$, the gelation time is explicitly calculable and $T_g = T_2$ where $T_2 = Y_2(0)^{-1}$ is the blow-up time of the second moment Y_2 [38, 90]. For other gelling coagulation kernels, fewer information seem to be known and only estimates of T_g from above and from below are available [38, 50]. In particular, it is not clear (though likely) whether the gelation time coincide with the blow-up time of some particular moment. Concerning the second question on the way gelation occurs, an open problem is which moments of the solution blow up at the gelation time. For instance, for the coagulation kernel (5) with $\lambda = \alpha+\beta \in (1,2]$, it is conjectured that $Y_k(t)$ blows up as $t \to T_g$ for $k > (\lambda+1)/2$ [50]. When $T_* = +\infty$, an interesting question is the speed at which the total number of particles Y_0 (or some moment Y_k, $k \in [0,1)$) decays as a function of time. Except for the constant kernel $a = 1$ (for which an exact computation gives $Y_0(t) = 1/(t+1)$) and for the additive kernel $a = y + y'$ (for which we may compute exactly $Y_0(t) = e^{-t}$) for an initial datum such that $Y_0(0) = Y_1(0) = 1$, the rate of convergence to zero is not known. Still, temporal decay estimates (which seem to be non-optimal) are available for $Y_k(t)$, $k \in (\lambda/2, \lambda)$ when $a = (y\,y')^{\lambda/2}$ [68].

A further step is to determine the"profile" of the solution at the gelation time T_g. This question has been thoroughly studied by physicists (see, e.g., [32, 38, 50, 74] and the references therein). For the coagulation kernel (5) with $\lambda = \alpha + \beta \in (1,2]$, it is conjectured that

$$f(T_g, y) \sim y^{-3/2-\lambda/2} \quad \text{when} \quad y \to +\infty \,. \tag{18}$$

A mathematical proof is still lacking, but it is shown in [42] that

$$Y_k \notin L^2(T_1, T_2) \qquad \text{for every} \;\; k > \frac{\lambda+1}{2} \quad \text{and} \quad T_1 < T_g < T_2 \,. \tag{19}$$

As a consequence of both (15) and (19), we see that the only polynomial decay at infinity compatible with these moments estimates at the gelation time is precisely the one suggested in (18), but of course this does not prove (18).

At last, one can look for a more precise description near T_*. On the grounds of physical experiments, physicists have suggested that the behaviour of any solution f to (2), (3) near the time T_* has a self-similar form. This is the so-called *dynamical scaling hypothesis* which asserts that

$$f(t, y) \sim \frac{1}{s(t)^\tau} \, \varphi\left(\frac{y}{s(t)}\right) \qquad \text{as} \quad t \to T_* \,. \tag{20}$$

The parameter τ, the mean particle mass $s(t)$ and the profile φ are to be determined and depend on the coagulation kernel a but not on the "details" of the initial data, the mean particle mass being such that $s(t) \to +\infty$ as $t \to T_*$ [32, 74]. Several formal and computational studies have already been performed for homogeneous coagulation kernels a (see [32, 33, 44, 59, 71, 83] and the references therein), but not very much is known from the rigorous point of view. Assuming that the coagulation kernel a is homogeneous

$$a(\xi y, \xi y') = \xi^\lambda \; a(y, y') \,, \qquad (y, y', \xi) \in Y^3,$$

for some $\lambda \le 2$, it is conjectured that the self-similar profile $s(t)^{-\tau} \, \varphi\,(y/s(t))$ is actually a self-similar solution to (2). Then, for (20) to comply with the total mass conservation (13) when $T_* = +\infty$, it is clear that $\tau = 2$ in that case. When gelation occurs ($T_* = T_g < +\infty$), the determination of τ is less clear and is performed in [32] by formal arguments, the resulting value being $\tau = (\lambda+3)/2$. Once τ is known, inserting the ansatz $s(t)^{-\tau} \, \varphi\,(y/s(t))$ in (2) yields an explicitly solvable ordinary differential equation for $s(t)$ and a nonlinear integro-differential equation for φ. Unfortunately, owing to the nonlinear and nonlocal character of the equation satisfied by φ, the existence of the profile φ is still an open problem, except for the constant kernel $a = 1$, the additive kernel $a = y + y'$ and the multiplicative kernel $a = y\,y'$, for which explicit formulae are available. Nevertheless, in spite of the lack of existence results for φ, several information have been obtained by formal arguments on the behaviour of φ for $x \sim 0$ or $x \sim +\infty$, and we refer to [32] for a detailed discussion. In the few cases where self-similar solutions are known to exist, the next question is whether (20) is valid or not. When $a = 1$, an affirmative answer has first been given by Kreer & Penrose for initial data f^{in} decaying exponentially at infinity [58] and extended to general initial data in [2, 28, 68]. When $a = y + y'$ and $a = y\,y'$, the validity of (20) is considered in [10, 28]. We shall return to a more precise description of the dynamical scaling hypothesis in Section 4.3 below.

1.2 Other models

In many cases, coalescence is not the only mechanism governing the dynamics of the system of particles and other effects should be taken into account. These mechanisms may act directly on the size (and on the growth!) of particles (that is fragmentation, condensation, evaporation) or they may act on other variables such as the position $x \in \Omega \subset \mathbb{R}^3$, the velocity $v \in \mathbb{R}^3$ or/and the charge $q \in \mathbb{R}$ of particles when particles are not solely identified by their size (that is diffusion, transport (inner or exterior), friction, ...). We list below additional mechanisms encountered in the literature.

1. Linear fragmentation. Fragmentation is the mechanism by which a single particle splits into two or several smaller pieces. In particular, binary spontaneous (or linear) fragmentation corresponds to the reaction

$$\{y\} \overset{b(y-y',y')}{\longrightarrow} \{y'\} + \{y-y'\}\,, \qquad y' \in (0,y) \tag{21}$$

at the microscopic level [33]. Multiple spontaneous fragmentation and collisional breakage can be considered as well, see, e.g., [78] for the former and [70, 109] for the latter. For a precise modeling of that mechanism, see equation (23) below.

2. Condensation-Evaporation. Another natural growth mechanism is the growth of particles by exchange of matter with the surrounding medium (condensation/evaporation): for instance, liquid droplets in its gaseous phase, such as raindrops. The distribution of particles is still given by the density $f = f(t,y)$ which satisfies the mass transport equation

$$\partial_t f + \partial_y (E\, f) = 0, \tag{22}$$

where $E = E(u,y)$ is the rate of clusters growth and depends on the size y and the density u of the medium. Condensation (transfer of matter from the medium towards the clusters) occurs when $E > 0$, while evaporation (transfer of matter from the clusters to the medium) takes place when $E < 0$. A particular case is the Lifshitz-Slyozov-Wagner (LSW) equation which describes the Ostwald ripening [75, 107]. The growth rate E is then $E = k(y)\,u - q(y)$ and one has to supplement (22) with the time evolution of u which is given by one of the following two equations:

$$u(t) + \int_0^\infty y\, f(t,y)\, dy = \rho \qquad \text{or} \qquad u(t) = \frac{\int_0^\infty q(y)\ f(t,y)\ dy}{\int_0^\infty k(y)\ f(t,y)\ dy}\,.$$

The LSW equation is in fact connected with coagulation-fragmentation equations [91, 92, 96].

3. Diffusion. Consider now particles which, at a microsopic level, move with respect to space in a domain $\Omega \subset \mathbb{R}^3$. Assuming that the motion of a particle of mass y obeys a Brownian motion (with a mass-dependent diffusion constant $d(y) > 0$), a diffusion $-d(y)\, \Delta_x f$ appears at the mesoscopic level, and the density $f = f(t,x,y)$ now depends on time $t \geq 0$, position $x \in \Omega$ and $y \in Y$.

4. Transport. Assuming next that particles are transported along a velocity field $v \in \mathbb{R}^3$, a transport term $v \cdot \nabla_x f$ is to be added at the mesoscopic level. Here, either $v = v(t,x,y)$ is a given velocity drift or v is the inner velocity of the particle. In the latter case, particles are identified by the mass-momentum pair (m,p), the velocity being given by $v = p/m$, and the distribution function $f = f(t,x,m,p)$ depends on time $t \geq 0$, position $x \in \Omega$, mass $m \in Y$ and momentum $p \in \mathbb{R}^3$.

5. Kinetic coalescence. In the situation described in the previous point, observe that, at a microscopic level, the coalescence between two particles with respective mass-momentum $\{m,p\}$ and $\{m',p'\}$ results in a particle of mass-momentum $\{m'',p''\}$ with $m'' = m + m'$ and $p'' = p + p'$. Such a mechanism can be seen as a multi-dimensional extension of the coalescence mechanism (1). Corresponding mesoscopic models have been recently investigated from a modeling and a mathematical point of view [8, 11, 40, 93, 106].

6. Friction. When liquid or solid particles are transported by a gaseous phase, the velocity of particles has the tendency to get closer to that of the gas because of friction. This phenomenon is taken into account by a friction term $\mathrm{div}_v(F\, f)$, with $F = F_0\,(v-u)$ and $u \in \mathbb{R}^3$. We refer to [52] for a mathematical analysis of such a model when $u = u(t,x)$ is a given vector field and to [54] for more complicated nonlinear friction mechanisms.

7. Maximal admissible mass. In some situations such as in liquid-liquid dispersions in a vessel with rotating impellers, it is experimentally observed that droplets beyond some mass y_0 cannot persist for any time. A model accounting for this phenomenon has been recently developed in [43]. Roughly speaking, the coalescence of two droplets $\{y\}$ and $\{y'\}$ with $y < y_0$, $y' < y_0$ and $y + y' > y_0$ is possible but the resulting droplet is instantaneously broken into smaller pieces with admissible masses below y_0.

A detailed description of the above mechanisms is out of the scope of this survey and we thus focus here on the situation where only the (binary) fragmentation mechanism comes into play and competes with the coalescence mechanism. Some results on the models where spatial diffusion is taken into account will also be discussed in the sequel.

Let us first observe that, at the microscopic level, fragmentation also conserves the total mass but acts in a reverse way on the distribution of particles.

At the mesoscopic level, the coagulation-fragmentation (CF) equation reads

$$\partial_t f = Q(f) = Q_c(f) - Q_f(f)\,, \qquad (t,y) \in (0,+\infty) \times Y\,, \tag{23}$$

where the coagulation term $Q_c(f)$ is still given by (2) and the fragmentation term $Q_f(f) := Q_3(f) + Q_4(f)$ by

$$\begin{aligned} Q_3(f)(y) &:= -\frac{1}{2} \int_0^y b(y', y-y')\ dy'\ f(y)\,, \\ Q_4(f)(y) &:= \int_0^\infty b(y,y')\ f(y+y')\ dy'\,. \end{aligned}$$

In the discrete setting ($Y = \mathbb{N} \setminus \{0\}$), the discrete version of (23) reads

$$\frac{df_i}{dt} = Q_i(f)\,, \qquad (t,i) \in (0,+\infty) \times \mathbb{N} \setminus \{0\}\,, \tag{24}$$

where $f = (f_i)_{i \geq 1}$,

$$Q_i(f) = \frac{1}{2} \sum_{j=1}^{i-1} (a_{j,i-j}\ f_j\ f_{i-j} - b_{j,i-j}\ f_i) - \sum_{j=1}^{\infty} (a_{i,j}\ f_i\ f_j - b_{i,j}\ f_{i+j})\ ,$$

and $(a_{i,j})$ and $(b_{i,j})$ denote the coagulation and fragmentation coefficients, respectively. A particular case of the discrete coagulation-fragmentation equation is the Becker-Döring (BD) equation which is obtained from (24) with the choice $a_{i,j} = b_{i,j} = 0$ if $\max\{i,j\} \geq 2$ (see [7, 96] and the references therein, and Sections 5.3 and 5.4 as well). From a physical point of view, it means that all coagulation and fragmentation events involve a cluster of size 1. Introducing $a_i = a_{i,1}$, $b_{i+1} = b_{i,1}$ for $i \geq 2$, and $a_1 = a_{1,1}/2$, $b_2 = b_{1,1}/2$, the BD equation then reads

$$\frac{df_1}{dt} = -W_1(f) - \sum_{i=1}^{\infty} W_i(f)\,, \tag{25}$$

$$\frac{df_i}{dt} = W_{i-1}(f) - W_i(f)\,, \qquad i \geq 2\,, \tag{26}$$

where $f = (f_i)_{i \geq 1}$ and $W_i(f) = a_i\, f_1\, f_i - b_{i+1}\, f_{i+1}$ for $i \geq 1$.

Besides existence and uniqueness results, nothing much is known on the qualitative behaviour of solutions to the coagulation-fragmentation equation (23), except when the coagulation and fragmentation coefficients are linked by the so-called *detailed balance condition*: there exists a nonnegative function $M \in L^1_1(Y) := L^1(Y, (1+y)\ dy)$, $M \not\equiv 0$, such that

$$a(y,y')\, M(y)\, M(y') = b(y,y')\, M(y+y')\,, \quad (y,y') \in Y \times Y\,. \tag{27}$$

Let us first point out that this condition is not fulfilled for arbitrary pair of coefficients a and b. Observe next that (27) implies that M is a stationary solution to (23), usually refered to as an *equilibrium*. It is then straightforward to check that, for $z \geq 0$, M_z defined by

$$M_z(y) := M(y)\, z^y\,, \quad y \in Y\,, \tag{28}$$

also satisfies (27) but does not necessarily belong to $L^1_1(Y)$. We therefore introduce

$$\begin{aligned} z_s &:= \sup\left\{z \geq 0,\ M_z \in L^1_1(Y)\right\} \in [1,+\infty]\,, \\ \varrho_s &:= Y_1(M_{z_s}) \in [0,+\infty]\,. \end{aligned} \tag{29}$$

Since no equilibrium with a total mass above ϱ_s can exist, ϱ_s is usually refered to as the *saturation mass*. An additional and interesting feature of the detailed balance condition (27) is the existence of a Liapunov functional H given by

$$H(f) := \int_Y f\, \left\{\ln \frac{f}{M} - 1\right\}\, dy\,. \tag{30}$$

With this definition of the entropy (or free energy), a solution f to the CF equation (23) satisfies (at least formally) the following *H-Theorem*

$$\frac{d}{dt} H(f) = -\frac{1}{2} D(f)\,, \tag{31}$$

where the so-called entropy dissipation term $D(f)$ is given by

$$D(f) := \int_Y \int_Y (a\, f\, f' - b\, f'')\, \left(\ln(a\, f\, f') - \ln(b\, f'')\right)\, dy dy' \geq 0\,. \tag{32}$$

Since $D(f)$ only vanishes when f is an equilibrium, we are naturally led to the following conjecture:

$$f(t,y) \to M_z(y) \quad \text{when} \quad t \to +\infty\,,$$

the parameter z being uniquely determined by the condition $Y_1(M_z) = Y_1(f^{in})$ if $Y_1(f^{in}) \leq \varrho_s$ and $z = z_s$ if $Y_1(f^{in}) > \varrho_s$. The interesting feature here is that, when $\varrho_s < +\infty$, there is a saturation phenomenon: mass is lost in infinite time. However, a mathematical proof of this conjecture is far from being complete and the only cases where complete proofs are available are the Becker-Döring equations [5, 7, 94] and their generalisations [13, 16, 22], or the strong fragmentation case [14, 67]. We will return more precisely to that point later on, in Section 5.

To go further, one may wonder how the saturation phenomena takes place. An answer to this question has been supplied in [91, 92, 88] for the Becker-Döring equations (25), (26) (see also the survey paper [96]). More precisely, assume that $\varrho_s = Y_1(M_{z_s}) < +\infty$ and that $\varrho := Y_1(f^{in}) > \varrho_s$. As already mentioned, it is expected that $f_i(t) \to M_i\, z_s^i$ as $t \to +\infty$ for $i \geq 1$, while the remaining fraction of mass $\varrho - \varrho_s$ accumulates on larger and larger clusters.

To obtain quantitative information on the latter process (saturation), Penrose introduces in [91] a new time variable $\tau = \varepsilon^{1-\alpha+\gamma}\, t$ and a cut i_ε between small and large masses, and studies the limiting behaviour as $\varepsilon \to 0$, $i_\varepsilon \to +\infty$ and $\varepsilon\ i_\varepsilon \to 0$ for the coefficients

$$a_i = a_1\ i^\alpha\,, \qquad b_i = a_i\ \left(z_s + q\ i^{-\gamma}\right)\,, \qquad i \ge 2\,,$$

with $\alpha \in (0,1]$, $\gamma \in [0,1)$, $a_1 > 0$, $z_s > 0$ and $q > 0$ (in [91], Penrose actually considers only the case $\alpha = \gamma = 1/3$. The extension presented here is performed by Niethammer in [88]). Recalling that solutions to the Becker-Döring equations (25), (26) satisfy $Y_1(f(t)) = Y_1(f^{in})$ for all $t \ge 0$ [7], an alternative formulation of the Becker-Döring equations (25), (26) reads

$$\sum_{i=1}^\infty i\ f_i(\tau) = \varrho \quad \text{and} \quad \frac{df_i}{dt} = \frac{1}{\varepsilon}\ \left(W_{i-1}(f) - W_i(f)\right)\,, \quad i \ge 2\,, \tag{33}$$

where

$$\begin{aligned} W_i(f) &= a_i\ \left(f_1 - \frac{b_i}{a_i}\right)\ f_i - \left(b_{i+1}\ f_{i+1} - b_i\ f_i\right) \\ &= a_1\ i^\alpha\ \left(f_1 - z_s - q\ i^{-\gamma}\right) - \left(b_{i+1}\ f_{i+1} - b_i\ f_i\right) \end{aligned} \tag{34}$$

Introducing

$$f(\tau,x) = \frac{1}{\varepsilon^2}\ c_i(\tau) \quad \text{and} \quad W(\tau,x) = \frac{1}{\varepsilon^{2+\alpha-\gamma}}\ W_i(f(\tau))$$

for $(\tau,x) \in (0,+\infty) \times ((i-1/2)\varepsilon,(i+1/2)\varepsilon))$, we may approximate the differences in (33) and (34) by derivatives for $i \ge i_\varepsilon$ and obtain, since $x \sim i\ \varepsilon$,

$$\partial_\tau f \sim -\partial_x W(f) \quad \text{and} \quad W(f)(\tau,x) \sim a_1\ \left(x^\alpha\ u(\tau) - q\ x^{\alpha-\gamma}\right)\,, \tag{35}$$

to first order in ε, where $u(\tau) := \varepsilon^{-\gamma}\ (f_1(\tau) - z_s)$. Also, for a suitable choice of i_ε (for instance, $i_\varepsilon = -\ln\varepsilon$),

$$\sum_{i=1}^{i_\varepsilon} i\ f_i(\tau) \sim \varrho_s$$

and the first equality in (33) becomes

$$\int_0^\infty x\ f(\tau,x)\ dx = \varrho - \varrho_s\,. \tag{36}$$

The system (35), (36) is the Lifschitz-Slyozov-Wagner (LSW) equation [75, 107] and a rigorous proof of the above formal arguments has been recently provided in [88]. We also refer to [17, 66] for connections between the Becker-Döring equations and the LSW equation in a similar spirit.

2 Existence and uniqueness

Since the pioneering works of Melzak [84] and McLeod [79, 80, 81], many works have investigated the existence of solutions to the coagulation-fragmentation equation (23) for initial data f^{in} satisfying at least

$$f^{in} \in L^1_1(Y) = L^1(Y,(1+y)dy) \quad \text{is nonnegative a.e. in } Y. \tag{37}$$

Basically, two different functional approaches have been used to study the existence of solutions to (23). On the one hand, fixed point and compactness methods in the space of continuous functions satisfying (37) have been introduced in [81, 84] and further developed in [35, 47]. On the other hand, weak and strong compactness methods in $L^1(Y)$ have been introduced by Ball, Carr & Penrose [7] in the discrete setting and by Stewart [100] for (23). They were subsequently developed in [6, 99] for (24) and in [41, 42, 61, 65] for (23). It turns out that the latter approach has proved to be more efficient and we briefly outline the strategy below. It relies on a Stability Principle which is the following: let (f_n) be a sequence of solutions to (23) (or to suitable approximations of (23)). If

$$(f_n) \ \text{ and } \ Q_i(f_n) \ \text{ belong to a weakly compact subset of } \ L^1_{\text{loc}}((0,T)\times Y)$$

for $i \in \{1,\dots,4\}$ and

$$t \longmapsto \int_Y f_n(t,y)\,\phi(y)\,dy \ \text{ belong to a strongly compact subset of } \ L^1(0,T)$$

for any $\phi \in \mathcal{C}_c(Y)$, there are a subsequence of (f_n) (not relabeled) and a function f such that $f_n \rightharpoonup f$ and $Q(f_n) \rightharpoonup Q(f)$ in $L^1_{\text{loc}}((0,T)\times Y)$. Thus f is a solution to the coagulation-fragmentation equation (23). Let us recall here that, by a solution to (23), we mean the following:

Definition 1. *Let f^{in} be such that (37) is satisfied. A (weak) solution to (23) with initial datum f^{in} is a nonnegative function $f \in L^\infty(0,T;L^1_1(Y))$ such that $Q_i(f) \in L^1((0,T)\times(0,R))$ for every $T>0$, $R>0$ and $i\in\{1,\dots,4\}$ which satisfies $Y_1(t) \le Y_1(0)$ for $t \ge 0$ and*

$$\int_0^\infty \int_Y f\,\partial_t\psi\,dydt + \int_Y f^{in}\,\psi(0,.)\,dy + \int_0^\infty \int_Y Q(f)\,\psi\,dydt = 0$$

for each $\psi \in \mathcal{C}_0^\infty([0,+\infty)\times Y)$.

In order to be able to apply the above mentioned stability principle, we basically need two estimates which we discuss now. Note that, in general, the only piece of information readily available is a uniform bound on $Y_1(f_n)$.

A. On the one hand, we need a control on the behaviour of $f_n(t,y)$ for small or large values of y to be able to pass to the limit in the integral terms $Q_i(f_n)$, $i \in \{1,\dots,4\}$.

1. If
$$\sup_{y\in(0,R)} \frac{a(y,y')}{y'}, \sup_{y\in(0,R)} \frac{b(y,y')}{y'} \to 0 \qquad \text{as } y' \to +\infty\,,$$
for $R > 0$, the bound on $Y_1(f_n)$ is sufficient [65, 73, 99, 100]. It also works in a spatially inhomogeneous setting for the diffusive coagulation-fragmentation equation [3, 9, 18, 26, 49, 63, 64, 85, 110]. Otherwise, a control of a moment of order larger than one is needed. Fortunately, such a control is available in several situations:
2. product kernel (5) [42, 61, 65]. In that case, the estimate is also useful in a spatially inhomogeneous setting for the diffusive coagulation-fragmentation equation [64];
3. weak coagulation $a \le A\,(1+y+y')$ [6, 41, 65];
4. strong fragmentation, that is, $a(y,y') \le A\ \left(y^\alpha\,(y')^\beta + (y')^\alpha\,y^\beta\right)$ with $0 \le \alpha \le \beta \le 1$ and $b(y,y') \ge B\,(1+y+y')^\gamma$ with $\gamma > \alpha+\beta-2$ [20, 41].
5. The coagulation coefficient a may also have a singularity for $y=0$ as the coagulation kernel (4) when $\gamma > 0$. In that case, a control on the behaviour of $f_n(t,y)$ for small values of y is needed, such as a moment of negative order [40, 85, 89].

B. On the other hand, we need to prevent concentration, that is the formation of Dirac masses. In other words, a uniform integrability estimate on f and $Q(f)$ is needed (except for the discrete coagulation-fragmentation equation (24)).
1. For the continuous coagulation-fragmentation equation (23), such an estimate can be obtained under mild growth conditions on a and b [41, 61, 65, 100];
2. In the spatially inhomogeneous setting, such a uniform integrability estimate is much harder to obtain because of the local dependence on the spatial variable x. Nevertheless, a uniform integrability estimate can be obtained in the general case for the discrete diffusive coagulation-fragmentation equation [63], see also [9, 18, 110] where L^∞-bounds are obtained under restrictive assumptions on a_{ij}, b_{ij} and d_i. For the continuous diffusive coagulation-fragmentation equation, additional structure conditions on the coagulation coefficient seem to be needed to obtain additional bounds. Three cases have been investigated recently:
   - the case of coalescence kernels satisfying (9) coupled with a sufficiently weak fragmentation: L^p-norms are Liapunov functionals (in the absence of fragmentation) or remain bounded on finite time intervals [12, 64, 85];
   - the case where the coagulation and fragmentation coefficients fulfil the detailed balance condition (27), for which the entropy H and the entropy dissipation term D defined by (30), (32) remain bounded [64].
   - for bounded coefficients, local existence and uniqueness have been established in [3].

Let us mention that the assumption (37) on the initial data can be weaken for coagulation coefficients satisfying $a(y,y') \le \varphi(y)\,\varphi(y')$, where φ is a subadditive function (i.e., $\varphi(y+y') \le \varphi(y) + \varphi(y')$). In that case, existence of a weak solution to the coagulation equation (2) is shown for any initial data f^{in} such that $f^{in}(y)\,\min(1+y,\varphi(y)) \in L^1(Y)$, see [85, 89]. We also point out that there are coefficients a and b (such as $a_{i,j} = i^\alpha + j^\alpha$, $\alpha > 1$) for which non-existence results are available [7, 15, 29].

Let us close this section with some comments about the uniqueness issue for the CF equation (23). Uniqueness results have been obtained by several authors. It turns out that they can be seen as a consequence of Theorem 1 below. Let us emphasize that a modified version of (39) used in the proof of Theorem 1 gives a strong stability result which in turn may be used to prove existence [45, 68] in a similar way as for the Boltzmann equation [86]. A strong connection between the existence and uniqueness proofs also appears in [89].

Theorem 1. *Assume that there are a subadditive function φ and nonnegative constants A, B such that*

$$\begin{aligned} &a(y,y') \le A\,\varphi(y)\,\varphi(y'),\\ &\int_0^y b(y',y-y')\,(\varphi(y') + \varphi(y-y') - \varphi(y))\,dy' \le B\,\varphi(y) \end{aligned} \tag{38}$$

for $(y,y') \in Y \times Y$. Then, there exists a unique solution to (23) in the class $\mathcal{C}([0,T], L^1_\varphi(Y)) \cap L^1(0,T; L^1_{\varphi^2}(Y))$ for each $T > 0$. Here $L^1_\psi(Y)$ denotes the space of functions g such that $g\,\psi \in L^1(Y)$.

Proof of Theorem 1. Consider two solutions f and g to (23) enjoying the properties stated in Theorem 1. We multiply the equation satisfied by $f-g$ by $\psi = \mathrm{sign}(f-g)\,\varphi$ and integrate over Y to obtain

$$\begin{aligned} &2\,\frac{d}{dt}\int_Y |f-g|\,\varphi\,dy\\ &\le \int_Y\int_Y a\ (f-g)\ (f'+g')\ (\psi'' - \psi - \psi')\ dydy'\\ &- \int_Y (f-g)(y)\ \int_0^y b(y',y-y')\ (\psi(y) - \psi(y') - \psi(y-y'))\ dy'\ dy \end{aligned}$$

On the one hand, the subadditivity of φ and (38) ensure that

$$a\ (f-g)\ (\psi'' - \psi - \psi') \le a\ |f-g|\ (\varphi'' - \varphi + \varphi') \le 2A\ |f-g|\ \varphi\ \varphi'^2\,.$$

On the other hand, we infer from (38) that

$$\begin{aligned} &(f-g)(y)\ \int_0^y b(y',y-y')\ (\psi(y) - \psi(y') - \psi(y-y'))\ dy'\\ &\ge |(f-g)(y)|\ \int_0^y b(y',y-y')\ (\varphi(y) - \varphi(y') - \varphi(y-y'))\ dy'\\ &\ge -B\ \varphi(y)\ |(f-g)(y)|\,. \end{aligned}$$

Therefore,

$$\frac{d}{dt}\int_Y |f-g|\,\varphi\,dy \le A\int_Y |f-g|\,\varphi\,dy \int_Y (f+g)\,\varphi^2\,dy + B\int_Y |f-g|\,\varphi\,dy\,, \quad (39)$$

whence $f = g$ thanks to the Gronwall Lemma. □

Observe that Theorem 1 requires that the solution to (23) belongs to $L^1(0,T;L^1_{\varphi^2}(Y))$, a fact which might not be true for arbitrary $T > 0$ and initial data $f_{in} \in L^1_1$. Uniqueness then reduces to the problem of getting moment estimates on solutions. We will come back to this question in the next section.

In the absence of fragmentation ($b = 0$), Theorem 1 has been established in [89], while the choice $\varphi(y) = (1+y)^{1/2}$ allows us to recover the uniqueness results from [6, 102]. Finally, with the choice $\varphi(y) = 1 + y$, we recover the uniqueness result from [20, 56] (strong fragmentation with $\gamma > 0$ and $a(y,y') \le A\,(1+y)^\alpha\,(1+y')^\alpha$ for some $\alpha \in (1/2,1]$) and [56, 62] ($a(y,y') \le A\,(1+y+y')$ and $f^{in} \in L^1_2(Y) := L^1(Y,(1+y^2)\,dy)$). The uniqueness of solutions to (23) with strong fragmentation and without the restriction $\gamma > 0$ is established in [13]. Let us finally point out that, for the Becker-Döring equations (25), (26), the conditions of Theorem 1 can be relaxed and uniqueness holds true for a large class of coefficients [7, 66]. The available uniqueness results only deal with mass-conserving solutions and none of them applies to cases where gelation takes place. In that case, there are uniqueness results which are valid up to the gelation time T_g but there is no global uniqueness result except for the multiplicative kernel $a = y\,y'$ for some initial data. More precisely, for initial data for which $Y_1(t)$ can be explicitly computed, there are uniqueness results past the gelation time [34, 57]. In the spatially inhomegeneous setting, the uniqueness issue is much harder and only a few results are available under strong assumptions on the reactions rates a, b, the diffusion coefficient d and the initial data [3, 111] (typically, the diffusion coefficient d does not depend on the size y for $y \ge y_0$ or the space dimension is equal to 1).

3 Mass conservation and gelation

In this section, we give a more detailed account of the available results concerning mass conservation and gelation for the solutions to the coagulation-fragmentation equation (23). Recall that a solution to (23) is mass-conserving if

$$Y_1(t) = Y_1(0) \qquad \text{for each} \quad t \ge 0\,,$$

or is a gelling solution if gelation occurs in finite time, that is,

$$\text{there exists} \quad T_g \in [0,+\infty) \quad \text{such that} \quad \begin{cases} Y_1(t) = Y_1(0) & \text{if} \;\; t < T_g\,, \\ Y_1(t) < Y_1(0) & \text{if} \;\; t > T_g\,. \end{cases}$$

From an historical point of view, the gelation phenomenon was already discussed in the forties (see, e.g., Stockmayer [105]). The fact that the Smoluchowski coagulation equation (2) (or (24) with $b_{i,j} \equiv 0$) could account for it did not seem to be clear at that time. Seemingly, this was pointed out later on by Ziff [112] by constructing coagulation kernels for which gelation was likely to occur. Nevertheless, Stockmayer's kernel $a_{i,j} = (A\ i + B)\,(A\ j + B)$ is not included in his analysis. Two important results were obtained at the beginning of the eighties: on the one hand, White showed that mass-conserving solutions do exist as soon as $a_{i,j} \le (i+j)$ [108]. On the other hand, Leyvraz & Tschudi considered the multiplicative kernel $a_{i,j} = i\,j$ and proved that gelation must occur for any solution to (24) in that case [73]. Furthermore, they succeeded in computing the solution corresponding to the monodisperse initial datum $c_1(0) = 1$ and $c_i(0) = 0$ for $i \ge 2$, which reads [73]:

$$c_i(t) = \begin{cases} \dfrac{i^{i-3}}{(i-1)!}\ t^{i-1}\ e^{-it} & \text{if } \ t \in [0,1]\,, \\[2ex] \dfrac{c_i(1)}{t} & \text{if } \ t \in [1,+\infty)\,, \end{cases}$$

and satisfies

$$\sum_{i=1}^{\infty} i\ c_i(t) = \min\left\{1, \frac{1}{t}\right\},$$

whence $T_g = 1$. Let us emphasize here that the above solution is unique [57], while a simpler way of computing it was later given by Slemrod [95]. For the coagulation kernel $a_{i,j} = (i\,j)^{\lambda/2}$, $\lambda \in [0,2]$, the conjecture was then that gelation occurs for $\lambda > 1$ [50, 74], since the result of White excludes the occurrence of gelation for $\lambda \in [0,1]$ [108]. A first step towards the proof of the above conjecture was done by Leyvraz, who showed in [72] that, if $\lambda \in (1,2)$, there exists a sequence $(\gamma_i)_{i\ge 1}$ of nonnegative real numbers such that

$$\sum_{i=1}^{\infty} i\ \gamma_i < +\infty\,,$$

and $c_i(t) = \gamma_i/(1+t)$, $i \ge 1$, $t \ge 0$, is a solution to (24) with $a_{i,j} = (i\,j)^{\lambda/2}$ and $b_{i,j} \equiv 0$ (see also [30] for a similar result for $a_{i,j} = i^\alpha\, j^\beta + i^\beta\, j^\alpha$ when $\alpha + \beta \in (1,2)$). Clearly, $T_g = 0$ for that particular solution. Therefore, there is at least one gelling solution to (24) with $a_{i,j} = (i\,j)^{\lambda/2}$ and $\lambda > 1$. The remaining question was then whether gelation occurs for any initial data in that case. A similar conjecture is stated in [38] for the continuous coagulation equation (2) for $a = (y\,y')^{\lambda/2}$ for $\lambda > 1$, and several explicit gelling solutions are computed there for the multiplicative kernel $a = y\,y'$. An important contribution towards the proof of this conjecture is due to Jeon and relies on a stochastic approach [55]. For a dense set of initial data, Jeon proves that there is at least a gelling solution to (24) with $a = (y\,y')^{\lambda/2}$ and $\lambda \in (1,2)$. At the same time, da

Costa extends the construction performed by Leyvraz in [72] and exhibit an infinite family of solutions to the discrete Smoluchowski equation of the form $c_i(t) = \gamma_i/(1+t)$, $i \geq 1$ and $t \geq 0$ [23]. A definitive and positive answer to the conjecture was recently provided by Escobedo, Mischler & Perthame [42]. For the coagulation kernel (5), they prove that gelation occurs in finite time for any initial data and any weak solution to (2) as soon as $\lambda = \alpha+\beta > 1$. The fact that this result is valid for any weak solution is important since no uniqueness results are available in that case. The approach employed in [42] relies on a tricky use of differential and integral inequalities and actually works for both discrete and continuous coagulation equations. It provides several additional information on the gelation phenomenon which we outline below. It also allows to study the occurrence of gelation for the coagulation-fragmentation equation (23) for which nothing was known or conjectured, besides some partial results in [55, 61].

On the other hand, the existence of mass-conserving solutions initiated in [108] was subsequently completed in [6, 35, 41, 65] for the coagulation-fragmentation equation (23) for weak coagulation kernels (i.e., $a(y,y') \leq A\,(1+y+y'))$ under mild assumptions on the fragmentation kernel b. It was also noticed that fragmentation can prevent the occurrence of gelation, as observed in [20] for the discrete model and extended to (23) in [41].

To illustrate the above discussion, let us now give a more precise statement for a particular class of kernels.

Theorem 2. *Assume that f^{in} fulfils (37) and put*

$$a(y,y') = A\,(y\,y')^{\lambda/2}\,, \qquad b(y,y') = B\,(1+y+y')^{\gamma}\,,$$

where $A > 0$, $B > 0$, $\lambda \in [0,2]$ and $\gamma \in \mathbb{R}$.

1. `weak coagulation`*: if $\lambda \leq 1$, there is at least a mass-conserving weak solution to (23).*
2. `strong fragmentation`*: if $\lambda > 1$ and $\gamma > \lambda - 2$, there is at least a mass-conserving weak solution to (23).*
3. `strong coagulation`*: if $\lambda > 1$ and $\gamma < \lambda - 2$ or $(\lambda,\gamma) = (2,0)$, there exists $Y^* \geq 0$ such that gelation occurs for any weak solution whenever $Y_1(f^{in}) > Y^*$. Furthermore, $Y^* = 0$ if either $\lambda > 1$ and $b \equiv 0$ or if $\lambda = 2$ and $\gamma < -1$. In that case, we have $Y_1(t) \to 0$ as $t \to \infty$.*

Let us first point out that the last assertion of Theorem 2 only gives a sufficient condition for gelation to occur for any non-zero initial data. Scaling arguments performed in [41] seem to indicate that Y^* should be equal to zero when $\gamma < (\lambda-3)/2$ (observe that $(\lambda-3)/2 < \lambda-2$ as $\lambda > 1$). We also mention that the "critical" case $\gamma = \lambda - 2$ is not included in Theorem 2, except when $\lambda = 2$.

Remark 1. In the strong fragmentation case $\gamma > \lambda - 2$, there are also unphysical solutions for which $Y_1(t)$ increases with time [6, 41].

We now give some arguments towards the proof of Theorem 2 and focus on the moment estimates needed to control the behaviour of f for large y (Point A in Section 2) and to prove or exclude gelation.

Case 1 - `weak coagulation`: we assume in addition that $f^{in} \in L^1_2(\mathbb{R}_+)$, the general case being handled in a similar way. We multiply (23) by $\phi(y) = y^2$ and notice that the contribution of the fragmentation term is non-positive, while (10) yields

$$\frac{d}{dt} Y_2 \le C\, Y_1\, (Y_2 + Y_1)\,,$$

whence $Y_2(t) \le e^{C\,(1+t)}$ for $t \ge 0$, and a strong control on the behaviour of f for large y which guarantees the existence of a mass-conserving solution.

Case 2 - `strong fragmentation`: multiplying again (23) by $\phi(y) = y^2$, we obtain

$$\frac{d}{dt} Y_2 \le C_1\, Y_1\, Y_{1+\lambda} - C_2\, Y_{3+\gamma}\,,$$

from which the bound $Y_2(t) \le C\, t^{-\nu}$ follows for some $\nu > 0$, since $Y_{1+\lambda}^{2+\gamma} \le Y_1^{2+\gamma-\lambda}\, Y_{3+\gamma}^{\lambda}$ and $Y_2^{2+\gamma} \le Y_1^{1+\gamma}\, Y_{3+\gamma}$ by the Hölder inequality.

Case 3 - `strong coagulation`: the cornerstone of the analysis is to establish that

$$\int_0^T Y_1^2(t)\, dt \le C_{\lambda,\gamma}\, (Y_0(0) + Y_1(0) + B^2\, T) \tag{40}$$

for each $T > 0$. The occurrence of gelation then follows from (40) as soon as the initial mass satisfies $Y_1^2(0) > C_{\lambda,\gamma}\, B^2$. We now sketch the proof of (40) for the coagulation equation (2) in the absence of fragmentation ($B = 0$) and also set $A = 1$ without loss of generality.

Proof of (40). On the one hand, it follows from (10) with $\phi = 1$ that

$$\int_0^T Y_{\lambda/2}^2(t)\, dt \le 2\, Y_0(0)\,. \tag{41}$$

As already pointed out in the Introduction, the above bound implies that $Y_1 \in L^2(0, +\infty)$ when $\lambda = 2$. Therefore, Y_1 cannot remain constant through time evolution and gelation occurs. When $\lambda \in (1, 2)$, the estimate (41) does not allow to conclude and more information are needed.

On the other hand, for $R > 0$, we infer from (10) with $\phi = y \wedge R := \min\{y, R\}$ that

$$\int_0^T \left(\int_R^\infty f(t,y)\, y^{\lambda/2}\, dy \right)^2 dt \le 2\, \frac{Y_1(0)}{R} \tag{42}$$

for $T > 0$, since $\phi(y) + \phi(y') - \phi(y + y') \ge R\, \mathbf{1}_{[R,+\infty)}(y)\, \mathbf{1}_{[R,+\infty)}(y')$.

We next consider $\Phi \in W^{1,1}_{loc}([0,+\infty))$ such that $\Phi(0) = 0$ and $C_\Phi := \|\Phi'(y)\, y^{-1/2}\|_{L^1} < \infty$. Using the Fubini theorem and the Cauchy-Schwarz inequality, we have

$$\begin{aligned}
&\int_0^T \left(\int_0^\infty f(t,y)\, y^{\lambda/2}\, \Phi(y)\, dy\right)^2 dt \\
&= \int_0^T \left(\int_0^\infty \Phi'(R) \int_R^\infty f(t,y)\, y^{\lambda/2}\, dy\, dR\right)^2 dt \\
&\le \int_0^T C_\Phi \int_0^\infty \Phi'(R)\, R^{1/2} \left(\int_R^\infty f(t,y)\, y^{\lambda/2}\, dy\right)^2 dR\, dt \\
&\le C_\Phi \int_0^\infty \Phi'(R)\, R^{1/2} \int_0^T \left(\int_R^\infty f(t,y)\, y^{\lambda/2}\, dy\right)^2 dt\, dR\,.
\end{aligned}$$

Using (42) to estimate the right-hand side of the above inequality, we obtain

$$\int_0^T \left(\int_0^\infty f(t,y)\, y^{\lambda/2}\, \Phi(y)\, dy\right)^2 dt \le 2\, C_\Phi \int_0^\infty \frac{\Phi'(R)}{R^{1/2}}\, Y_1(0)\, dR = 2\, C_\Phi^2\, Y_1(0)\,.$$

The choice $\Phi(y) = (y-1/2)_+^{1-\lambda/2}$ in the previous estimate implies that

$$\int_0^T \left(\int_1^\infty f(t,y)\, y\, dy\right)^2 dt \le C\, Y_1(0)\,,$$

which, together with (41), yields (40). □

4 Time asymptotics for the coagulation equation

In this section, we gather further information on the behaviour of solutions to the coagulation equation (2), (3) as $t \to +\infty$ or $t \to T_*$. We actually aim at a more precise description of how the loss of mass occurs as $t \to T_*$ and first analyze the behaviour of moments of f near T_*. We next briefly present the conjectured self-similar behaviour.

4.1 Decay of the total number of particles Y_0

From a physical point of view, coagulation process reduce the number of particles until only one particle remains (with an infinite mass), and we thus expect the total number of particles to converge to zero for large times.

Proposition 1. *Assume that*

$$a(y,y') > 0\,, \qquad (y,y') \in Y \times Y,\ y \neq y'. \tag{43}$$

Then, $Y_k(t) \longrightarrow 0$ *as* $t \to +\infty$ *for* $k \in [0,1)$.

Since solutions to (2), (3) satisfy $Y_1(t) \le Y_1(0)$ by Definition 1, it suffices to prove Proposition 1 for $k = 0$. We prove Proposition 1 under the additional assumption (9) on a. We refer to [16] when the coalescence kernel satisfies $a > 0$ on Y^2 and to [45, 68] for the general case in the continuous setting and for some extensions in the discrete setting. When a satisfies (9), the proof relies on the availability of several Liapunov functionals, a fact which is an interesting property by its own and can also be used in a spatially inhomogeneous setting, and for the existence theory as well. The cornerstone of the proof is the following result [40, 85].

Theorem 3. *Assume a satisfies (9). Let f be a solution to (2), (3) and Φ be a nonnegative increasing and convex function such that $\Phi(0) = 0$. We have*

$$\int_Y \Phi(f(t,y))\ dy + \int_0^t D_\Phi(f(\tau))\ d\tau \le \int_Y \Phi(f^{in}(y))\ dy\,, \tag{44}$$

where $D_\Phi(f) := D^1_\Phi(f) + D^2_\Phi(f)$,

$$D^1_\Phi(f) := \frac{1}{2}\int_{Y^2} a(y,y')\ (f \vee f')\ \Phi(f \wedge f')\ dydy' \ge 0\,, \tag{45}$$

$$D^2_\Phi(f) := \int_{Y^2} a(y,y')\ \Psi(f)\ f'\ \mathbf{1}_{y' \ge y}\ dy'dy \ge 0\,,$$

and $\Psi(s) := s\ \Phi'(s) - \Phi(s) \ge 0$ for $s \ge 0$. Here and below, we use the notations $f \vee f' = \max\{f, f'\}$ and $f \wedge f' = \min\{f, f'\}$.

Proof of Theorem 3. Fo the sake of simplicity we only present the proof in the case $\Phi(s) = s^2$ and refer to [40, 85] for the general case. It follows from the Young inequality that

$$\begin{aligned} 2\int_{Y^2} a\ f\ f'\ f''\ dy'dy &= 2\int_{Y^2} a\ (f \wedge f')\ (f \vee f')\ f''\ dy'dy \\ &\le \int_{Y^2} a\ (f \wedge f')\ \left\{(f \vee f')^2 + (f'')^2)\right\}\ dy'dy \end{aligned}$$

We now use (9) to bound the second term of the right-hand side of the above inequality and deduce that

$$\begin{aligned} &2\int_{Y^2} a\ f\ f'\ \ f''\ dy'dy \\ &\le \int_{Y^2} a\ (f \wedge f')\ (f \vee f')^2\ dy'dy \\ &\quad + \int_{Y^2} (a(y,y'') + a(y',y''))\ (f \wedge f')\ (f'')^2\ dy'dy \\ &\le \int_{Y^2} a\ (f \wedge f')\ (f \vee f')^2\ dy'dy + 2\int_{Y^2} a(y',y'')\ f'\ (f'')^2\ dy'dy \\ &\le \int_{Y^2} a\ (f \wedge f')\ (f \vee f')^2\ dy'dy + 2\int_{Y^2} a\ f'\ (f)^2\ \mathbf{1}_{(0,y)}(y')\ dy'dy\,. \end{aligned}$$

Consequently,

$$
\begin{aligned}
& 2 \int_Y Q(f)\, f^2\, dy = \int_{Y^2} a\, f\, f'\, (f'' - f - f')\, dy' dy \\
\le\ & \frac{1}{2} \int_{Y^2} a\, (f \wedge f')\, (f \vee f')^2\, dy' dy + \int_{Y^2} a\, f'\, f^2\, \mathbf{1}_{(0,y)}(y')\, dy' dy \\
& -2 \int_{Y^2} a\, f^2\, f'\, dy' dy\,,
\end{aligned}
$$

whence (44). □

Proof of Proposition 1 (when a fulfils (9)). We assume here again for simplicity that $f^{in} \in L^2(Y)$. On the one hand, Theorem 3 with $\Phi(s) = s^2$ and the bound on Y_1 in Definition 1 imply that $\{f(t)\,, t \ge 0\}$ is weakly sequentially compact in $L^1(Y)$. On the other hand, Theorem 3 with $\Phi(s) = s$ entails that $(t, y, y') \longmapsto a(y, y')\, f(t, y)\, f(t, y')$ belongs to $L^1((0, \infty) \times Y^2)$. A weak lower semicontinuity argument then ensures that $(f(t))$ converges weakly to zero in $L^1(Y)$ as $t \to +\infty$, which completes the proof. □

The next question to be solved is whether we can estimate the speed of this process. Besides the cases $a = 1$ and $a = y + y'$ where Y_0 is explicitly calculable, we have also the following result [68].

Proposition 2. *Assume that there are $\lambda \in [0, 1)$ and $\delta > 0$ such that*

$$
a(y, y') \ge (y\, y')^{\lambda/2} \quad \textit{for} \quad (y, y') \in Y^2\,,
$$

and $f^{in} \equiv 0$ a.e. on $(0, \delta)$. Then, for each $k \in (0, 1)$, there is a constant C_k such that $Y_\lambda(t) \le C_k\, t^{-k}$ for $t > 0$.

It is likely that, in fact, $Y_\lambda(t)$ decays as $C\, t^{-1}$, but we have been unable to prove it. On the other hand, it can be shown that $Y_\lambda(t)$ cannot decay at a faster algebraic rate if $a(y, y') = y^\lambda + (y')^\lambda$, $\lambda \in (0, 1)$.

4.2 Profile at the gelation time

In this section, we assume that a is given by (5) with $\lambda = \alpha + \beta \in (1, 2]$ and consider a solution f to (2), (3). According to Theorem 2, gelation takes place and $T_* = T_g < \infty$. A more precise result is actually available [42].

Theorem 4. *Consider $T_1 > T_0 \ge 0$ such that $Y_1(T_1) < Y_1(T_0)$. Then,*

$$
\int_{T_0}^{T_1} \left(\int_e^\infty \frac{y^{(1+\lambda)/2}}{(\ln y)^{1/2}}\, f(t, y)\, dy \right)^2 dt = +\infty\,, \tag{46}
$$

while

$$
\int_{T_0}^{T_1} \left(\int_e^\infty \frac{y^{(1+\lambda)/2}}{(\ln y)^{\delta}}\, f(t, y)\, dy \right)^2 dt < +\infty\,, \tag{47}
$$

for any $\delta > 1$.

In particular, Theorem 4 applies when $T_0 = T_g - \tau$ and $T_1 = T_g + \tau$ for any $\tau > 0$ and indicates that a singularity takes place at the gelation time T_g. More precisely, it somehow (of course formally) implies that

$$Y_{\lambda/2+1/2+\varepsilon}(T_g) = +\infty \quad \text{and} \quad Y_{\lambda/2+1/2-\varepsilon}(T_g) < +\infty$$

at the gelation time T_g for any $\varepsilon > 0$. In other words, it means *in a weak sense* that the distribution function $f(T_g)$ at the gelation time behaves as follows for large sizes

$$f(T_g, y) \underset{y \to +\infty}{\sim} C\, y^{-(\lambda+3)/2},$$

which is actually the behaviour conjectured by physicists. Further information of the same kind as that of Theorem 4 can also be obtained in terms of Morrey-Campanato norms [42]. Also, Theorem 4 extends to the coagulation-fragmentation equation (23) under the same assumption on a when b is given by $b(y, y') = (1 + y + y')^\gamma$ and $\gamma < (\lambda - 3)/2$ [42]. However, when $\gamma \in ((\lambda-3)/2, \lambda-2)$ for which gelation also occurs by Theorem 2 for "large" initial data, the situation seems likely to be of a different nature, the fragmentation having a stronger influence on the dynamics as suggested by scaling arguments [41].

4.3 Dynamical scaling hypothesis

We close this section with a short discussion on the more precise behaviour of f near T_* conjectured by physicists and focus for simplicity on the case where the coagulation coefficient is given by (5), that is,

$$a(y, y') = y^\alpha\, (y')^\beta + (y')^\alpha\, y^\beta,$$

where $0 \le \alpha \le \beta \le 1$. The formal analysis performed in [32] which we present below actually includes a wider class of coagulation coefficients and we refer to [32] for a more complete account. As previously mentioned, physicists conjecture that the distribution function f behaves in a self-similar way as time approaches T_*, forgetting the details of the initial datum as times goes by. It is however not completely clear which features of the initial datum are retained in the large time. The main conjecture is that

$$f(t, y) \sim f_S(t, y) := \frac{1}{s(t)^\tau}\, \varphi\left(\frac{y}{s(t)}\right) \quad \text{as } t \to T_*, \tag{48}$$

the function f_S being a self-similar solution to (2) and the mean particle size satisfying $s(t) \to +\infty$ as $t \to T_*$. The first step is to identify the parameter τ: if $\lambda := \alpha + \beta \in [0, 1]$, then $T_* = +\infty$ by Theorem 2 and the conservation of mass implies that $\tau = 2$. If $\lambda \in (1, 2]$, gelation takes place and $T_* = T_g < +\infty$. In that case, formal arguments are given in [32] and lead to $\tau = (\lambda + 3)/2$. Thus

$$\tau = 2 \quad \text{if} \quad \lambda \in [0,1] \quad \text{and} \quad \tau = \frac{\lambda+3}{2} \quad \text{if} \quad \lambda \in (1,2]\,. \tag{49}$$

Inserting the ansatz for f_S in (2) yields an ordinary differential equation for s

$$s^{\tau-\lambda-2}\,\frac{ds}{dt} = w\,, \qquad s(T_*) = +\infty\,, \tag{50}$$

and a nonlinear integro-differential equation for φ

$$w \int_y^\infty \left(\tau\, y_*\, \varphi(y_*) + y_*^2\, \frac{d\varphi}{dy}(y_*) \right)\, dy_* \tag{51}$$

$$+ \int_0^y \int_{y-u}^\infty u\, a(u,v)\, \varphi(u)\, \varphi(v)\, dvdu = 0\,, \qquad y \in Y\,, \tag{52}$$

the separation constant w being a positive real number. While (50) is explicitly solvable, the analysis of (52) is less obvious and is currently one of the main open questions in the field. In the absence of existence results for (52), the validity of (48) is still pending. Let us however mention that qualitative properties of φ are derived in [25, 32, 59, 71, 83] by formal arguments and/or numerical simulations, while numerical evidence of the validity of (48) is reported in [44, 46, 59, 71].

Remark 2. According to [32], the ansatz (48) for f_S is not correct when $\lambda = 1$ and $\alpha > 0$ and has to be modified.

There are however three cases for which explicit solutions to (52) are available, and for which the validity of (48) has been investigated. Let us begin with the constant coefficient case $a = 1$. In that case, $\tau = 2$ and given $\varrho > 0$, we have

$$s(t) = 1 + t\,, \qquad \varphi(y) = \varphi_\varrho(y) = \frac{4}{\varrho}\, e^{-2\,y/\varrho}\,, \qquad y \in Y\,, \tag{53}$$

and $Y_1(\varphi_\varrho) = \varrho$. Then, we have

$$(t+1)^2\, f(t+1, (t+1)\, y) \underset{t\to\infty}{\longrightarrow} \varphi_\varrho(y) \quad \text{with} \;\; \varrho := Y_1(0)\,, \tag{54}$$

The first proof of (54) has been provided by Kreer & Penrose for initial data f^{in} decaying exponentially at infinity [58], the convergence being uniform on compacts subsets of Y (see also [21] for the discrete model). Different proofs have been subsequently supplied by Aldous [2, Section 3.1] and Deaconu & Tanré [28, Theorem 3.6] by a probabilistic approach, the convergence being in the weak topology of $L^1(Y)$. The proofs performed in the above mentioned papers rely on the Laplace transform which can be computed explicitly in that case. We have proposed a different approach in [68] where we construct suitable Liapunov functions for the coagulation equation (2) written in self-similar variables and also prove that (54) holds true for the weak topology of $L^1(Y)$. Let us emphasize here that the large time behaviour is uniquely determined by the initial mass $Y_1(0)$.

We next consider the case of the additive kernel $a = y + y'$. Here again, $\tau = 2$ and, for $\varrho > 0$ and $\sigma > 0$, we have

$$s(t) = e^{2\varrho t}, \qquad \varphi(y) = \varphi_{\varrho,\sigma}(y) = \frac{\varrho\, \sigma^{3/2}}{(2\pi)^{1/2}}\, y^{-3/2}\, e^{-y/(2\sigma)} \tag{55}$$

for $y \in Y$, with

$$Y_1(\varphi_{\varrho,\sigma}) = \varrho \quad \text{and} \quad Y_2(\varphi_{\varrho,\sigma}) = \varrho\, \sigma\,.$$

However, as pointed out in [10, Section 3.3], this is not the only family of self-similar solutions to (2): in particular, given $\alpha \in (1,2)$ and $\varrho > 0$, the function $(t,y) \longmapsto (\varrho/s_\alpha(t)^2)\, \psi_{\alpha,\varrho}(y/s_\alpha(t))$ with

$$s_\alpha(t) = e^{(\alpha\, \varrho\, t)/(\alpha-1)}, \qquad \psi_{\alpha,\varrho}(y) = y^{-(1+\alpha)/\alpha} R_\alpha\left(-y^{(\alpha-1)/\alpha}\right), \tag{56}$$

is a self-similar solution to (2), where R_α denotes the completely asymmetric α-stable density [10].

As for the validity of (48), it is shown in [10, 28] that, if $Y_2(f^{in}) < +\infty$,

$$e^{4\varrho t}\, f(2\,\varrho\, t, e^{2\varrho t}\, y) \underset{t\to\infty}{\longrightarrow} \varphi_{\varrho,\sigma}(y) \quad \text{with } \varrho := Y_1(0) \text{ and } \sigma = \frac{Y_2(0)}{Y_1(0)}, \tag{57}$$

the convergence being with respect to the weak topology of $L^1(Y)$. The proof still relies on a probabilistic approach together with the Laplace transform. We refer to [10] for results when $Y_2(f^{in}) = +\infty$.

We finally consider the multiplicative kernel $a = y\, y'$. In that case, gelation occurs and the gelation time T_g can be explicitly computed and is equal to $1/Y_2(0)$ [38, 90]. It turns out that there is a simple connection between solutions of (2) with $a = y + y'$ and $a = y\, y'$ which has been noticed in [28]: let f be a solution to (2) with $a = y + y'$, $T > 0$ and put

$$F(t,y) = \frac{1}{Y_1(f^{in})^3}\, \frac{1}{x\,(T-t)}\, f\left(\frac{\ln(T) - \ln(T-t)}{Y_1(f^{in})}, \frac{y}{Y_1(f^{in})}\right)$$

for $(t,y) \in (0,T) \times Y$. Then F is a solution to (2) with $a = y\, y'$. Thanks to this transformation, convergence results for the multiplicative kernel $a = y\, y'$ readily follow from that obtained for the additive kernel $a = y + y'$ since T_g is known.

5 Convergence to equilibrium under the detailed balance condition

In this section, we assume that the coagulation and fragmentation coefficients fulfil the *detailed balance condition* (27). In that case, we may define a Liapunov functional H by (30) which decreases along the trajectory by the

H-Theorem (31). We refer to (27)–(32) in the Introduction for the notations used in this section.

Let f^{in} be such that (37) holds true and $H(f^{in}) < +\infty$. We next consider a solution f to (23) such that $f(0) = f^{in}$ and recall that the expected result is:

$$\begin{cases} \bullet \quad \text{if } Y_1(f^{in}) \le \varrho_s, \text{ then } f(t) \longrightarrow M_z \text{ in } L^1_1(Y) \text{ as } t \to +\infty, \text{ where} \\ \quad\ z \text{ is such that } Y_1(M_z) = Y_1(f^{in}). \\ \bullet \quad \text{if } Y_1(f^{in}) > \varrho_s, \text{ then } f(t) \rightharpoonup M_{z_s} \text{ in } L^1(Y) \text{ as } t \to +\infty. \end{cases} \tag{58}$$

As already mentioned, the assertion (58) is far from being proved completely in all cases. We briefly summarize now the available results, together with the main tools used for the proof. Roughly speaking, it is in general possible to prove that the only cluster points of $\{f(t)\}$ as $t \to +\infty$ are equilibria. The next step would be to identify uniquely the mass of the cluster points as conjectured in (58) but this turns out to be quite difficult. In some cases, using the LaSalle invariance principle allows to bypass this difficulty and prove that $f(t)$ has a limit as $t \to +\infty$. This method however does not allow to identify the mass of the limit.

5.1 Weak lower semicontinuity of the entropy dissipation

The H-Theorem (31) formally holds, but in general, it is only possible to prove a weaker assertion, namely that,

$$\sup_{t\ge 0} H(f(t)) < +\infty \quad \text{and} \quad D(f) \in L^1(0,+\infty)\,. \tag{59}$$

Since $Y_1(f(t)) \le Y_1(f^{in})$ by Definition 1, the first bound in (59) and the Dunford-Pettis theorem ensure that $\{f(t)\}$ is weakly sequentially compact in $L^1(Y)$. Consequently, if (t_n) is an increasing sequence such that $t_n \to +\infty$, there are a function F and a subsequence $(t_{n'})$ of (t_n) such that $f(t_{n'} + .) \rightharpoonup F(.)$ in $L^1((0,1)\times Y)$. The weak lower semicontinuity of D, the second estimate in (59) and the Fatou lemma then allow to conclude that $D(F) = 0$, and thus $a\,F\,F' = b\,F''$. Classical arguments finally entail that there is $z \in [0, z_s]$ such that

$$f(t_{n'}) \rightharpoonup M_z \quad \text{in} \quad L^1(Y) \quad \text{with} \quad Y_1(M_z) \le Y_1(f^{in})\,.$$

At this stage, the parameter z can depend on $(t_{n'})$ and (t_n). Using an argument from [76], the above weak convergence can be improved to strong convergence in $L^1(Y)$ [64]. Of course, this step is useless in the discrete setting.

For the above method to be justified, rather mild assumptions on a, b and f^{in} are needed, so that the above result is true in most cases and it also works in a spatially inhomogeneous setting. This approach has been used for the Becker-Döring equations (25), (26) [7], the discrete coagulation-fragmentation equations (24) [16], the continuous coagulation-fragmentation equations (23) [67], the discrete diffusive Becker-Döring equations [69], the discrete diffusive coagulation-fragmentation equations [19] and the diffusive discrete or continuous coagulation-fragmentation equations [64].

5.2 The LaSalle invariance principle

The main drawback of the above method is that it does not guarantee the convergence of $f(t)$ as $t \to +\infty$. It however only uses a weak form (59) of the H-Theorem (31). It turns out that the conservation of mass and the H-Theorem (31) allow us to conclude that a modified version of H is a Liapunov functional as first pointed out in [7]. One may next apply the LaSalle invariance principle. More precisely, assume that f satisfies

$$Y_1(f(t)) = Y_1(f^{in}) \quad \text{and} \quad H(f(t)) - H(f^{in}) = -\int_0^t D(f(s)\, ds$$

for $t \geq 0$. Then, on the one hand, $t \longmapsto H(f(t))$ is a non-increasing function on time. On the other hand, $\psi \longmapsto H(\psi)$ is not continuous in $L^1(Y)$ but the modified entropy

$$H_{z_s}(\psi) := H(\psi) - Y_1(\psi)\, \ln z_s$$

is continuous in $L^1(Y)$ on bounded subsets of $L^1_1(Y)$ under the additional assumption

$$\lim_{y\to+\infty} M(y)^{1/y} = \frac{1}{z_s}\,. \tag{60}$$

Combining the above two properties allows to proceed as in the proof of the classical LaSalle invariance principle and conclude that there is a unique $z \in [0, z_s]$ such that

$$Y_1(M_z) \leq Y_1(f^{in}) \quad \text{and} \quad f(t) \longrightarrow M_z \ \text{ in } \ L^1(Y)\,.$$

Still, let us emphasize that it does not allow to identify z as conjectured in (58).

This approach works under stronger assumptions on a, b and f^{in} and has been used for the Becker-Döring equations (25), (26) [7], the discrete coagulation-fragmentation equations (24) [16], the continuous coagulation-fragmentation equations (23) [67, 104], the discrete diffusive Becker-Döring equations [69]. Up to now, no result of this kind is available for the general diffusive coagulation-fragmentation equations, the main reason being that it does not seem obvious to prove the conservation of mass and the entropy equality in that case. If one could justified these two properties, the above method could also be used.

5.3 Strong compactness

Fortunately, there are some cases for which one can prove (58). The easiest case is when $z_s = +\infty$, which in turn implies that $\varrho_s = +\infty$. This assumption warrants that

$$\lim_{y\to+\infty} \sup_{t\geq 0} \int_y^\infty y_* \, f(t,y_*) \, dy_* = 0 \,,$$

which, together with the entropy bound, entail that $(f(t))$ is weakly sequentially compact in $L_1^1(Y)$. It is then clear that f is mass-conserving and that any cluster point F of $(f(t))$ as $t\to+\infty$ satisfies $Y_1(F) = Y_1(f^{in})$. Combining this fact with the result of Section 5.1 yields the expected convergence (58) (see, e.g., [7, 19, 24, 64] and the references therein).

A similar situation is met under the strong fragmentation assumption (see case 2 of Theorem 2). In that case, $\varrho_s = +\infty$ and $Y_2(f(t))$ becomes finite for positive times [14, 20, 41], from which the weak sequential compactness of $(f(t))$ in $L_1^1(Y)$ readily follows, again with the help of the entropy bound. A similar argument as above then leads to (58) [14, 24, 67].

Observe that, in the previous two situations, $\varrho_s = +\infty$, and no saturation phenomenon occurs.

Let us finally mention a third case for which (58) can be proved by constructing supersolutions. Up to now, this method only works successfully for the Becker-Döring equations (25)–(26), see [5, 7]. An extension of this method to the generalized Becker-Döring equations (that is, the discrete coagulation-fragmentation equations (24) with $a_{i,j} = b_{i,j} = 0$ if $\max\{i,j\} \geq N$ for some given $N\geq 3$) has been performed in [16, 22] for initial data f^{in} with a sufficiently small mass, $Y_1(f^{in}) \leq c_N$. Unfortunately, $c_N \to 0$ as $N\to+\infty$. This assumption has been removed recently in [13]. We emphasize here that z_s and ϱ_s can be finite in that case.

We now give a sketch of the proof for the Becker-Döring equations (25), (26), following the arguments of [5]. Introducing

$$G_i := \sum_{j=i}^\infty j\, f_j \,, \quad i\geq 2 \,,$$

the specific structure of (25)-(26) allows us to construct a supersolution to the equation satisfied by (G_i) and deduce that $(f_i(t))_{i\geq 1}$ is compact in $L_1^1(\mathbb{N}\backslash\{0\})$, whence (58) [5]. Indeed, by Section 5.2, we know that there is $z\in[0,z_s]$ such that $f_i(t) \to M_i\, z^i$ for $i\geq 1$ as $t\to+\infty$. Assume that

$$z < z_s \,. \tag{61}$$

Then, there exists $\delta>0$, $T>0$, $i_0\geq 1$ and a sequence $(r_i)_{i\geq 1}$ of positive real numbers such that $r_i\to 0$,

$$f_1(t) \leq z+\delta < z_s \,, \quad G_i(T) \leq r_i \quad \text{for} \quad t\geq T \,,$$

and $G_{i_0}(t) \le r_{i_0}$ for every $t \ge T$. The cornerstone of the proof is to notice that (r_i) can be constructed so that a direct computation (using the particular structure of the BD equations) yields

$$\frac{\partial}{\partial t}(G_i - r_i)_+ \le (G_{i_0} - r_{i_0})_+ + C\,(G_i - r_i)_+$$

for $i \ge i_0$ and $t \ge T$. Therefore, $G_i(t) \le r_i$ for for $i \ge i_0$ and $t \ge T$, and $(i\, f_i)_{i \ge 1}$ is equi-summable, from which we readily conclude that

$$\sum_{i=1}^{\infty} i\, M_i\, z^i = \lim_{t \to +\infty} \sum_{i=1}^{\infty} i\, f_i(t) = \varrho_0 := \sum_{i=1}^{\infty} i\, f_i(0)\,.$$

Then, either $\varrho_0 < \varrho_s$ and we have proved (58). Or $\varrho_0 \ge \varrho_s$, and the assumption (61) leads to a contradiction. Therefore, $z = z_s$ in that case, which completes the proof of (58).

5.4 Convergence rates by entropy dissipation methods

Another approach to the trend to equilibrium is to estimate the distance between $f(t)$ and its expected limit equilibrium. This method has the advantage of providing convergence as well as rates of convergence, but usually requires to establish non-obvious functional inequalities. Still, it has been successfully worked out for the continuous coagulation-fragmentation equation (23) with constant coefficients a and b [1] and for the Becker-Döring equations (25)-(26) [53].

The basic underlying idea is to exploit further the H-theorem (31) and estimate from below the entropy dissipation $D(f)$ in terms of the relative entropy $H(f|M_z) = H(f) - H(M_z)$, M_z being the equilibrium associated to f in (58). For instance, if there is a nonnegative function Ψ (depending possibly on f^{in}) such that

$$D(f) \ge \Psi(H(f|M_z)) \quad \text{and} \quad \int_0^1 \frac{ds}{\Psi(s)} = +\infty\,, \tag{62}$$

the H-theorem (31) then yields a differential inequality for the relative entropy from which a time-dependent estimate $H(f(t)|M_z) \le \omega(t)$ follows by direct integration, with $\omega(t) \to 0$ as $t \to +\infty$. A temporal decay estimate for $\|f(t) - M_z\|_{L^1(Y)}$ is then recovered by the Csiszár-Kullback inequality (see, e.g., [4] and the references therein)

$$\|f(t) - M_z\|_{L^1(Y)}^2 \le \left(\frac{2\,Y_0(f(t))}{3} + \frac{4\,Y_0(M_z)}{3} \right)\, H(f(t)|M_z)\,, \qquad t \ge 0\,,$$

provided a control on $Y_0(f)$ is available.

Let us now be more precise about the inequality (62) obtained in [1, 53].

The continuous coagulation-fragmentation equation (23) with $a = b = 1$

In that case, it is plain that the detailed balance condition (27) is satisfied with $M(y) := e^{-y}$. Then $z_s = e$ and $\varrho_s = +\infty$. To simplify notations, we however use a slightly different way of denoting the equilibria and define $M_0 = 0$ and

$$M_m(y) = e^{-y\, m^{-1/2}}\,, \qquad y \in Y\,,$$

for $m > 0$, so that $Y_1(M_m) = m$. The lower bound for the entropy dissipation $D(f)$ established in [1] reads

$$D(f(t)) \geq Y_0(f(t))\, H\left(f(t)|M_{Y_1(f^{in})}\right)\,, \qquad t \geq 0\,.$$

Since $Y_0(f(t)) \to 2$ as $t \to +\infty$ in that case, we end up with an exponential temporal decay estimate for the relative entropy $H\left(f(t)|M_{Y_1(f^{in})}\right) \leq C_1\, e^{-C_2\, t}$, where C_1 and C_2 depend on f^{in}. We now give a proof of the above lower bound for $D(f)$. Though it follows the lines of [1], we state it in a slightly more precise form.

Lemma 1. *Let f be a nonnegative function in $L^1_1(Y)$ and put $m_0 := Y_0(f)$ and $m_1 := Y_1(f)$. We denote by $M^f = M_{m_1}$ the equilibrium with the same mass, the relative entropy being*

$$H(f|M^f) := \int_0^\infty M^f\, \left(\frac{f}{M^f}\, \ln\left(\frac{f}{M^f}\right) + 1 - \frac{f}{M^f}\right)\, dy\,,$$

and the entropy dissipation

$$D_1(f) := \int_0^\infty \int_0^\infty (f\, f' - f'')\, (\ln(f\, f') - \ln f'')\, dy dy'\,.$$

There holds

$$D_1(f) \geq m_0\;\, H(f|M^f) + \left(m_0 - m_1^{1/2}\right)^2 + m_0^2\, \left(\frac{m_1}{m_0^2}\, \ln\left(\frac{m_1}{m_0^2}\right) + 1 - \frac{m_1}{m_0^2}\right)\,. \tag{63}$$

Observe that the three terms of the right-hand side of (63) are nonnegative.

Proof. We define

$$g = \frac{f}{M^f} \quad \text{and} \quad F(y) := \int_y^\infty f(y')\; dy' = \int_0^\infty f(y+y')\; dy'\,.$$

We have

$$\begin{aligned} D_1(f) &= \int_0^\infty \int_0^\infty M^f\, {M^f}'\, g'\, g\, \ln g\, dy dy' \quad (=: D_{11}(g)) \\ &+ \int_0^\infty \int_0^\infty M^f\, {M^f}'\, g\, g'\, \ln\left(\frac{g'}{g''}\right)\, dy dy' \quad (=: D_{12}(g)) \\ &+ \int_0^\infty \int_0^\infty M^f\, {M^f}'\, g''\, \ln\left(\frac{g''}{g\, g'}\right)\, dy dy' \quad (=: D_{13}(g)), \end{aligned}$$

and estimate each term $D_i(g)$ separately. First,

$$D_{11}(g) = m_0 \int_0^\infty M^f \, \frac{f}{M^f} \, \ln\left(\frac{f}{M^f}\right) \, dy = m_0 \, \left(H(f|M^f) + m_0 - m_1^{1/2}\right) \, .$$

Next, since $\Phi(s) = s \ln s$ is a convex function and $M \, M' = M''$, we infer from Jensen's inequality that

$$\begin{aligned} D_{12}(g) &= \int_0^\infty g \int_0^\infty \frac{M^{f''} \, g''}{F} \, \Phi\left(\frac{g'}{g''}\right) \, dy' \, F \, dy \\ &\geq \int_0^\infty g \, F \, \Phi\left(\frac{\int_0^\infty M^{f''} \, g' \, dy'}{F}\right) \, dy \, . \end{aligned}$$

Noticing that

$$\int_0^\infty M^{f''} \, g' \, dy' = m_0 \, M(y) \, ,$$

we obtain

$$D_{12}(g) \geq \int_0^\infty g \, m_0 \, M \, \ln\left(\frac{m_0 \, M}{F}\right) \, dy \geq m_0 \, \int_0^\infty f \, \left(\ln m_0 - \frac{y}{m_1^{1/2}} - \ln F\right) \, dy \, .$$

Now, $dF/dy = -f$, $F(0) = m_0$, and $F(y) \to 0$ as $y \to +\infty$, from which we deduce that

$$-\int_0^\infty f \, \ln F \, dy = \int_0^\infty \frac{dF}{dy} \, \ln F \, dy = -m_0 \, (\ln m_0 - 1) \, .$$

Consequently,

$$D_{12}(g) \geq m_0 \, \left(m_0 \, \ln m_0 - m_1^{1/2} - m_0 \, (\ln m_0 - 1)\right) = m_0 \, \left(m_0 - m_1^{1/2}\right) \, .$$

Finally, using once more Jensen's inequality, we obtain

$$\begin{aligned} D_{13}(g) &= m_0^2 \int_0^\infty \int_0^\infty \frac{M^f \, M^{f'} \, g \, g'}{m_0^2} \, \Phi\left(\frac{g''}{g \, g'}\right) \, dy dy' \\ &\geq m_0^2 \, \Phi\left(\int_0^\infty \int_0^\infty \frac{M \, M^{f'} \, g''}{m_0^2} \, dy dy'\right) = m_0^2 \, \Phi\left(\frac{m_1}{m_0^2}\right) \, . \end{aligned}$$

Inserting the bounds from below for $D_{11}(g)$, $D_{12}(g)$ and $D_{13}(g)$ in $D_1(f)$ leads to (63). □

With the help of Lemma 1, it is actually possible to adapt the approach used in [1] and obtain rates of convergence to the equilibrium when $a = b$ but not necessarily constants [68].

The Becker-Döring equations (25)-(26)

Here again, it is clear that the detailed balance condition is satisfied. Under suitable assumptions on the coefficients (a_i) and (b_i), and if the initial datum $f^{in} = (f_i^{in})$ satisfies

$$Y_1(f^{in}) < \varrho_s \quad \text{and} \quad \sum_{i=1}^{\infty} e^{\eta\, i}\, f_i^{in} < +\infty$$

for some $\eta > 0$, it is shown in [53] that there is a constant C (depending on f^{in}) such that

$$D(f) \geq C\, \frac{H(f|M_z)}{(\ln H(f|M_z))^2}\,,$$

M_z being the equilibrium such that $Y_1(M_z) = Y_1(f^{in})$. This inequality then yields a temporal decay estimate $e^{-ct^{1/3}}$ for $H(f(t)|M_z)$.

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