

Some problems related to  
the study of interaction kernels:  
coagulation, fragmentation and diffusion  
in kinetic and quantum equations

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*Algunos problemas relacionados  
con el estudio de núcleos de interacción:  
coagulación, fragmentación y difusión  
en ecuaciones cinéticas y cuánticas*

José Alfredo Cañizo Rincón

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V. B. El Director

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# Introducción

Este trabajo trata principalmente el problema de la existencia de soluciones para dos ecuaciones diferentes: las ecuaciones continuas de coagulación-fragmentación y la ecuación de Wigner-Poisson-Fokker-Planck. Además, se estudian algunos aspectos del comportamiento cualitativo de las ecuaciones de coagulación-fragmentación. La tesis está organizada de la siguiente forma: en esta introducción presentamos brevemente el contexto de ambas ecuaciones y los principales resultados obtenidos. En los capítulos 2–4 damos algunos resultados preliminares que son necesarios para el tratamiento posterior de las ecuaciones continuas de coagulación-fragmentación; en el capítulo 5 se enuncian y demuestran los resultados de existencia mencionados, y al mismo tiempo se recuperan algunos resultados ya conocidos sobre el tema, ya que las técnicas involucradas son parecidas. En particular, la sección 5.7.3 contiene resultados que muestran la interacción entre coeficientes de coagulación y fragmentación singulares. El capítulo 6 contiene un resultado nuevo sobre el comportamiento asintótico del sistema de ecuaciones generalizado de Becker-Döring (que es un caso particular de las ecuaciones discretas de coagulación-fragmentación, como se explica a continuación), y el capítulo 7 presenta una aproximación explícita al comportamiento de las soluciones de las ecuaciones de Becker-Döring en un caso particular, junto con soluciones numéricas que respaldan la validez de la aproximación. Finalmente, el capítulo 8 contiene nuestro resultado sobre la ecuación de Wigner-Poisson-Fokker-Planck, que consiste esencialmente en una teoría de existencia en  $L^1$ . Se incluyen también algunos apéndices que contienen un resumen de algunos resultados conocidos que son necesarios en el desarrollo de este trabajo. En el resto de esta introducción se presenta más ampliamente cada uno de los temas tratados. Por supuesto, una gran parte del contenido está aquí gracias al trabajo de otras personas y ha sido hecho con su colaboración, y me gustaría nombrarlos aquí. Quiero agradecer a Juan Soler su dirección y su ayuda con las ecuaciones de transporte y en general en el tema de las ecuaciones de evolución, y también su trabajo en la preparación de esta tesis. El trabajo recogido en los capítulos 5 y 6 fue llevado a cabo junto con Stéphane Mischler, y quiero agradecerle sus sugerencias y su ayuda; el trabajo contenido en el capítulo 6 fue publicado en [14]. Asimismo, me gustaría agradecer a Luis Bonilla y John Neu el darme la oportunidad de trabajar con ellos en la solución numérica y el análisis asintótico del caso particular de las ecuaciones recogido en el capítulo 7, y que fue publicado en [73]. José Luis López y Juan José Nieto me enseñaron sobre la ecuación de Wigner y me animaron a trabajar

con ellos, y estoy muy agradecido por eso; los resultados obtenidos, recogidos en el capítulo 8, también han sido publicados en [13]. También quiero agradecer a P. E. Jabín sus explicaciones y su ayuda sobre modelos de acoplamiento fluido-partícula, y a Magdalena Rodríguez por el diseño de las ilustraciones en los apéndices.

## Las ecuaciones de coagulación-fragmentación

Muchos fenómenos físicos consisten en un gran número de partículas pequeñas que pueden unirse de alguna forma para formar unidades mayores. Por ejemplo, cuando una sustancia cambia de la fase líquida a la gaseosa, las moléculas del gas empiezan a agruparse para formar gotas cada vez mayores de la fase líquida; procesos análogos ocurren en otros tipos de cambios de fase [59] y en el comportamiento de los aerosoles (partículas líquidas o sólidas suspendidas en un gas) [27]. La cristalización en coloides [39] y la separación de aleaciones binarias [60, 89, 65] son otros ejemplos de esta situación. En biología, la formación de cristales de proteínas de la fase cúbica de membranas lipídicas [42] y la agregación de ciertos lípidos formando agregados esféricos (*micelas*) o bicapas lipídicas (*membranas*) siguen un proceso parecido. [73, 46]. Estos ejemplos son muy generales, pero el punto sorprendente es que en muchos casos tienen características que permiten una descripción común útil.

Merece la pena tener una buena comprensión de estos fenómenos, y se ha intentado desde varios puntos de vista: la termodinámica y la mecánica estadística dan información muy útil sobre las situaciones de equilibrio, pero no pueden decir mucho fuera de ellas (ver la sección 2.5 y [46, 81]). Se han propuesto algunas ecuaciones cinéticas como modelo para estos procesos, de las cuales damos a continuación un breve resumen; referimos a los artículos [58, 1, 27, 28] para más información sobre el tema. Dichos modelos pueden clasificarse según la escala de la descripción que intentan dar: las *descripciones microscópicas* intentan modelizar la evolución de un conjunto finito de partículas individuales, y normalmente suponen que los sucesos por los que dos partículas se unen ocurren al azar. El primer modelo de este tipo fue propuesto por Marian Smoluchowski [83, 84]; otro ejemplo es el proceso de Marcus-Lushnikov [63, 64]. Las *descripciones mesoscópicas* o *modelos de campo medio* tratan la evolución del número de partículas de cada tamaño posible, y no la de cada partícula individual; estas descripciones son válidas cuando el número de partículas es suficientemente alto. Los modelos mesoscópicos pueden incluir o no la distribución espacial de las partículas. En este trabajo nos centraremos en este nivel de descripción, así que algunos modelos de este tipo serán descritos en detalle más adelante; en particular estudiaremos ampliamente algunos problemas matemáticos relacionados con la *ecuación de coagulación-fragmentación*. Finalmente, los *modelos macroscópicos* describen la evolución de ciertas cantidades macroscópicas que representan algún tipo de media de las propiedades microscópicas del sistema en consideración (como el tamaño medio de las partículas).

Entre los modelos de campo medio, probablemente el mejor conocido es el de las

*ecuaciones de coagulación de Smoluchowski*, propuesto en 1917 por Smoluchowski en su versión discreta [84], y extendidas al planteamiento continuo por Müller en 1928 [72]:

$$\frac{d}{dt}c_i = \sum_{j=1}^{i-1} a_{j,i-j}c_jc_{i-j} - \sum_{j=1}^{\infty} a_{ij}c_ic_j \quad \text{for } i \geq 1.$$

Aquí los  $a_{ij}$ , para  $i, j \geq 1$  enteros, son números no negativos llamados *coeficientes de coagulación*; el anterior es un sistema de infinitas ecuaciones diferenciales ordinarias en las incógnitas  $c_i = c_i(t)$  para  $i \geq 1$ , que representan las densidades de clusters (agregados de partículas) de tamaño  $i$ , dependiendo del tiempo  $t$ . El supuesto básico es que la frecuencia con la que tiene lugar la reacción de coagulación en la que un cluster de tamaño  $i$  y un cluster de tamaño  $j$  se unen es proporcional a las concentraciones  $c_i, c_j$  de clusters de tamaño  $i$  y  $j$ ; esto se conoce como la *ley de acción de masas*. Así, el término positivo a la derecha de la ecuación anterior representa el número de las reacciones de coagulación cuyo producto es un cluster de tamaño  $i$  que tienen lugar; el término negativo representa el número de reacciones en las que un cluster de tamaño  $i$  se une a algún otro cluster, produciendo así un cluster de tamaño mayor que  $i$ . Una generalización de esta ecuación se describe con precisión en el capítulo 2, así que no nos extendemos aquí sobre eso.

La ecuación de coagulación de Smoluchowski sólo tiene en cuenta las posibles reacciones de *coagulación* entre pares de clusters, pero no incluye la posible fragmentación de las partículas. Por el contrario, las *ecuaciones de Becker-Döring*, dadas por el siguiente sistema de ecuaciones, describen sucesos de fragmentación binaria y coagulación, pero incluyen sólo aquéllos que involucran reacciones entre partículas individuales y otros clusters (de forma que no tienen en cuenta, por ejemplo, reacciones entre dos clusters de tamaño tres):

$$\frac{d}{dt}c_i = J_{i-1} - J_i, \quad r \geq 2 \tag{1}$$

$$\frac{d}{dt}c_1 = -J_1 - \sum_{i=1}^{\infty} J_i, \tag{2}$$

donde  $J_i := a_i c_1 c_i - b_{i+1} c_{i+1}$  para  $i \geq 1$  y  $a_i, b_i$  son los *coeficientes de coagulación y fragmentación*, respectivamente. ( $a_i$  se corresponde con  $a_{i,1}$  en la ecuación de Smoluchowski, ya que ahora sólo consideramos reacciones que involucran una partícula individual y un cluster de cualquier tamaño). Estas ecuaciones fueron propuestas originalmente por Becker y Döring [6] en 1935; un resumen de los resultados principales sobre ellas puede encontrarse en el artículo de Slemrod [82]. Una generalización directa tanto de las ecuaciones de Smoluchowski como de la de Becker-Döring son las *ecuaciones discretas de coagulación-fragmentación*:

$$\frac{d}{dt}c_i = \frac{1}{2} \sum_{j=1}^{i-1} W_{j,i-j} - \sum_{j=1}^{\infty} W_{ij} \quad \text{for } i \geq 1, \tag{3}$$

donde  $W_{ij} := a_{ij}c_i c_j - b_{ij}c_{i+j}$ . Las *ecuaciones de Becker-Döring generalizadas* son el caso particular de este sistema en el que, para cierto  $N \in \mathbb{N}$ ,  $a_{ij} = b_{ij} = 0$  siempre que  $\min\{i, j\} \geq N$ ; esto es, sólo consideramos las reacciones en las que al menos una de las partículas es de tamaño menos que  $N$ .

Parte de este trabajo trata algunos problemas en la teoría matemática de la versión continua de las ecuaciones de coagulación-fragmentación, dada por la siguiente ecuación integro-diferencial:

$$\frac{\partial}{\partial t} f = C(f) + F(f), \quad t, y \in (0, +\infty) \quad (4)$$

$$f(0, y) = f^0(y), \quad y \in (0, +\infty), \quad (5)$$

donde los términos de coagulación y fragmentación están dados por

$$C(f) := C_1(f) - C_2(f)$$

$$F(f) := F_1(f) - F_2(f)$$

$$C_1(f)(y) := \frac{1}{2} \int_0^y a(y', y - y') f(y') f(y - y') dy'$$

$$C_2(f)(y) := f(y) \int_0^\infty a(y, y') f(y') dy'$$

$$F_1(f)(y) := \int_y^\infty b(y', y - y') f(y') dy'$$

$$F_2(f)(y) := f(y) \frac{1}{2} \int_0^y b(y', y - y') dy'.$$

Observamos que este sistema es la versión continua de (3), lo cual se ve más fácilmente si uno escribe  $a_{ij}c_i c_j - b_{ij}c_{i+j}$  en lugar de  $W_{ij}$  en (3). De hecho, trabajaremos con una forma más general que permite reacciones de fragmentación múltiple (en las que un cluster puede romperse en cualquier número de trozos, no únicamente dos). Ver chapter 2 para una descripción más detallada de estas ecuaciones. También es posible incluir en este modelo una descripción de la distribución espacial de las partículas; entre los trabajos en esta dirección se cuentan los de Laurençot y Mischler [54, 57], Herrero y Rodrigo [44] y Herrero, Velázquez y Wrzosek [45].

Un modelo obtenido por un acercamiento distinto es el de las *ecuaciones de Lifshitz-Slyozov* (inicialmente deducidas in [60]):

$$\partial_t f + \partial_x(Vf) = 0, \quad t, x \geq 0$$

$$u(t) + A \int_0^\infty x f(t, x) dx = Q, \quad t \geq 0,$$

donde  $x \geq 0$  representa el volumen de las partículas (que es una variable continua, en lugar de una discreta como antes),  $t \geq 0$  es la variable temporal,  $Q$  es la *super-saturación inicial total*,  $A > 0$  es un parámetro y  $V = V(t, x)$  es la velocidad de crecimiento de los clusters, dada por

$$V(t, x) = k(x)u(t) - q(x).$$

Aquí,  $k$  y  $q$  son funciones reales que dependen del mecanismo de transferencia de masa entre los clusters. En la evolución de los procesos de coagulación-fragmentación, estas ecuaciones describen un estadio posterior al descrito por las ecuaciones de Becker-Döring. De hecho, la conexión entre estos sistemas es conocida [78, 55, 19, 74]: bajo condiciones apropiadas sobre los coeficientes de coagulación y fragmentación  $a_i, b_i$  y las velocidades de crecimiento  $k, q$ , las soluciones de un reescalamiento de las ecuaciones de Becker-Döring convergen para tiempos grandes hacia soluciones en medidas de las ecuaciones de Lifshitz-Slyozov.

Hay también enfoques cinéticos a los fenómenos de coagulación y fragmentación, que tienen en cuenta los efectos del movimiento y las trayectorias de las partículas. Un enfoque difusivo donde se considera un núcleo de tipo Fokker-Planck puede encontrarse en el artículo clásico de Caffisch y Papanicolau [11]. Un estudio del límite hidrodinámico de este modelo ha sido hecho recientemente por Goudon, Jabin y Vasseur en [41, 40], y la interacción fluido-partícula ha sido analizada por varios autores (ver [49] y las referencias allí indicadas); en particular mencionamos aquí el caso en el que el fluido se rige por la ecuación de Stokes; para esto nos remitimos al artículo de Jabin y Otto [48]. Un estudio de modelos de núcleos de fragmentación en un contexto cinético ha sido hecho por Jabin y Soler [49], los cuales tienen una estructura similar a la que aparece en modelos biológicos de procesos multicelulares en la competición de células inmunes en tumores [7]. Un resumen de algunos modelos estadísticos en el contexto de la interacción fluido-partícula puede encontrarse en el artículo de Lasheras, Eastwood, Martínez-Bazán y Montañés [51].

Hay varios problemas relacionados con estas ecuaciones y los procesos para los cuales sirven como modelo. Uno querría saber, por ejemplo, si describen de forma precisa cierto fenómeno dado, y para qué coeficientes de coagulación y fragmentación, de forma que se puede predecir el comportamiento del objeto de estudio y posiblemente inferir las características microscópicas de las reacciones que tienen lugar. Para esto es útil desarrollar una comprensión aproximada del comportamiento de las soluciones de las ecuaciones relevantes, como su convergencia o no a un equilibrio; obtener aproximaciones asintóticas útiles de las soluciones en límites apropiados, que sean más simples que las propias ecuaciones o den información nueva sobre ellas; encontrar soluciones particulares; ser capaz de simular las soluciones experimentales; y finalmente, alcanzar una comprensión matemática precisa de la estructura de la ecuación que ayude en los problemas anteriores, y también como manera de poner a prueba y desarrollar las herramientas usadas en el estudio de las ecuaciones diferenciales.

Nuestro objeto de estudio en algunos de los capítulos siguientes serán las ecuaciones de coagulación-fragmentación, ya sea en su versión discreta (3) o continua (4). Este modelo incluye algunos otros que han sido ampliamente estudiados (como el sistema de Becker-Döring presentado anteriormente) y es apropiado para el estudio matemático que queremos llevar a cabo. A continuación detallamos nuestros objetivos y algunas de las dificultades a superar.

## Existencia de soluciones

Desde el punto de vista matemático, una de las primeras preguntas en el estudio de cualquier ecuación es la de la existencia de soluciones. Para las ecuaciones de coagulación-fragmentación esto se ha estudiado en varios trabajos, que dan un conocimiento bastante preciso de las condiciones bajo las cuales la ecuación de coagulación-fragmentación está bien planteada, ya sea en la forma discreta o continua; las condiciones usuales incluyen el requerimiento básico de que la función de distribución inicial  $f^0$  tenga masa finita  $\int_0^\infty y f^0(y) dy$  y que el número total de partículas  $\int_0^\infty f^0(y) dy$  sea también finite, así como algunas cotas sobre los coeficientes. Melzak y McLeod fueron los primeros en estudiar el problema [69, 66, 67, 68]; Galkin, Dubovskii y Stewart extendieron sus resultados en [38, 29] usando técnicas de compacidad en el espacio de funciones continuas en las condiciones anteriores. Ball, Carr, Penrose y Spouge estudiaron el sistema discreto de ecuaciones [5, 4, 85], y Stewart, Escobedo, Laurençot, Mischler y Perthame [86, 33, 35, 52, 56] trataron las ecuaciones continuas usando métodos de compacidad en el espacio de funciones integrables. Sus resultados para las ecuaciones continuas pueden enunciarse aproximadamente como sigue: definimos una solución débil de las ecuaciones de coagulación-fragmentación como una función  $f : (0, +\infty) \times [0, T) \rightarrow \mathbb{R}$  tal que (4) es cierta en el sentido de las distribuciones (ver la sección 5.1 para una definición precisa); entonces, el sistema tiene una solución débil no negativa cuando el coeficiente de coagulación  $a$  es menor que un múltiplo constante de  $1 + y + y'$ , el coeficiente de fragmentación  $b$  está localmente acotado en  $[0, +\infty) \times [0, +\infty)$  y el dato inicial  $f^0$  es una función integrable no negativa con momento de orden 1 finito; es decir,

$$\int_0^\infty (1 + y) f^0(y) dy < +\infty.$$

Una motivación del interés en extender estos resultados viene dada por lo siguiente: teniendo en cuenta que tanto las reacciones de coagulación como las de fragmentación conservan la masa total del sistema, una propiedad natural del comportamiento de las soluciones es la *conservación de la masa*: la masa total, dada por  $\int_0^\infty y f(y) dy$ , se mantiene constante a lo largo de la evolución temporal. Se sabe que esta propiedad *no* se cumple bajo ciertas condiciones sobre el tamaño de los coeficientes: por ejemplo, si el coeficiente de coagulación crece demasiado rápido con el tamaño de los clusters y la fragmentación no contrarresta esto, entonces la solución de las ecuaciones conserva la masa sólo hasta un tiempo crítica después del cual la masa es menor que la inicial; este fenómeno se conoce como *gelación* (ver los artículos [33, 35] de Escobedo, Laurençot, Mischler y Perthame), y puede interpretarse como la aparición de “partículas de tamaño infinito”. De forma parecida, cuando la fragmentación es demasiado fuerte para clusters de tamaño cercano a 0 (en el caso continuo), la masa puede también perderse; este fenómeno se conoce como *pulverización (shattering)* y puede pensarse causado por la creación de “partículas de tamaño 0”. Sin embargo, este fenómeno no ocurre a no ser que se permita un coeficiente de fragmentación

$b(y, y')$  no acotado cerca de  $y' = y = 0$ , de forma que deben extenderse las condiciones sobre los coeficientes para poder estudiarlo. La gelación y la pulverización son efectos matemáticos, interesantes por derecho propio, de los que merece la pena tener una mejor comprensión.

En este trabajo extendemos los resultados conocidos para incluir datos iniciales que no necesariamente satisfacen  $\int_0^\infty f^0(y) dy < +\infty$ , y coeficientes de coagulación y fragmentación que pueden ser no acotados para partículas pequeñas. Cuando sólo se tienen en cuenta efectos de coagulación, esto ha sido hecho por Escobedo y Mischler [34]; aquí incluimos la fragmentación en esta teoría de existencia, de forma que la interacción de ambos efectos puede estudiarse. En particular, demostramos que cuando la coagulación es suficientemente fuerte para partículas pequeñas en comparación con la fragmentación, la pulverización no puede ocurrir y la masa se conserva, mientras que puede haber pulverización cuando la fragmentación es más fuerte. Estos resultados se han obtenido en colaboración con Stéphane Mischler. Para dar un enunciado concreto y sencillo, demostramos lo siguiente:

**Teorema 1.** *Supongamos que:*

1. *Para algún  $\gamma \in \mathbb{R}$ ,  $0 < k_0 < 1$ , y  $C > 0$ , el coeficiente de fragmentación  $b$  está dado por*

$$b(y, y') = C \phi_\gamma(y) \frac{1}{y} \left( \frac{y'}{y} \right)^{-1-k_0}$$

*para todo  $0 < y' < y$ , donde para  $y > 0$  definimos*

$$\begin{aligned} \phi_\gamma(y) &= y^\gamma && \text{if } \gamma \leq 0, \\ \phi_\gamma(y) &= \min\{y^\gamma, y^{-l}\} && \text{if } \gamma > 0, \end{aligned}$$

*para algún número  $l > 0$ .*

2. *Para algún  $\alpha < \beta \in \mathbb{R}$ , el coeficiente de coagulación  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  está dado por*

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

*para todo  $y, y' > 0$ . Suponemos que*

$$\begin{aligned} \alpha &< \beta < 1 \\ 0 &< \lambda := \alpha + \beta < 1 \\ \beta - \alpha &< 1. \end{aligned}$$

*Si, además,*

$$\gamma < \lambda - 1 \quad \text{o} \quad \frac{\lambda - 1}{2} < \gamma,$$

*entonces para todo  $0 < T \leq +\infty$  hay una solución en medidas  $f$  de las ecuaciones de coagulación-fragmentación (descritas en el capítulo 2) con dato inicial  $f^0$ , y tal que  $f \in L^\infty([0, T], \dot{M}_1)$ . En el caso  $\frac{\lambda-1}{2} < \gamma$ , la masa total se conserva.*



De hecho, demostramos este resultado para un tipo más general de coeficientes de coagulación y fragmentación, a saber, coeficientes que están acotados superior e inferiormente por funciones de la forma anterior.

## Comportamiento asintótico

Bajo la condición de *balance detallado* (una condición física motivada por el requerimiento de que las reacciones microscópicas deben ser reversibles; ver el capítulo 6) y condiciones adicionales que aseguran que la masa se conserva, se conoce desde hace tiempo que las ecuaciones de Becker-Döring muestran el siguiente comportamiento: cuando la masa inicial total es menor que cierto valor crítico  $\rho_s$ , todas las soluciones convergen de forma fuerte a una solución de equilibrio con la misma masa total, la cual es también el único equilibrio con esa masa. Por otra parte, cuando la masa inicial está por encima de ese valor crítico, entonces todas las soluciones convergen en un sentido débil al único equilibrio cuya masa es igual a la crítica, mientras que el exceso de masa  $\rho - \rho_s$  se concentra en clusters cada vez mayores según pasa el tiempo. Esto fue demostrado por Ball, Carr y Penrose en [5, 3], y ha habido intentos de extender este importante resultado a modelos más generales: Carr y da Costa [16] lo probaron para las ecuaciones de Becker-Döring generalizadas cuando el dato inicial decrece suficientemente rápido para tamaños grandes de las partículas; da Costa [20] demostró lo mismo para datos iniciales suficientemente pequeños. Se esperaba que estas condiciones adicionales sobre el dato inicial pudieran eliminarse, y se espera que el mismo resultado sea cierto en condiciones generales para las ecuaciones de coagulación-fragmentación, pero esto es todavía una conjetura. En el capítulo 6 extendemos los resultados de Carr y da Costa probando que las restricciones sobre el dato inicial no son necesarias para las ecuaciones de Becker-Döring generalizadas. Nuestro principal resultado es el siguiente:

**Teorema 2.** *Supongamos las hipótesis 6.2.6-6.2.12 del capítulo 6, y sea  $c = \{c_j\}_{j \geq 1}$  una solución admisible de las ecuaciones de Becker-Döring generalizadas (3) (las hipótesis consisten esencialmente en suponer una hipótesis de balance detallado y condiciones suficientes para asegurar que se conserva la masa; recordemos que las ecuaciones generalizadas de Becker-Döring son un caso particular de las ecuaciones de Becker-Döring en el que sólo se consideran reacciones en las que uno de los clusters implicados tiene tamaño menos que un cierto  $N$ ), Llamemos  $\rho_0 := \sum_{j=1}^{\infty} j c_j(0)$ , la densidad inicial.*

1. *Si  $0 \leq \rho_0 \leq \rho_s$  entonces  $c$  converge fuertemente al equilibrio con densidad  $\rho_0$ .*
2. *Si  $\rho_s < \rho_0$  entonces  $c$  converge débilmente al equilibrio con densidad  $\rho_s$ .*

Una descripción más precisa de la convergencia de las soluciones se da en el capítulo 6. La demostración de este resultado se apoya en una cuidadosa estimación del tamaño de la cola de una solución, la cual está inspirada en un método inicialmente usado por Laurençot y Mischler en [55] para probar la unicidad de

las soluciones. La estimación en sí es interesante porque es posible que pueda ser mejorada para obtener información adicional sobre el comportamiento de las soluciones; tal como está, depende fuertemente del hecho de que no ocurren reacciones en las que los dos clusters son de más de un cierto tamaño  $N$ , así que no puede generalizarse directamente para dar una demostración del resultado correspondiente para las ecuaciones generales de coagulación-fragmentación. Sin embargo, proporciona una nueva técnica para atacar el problema y podría ayudar a encontrar una generalización de nuestros resultados.

## Simulación numérica y aproximación asintótica

Existen grandes dificultades para simular numéricamente las ecuaciones de coagulación-fragmentación debido al enorme número de variables necesarias y las escalas de tiempo tan distintas que influyen en la evolución de las soluciones; se necesita una comprensión previa del comportamiento esperado. En el capítulo 7 damos una aproximación asintótica de las soluciones de las ecuaciones de Becker-Döring en un caso en el que la forma de los coeficientes de coagulación y fragmentación es suficientemente sencilla como para que se pueda presentar una teoría limpia del comportamiento de las soluciones y ésta pueda compararse a una solución numérica de las ecuaciones. Se espera que el método sea aplicable a situaciones más complejas, y de hecho ha sido usado posteriormente por Bonilla, Carpio y Neu [8] para estudiar el caso en el que hay una densidad crítica, de forma que la nucleación y el “coarsening” tienen lugar.

El modelo concreto que usamos es el caso en el que la *energía de enlace* de los clusters, una cantidad relacionada con la proporción entre los coeficientes de coagulación y fragmentación (ver la sección 2.5), depende linealmente del tamaño del cluster, y donde suponemos que la fragmentación no depende del tamaño del cluster; esto es, estamos suponiendo que todos los clusters tienen la misma tendencia a desprenderse de una partícula, la cual es independiente de su tamaño. Se piensa que este caso es un modelo adecuado para la agregación de lípidos en disolución acuosa formando *micelas* cilíndricas, que se forman debido al hecho de que las moléculas de los lípidos implicadas tienen una parte hidrófoba (“cola”) y una hidrófila (“cabeza”), de manera que tienen tendencia a mantenerse cerca de forma tal que las colas están juntas y alejadas del agua, mientras que las cabezas apuntan hacia el agua. Debido al tamaño de la molécula concreta de la que se trate, los lípidos pueden agruparse en clusters esféricos, cilíndricos o en membranas; cada forma de agrupación tiene una energía de enlace distinta, y parece que una dependencia lineal del tamaño es una buena aproximación para las micelas cilíndricas [46, chapter 15].

Desarrollamos una aproximación analítica para el comportamiento de la solución en el límite en el cual la concentración inicial es mucho mayor que la *concentración micelar crítica* (ver capítulo 7 para más detalles) mediante el método de expansiones asintóticas acopladas (“matched asymptotic expansions”). Mostramos que durante la evolución de la solución aparecen tres partes distinguidas o “eras”, en las cuales

las escalas temporales son muy distintas: durante la primera parte, el número de monómeros (partículas individuales) decrece muy rápidamente y se crea un gran número de clusters pequeños, de forma que la distribución de tamaños comienza a parecerse a una función continua; durante la segunda parte, esta función evoluciona como una solución de la ecuación del calor; finalmente, la solución se aproxima lentamente a una distribución de equilibrio en la que clusters de tamaños muy distintos coexisten. Estos resultados se comparan a una solución numérica y mostramos que coinciden bien con ella.

## La ecuación de Wigner-Poisson-Fokker-Planck

La modelización de la difusión cuántica es uno de los campos de interés matemáticos en mecánica cuántica que no está bien entendido por completo actualmente. Algunos trabajos destacados que apuntan a un análisis de correcciones difusivas en modelos surgidos de la cinética cuántica se deben a Caldeira y Leggett [12], Diósi [24, 25] y Diósi *et al.* [26]. El contexto apropiado para este tipo de modelos difusivos es el de sistemas cuánticos abiertos, esto es, un conjunto de electrones interactuando con un baño térmico (un conjunto infinito de osciladores armónicos en equilibrio termodinámico) y que pueden intercambiar masa con su entorno (ver [12], [21], [37], [18]).

La ecuación de Wigner-Fokker-Planck es:

$$\begin{aligned} \frac{\partial W}{\partial t} + (\xi \cdot \nabla_x)W + \Theta[V]W \\ = \frac{D_{pp}}{m^2} \Delta_\xi W + 2\lambda \operatorname{div}_\xi(\xi W) + 2 \frac{D_{pq}}{m} \operatorname{div}_x(\nabla_\xi W) + D_{qq} \Delta_x W, \end{aligned} \quad (6)$$

donde  $W$  es la distribución de (quasi)-probabilidad,  $D_{pp}$ ,  $D_{pq}$ ,  $D_{qq}$ ,  $m$  y  $\lambda$  son constantes físicas y  $\Theta[V]W$  es el término cuadrático no lineal asociado con el potencial autoconsistente de Hartree en 3D (ver (1.12) más abajo). En un artículo reciente [2] se estudia el buen planteamiento del sistema conocido como de Wigner-Poisson-Fokker-Planck (WPFPP) en el enfoque Markoviano más sencilla para el caso (a temperatura alta) sin fricción ( $\lambda = 0$ ). Éste es un modelo cinético-cuántico (en la representación de Wigner) con mecanismo disipativo de Fokker-Planck sólo en la dirección  $\xi$  (es decir,  $D_{pq} = D_{qq} = 0$ ):

$$\frac{\partial W}{\partial t} + (\xi \cdot \nabla_x)W + \Theta[V]W = \frac{D_{pp}}{m^2} \Delta_\xi W, \quad x, \xi \in \mathbb{R}^3, t > 0. \quad (7)$$

La forma de Lindblad [61] de este operador cinético a nivel de la matriz de densidad implica que el problema es matemáticamente consistente, en el sentido de que la ecuación preserva la positividad de la matriz de densidad inicial. Los problemas de existencia local, unicidad, estabilidad, regularidad y comportamiento para tiempos grandes (en el caso de soluciones globales) de soluciones “mild” de (7) se

atacan también en [2]. En [18], los autores llevan a cabo una deducción matemáticamente rigurosa de la ecuación de Fokker-Planck sin fricción a partir del modelo de Caldeira-Leggett presentado en [12]. Además, investigan otras ecuaciones de tipo Fokker-Planck obtenidas del Hamiltoniano de Caldeira-Leggett mediante diferentes mecanismos de difusión y reescalamientos (temperatura fija y límite para tiempos grandes), especialmente una ecuación del calor con un término de fricción para el proceso radial en el espacio de fases. Asimismo, la velocidad de decrecimiento en tiempo de las soluciones al modelo hidrodinámico con viscosidad (esto es, las ecuaciones de momentos para las densidades de carga y corriente acopladas a la ecuación de Poisson para el potencial electrostático) asociadas a la ecuación de WFPF en 1D se estudian en a través del método de disipación de la entropía.

El capítulo 8 está dedicado a demostrar existencia de soluciones globales de tipo “mild” (esto es, soluciones de la ecuación de WFPF escrita en una forma integral equivalente, definidas en  $[0, \infty)$ ) para el tipo más general de modelos de WFPF físicamente relevantes (sólo requerimos  $D_{pq} = 0$ ). Se basa en los resultados de J. L. López, Juan José Nieto y el autor que han sido publicados en [13]. Tratamos el análisis del siguiente problema de valores iniciales:

$$\frac{\partial W}{\partial t} + (\xi \cdot \nabla_x)W + \Theta[V]W = \frac{D_{pp}}{m^2} \Delta_\xi W + 2\lambda \operatorname{div}_\xi(\xi W) + D_{qq} \Delta_x W \quad (8)$$

$$W(x, \xi, 0) = W_0(x, \xi), \quad (9)$$

acoplado a la ecuación de Poisson para la determinación del potencial electrostático autoconsistente: c potential:

$$V(x, t) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{n(y, t)}{|x - y|} dy, \quad (10)$$

con

$$n(x, t) = \int_{\mathbb{R}_\xi^3} W(x, \xi, t) d\xi. \quad (11)$$

Aquí,  $\Theta[V]$  representa el operador pseudo-diferencial

$$\begin{aligned} \Theta[V]W(x, \xi, t) &= \frac{i}{(2\pi)^3} \int_{\mathbb{R}_\eta^3} \int_{\mathbb{R}_{\xi'}^3} \frac{V(x + \frac{\hbar}{2m}\eta, t) - V(x - \frac{\hbar}{2m}\eta, t)}{\hbar} \\ &\quad \times W(x, \xi', t) e^{-i(\xi - \xi') \cdot \eta} d\xi' d\eta, \end{aligned} \quad (12)$$

donde  $\hbar$  denota la constante de Planck reducida y  $m$  la masa efectiva de las partículas, con  $\lambda, D_{pp}, D_{qq}$  constantes positivas relacionadas con las interacciones entre las partículas y el baño térmico (ver [24]):

$$\lambda = \frac{\eta}{2m}, \quad D_{pp} = \eta k_B T, \quad D_{qq} = \frac{\eta \hbar^2}{12m^2 k_B T}, \quad (13)$$

donde  $\eta > 0$  es la constante de acoplamiento (amortiguamiento) del baño,  $k_B$  la constante de Boltzmann y  $T$  la temperatura del baño. Asimismo,

$$Q = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} W(x, \xi, t) d\xi dx$$

es la carga total del sistema, que se conserva durante la evolución. Esta ecuación es la aproximación Markoviana más simple que tiene en cuenta efectos de fricción y disipación, tal que la correspondiente ecuación maestra para la matriz de densidad del conjunto de partículas pertenece a la clase de Lindblad (como se demuestra en [25]), asegurando la conservación de la positividad para todas las condiciones iniciales y todo tiempo. De hecho, si se quita el término elíptico que involucra  $\Delta_x W$  en la ecuación (8), entonces el núcleo de colisión de Fokker-Planck sobrante (que tiene en cuenta sólo fricción y efectos de difusión en  $\xi$ ) impide que la ecuación pertenezca a la familia de Lindblad. Así, es este caso el problema no sería matemáticamente consistente ni significativo en un contexto físico.

La ecuación de WFPF (8) surge del siguiente modelo de evolución (ver [2]) para la matriz de densidad  $\rho(x, y, t) \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ :

$$\begin{aligned} \frac{\partial \rho}{\partial t} = & -\frac{i}{\hbar}(H_x - H_y)\rho - \lambda(x - y) \cdot (\nabla_x - \nabla_y)\rho \\ & + \left( D_{qq} |\nabla_x + \nabla_y|^2 - \frac{D_{pp}}{\hbar^2} |x - y|^2 \right) \rho, \end{aligned}$$

donde  $H_x$  y  $H_y$  son copias del Hamiltoniano del electrón

$$H_z = -\frac{\hbar^2}{2m}\Delta_z + V(z, t)$$

actuando sobre las variables  $x$  e  $y$ , respectivamente. De hecho, teniendo en cuenta que la función de Wigner del conjunto de electrones  $W : \mathbb{R}_x^3 \times \mathbb{R}_\xi^3 \times [0, \infty) \rightarrow \mathbb{R}$  está definida por

$$W(x, \xi, t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}_\eta^3} \rho\left(x + \frac{\hbar}{2m}\eta, x - \frac{\hbar}{2m}\eta, t\right) e^{-i\xi \cdot \eta} d\eta,$$

se puede deducir fácilmente que la ley de evolución para  $W(x, \xi, t)$  está descrita por la ecuación (8). La positividad del operador de matriz de densidad

$$[R(t)f](x) = \int_{\mathbb{R}_y^3} f(y)\rho(x, y, t) dy \in L^2(\mathbb{R}^3)$$

(garantizada por la condición de Lindblad) implica que la transformada de Husimi, definida por la siguiente convolución de la función de Wigner con un núcleo Gaussiano

$$W^H(x, \xi, t) = W(x, \xi, t) *_{x, \xi} \left( \frac{m}{\hbar\pi} \right)^3 \exp \left\{ -\frac{m}{\hbar} (|x|^2 + |\xi|^2) \right\}, \quad (14)$$

es no negativa en cada punto en  $\mathbb{R}_x^3 \times \mathbb{R}_\xi^3$ . Asimismo, la condición de Lindblad y una fricción no nula ( $\lambda > 0$ ) implican que el operador de Fokker-Planck es uniformemente elíptico en  $\mathbb{R}_x^3 \times \mathbb{R}_\xi^3$ .

Contrariamente a las técnicas comunes que conducen a la existencia global, regularidad y comportamiento asintótico de las soluciones a sistemas clásicos de (Vlasov)-Fokker-Planck, nuestras técnicas evitan el uso explícito de normas  $S_p$  (ver [17, 9, 76] por ejemplo) para controlar la función de distribución. En realidad, nuestra demostración no requiere más regularidad que  $L^1(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3) \cap L^1(\mathbb{R}_\xi^3; L^2(\mathbb{R}_x^3))$  y el control de la energía cinética de la función de Wigner inicial. Notemos también que el espacio natural donde vive la función de Wigner es  $L^2(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)$ , lo cual puede verse a partir de la formulación original con la matriz de densidad en el contexto más amplio de los problemas de Wigner. De hecho, multiplicando formalmente la ecuación (8) por  $W$  e integrando en  $x$  y  $\xi$  tenemos

$$\|W(t)\|_{L^2(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)} \leq \|W_0\|_{L^2(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)} e^{6\lambda t}.$$

Sin embargo, la presencia de un núcleo de regularización de Fokker-Planck en el modelo a estudiar nos permite desarrollar una teoría en  $L^1$  para la ecuación de WFPF y explotar las propiedades de regularización del operador de Fokker-Planck para obtener soluciones regulares. El hecho de que no se dispone de un principio del máximo para ecuaciones del tipo Wigner es significativo, de forma que en general la función de Wigner cambia de signo incluso si empezamos con un dato inicial positivo. Éste es el motivo de que la función de Husimi (14), junto con la regularización elíptica en la variable  $x$ , tengan un papel esencial en nuestro análisis.

En el capítulo 8 demostramos el siguiente resultado de existencia global en tiempo:

**Teorema 3.** *Sea  $W_0 \in L^1(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3) \cap L^1(\mathbb{R}_\xi^3; L^2(\mathbb{R}_x^3))$  tal que*

$$\int_{\mathbb{R}_x^3} \int_{\mathbb{R}_\xi^3} |\xi|^2 W_0(x, \xi) d\xi dx < \infty.$$

*Entonces, la ecuación de the Wigner-Poisson-Fokker-Planck equation (8)–(13) admite una única solución global de tipo “mild”*

$$W \in C([0, \infty); L^1(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)) \cap C([0, \infty); L^1(\mathbb{R}_\xi^3; L^2(\mathbb{R}_x^3))).$$

*Además,*

$$W \in C((0, \infty); W^{1,1} \cap W^{1,\infty}(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)).$$

*Asimismo, la densidad de carga (11) y el potencial eléctrico (10) satisfacen las siguientes propiedades de regularidad de tipo Hölder: para todo  $t > 0$ ,*

$$n(\cdot, t) \in C^{0,\alpha}(\mathbb{R}_x^3) \text{ con } 0 < \alpha < \frac{1}{2}, \quad V(\cdot, t) \in C^{1,\beta}(\mathbb{R}_x^3) \text{ con } 0 < \beta < \frac{1}{3}.$$



# Chapter 1

## Introduction

This work treats mainly the problem of existence of solutions for two different equations: the continuous coagulation-fragmentation equations and the Wigner-Poisson-Fokker-Planck equation. In addition, some aspects of the qualitative behavior of the coagulation-fragmentation equations are studied. The thesis is organized as follows: in this introduction we briefly present the context of both equations and the main results obtained. In chapters 2–4 we give some preliminar results and background which is needed for the later treatment of the continuous coagulation-fragmentation system of equations; in chapter 5 we state and prove our existence results, and on the way we rederive some of the already known results on the topic, as the techniques involved are similar. In particular, section 5.7.3 contains results which show the interplay between singular coagulation and fragmentation coefficients. Chapter 6 contains a new result on the asymptotic behavior of the generalized Becker-Döring system of equations (which is a particular case of the discrete coagulation-fragmentation equations, as explained below), and chapter 7 shows an explicit approximation to the behavior of solutions of the Becker-Döring equations in a particular case, together with numerical solutions that back up the validity of the approximation. Finally, chapter 8 contains our result on the Wigner-Poisson-Fokker-Planck equation, which essentially consists of an existence theory in  $L^1$ . Some appendices are given which contain a summary of known results which are necessary in the development of the rest of this work. Below we give a short introduction to each of the topics treated. Of course, a good part of the content is here thanks to the work of other people and has been done with their collaboration, and I would like to name them here. I want to thank Juan Soler for his guidance and help on the topic of transport and evolution equations in general, and for his work on the preparation of this thesis. The work gathered in chapters 5 and 6 was carried out together with Stéphane Mischler, and I wish to thank him for his suggestions and help; that in chapter 6 was published in [14]. Also, I would like to thank Luis Bonilla and John Neu for giving me the opportunity to work with them on the numerical solution and asymptotic analysis of the particular case of the equations which is collected in chapter 7, and which was published in [73]. José Luis López



and Juan José Nieto taught me about the Wigner equation and encouraged me to work with them, and I'm very grateful for that; the results obtained, gathered in chapter 8, have also been published in [13]. I also want to thank P. E. Jabin for his explanations and help on the modelling of particle-fluid coupling, and Magdalena Rodríguez for the design of the figures in the appendices.

## 1.1. The coagulation-fragmentation equations

Many physical phenomena consist of a great number of small particles that can stick together in some way to form larger units. For example, when a substance changes from its gas phase to a liquid phase, the molecules in the gas start to come together to form larger and larger droplets of the liquid phase; analogous processes occur in other kinds of phase changes [59] and in the behavior of aerosols (liquid or solid particles suspended in a gas) [27]. Crystallization in colloids [39] and the segregation of binary alloys [60, 89, 65] are other examples of this situation. In biology, the formation of protein crystals from the lipidic cubic phase of membranes [42] and the aggregation of certain lipids to form spherical clusters (*micelles*) or lipid bilayers (*membranes*) follow a similar process [73, 46]. These examples are very general, but the surprising point is that in many cases they have characteristics that allow a useful common description.

A good understanding of these phenomena is worth having, and it has been attempted from several standpoints: thermodynamics and statistical mechanics give very useful information on equilibrium situations, but can say little away from them (see section 2.5 and [46, 81]). Some kinetic equations have been proposed as a model for these processes, of which we give next a short account; we can refer to the reviews [58, 1, 27, 28] for more information on the topic. The models can be classified according to the scale of the description they intend to give: *microscopic descriptions* try to model the evolution of a finite set of individual particles, and usually suppose that events in which two particles stick together occur in a random way. The first model of this kind was proposed by Marian Smoluchowski [83, 84]; another example is the Marcus-Lushnikov process [63, 64]. *Mesosopic descriptions* or *mean-field models* are concerned with the evolution of the number of particles of each possible size, and not that of the individual particles; these descriptions are valid when the number of particles is sufficiently high. Mesoscopic models may or may not include the spatial distribution of the particles. In the present work we will focus on this level of description, so some models of this type will be described later in detail; in particular we will study mathematical issues related to the *coagulation-fragmentation equation* at length. Finally, *macroscopic models* describe the evolution of some macroscopic quantities, which represent some kind of average of the microscopic properties of the system (such as the mean cluster size).

Among the mean-field models, probably the best-known are the *Smoluchowski coagulation equations*, proposed in 1917 by Smoluchowski in their discrete version

[84], and extended to the continuous setting by Müller in 1928 [72]:

$$\frac{d}{dt}c_i = \sum_{j=1}^{i-1} a_{j,i-j}c_jc_{i-j} - \sum_{j=1}^{\infty} a_{ij}c_ic_j \quad \text{for } i \geq 1.$$

Here the  $a_{ij}$  for integers  $i, j \geq 1$  are nonnegative numbers called *coagulation coefficients*; this is an infinite system of ordinary differential equations in the unknowns  $c_i = c_i(t)$  for  $i \geq 1$ , which represent the densities of clusters (aggregates of particles) of size  $i$  depending on the time  $t$ . The basic assumption is that the rate of occurrence of the coagulation reaction where a cluster of size  $i$  joins a cluster of size  $j$  is proportional to both the concentrations  $c_i, c_j$  of  $i$ - and  $j$ -clusters; this is known as the *law of mass action*. Then, the positive term on the right hand side of the above equation represents the number of coagulation reactions taking place that have a cluster of size  $i$  as their product; the negative term represents the number of reactions in which a cluster of size  $i$  joins some other cluster, thus giving a cluster of size greater than  $i$ . A generalization of this equation will be carefully described in chapter 2, so we do not extend here on the matter.

The Smoluchowski coagulation equation only takes into account all possible *coagulation* reactions between pairs of clusters but does not include the possible *fragmentation* of clusters. In turn, the *Becker-Döring cluster equations*, which are given by the following infinite set of equations, describe coagulation and binary fragmentation events, but include only those that involve reactions between individual particles and other clusters (so they do not take into account, for example, reactions between two clusters of size three):

$$\frac{d}{dt}c_i = J_{i-1} - J_i, \quad r \geq 2 \tag{1.1}$$

$$\frac{d}{dt}c_1 = -J_1 - \sum_{i=1}^{\infty} J_i, \tag{1.2}$$

where  $J_i := a_i c_1 c_i - b_{i+1} c_{i+1}$  for  $i \geq 1$  and  $a_i, b_i$  are the *coagulation* and *fragmentation coefficients*, respectively ( $a_i$  corresponds to  $a_{i,1}$  in the Smoluchowski equation, as now we only consider reactions involving an individual particle and a cluster of arbitrary size). These equations were originally proposed by Becker and Döring [6] in 1935; a review by M. Slemrod can be found in [82]. A straightforward generalization of both the Smoluchowski and Becker-Döring equations are the *discrete coagulation-fragmentation equations*:

$$\frac{d}{dt}c_i = \frac{1}{2} \sum_{j=1}^{i-1} W_{j,i-j} - \sum_{j=1}^{\infty} W_{ij} \quad \text{for } i \geq 1, \tag{1.3}$$

where  $W_{ij} := a_{ij}c_ic_j - b_{ij}c_{i+j}$ . The *generalized Becker-Döring equations* are the particular case of this system where, for some  $N \in \mathbb{N}$ ,  $a_{ij} = b_{ij} = 0$  whenever

$\min\{i, j\} \geq N$ ; this is to say that we only consider reactions in which at least one of the involved clusters has a size less than  $N$ .

Part of our work deals with some issues related to the mathematical theory of the continuous version of the coagulation-fragmentation equations, given by the following integro-differential equation:

$$\frac{\partial}{\partial t} f = C(f) + F(f), \quad t, y \in (0, +\infty) \quad (1.4)$$

$$f(0, y) = f^0(y), \quad y \in (0, +\infty), \quad (1.5)$$

where the coagulation and fragmentation terms are given by:

$$C(f) := C_1(f) - C_2(f)$$

$$F(f) := F_1(f) - F_2(f)$$

$$C_1(f)(y) := \frac{1}{2} \int_0^y a(y', y - y') f(y') f(y - y') dy'$$

$$C_2(f)(y) := f(y) \int_0^\infty a(y, y') f(y') dy'$$

$$F_1(f)(y) := \int_y^\infty b(y', y - y') f(y') dy'$$

$$F_2(f)(y) := f(y) \frac{1}{2} \int_0^y b(y', y - y') dy'.$$

Note that this system is the continuous version of (1.3), which is seen more easily if one writes  $a_{ij}c_i c_j - b_{ij}c_{i+j}$  instead of  $W_{ij}$  in (1.3). Actually, we will work with a more general form that allows multiple fragmentation reactions (where a cluster may break into any number of pieces, and not only two). See chapter 2 for a more detailed description of these equations. It is also possible to include in this model a description of the spatial distribution of the particles; works in this direction include those by Laurençot and Mischler [54, 57], Herrero and Rodrigo [44] and Herrero, Velázquez and Wrzosek [45].

A model obtained from a different approach are the *Lifshitz-Slyozov equations* (initially derived in [60]):

$$\begin{aligned} \partial_t f + \partial_x(Vf) &= 0, & t, x \geq 0 \\ u(t) + A \int_0^\infty x f(t, x) dx &= Q, & t \geq 0, \end{aligned}$$

where  $x \geq 0$  represents the volume of the clusters (which is a continuous variable, rather than a discrete one as before),  $t \geq 0$  is the time variable,  $Q$  is the *total initial supersaturation*,  $A > 0$  is a parameter and  $V = V(t, x)$  is the rate of growth of the clusters, given by

$$V(t, x) = k(x)u(t) - q(x).$$

Here,  $k$  and  $q$  are real functions that depend on the mechanism of mass transfer between the clusters. In the evolution of coagulation-fragmentation processes, these equations describe a later stage than the Becker-Döring equations. In fact, the connection between these systems is known [78, 55, 19, 74]: under suitable conditions on the coagulation and fragmentation coefficients  $a_i, b_i$  and the rates of growth  $k, q$ , solutions to a rescaling of the Becker-Döring equations converge for large times to measure-valued solutions to the Lifshitz-Slyozov equations.

There are also kinetic approaches to the phenomenon of coagulation and fragmentation, which take into account the effects of the movement and trajectories of the particles. A diffusive approach where a Fokker-Planck-type kernel is considered can be found in the classical Caffisch and Papanicolau's paper [11]. A study of the hydrodynamic limits of this model has recently been given by Goudon, Jabin and Vasseur in [41, 40], and particle-fluid interaction has been analyzed by several authors (see [49] and the references therein); in particular we mention here the case where the fluid is governed by the Stokes equation; for this we refer to the paper by Jabin and Otto [48]. A study in a kinetic context of fragmentation kernels has been given by Jabin and Soler [49], which have a similar structure to those in models for biological processes of multicellular systems in tumor immune cells competition [7]. A review of some statistical models in the context of bubble-fluid interaction can be found in the paper by Lasheras, Eastwood, Martínez-Bazán and Montañés [51].

There are a number of problems related to these equations and the processes they serve as a model for. One would like to know, for example, whether they accurately describe a given phenomenon, and for which choice of coagulation and fragmentation coefficients, so that one can predict the behavior of the object of study and possibly infer the microscopic characteristics of the reactions taking place. For this it is helpful to develop a rough understanding of the behavior of the solutions of the relevant equations, such as their convergence or not to an equilibrium; to obtain useful asymptotic approximations to the solutions in some suitable limits, which are simpler than the equations themselves or give new information on them; to find particular solutions; to be able to simulate the solutions numerically in order to compare them to experimental data; and finally, to have a precise mathematical understanding of the structure of the equation to help in the previous matters, and also as a way to test and develop the tools used in the study of differential equations.

The object of our study in some of the following chapters will be the coagulation-fragmentation equations, either in their discrete form (1.3) or the continuous one (1.4). This model includes some others that have been widely studied (such as the Becker-Döring system presented above) and is well-suited for the mathematical study we want to carry out. In the following we detail some of the difficulties to overcome and our aims.

### 1.1.1. Existence of solutions

From the mathematical point of view, one of the first questions in the study of any equation is that of the existence of solutions. For the coagulation-fragmentation equations this has been studied in a number of papers, which give a quite precise knowledge on the conditions under which the coagulation-fragmentation equation is well-posed either in the continuous or the discrete form; the usual conditions include the basic requirement that the initial distribution function  $f^0$  should have a finite mass  $\int_0^\infty y f^0(y) dy$  and that the total number of particles  $\int_0^\infty f^0(y) dy$  is also finite, as well as some bounds on the coefficients. Melzak and McLeod first studied the issue [69, 66, 67, 68]; Galkin, Dubovskii and Stewart extended their results in [38, 29] using compactness techniques in the space of continuous functions in the above conditions. Ball, Carr, Penrose and Spouge studied the discrete system of equations [5, 4, 85], and Stewart, Escobedo, Laurençot, Mischler and Perthame [86, 33, 35, 52, 56] treated the continuous equations using compactness methods in the space of integrable functions. Their results for the continuous equations can be roughly stated as follows: we define a weak solution to the coagulation-fragmentation system of equations as a function  $f : (0, +\infty) \times [0, T) \rightarrow \mathbb{R}$  such that (1.4) holds in the sense of distributions (see section 5.1 for the precise definition); then, the system has a nonnegative weak solution when the coagulation coefficient  $a$  is less than a constant multiple of  $1 + y + y'$ , the fragmentation coefficient  $b$  is locally bounded on  $[0, +\infty) \times [0, +\infty)$  and the initial data  $f^0$  is a nonnegative integrable function with finite moment of order one; this is,

$$\int_0^\infty (1 + y) f^0(y) dy < +\infty.$$

A motivation of the interest in extending these results is given by the following: considering that both the coagulation and fragmentation reactions preserve the total mass in the system, a natural property of the behavior of solutions to this system is *mass conservation*: the total mass, given by  $\int_0^\infty y f(y) dy$ , remains constant during time evolution. This property is known *not* to hold under certain conditions on the size of the coefficients: for example, if the coagulation coefficient grows too rapidly with cluster size and fragmentation does not counter this, then the solution to the equations conserves mass only up to a given critical time, after which the mass is less than the initial one; this phenomenon is known as *gelation* (see the papers [33, 35] by Escobedo, Laurençot, Mischler and Perthame), and can be interpreted as the apparition of “particles of infinite size”. In a similar way, when fragmentation is too strong for clusters of size close to 0 (in the continuous case), mass may also be lost; this phenomenon is known as *shattering*, and can be thought of as caused by the creation of “particles of size 0”. However, this phenomenon does not happen unless one allows for a fragmentation coefficient  $b(y, y')$  which is unbounded near  $y' = y = 0$ , so one must extend the conditions on the coefficients in order to study it. Gelation and shattering are mathematical effects, interesting in their own right, and which are worth to have a better understanding of.

In this work we extend the known existence results to include initial data that does not necessarily satisfy  $\int_0^\infty f^0(y) dy < +\infty$ , and coagulation and fragmentation coefficients that can be unbounded for small particles. When only coagulation effects are taken into account, this has been done by Escobedo and Mischler [34]; here we include fragmentation in this existence theory, so that the interaction of both effects can be studied. In particular, we prove that when coagulation is strong enough for small particles when compared to fragmentation, shattering does not take place and mass is conserved, while shattering may happen when fragmentation is stronger. These results were obtained in collaboration with Stéphane Mischler. To give a concrete and simple statement, we prove the following:

**Theorem 1.1.1.** *Assume that:*

1. *For some  $\gamma \in \mathbb{R}$ ,  $0 < k_0 < 1$ , and  $C > 0$ , the fragmentation coefficient  $b$  is given by*

$$b(y, y') = C \phi_\gamma(y) \frac{1}{y} \left( \frac{y'}{y} \right)^{-1-k_0}$$

*for all  $0 < y' < y$ , where for  $y > 0$  we set*

$$\begin{aligned} \phi_\gamma(y) &= y^\gamma && \text{if } \gamma \leq 0, \\ \phi_\gamma(y) &= \min\{y^\gamma, y^{-l}\} && \text{if } \gamma > 0, \end{aligned}$$

*for some number  $l > 0$ .*

2. *For some  $\alpha < \beta \in \mathbb{R}$ , the coagulation coefficient  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  is given by*

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

*for all  $y, y' > 0$ . We assume that*

$$\begin{aligned} \alpha &< \beta < 1 \\ 0 &< \lambda := \alpha + \beta < 1 \\ \beta - \alpha &< 1. \end{aligned}$$

*If, in addition,*

$$\gamma < \lambda - 1 \quad \text{or} \quad \frac{\lambda - 1}{2} < \gamma,$$

*then for all  $0 < T \leq +\infty$  there is a measure solution  $f$  to the coagulation-fragmentation equations (described in chapter 2) with initial data  $f^0$ , and such that  $f \in L^\infty([0, T], \dot{M}_1)$ . In the case  $\frac{\lambda-1}{2} < \gamma$ , the total mass is conserved.*

Actually, we prove the above result for a more general class of coagulation and fragmentation coefficients; namely, coefficients which are bounded above and below by functions of the above form.

### 1.1.2. Asymptotic behavior

Under the condition of *detailed balance* (a physical condition motivated by the requirement that microscopic reactions should be reversible; see chapter 6) and further conditions that ensure that mass is conserved, it has been known for some time that the Becker-Döring equations exhibit the following behavior: when the initial total mass is less than some critical value  $\rho_s$ , all solutions converge in a strong way to an equilibrium solution with the same total mass, which is also the only equilibrium with that mass. On the other hand, when the initial mass  $\rho$  is above that critical value, then all solutions converge in a weak sense to the only equilibrium whose mass is the critical one, while the excess mass  $\rho - \rho_s$  is concentrated in larger and larger clusters as time passes. This was proved by Ball, Carr and Penrose in [5, 3], and there have been attempts to extend this important result to more general models: Carr and da Costa [16] proved it for the generalized Becker-Döring equations when the initial data decays rapidly enough for large cluster sizes; da Costa [20] then proved the same for small enough initial data. It was expected that these additional conditions on the initial data could be removed, and the same result is expected to hold under general conditions for the coagulation-fragmentation equations, but this is still a conjecture. In chapter 6 we extend Carr and da Costa's results by showing that the restrictions on the initial data are indeed not necessary for the generalized Becker-Döring equations. Our main result is the following:

**Theorem 1.1.2.** *Assume hypotheses 6.2.6-6.2.12 in chapter 6, and let  $c = \{c_j\}_{j \geq 1}$  be an admissible solution of the generalized Becker-Döring equations (1.3) (the hypotheses essentially consist in assuming a detailed balance hypotheses and sufficient conditions that ensure mass conservation; recall that the generalized Becker-Döring equations are a particular case of the Becker-Döring equations in which only reactions where one of the involved clusters is of size less than a certain  $N$  are considered). Call  $\rho_0 := \sum_{j=1}^{\infty} j c_j(0)$ , the initial density.*

1. *If  $0 \leq \rho_0 \leq \rho_s$  then  $c$  converges strongly to the equilibrium with density  $\rho_0$ .*
2. *If  $\rho_s < \rho_0$  then  $c$  converges weakly to the equilibrium with density  $\rho_s$ .*

A more precise description of the convergence of the solutions is given in chapter 6. The proof of this result relies on a careful estimate on the size of the tail of a solution, which is inspired in a method initially used by Laurençot and Mischler in [55] to prove uniqueness of solutions. The estimate itself is of interest because it can possibly be improved to obtain further information on the behavior of solutions; as it stands, it depends strongly on the fact that reactions where both clusters are of size greater than some fixed  $N$  do not take place, so it cannot be directly generalized to provide a proof of the corresponding result for the general coagulation-fragmentation equations. However, it gives a new technique to attack the problem and could help find a generalization of our results.

### 1.1.3. Numerical simulation and asymptotic approximation

There is a great difficulty in simulating the coagulation-fragmentation equations numerically due to the huge number of variables that are necessary and the very different time scales that play a role in the evolution of the solutions; a previous understanding of their expected behavior is needed. In chapter 7 we give an asymptotic approximation of the solutions of the Becker-Döring equations in a case in which the form of the coagulation and fragmentation coefficients is simple enough so that a clean theory of the behavior of the solutions can be presented and compared to a numerical simulation of the equations. The method is expected to be applicable to more complicated situations, and in fact it has been used later by Bonilla, Carpio and Neu [8] to study the case in which there is a critical density, so nucleation and coarsening can take place.

The concrete model we use is the case in which the *binding energy* of clusters, a quantity which is related to the ratio between the coagulation and fragmentation coefficients (see section 2.5), depends linearly on the cluster size, and we assume that the fragmentation does not depend on the size of the cluster; this is, we are assuming that all clusters have the same tendency to shed a particle, which is independent of their size. This case is thought to be a model for the aggregation of lipids in aqueous solution into cylindrical *micelles*, which form due to the fact that the involved lipid molecules have a hydrophobic part (tail) and a hydrophilic one (head), so they have a tendency to stay close so that tails are together and away from the water, while heads are pointing towards the water. Due to the shape of the particular molecule at hand, lipids can pack into cylindrical, spherical clusters, or membranes; each way of packing has a different cluster binding energy, and it seems that a linear dependence on the size is a good approximation for cylindrical micelles [46, chapter 15].

We develop an analytic approximation to the behavior of the solution in the limit where the initial concentration is much larger than the *critical micelle concentration* (see chapter 7 for details) by the method of matched asymptotic expansions. The evolution of the solution is shown to exhibit three distinguished parts or eras, in which the time scales are very different: during the first part, the number of monomers (single particles) decreases very fast and a high number of small clusters are created, so that the size distribution starts to resemble a continuous function; during the second part, this function evolves as a solution of the heat equation; finally, the solution slowly approaches an equilibrium distribution where clusters of very different sizes coexist. These results are compared to numerical simulations and are shown to agree very well with them.

## 1.2. The Wigner-Poisson-Fokker-Planck equation

The modeling of quantum diffusion is one of the fields of mathematical interest in quantum mechanics that is not completely well understood at present. Some remarkable works aiming to an earlier analysis of diffusive corrections in models



arising from quantum kinetics are due to Caldeira and Leggett [12], Diósi [24, 25] and Diósi *et al.* [26]. The proper framework of such sort of diffusive models is that of open quantum systems, i.e. an ensemble of electrons interacting with a heat bath (an infinite set of harmonic oscillators in thermodynamic equilibrium) that can exchange matter (conserved particles) with their environment (see [12], [21], [37], [18]).

The quantum Wigner-Fokker-Planck equation reads

$$\begin{aligned} \frac{\partial W}{\partial t} + (\xi \cdot \nabla_x)W + \Theta[V]W \\ = \frac{D_{pp}}{m^2} \Delta_\xi W + 2\lambda \operatorname{div}_\xi(\xi W) + 2\frac{D_{pq}}{m} \operatorname{div}_x(\nabla_\xi W) + D_{qq} \Delta_x W, \end{aligned} \quad (1.6)$$

where  $W$  is the (quasi)-probability distribution function,  $D_{pp}$ ,  $D_{pq}$ ,  $D_{qq}$ ,  $m$  and  $\lambda$  are physical constants and  $\Theta[V]W$  is the (quadratic) nonlinear term associated with the 3D Hartree self-consistent potential (cf. (1.12) below). In a recent paper [2], the well-posedness of the so-called Wigner-Poisson-Fokker-Planck (WPF) system in the simplest Markovian approach for the (high temperature) frictionless case ( $\lambda = 0$ ) is studied. This is a quantum-kinetic model (in the Wigner representation) with Fokker-Planck dissipation mechanism only in the  $\xi$ -direction (that is,  $D_{pq} = D_{qq} = 0$ ):

$$\frac{\partial W}{\partial t} + (\xi \cdot \nabla_x)W + \Theta[V]W = \frac{D_{pp}}{m^2} \Delta_\xi W, \quad x, \xi \in \mathbb{R}^3, t > 0. \quad (1.7)$$

The Lindblad form [61] of this kinetic operator at the density matrix level implies that the problem is mathematically consistent, in the sense that the equation preserves the positivity of the initial density matrix. The problems of local existence, uniqueness, stability, regularity and long-time behaviour (in the case of global solutions) of mild solutions of (1.7) are also tackled in [2]. In [18], the authors make a mathematically rigorous derivation of the frictionless Fokker-Planck equation from the Caldeira-Leggett model introduced in [12]. Furthermore, they investigate other Fokker-Planck-type equations obtained from the Caldeira-Leggett Hamiltonian through different diffusion mechanisms and scalings (fixed temperature and long-time limit), especially a heat equation with a friction term for the radial process in phase space. Also, the rate of time decay of solutions to the viscous hydrodynamic model (i.e. the moment equations for the charge density and the current coupled to the Poisson equation for the electric potential) associated with the 1D WPF equation is studied in [43] via the entropy dissipation method.

Chapter 8 is devoted to prove the existence of global mild solutions (i.e. solutions of the WPF equation written in an equivalent integral form, defined in  $[0, \infty)$ ) to the most general physically relevant class of WPF models (we only set  $D_{pq} = 0$ ). It is based on the results by José Luis López, Juan José Nieto and the author that have been published in [13]; some closely related results have been recently published in

[75]. We are concerned with the analysis of the following initial value problem:

$$\frac{\partial W}{\partial t} + (\xi \cdot \nabla_x)W + \Theta[V]W = \frac{D_{pp}}{m^2} \Delta_\xi W + 2\lambda \operatorname{div}_\xi(\xi W) + D_{qq} \Delta_x W \quad (1.8)$$

$$W(x, \xi, 0) = W_0(x, \xi), \quad (1.9)$$

coupled to the Poisson equation for the determination of the self-consistent electrostatic potential:

$$V(x, t) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{n(y, t)}{|x - y|} dy, \quad (1.10)$$

with

$$n(x, t) = \int_{\mathbb{R}^3} W(x, \xi, t) d\xi. \quad (1.11)$$

Here,  $\Theta[V]$  stands for the pseudo-differential operator

$$\begin{aligned} \Theta[V]W(x, \xi, t) &= \frac{i}{(2\pi)^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{V(x + \frac{\hbar}{2m}\eta, t) - V(x - \frac{\hbar}{2m}\eta, t)}{\hbar} \\ &\quad \times W(x, \xi', t) e^{-i(\xi - \xi') \cdot \eta} d\xi' d\eta, \end{aligned} \quad (1.12)$$

with  $\hbar$  denoting the reduced Planck constant and  $m$  the effective mass of the particles, while  $\lambda, D_{pp}, D_{qq}$  are positive constants related to the interactions between the particles and the reservoir (cf. [24]):

$$\lambda = \frac{\eta}{2m}, \quad D_{pp} = \eta k_B T, \quad D_{qq} = \frac{\eta \hbar^2}{12m^2 k_B T}, \quad (1.13)$$

where  $\eta > 0$  is the coupling (damping) constant of the bath,  $k_B$  the Boltzmann constant and  $T$  the temperature of the bath. Also,

$$Q = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} W(x, \xi, t) d\xi dx$$

is the total charge of the system, which is preserved along the evolution. This equation is the simplest systematic Markovian approximation taking friction and dissipation effects into account, such that the corresponding master equation for the density matrix of the particle ensemble still belongs to the Lindblad class (as shown in [25]), ensuring preservation of positivity for all initial conditions and for all times. Indeed, if the elliptic term involving  $\Delta_x W$  is removed from Eq. (1.8), then the remaining Fokker-Planck collision kernel (accounting only for friction and  $\xi$ -diffusion effects) prevents the equation from belonging to the Lindblad family. Thus, in this case the problem would be neither mathematically consistent nor meaningful in a physical context.

The WFPF equation (1.8) stems from the following evolution model (see [2]) for the density matrix function  $\rho(x, y, t) \in L^2(\mathbb{R}_x^3 \times \mathbb{R}_y^3)$ :

$$\begin{aligned} \frac{\partial \rho}{\partial t} = & -\frac{i}{\hbar}(H_x - H_y)\rho - \lambda(x - y) \cdot (\nabla_x - \nabla_y)\rho \\ & + \left( D_{qq}|\nabla_x + \nabla_y|^2 - \frac{D_{pp}}{\hbar^2}|x - y|^2 \right)\rho, \end{aligned}$$

where  $H_x$  and  $H_y$  are copies of the electron Hamiltonian

$$H_z = -\frac{\hbar^2}{2m}\Delta_z + V(z, t)$$

acting on the variables  $x$  and  $y$ , respectively. Indeed, taking into account that the Wigner function of the electron ensemble  $W : \mathbb{R}_x^3 \times \mathbb{R}_\xi^3 \times [0, \infty) \rightarrow \mathbb{R}$  is defined by

$$W(x, \xi, t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}_\eta^3} \rho\left(x + \frac{\hbar}{2m}\eta, x - \frac{\hbar}{2m}\eta, t\right) e^{-i\xi \cdot \eta} d\eta,$$

one can easily deduce that the evolution law for  $W(x, \xi, t)$  is described by Eq. (1.8). The positivity of the density matrix operator

$$[R(t)f](x) = \int_{\mathbb{R}_y^3} f(y)\rho(x, y, t) dy \in L^2(\mathbb{R}^3)$$

(guaranteed by the Lindblad condition) implies that the Husimi transform, defined by the following convolution of the Wigner function with a Gaussian kernel

$$W^H(x, \xi, t) = W(x, \xi, t) *_{x, \xi} \left( \frac{m}{\hbar\pi} \right)^3 \exp \left\{ -\frac{m}{\hbar} \left( |x|^2 + |\xi|^2 \right) \right\}, \quad (1.14)$$

is pointwise nonnegative on  $\mathbb{R}_x^3 \times \mathbb{R}_\xi^3$ . Also, the Lindblad condition and a nonvanishing friction ( $\lambda > 0$ ) imply that the Fokker–Planck operator is uniformly elliptic in  $\mathbb{R}_x^3 \times \mathbb{R}_\xi^3$ .

Contrary to the common techniques leading to the global existence, regularity and asymptotic behaviour of solutions to classical (Vlasov)-Fokker-Planck systems, our techniques avoid the explicit use of  $S_p$  norms (see [17, 9, 76] for example) to control the position density. Actually, our proof does not require more regularity than  $L^1(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3) \cap L^1(\mathbb{R}_\xi^3; L^2(\mathbb{R}_x^3))$  and the control of the kinetic energy for the initial Wigner function. We also remark that the natural space where the Wigner function lives is  $L^2(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)$ , which can be seen from the original density matrix formulation in the widest context of Wigner problems. Actually, by formally multiplying Eq. (1.8) by  $W$  and integrating against  $x$  and  $\xi$  we have

$$\|W(t)\|_{L^2(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)} \leq \|W_0\|_{L^2(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)} e^{6\lambda t}.$$

However, the presence of a regularizing Fokker-Planck kernel in the model under study allows us to develop an  $L^1$  theory for the WFPF equation and exploit the smoothing properties of the Fokker-Planck operator to get regular solutions. The fact that no maximum principle is available for equations of Wigner type is significant, so that in general the Wigner function changes sign even if we start from positive initial data. This is why the Husimi function (1.14) together with the elliptic regularization in the  $x$ -variable will play an essential role in our analysis.

In chapter 8 we prove the following global-in-time existence result:

**Theorem 1.2.1.** *Let  $W_0 \in L^1(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3) \cap L^1(\mathbb{R}_\xi^3; L^2(\mathbb{R}_x^3))$  be such that*

$$\int_{\mathbb{R}_x^3} \int_{\mathbb{R}_\xi^3} |\xi|^2 W_0(x, \xi) d\xi dx < \infty.$$

*Then, the Wigner-Poisson-Fokker-Planck equation (1.8)–(1.13) admits a unique global mild solution*

$$W \in C([0, \infty); L^1(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)) \cap C([0, \infty); L^1(\mathbb{R}_\xi^3; L^2(\mathbb{R}_x^3))).$$

*Moreover,*

$$W \in C((0, \infty); W^{1,1} \cap W^{1,\infty}(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)).$$

*Also, the charge density (1.11) and the electric potential (1.10) satisfy the following Hölder-regularity properties: for all  $t > 0$ ,*

$$n(\cdot, t) \in C^{0,\alpha}(\mathbb{R}_x^3) \text{ with } 0 < \alpha < \frac{1}{2}, \quad V(\cdot, t) \in C^{1,\beta}(\mathbb{R}_x^3) \text{ with } 0 < \beta < \frac{1}{3}.$$



# Chapter 2

## Preliminaries

In this chapter we present in detail the coagulation-fragmentation equations which will be studied in subsequent chapters. It contains no new results, and it is intended to introduce some of the concepts used later. References to the sources can be found inside the chapter.

### 2.1. Derivation of the equations

Suppose that we have a group of things distributed in space, which we call *units* or *particles*, that can stick together to form groups of several units, which we call *clusters*. The easiest example to think of and to which the following applies is a dilute solution of some kind of molecules that may interact and form groups of several molecules. The *size* of a cluster is the number of units that form it, so it can be any positive integer. We are interested in the evolution of the *size distribution* of these clusters: we want to know the number of clusters of size  $j$  at any time  $t$ . Actually, instead of studying directly the number of clusters of size  $j$ , it is easier to make an approximation and study the *density* of clusters of size  $j$ ; this is, the number of clusters per unit of volume (also called *number density* to distinguish it from other measures of density). In this approximation, we suppose that the clusters are distributed homogeneously enough so that this average density gives a reasonable description of the size distribution of clusters. It can take any nonnegative value.

We denote by  $c_j$  the number density of clusters of size  $j$ . Usually we will abuse language by saying “number of clusters” instead of “number density of clusters” because ideas are explained more easily, but the proper units for  $c_j$  are clusters per unit of volume.

We assume that these clusters can join to form larger clusters, and that they may break into smaller pieces; the first process is called *coagulation* and the second is *fragmentation* (the former is also often referred to as *coalescence* or *clustering*, and the latter as *breakage*). We will sometimes refer to these as *reactions*. In a coagulation reaction, a cluster of size  $j$  can stick to a cluster of size  $i$  to form a cluster of size  $i + j$ ; we refer to this process symbolically as  $i, j \rightarrow i + j$ . We

disregard coagulation processes that involve three or more clusters sticking together at the same time as these events are extremely infrequent or they do not happen at all in most of the situations where we want to apply our equation. A fragmentation reaction is more complicated: it can be a *binary* fragmentation reaction where a cluster of size  $k$  breaks into a cluster of size  $j < k$  and a cluster of size  $k - j$ ; we represent this reaction as  $k \rightarrow j, k - j$ ; it can also be a *multiple fragmentation* reaction where a cluster breaks into more than two pieces, which will be represented in an analogous way.

To be able to describe the dynamics of the size distribution we need to know how often and under which conditions these processes happen: we need to keep track of which of them happen at which moments. As before we will make an approximation and use the *rate of occurrence* of a given process, which is the number of times it happens per unit of time, per unit of volume. Again, we suppose that reactions happen uniformly enough for this to be a useful approximation. This rate can be any positive number.

A fundamental assumption is that these processes occur according to the *law of mass action*: we suppose that the rate of occurrence of the reaction  $i, j \rightarrow i + j$  is proportional both to the density of clusters of size  $i$  and the density of clusters of size  $j$  (and the constant of proportionality does not change in time). It is a well-known (approximated) principle in chemistry that the rate of a reaction is proportional to the concentration of the reacting substances, and this assumption is in agreement with this. In the same way, we suppose that the rate of occurrence of a fragmentation reaction in which a cluster of size  $j$  fragments into two or more pieces is proportional to the density of clusters of size  $j$ .

We will write  $a_{ij}$  to denote the constant of proportionality for the coagulation reaction  $i, j \rightarrow i + j$ , so that its rate of occurrence is  $a_{ij}c_i c_j$ . For now, consider only binary fragmentation and denote by  $b_{ij}$  its constant of proportionality, so that the rate of occurrence of the fragmentation reaction  $i + j \rightarrow i, j$  is  $b_{ij}c_{i+j}$ . We call the  $a_{ij}$  the *coagulation coefficients* and the  $b_{ij}$  the *fragmentation coefficients*. Note that they must be symmetric in  $i, j$ :  $a_{ij} = a_{ji}$ ,  $b_{ij} = b_{ji}$  for all  $i, j$ . With these we are able to write an evolution equation for the size distribution of clusters given by the  $c_j$ . The *net rate* of the reaction  $i, j \rightarrow i + j$  is

$$W_{ij} := a_{ij}c_i c_j - b_{ij}c_{i+j}.$$

It represents the net rate at which pairs of clusters of sizes  $i, j$  are converted to clusters of size  $i + j$ ; it is *net* in the sense that we are taking into account both the forward and backward reactions (due to coagulation and fragmentation, respectively). The  $W_{ij}$  are also symmetric in  $i, j$ . The number of clusters of size  $i$  is increased by reactions of the form  $j, i - j \rightarrow i$  and decreased by reactions of the form  $i, j \rightarrow i + j$ . Hence, the rate of change in time of the density  $c_i$  is

$$\frac{d}{dt}c_i = \sum_{j=1}^{\lfloor \frac{i}{2} \rfloor} W_{j, i-j} - \sum_{j=1}^{\infty} W_{ij} \quad \text{for } i \geq 1,$$

where  $[x]$  denotes the integer part of a number  $x$ . The first sum includes all possible reactions where two clusters stick to form a cluster of size  $i$ ; the second sum takes into account all possible reactions in which a cluster of size  $i$  joins some other cluster. In order to be able to write the equations in a more convenient way, it is customary to define the coefficient  $a_{ii}$  for  $i \geq 1$  so that the rate of the reaction  $i, i \rightarrow 2i$  is  $\frac{1}{2}a_{ii}c_i^2$  instead of  $a_{ii}c_i^2$ , and do the same for  $b_{ii}$ . We will follow this convention here. Then, with this slight modification of the  $a_{ii}$  and  $b_{ii}$  one can write the above equations as

$$\frac{d}{dt}c_i = \frac{1}{2} \sum_{j=1}^{i-1} W_{j,i-j} - \sum_{j=1}^{\infty} W_{ij} \quad \text{for } i \geq 1.$$

(Note that we have added the  $1/2$  factor because each possible reaction of the kind  $j, i-j \rightarrow i$  is counted *twice* in the sum except for the reaction  $i/2, i/2 \rightarrow i$  when  $i$  is even; this is the reason for our renaming of the coefficients with repeated indices). This infinite system of ordinary differential equations where the unknowns are the  $c_i$  is the *discrete binary coagulation-fragmentation system of equations*.

One can make a different approximation where the size of a cluster can be any positive number and not necessarily an integer; this can be reasonable if one measures the size of a cluster by its mass or its radius instead of the number of clusters that form it. Then, the size distribution at any given moment can be described by a function  $f = f(y)$  for  $y \geq 0$ , where  $y$  represents the size of the cluster (measured in any useful unit) and  $f(y)$  is the density of clusters of that size (again measured in some adequate way). The function  $f$  should be viewed as a density function, so that

$$\int_a^b f(y) dy$$

represents the density of clusters whose size is between  $a$  and  $b$ . The function  $f$  is called the *size distribution of clusters*. Analogously we can talk about coagulation reactions  $y, y' \rightarrow y + y'$ , where now  $y, y'$  are positive numbers (not necessarily integers); and fragmentation reactions, where a cluster of size  $y$  breaks into clusters of positive sizes  $y', y'', y''', \dots$  such that  $y' + y'' + y''' + \dots = y$ . Now the rate of occurrence of the coagulation reaction  $y, y' \rightarrow y + y'$  is determined (by the law of mass action) by the *coagulation coefficient*  $a(y, y')$  and the rate of occurrence of the fragmentation reaction  $y + y' \rightarrow y, y'$  is given by the *fragmentation coefficient*  $b(y, y')$ . Then,  $a(y, y')f(y)f(y')$  is the number of times the corresponding coagulation reaction happens per unit of time, per unit of volume, *per unit of cluster size*, as now the values of  $f$  are densities of clusters *per unit of cluster size*. Again, we will not always mention this and instead will talk about  $f$  as measuring densities of clusters just because the language becomes easier to understand.

Then we can write down the continuous analogue of the discrete binary coagulation-fragmentation equations, which is expectedly called *the continuous binary coagulation-fragmentation equations*, already introduced in chapter 1:

$$\frac{\partial}{\partial t}f = C(f) + F(f), \quad t, y \in (0, +\infty) \quad (2.1)$$



where the coagulation and fragmentation terms are given by:

$$C(f) := C_1(f) - C_2(f) \quad (2.2)$$

$$F(f) := F_1(f) - F_2(f) \quad (2.3)$$

$$C_1(f)(y) := \frac{1}{2} \int_0^y a(y', y - y') f(y') f(y - y') dy' \quad (2.4)$$

$$C_2(f)(y) := f(y) \int_0^\infty a(y, y') f(y') dy' \quad (2.5)$$

$$F_1(f)(y) := \int_y^\infty b(y', y - y') f(y') dy' \quad (2.6)$$

$$F_2(f)(y) := f(y) \frac{1}{2} \int_0^y b(y', y - y') dy'. \quad (2.7)$$

One can also take into account multiple fragmentation reactions. In this case it is useful to define a new coefficient  $b(y, y')$  so that  $b(y, y')f(y)$  represents the rate of formation of clusters of size  $y'$  from clusters of size  $y$ , this is: how many clusters of size  $y'$  are formed from the breakage of clusters of size  $y$  per unit of time, per unit of volume, per unit of cluster size. When one takes this into account, the fragmentation term from (2.1) must be changed to

$$F(f) := F_1(f) - F_2(f) \quad (2.8)$$

$$F_1(f)(y) := \int_y^\infty b(y'', y) f(y'') dy'' \quad (2.9)$$

$$F_2(f)(y) := f(y) \int_0^y \frac{y'}{y} b(y, y') dy', \quad (2.10)$$

and the resulting equation is called *the continuous coagulation-fragmentation equation*. Below we explain further the meaning and the derivation of this fragmentation term.

## 2.2. Interpretation of the fragmentation coefficient

As explained above, the multiple fragmentation coefficient  $b(y, y')$  is defined so that  $b(y, y')f(y)$  represents the rate of formation of clusters of size  $y'$  from clusters of size  $y$  (where  $f$  is the size distribution of clusters). Any kind of breakage of a cluster into a finite number of pieces is allowed here, and the fact that the fragmentation term in an evolution equation with this kind of fragmentation should be (2.8)–(2.10) is not obvious. Here we derive it from the more basic assumption that a cluster of a given size breaks in a certain way at a rate given by a distribution on the space of possible “ways of breaking”. This derivation is taken from [36], and we include it here for completeness.

Consider, for  $y > 0$ , the space  $S(y)$  of nonincreasing finite sequences  $Y = \{y_1, \dots, y_n\}$  with  $n \geq 2$ ,  $y_i > 0$  for all  $i$  and such that  $y_1 + \dots + y_n = y$ . Each

of these sequences represents a possible fragmentation reaction  $y \rightarrow y_1 + \dots + y_n$ , and the condition that  $y_1 + \dots + y_n = y$  ensures that mass is conserved in the reaction. The rate at which each of them occurs (per cluster of size  $y$ ) is given by a positive measure  $\nu(y)$  on  $S(y)$ , which clearly comprises all the information on the rate and type of fragmentation reactions that can take place. The *total fragmentation rate* for a cluster of size  $y$  can then be written as

$$\beta(y) := \int_{S(y)} \nu(y).$$

Now we would like to express the rate at which clusters of size  $y'$  are obtained from the fragmentation of clusters of size  $y$  in terms of  $\nu$ . For this, define the marginal measure  $\nu_i(y)$  on the interval  $(0, y)$  (with  $i \geq 1$  an integer) as

$$\int_0^y \phi(y') \nu_i(y, y') = \int_{S(y)} \phi(y_i) \nu(y, Y) \quad \text{for all } \phi \in \mathcal{C}_c(0, y).$$

The integral on the right is the integral on  $S(y)$  of the measure  $\nu(y)$  times the function on  $S(y)$  given by  $Y = \{y_1, \dots, y_n\} \mapsto \phi(y_i)$  (or zero if  $n < i$ ). This  $\nu_i(y)$  represents the rate at which a cluster of a given size is obtained as the  $i$ -th piece in the breakage of a cluster of size  $y$ . The rate at which a cluster of a given size is obtained as *any* of the pieces resulting from the breakage of a cluster of size  $y$  is then the measure given by

$$b(y) := \sum_{i=1}^{\infty} \nu_i(y).$$

This is a measure on  $(0, y)$ , but we can consider it as a measure on  $(0, +\infty)$  extending it by 0. Now, if the size distribution function is  $f$  then the gain and loss terms in the evolution of the density of clusters of size  $y$  are <sup>1</sup>

$$Ff(y) = \int_0^{\infty} f(y') b(y', y) dy' - f(y) \int_{S(y)} \nu(y). \quad (2.11)$$

In the above, the *gain term* (positive) is due to clusters of size  $y' > y$  breaking to give a cluster of size  $y$  as one of the results, and the *loss term* (negative) is due to the fragmentation of clusters of size  $y$  (so it is  $f(y)$  times the total fragmentation rate). To write the above as (2.8), note that the total fragmentation rate can be

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<sup>1</sup>In the first integral we are integrating the function  $y' \mapsto b(y')$ , which is measure-valued, and hence the integral gives a measure. We write it as if evaluated on  $y$ , which is an abuse of notation, but we will not worry about the technical details here, as the aim is to provide a plausible derivation of the fragmentation term to be used later (one can always think that  $b(y)$  is regular enough for  $b(y, y')$  to be representable as a function).

expressed in terms of  $b$  as follows:

$$\begin{aligned} y \int_{S(y)} \nu(y) &= \int_{S(y)} \nu(y, Y) \sum_{i=1}^{\infty} y_i = \sum_{i=1}^{\infty} \int_{S(y)} y_i \nu(y, Y) \\ &= \sum_{i=1}^{\infty} \int_0^{\infty} y' \nu_i(y, y') = \int_0^{\infty} y' \sum_{i=1}^{\infty} \nu_i(y, y') = \int_0^{\infty} y' b(y, y'), \end{aligned}$$

so

$$\int_0^y \frac{y'}{y} b(y, y') = \int_{S(y)} \nu(y)$$

and the fragmentation term in (2.11) can be written as

$$Ff(y) = \int_0^{\infty} f(y') b(y', y) dy' - f(y) \int_0^y \frac{y'}{y} b(y', y),$$

which is the same as (2.8).

As we have seen,

$$\beta(y) := \int_0^y \frac{y'}{y} b(y, y') dy' \quad (2.12)$$

represents the total fragmentation rate of a cluster of size  $y$ . We will define  $\beta(y)$  as above for any  $y > 0$  for which the integral makes sense (under the technical conditions imposed later), and will define  $\beta(y) = 0$  otherwise. Then we can call

$$P(y, y') := b(y, y') / \beta(y). \quad (2.13)$$

As before, we make this definition whenever it makes sense and define  $P(y, y') = 0$  otherwise. This  $P(y, y')$  represents *the probability* that a cluster of size  $y'$  is obtained by fragmentation of a cluster of size  $y$ .

### 2.3. Binary fragmentation

If we only allow binary fragmentation reactions, then the measure  $\nu(y)$  is concentrated on the set of sequences in  $S(y)$  with two terms. For every  $Y = \{y_1, y_2\}$  in this set,  $y_1 = y - y_2$  and we find a relation between  $\nu_1(y)$  and  $\nu_2(y)$ : for all  $\phi \in \mathcal{C}_c(0, y)$ ,

$$\begin{aligned} \int_0^y \phi(y') \nu_1(y, y') &= \int_{S(y)} \phi(y_1) \nu(y, Y) = \int_{S(y)} \phi(y - y_2) \nu(y, Y) \\ &= \int_0^y \phi(y - y') \nu_2(y, y') = \int_0^y \phi(y') \nu_2(y, y - y'). \end{aligned}$$

Hence,

$$\nu_1(y, y') = \nu_2(y, y - y').$$

For  $i \geq 3$ ,  $\nu_i(y) \equiv 0$  for all  $y$  by definition (as the measure  $\nu(y)$  is zero on the set of sequences in  $S(y)$  with more than 2 terms). As a consequence of the previous identity,  $b(y) = \nu_1(y) + \nu_2(y)$  satisfies the following symmetry property:

$$b(y, y') = b(y, y - y').$$

When only binary fragmentation is considered it is usual to define

$$\tilde{b}(y, y') := b(y + y', y) = b(y + y', y').$$

Then  $\tilde{b}$  is symmetric:  $\tilde{b}(y, y') = \tilde{b}(y', y)$ . Thanks to this symmetry,

$$\int_0^y \frac{y'}{y} \tilde{b}(y', y - y') dy' = \int_0^y \frac{y - y'}{y} \tilde{b}(y - y', y') dy',$$

so

$$\int_0^y \frac{y'}{y} \tilde{b}(y', y - y') dy' = \frac{1}{2} \int_0^y \tilde{b}(y - y', y') dy',$$

and we get the expression of the binary fragmentation term from (2.6)–(2.7).

## 2.4. Self-similar coefficients

We can also impose some additional requirements of the fragmentation coefficient. One of them is to ask for it to be *self-similar*: this is, that the *probability* (see (2.13)) at which clusters of size  $y'$  are obtained by fragmentation of clusters of size  $y$  depends only on their relative sizes. This means that  $b$  is of the form

$$b(y, y') = \beta(y) \frac{1}{y} B\left(\frac{y'}{y}\right), \quad (2.14)$$

where  $B$  is a positive function or a positive measure on  $(0, 1)$  (depending on the mathematical model we are interested in) such that

$$\int_0^1 zB(z) dz = 1. \quad (2.15)$$

The probability distribution of cluster sizes obtained from the breakage of a particle of size  $y$  is here  $P(y, y') = 1/y B(y'/y)$ . What we mean by saying that the probability of obtaining a cluster some given size from a given cluster depends only on their relative sizes is that the *probability* of obtaining clusters whose size is within some given fractions of  $y$  *does not depend on  $y$* . For example, the probability of obtaining clusters whose size is less than a third of  $y$  is, making the change of variables  $z = y'/y$ ,

$$\int_0^{\frac{y}{3}} 1/y B(y'/y) dy' = \int_0^{\frac{1}{3}} B(z) dz.$$

Observe that the coefficient  $\beta$  which appears in equation (2.14) is indeed the total fragmentation rate for this  $b$ :

$$\int_0^y \frac{y'}{y} b(y, y') dy' = \int_0^y \frac{y'}{y} \beta(y) \frac{1}{y} B\left(\frac{y'}{y}\right) dy' = \beta(y) \int_0^1 zB(z) dy' = \beta(y).$$

## 2.5. Statistical mechanics for steady states

The coagulation-fragmentation equations are expected to model certain physical situations in which a very high number of particles in a dilute solution are reacting and forming aggregates. Hence, if the model is appropriate, equilibrium states (solutions which do not depend on time) should agree with equilibrium statistical mechanics for the particular physical system we are considering. This gives a useful insight on the connection of these equations with physical phenomena and provides a new interpretation of some quantities involved in the equations.

We will deal with statistical mechanics of a dilute solution of particles that can form clusters as a limit of ideal systems in which particles can occupy only a finite number of places in space and where two or more particles are allowed to occupy the same place. This idealized situation is called *lattice nucleation*. The following is based on personal notes by John Neu and appears in the introduction in [73].

Suppose we have  $n$  indistinguishable particles which can occupy  $M$  different places, called *binding sites*. As they are indistinguishable, the possible states of the system are  $M$ -tuples of nonnegative integers  $\{n_1, n_2, \dots, n_M\}$  such that  $n_1 + \dots + n_M = N$ , where  $n_i$  represents the number of particles in the space  $i$  (forming a cluster of  $n_i$  particles). The  $n_i$  are called *occupation numbers*.

In order to study the statistical mechanics of the system we need to give the energies of all possible configurations. We assume that the energy of a state  $A_j$  can be written as

$$E \equiv E(A_j) = \sum_{i=1}^{\infty} e_i c_i,$$

where  $c_i$  is the number of clusters with exactly  $i$  particles in the state  $A_j$  (this is, the number of binding sites with exactly  $i$  particles) and  $e_i$  is the energy of an  $i$ -particle cluster. The zero level is chosen so that  $e_0$ , the energy of an empty space, is zero. We will write  $E$  instead of  $E(A_j)$  when the state it refers to is implied. Let us further assume that the system is in a state with known size distribution  $\{c_i\}$ . Then the possible states are the occupation numbers  $\{n_1, \dots, n_M\}$  that agree with this. Let us calculate their number.

The number of ways to place  $c_1$  indistinguishable 1-clusters (particles) in  $M$  spaces is

$$\frac{M!}{c_1!(M - c_1)!}.$$

The number of ways to place to place  $c_2$  indistinguishable 2-clusters in the remaining  $M - c_1$  spaces is

$$\frac{(M - c_1)!}{c_2!(M - c_1 - c_2)!},$$

and so on. One can see that the number of ways to place all the clusters ( $c_1$  1-

clusters,  $c_2$  2-clusters,...) is their product:

$$\begin{aligned} \frac{M!}{c_1!(M-c_1)!} \cdot \frac{(M-c_1)!}{c_2!(M-c_1-c_2)!} \cdots \frac{(M-\sum_{i=1}^{N-1} c_i)!}{c_N!(M-\sum_{i=1}^N c_i)!} \\ = \frac{M!}{c_1! \cdots c_N!(M-\sum_{i=1}^N c_i)!}. \end{aligned}$$

Note that we only write the terms up to  $N$  because there can be no clusters of more than  $N$  particles (as we have exactly  $N$  particles). Then, this is the number of possible states with given size distribution  $\{c_i\}$ . As all of them have the same energy, the entropy  $S$  of the system in this state is given by  $k$  times the logarithm of this number (where  $k$  is Boltzmann's constant):

$$S = k \log M! - k \sum_{i=1}^N \log c_i! - k \log \left( M - \sum_{i=1}^N c_i \right)!.$$

Now we take a sequence of systems like the one just described, with higher and higher number of particles, so for each  $N \geq 1$  we consider a certain system with  $N$  particles,  $M$  binding sites and given size distribution  $\{c_i\}$  (and we do not explicitly write the dependence on  $N$  of both  $M$  and the  $c_i$ ). We will choose the sequence so that

$$\begin{aligned} N/M &\rightarrow \rho > 0 \\ \frac{c_i}{M} &\rightarrow \rho_i, \quad i \geq 1 \end{aligned}$$

for some  $\rho \geq 0$ ,  $\rho_i \geq 0$ . In the limit  $N \rightarrow \infty$ , the relation  $\sum_{i=1}^N i c_i = N$  gives the following when divided by  $M$ :

$$\sum_{i=1}^{\infty} i \rho_i = \rho. \quad (2.16)$$

We will also choose our sequence so that, for a fixed  $i$ ,  $c_i$  is always zero if  $\rho_i$  is zero. Hence, for a fixed  $i$ , either  $c_i$  is always zero or it tends to infinity, so we can use Stirling's approximation for the factorial:

$$\begin{aligned} \log c_i! &\sim c_i \log c_i \\ \log M! &\sim M \log M. \end{aligned}$$

Hence the entropy density  $\mathcal{S} = S/M$  can be approximated by

$$\begin{aligned} \mathcal{S} := \frac{S}{M} &\sim k \log M - k \sum_{i=1}^N \frac{c_i}{M} \log c_i - k \frac{1}{M} \left( M - \sum_{i=1}^N c_i \right) \log \left( M - \sum_{i=1}^N c_i \right) \\ &= -k \sum_{i=1}^N \frac{c_i}{M} \log \frac{c_i}{M} - k \left( 1 - \sum_{i=1}^N \frac{c_i}{M} \right) \log \left( 1 - \sum_{i=1}^N \frac{c_i}{M} \right), \end{aligned}$$

so in the limit  $N \rightarrow \infty$  the entropy density can be written as

$$\begin{aligned} \mathcal{S} &= -k \sum_{i=1}^{\infty} \rho_i \log \rho_i - k \left(1 - \sum_{i=1}^{\infty} \rho_i\right) \log \left(1 - \sum_{i=1}^{\infty} \rho_i\right) \\ &= -k \sum_{i=1}^{\infty} \rho_i \log \rho_i - k(1-r) \log(1-r), \end{aligned}$$

where we have called

$$r := \sum_{i=1}^{\infty} \rho_i.$$

In the limit, the *energy density*  $\mathcal{E} = E/M$  is

$$\mathcal{E} = \sum_{i=1}^{\infty} e_i \rho_i$$

and the *free energy density* is  $\mathcal{F} := \mathcal{E} - T\mathcal{S}$ , where  $T$  is the absolute temperature:

$$\mathcal{F} := \mathcal{E} - T\mathcal{S} = \sum_{i=1}^{\infty} e_i \rho_i + kT \sum_{i=1}^{\infty} \rho_i \log \rho_i + kT(1-r) \log(1-r).$$

In thermal equilibrium this should be a minimum among all possible configurations; the possible ones are those with  $\sum_{i=1}^{\infty} i \rho_i = \rho$  fixed, as (2.16) must hold. We can find this minimum using the method of Lagrange multipliers with this constraint; if a minimum exists, the  $\{\rho_i\}$  for which  $\mathcal{F}$  attains the minimum value must satisfy the following set of equations for some  $\lambda \in \mathbb{R}$ :

$$\begin{cases} \frac{\partial \mathcal{F}}{\partial \rho_i} = \lambda \frac{\partial}{\partial \rho_i} \left( \sum_{i=1}^{\infty} i \rho_i \right), & i \geq 1 \\ \sum_{i=1}^{\infty} i \rho_i = \rho. \end{cases}$$

Calculating the derivatives, the equations are

$$\begin{cases} e_i + kT \log \rho_i - kT \log(1-r) = \lambda i, & i \geq 1 \\ \sum_{i=1}^{\infty} i \rho_i = \rho. \end{cases}$$

If we eliminate  $\lambda$  and write the equations in terms of  $\rho_1$  we get

$$\lambda = kT \log \frac{\rho_1}{1-r} + e_1$$

so  $\rho_i$  is given by

$$\rho_i = (1-r) \exp \frac{1}{kT} \left( kT i \log \frac{\rho_1}{1-r} + i e_1 - e_i \right) = (1-r)^{i-1} \rho_1^i e^{-\epsilon_i/kT},$$

where we have defined the *binding energy*  $\epsilon_i$  as the difference between the energy of an  $i$ -cluster and the energy of the  $i$  particles taken separately:

$$\epsilon_i := e_i - i e_1.$$

In the cases we will be later interested in,  $r$  is very small, so the above is well approximated by

$$\rho_i = \rho_1^i e^{-\frac{\epsilon_i}{kT}},$$

and the entropy density  $\mathcal{S}$  can also be approximated for small  $r$ , using that  $(1-r)\log(1-r) \sim 1-r$ :

$$\mathcal{S} = -k \sum_{i=1}^{\infty} \rho_i \log \rho_i - k(1 - \sum_{i=1}^{\infty} \rho_i). \quad (2.17)$$

This reasoning leads to the conclusion that in equilibrium the size distribution of clusters should be given by

$$\rho_i = \rho_1^i e^{-\frac{\epsilon_i}{kT}} \quad \text{for } i \geq 1,$$

for some  $\rho_1 \geq 0$  which is determined by the condition that the total mass is  $\rho$ :

$$\sum_{i=1}^{\infty} i \rho_i = \sum_{i=1}^{\infty} \rho_1^i e^{-\frac{\epsilon_i}{kT}} = \rho.$$

This suggests that we identify the coefficients  $Q_i$  in the detailed balance condition (see chapter 6) according to this:

$$Q_i = e^{-\frac{\epsilon_i}{kT}}. \quad (2.18)$$

It also gives a good candidate for an entropy functional for the coagulation-fragmentation equations, given by equation (2.17), which is crucial when studying the asymptotic behavior of these equations.





## Chapter 3

# The fragmentation operator

In this chapter we want to define precisely the fragmentation operator  $F$  given in (2.8)–(2.10), this is:

$$Ff := F_1f - F_2f \quad (3.1)$$

$$F_1f(y) := \int_y^\infty b(y'', y)f(y'') dy'' \quad (3.2)$$

$$F_2f(y) := f(y) \int_0^y \frac{y'}{y} b(y, y') dy'. \quad (3.3)$$

The results in this chapter are not new, but are scattered among previous mathematical works on the topic of continuous coagulation-fragmentation equations (e.g. [33, 52, 29, 86] and their references), sometimes for coefficients of a slightly different kind from the one we use here (for example, binary fragmentation is usually considered instead of multiple fragmentation). Hence, though most of the results here can be easily deduced from the existing ones in the literature, we include them for completeness, as it would be difficult to find in the references the precise statements which are needed.

We want to know what conditions on  $f$  and  $b$  ensure  $Ff$  is well-defined, and what additional conditions ensure it has certain regularity. Particularly, later we will be interested in quantities of the form  $\int_0^\infty \phi(y)Ff(y) dy$  for some function  $\phi$  (e.g., moments of  $f$ ), so we will try to find requirements on  $f$  and  $b$  that guarantee some of these integrals make sense. We are not looking for the best possible results on the matter, but instead intend to adopt a compromise between simplicity and later applications.

The fragmentation coefficient  $b(y, y')$  (for  $0 < y' \leq y$ ) represents, as explained in previous chapters, the rate of formation of clusters of size  $y'$  from clusters of size  $y$ . Of course, sizes are always positive, as is the rate of formation of clusters of any size, and clusters resulting from fragmentation must have a smaller size than the cluster which breaks. So, in our mathematical models  $b$  will be a real positive function defined for  $y > y' > 0$ . Also, if we want (3.3) to make sense we must impose that

the integral that appears there is defined. To be precise, call

$$\mathbb{T} := \{(y, y') \in \mathbb{R}^2 \mid y > y' > 0\}.$$

The following conditions on  $b$  will be imposed frequently:

$$\begin{aligned} b : \mathbb{T} \rightarrow \mathbb{R} \text{ is a positive measurable function and} \\ \text{for almost all } y > 0, \text{ the function } y' b(y, y') \text{ is integrable in } y'. \end{aligned} \quad (3.4)$$

Whenever it is convenient we may consider  $b$  as defined on  $(0, +\infty) \times (0, +\infty)$  (or even  $\mathbb{R}^2$ ) extending it by 0.

When (3.4) holds we will define  $\beta(y)$  as in (2.12):

$$\beta(y) := \int_0^y \frac{y'}{y} b(y, y') dy' \quad (3.5)$$

for any  $y > 0$  for which the integral makes sense, and  $\beta(y) = 0$  otherwise. Note that by Fubini's theorem, the total fragmentation rate  $\beta$  thus defined is a positive measurable function.

**Definition 3.0.1 (Fragmentation operator).** Let  $b : \mathbb{T} \rightarrow \mathbb{R}$  be a positive measurable function, and let  $f : (0, +\infty) \rightarrow \mathbb{R}$  be a measurable function. We define  $Ff$ , the *fragmentation operator acting on  $f$* , as the following function, defined for almost all  $y > 0$ , whenever both integrands below are integrable in the sense of Lebesgue for almost all  $y > 0$ :

$$Ff(y) := \int_y^\infty b(y'', y) f(y'') dy'' - f(y) \int_0^y \frac{y'}{y} b(y, y') dy' \quad (3.6)$$

$$= \int_y^\infty b(y'', y) f(y'') dy'' - f(y) \beta(y). \quad (3.7)$$

When all these integrals have a meaning in the sense of Lebesgue for almost all  $y > 0$  we will say that  $Ff$  is *well-defined*.

### 3.1. Conditions for the definition of $F$

The following lemma gives a simple requirement for  $Ff$  to be well-defined:

**Lemma 3.1.1.** *Assume (3.4). If  $f : (0, +\infty) \rightarrow \mathbb{R}$  is a measurable function such that*

$$\int_\epsilon^\infty |f(y')| \int_\epsilon^R b(y, y') dy dy' < +\infty \quad \text{for all } 0 < \epsilon < R,$$

*then  $Ff$  is well-defined (as in definition 3.0.1). If  $\beta$  is locally integrable on  $(0, +\infty)$ , then  $Ff$  is a locally integrable function (actually, both  $F_1f$  and  $F_2f$  are).*

*Proof.* The second term in (3.7) is well defined and measurable as both  $\beta$  and  $f$  are. For the first term, we know that  $b(y'', y) |f(y'')|$  is measurable as a function of two variables. Then, applying Fubini's theorem for a positive measurable function we have for any  $0 < \epsilon < R$ :

$$\int_{\epsilon}^R \int_y^{\infty} b(y'', y) |f(y'')| dy'' dy = \int_{\epsilon}^{\infty} |f(y'')| \int_{\epsilon}^R b(y'', y) dy dy'' < +\infty$$

(recall that we set  $b(y, y') = 0$  whenever  $y < y'$ ). Hence, again by Fubini's theorem, the first term in (3.7) is also locally integrable (and in particular finite a.e.).  $\square$

The next lemma gives a stronger condition which is nevertheless simpler to understand, as usually one knows the size of  $\beta$  but not of the above integral:

**Lemma 3.1.2.** *Assume (3.4). If  $f : (0, +\infty) \rightarrow \mathbb{R}$  is a measurable function such that*

$$\int_{\epsilon}^{\infty} y \beta(y) |f(y)| dy < +\infty \quad \text{for all } \epsilon > 0,$$

*then  $Ff$  is well-defined (as in definition 3.0.1). If  $\beta$  is locally integrable on  $(0, +\infty)$ , then  $Ff$  is a locally integrable function (actually, both  $F_1f$  and  $F_2f$  are).*

*Proof.* It is easy to see that the conditions in the lemma imply those in 3.1.1, so this is really a corollary. However, we can also give a direct proof in the same way as before. The second term in (3.7) is no problem, and for the first term we have for any  $\epsilon > 0$ :

$$\begin{aligned} \int_{\epsilon}^{\infty} y \int_y^{\infty} b(y', y) |f(y')| dy' dy \\ = \int_{\epsilon}^{\infty} |f(y')| \int_{\epsilon}^{y'} y b(y'', y) dy dy' \leq \int_{\epsilon}^{\infty} |f(y')| \beta(y') y' dy' < +\infty, \end{aligned}$$

and we see as above that  $y \mapsto \int_y^{\infty} b(y', y) |f(y')| dy'$  is locally integrable.  $\square$

Sometimes we will need to impose some additional regularity on the fragmentation coefficient  $b$ . For example, the following hypothesis is often useful:

For some  $k \leq 1$  there is a constant  $C \geq 0$  such that

$$\int_0^y \left(\frac{y'}{y}\right)^k b(y, y') dy' \leq C \beta(y) \quad \text{a.e. } y > 0. \quad (3.8)$$

Note that for  $k \geq 1$ , (3.8) is implied by (3.4), as for  $k = 1$  this is just the definition of  $\beta$  and if (3.8) is true of any  $k \in \mathbb{R}$ , then it is true for any greater  $k$  and the same constant.

*Remark 3.1.3.* If the fragmentation is self similar (as in equation (2.14)) then the condition (3.8) is translated to a condition on  $B$ , as

$$\int_0^y \left(\frac{y'}{y}\right)^k b(y, y') dy' = \beta(y) \int_0^y \left(\frac{y'}{y}\right)^k \frac{1}{y} B\left(\frac{y'}{y}\right) dy' = \beta(y) \int_0^1 z^k B(z) dz$$

and the constant  $C$  is in this case  $\int_0^1 z^k B(z) dz$ , when this integral is finite (of course, it is when  $k \geq 1$  by (2.15)).

If  $b$  satisfies the previous assumption for some  $k \leq 1$ , then  $Ff$  is well-defined under slightly weaker conditions than in lemma 3.1.2:

**Lemma 3.1.4.** *Assume (3.4), and suppose (3.8) holds for some  $k \leq 1$ . If  $f : (0, +\infty) \rightarrow \mathbb{R}$  is a measurable function such that*

$$\int_\epsilon^\infty y^k \beta(y) |f(y)| dy < +\infty \quad \text{for all } \epsilon > 0,$$

*then  $Ff$  is well-defined (as in definition 3.0.1), and both  $F_1f$  and  $F_2f$  are locally integrable functions.*

*Proof.* The proof is the same as that of lemma 3.1.2; the only difference is that this time we multiply by  $y^k$ , integrate and then use (3.8): for any  $\epsilon > 0$ ,

$$\begin{aligned} & \int_\epsilon^\infty \int_y^\infty y^k b(y'', y) |f(y'')| dy'' dy \\ &= \int_\epsilon^\infty |f(y'')| \int_\epsilon^{y''} y^k b(y'', y) dy dy'' \leq C \int_\epsilon^\infty |f(y'')| \beta(y'')(y'')^k dy'' < +\infty. \end{aligned}$$

□

## 3.2. Some notation

We denote the usual space of  $p$ -integrable functions ( $1 \leq p \leq \infty$ ) on an open set  $\Omega \subseteq \mathbb{R}^N$  as  $L^p(\Omega)$  (where two functions which are almost everywhere equal are considered as the same one). The space of  $p$ -integrable functions for a measure  $\mu$  which is not the usual Lebesgue measure is denoted as  $L^p(\Omega, \mu)$ . As we will use  $L^p(0, +\infty)$  most often, when we write  $L^p$  with no other indication,  $L^p(0, +\infty)$  is understood.

For  $k \in \mathbb{R}$ , we write  $\dot{L}_k^1$  to denote the space  $L^1((0, +\infty), y^k dy)$ ; this is, the space of functions  $f : (0, +\infty) \rightarrow \mathbb{R}$  such that  $y \mapsto y^k f(y)$  is integrable. For  $f$  in this space, we write

$$M_k(f) := \int_0^\infty y^k f(y) dy.$$

$M_k$  is a norm in  $\dot{L}_k^1$  which makes it a complete normed space.

Analogously, we define the space  $\dot{L}_k^\infty$  as the space of functions  $f : (0, +\infty) \rightarrow \mathbb{R}$  such that  $y \mapsto y^k f(y)$  is in  $L^\infty(0, +\infty)$  (and as usual, two functions which are almost everywhere equal are considered as the same one). For  $f$  in this space, we write

$$\|f\|_{\dot{L}_k^\infty} := \|y^k f\|_\infty.$$

This defines a norm in  $\dot{L}_k^\infty$  which makes it a Banach space, as  $f \mapsto y^m f$  is an isometry from it to  $L^\infty(0, +\infty)$ .

We define the space  $M_k$  as the space of measures  $\mu$  on  $(0, +\infty)$  such that  $y^k \mu(y)$  is a finite measure. Its norm is defined by the expression

$$M_k(\mu) := \int_0^\infty y^k \mu(y).$$

With this norm,  $M_k$  is a complete normed space. Using the same notation as for the norm in  $\dot{L}_k^1$  is justified, as  $\dot{L}_k^1 \subseteq M_k$  — with the usual identification — and the inclusion is an isometry.

The space  $M_{\text{loc}}$  is the set of Borel measures on  $(0, +\infty)$  for which compact sets of  $(0, +\infty)$  have finite measure.

### 3.3. Moments of $Ff$

For later use we are interested in knowing when  $Ff$  has finite moments of a given order; this is, when  $Ff \in \dot{L}_k^1$  for some  $k \in \mathbb{R}$ .

**Lemma 3.3.1 (Moments of  $Ff$ ).** *Assume (3.4) holds and let  $f : (0, +\infty) \rightarrow \mathbb{R}$  be a measurable function.*

- *If  $y \mapsto y \beta(y) f(y)$  is integrable, then  $Ff$  is in  $\dot{L}_1^1$  and*

$$M_1(Ff) \leq 2 \int_0^\infty y \beta(y) |f(y)| dy.$$

- *Suppose that (3.8) holds for some  $k \leq 1$ . If for some  $m \geq k$  the function  $y \mapsto y^m \beta(y) f(y)$  is integrable, then  $Ff$  is in  $\dot{L}_m^1$  and*

$$M_m(Ff) \leq (C + 1) \int_0^\infty y^m \beta(y) |f(y)| dy,$$

where  $C$  is the constant in (3.8).

*Proof.* Observe that the conditions on both statements imply those in lemma 3.1.2, so  $Ff$  is well-defined and measurable. Also, the second statement includes the first one in the case  $k = 1$ , so we only need to prove the second one.

It is obvious that the second term in (3.7) is in  $\dot{L}_m^1$ . For the first term we can directly calculate the integral:

$$\begin{aligned} \int_0^\infty \int_y^\infty y^m b(y'', y) |f(y'')| dy'' dy &= \int_0^\infty |f(y'')| \int_0^{y''} y^m b(y'', y) dy dy'' \\ &\leq \int_0^\infty |f(y'')| (y'')^{m-k} \int_0^{y''} y^k b(y'', y) dy dy'' \\ &= \int_0^\infty |f(y'')| (y'')^m \int_0^{y''} \left(\frac{y}{y''}\right)^k b(y'', y) dy dy'' \\ &\leq C \int_0^\infty |f(y'')| a(y'') (y'')^m dy'' \end{aligned}$$

so the first term in (3.7) is in  $\dot{L}_m^1$ . With this, the bound in the statement is straightforward.  $\square$

**Corollary 3.3.2.** *Assume (3.4). Suppose that  $\beta$  is in  $L^\infty$ . Then  $F$  is a well defined continuous operator*

$$F : \dot{L}_M^1 \rightarrow \dot{L}_M^1 \quad \text{for } M \geq 1.$$

*In general, if (3.8) holds for some  $k \leq 1$ , then  $F$  is a well defined continuous operator*

$$F : \dot{L}_M^1 \rightarrow \dot{L}_M^1 \quad \text{for } M \geq k.$$

### 3.4. Adjoint of $F$

Most of the previous proofs in this chapter are based on the fact that we can write the operator  $F$  in a very useful form, which we will call *the fundamental identity*: for a sufficiently regular function  $\phi$  we have

$$\begin{aligned} \int_0^\infty \phi(y) F_1 f(y) dy &= \int_0^\infty \int_y^\infty \phi(y) b(y'', y) f(y'') dy'' dy \\ &= \int_0^\infty f(y'') \int_0^{y''} \phi(y) b(y'', y) dy dy'' \quad (3.9) \end{aligned}$$

and

$$\begin{aligned} \int_0^\infty \phi(y) F_2 f(y) dy &= \int_0^\infty \int_0^y \phi(y) f(y) \frac{y'}{y} b(y, y') dy' dy \\ &= \int_0^\infty f(y) \int_0^y \phi(y) \frac{y'}{y} b(y, y') dy' dy. \quad (3.10) \end{aligned}$$

So we get

$$\int_0^\infty \phi(y) F f(y) dy = \int_0^\infty f(y) F^* \phi(y) dy,$$

where

$$F^* \phi(y) := \int_0^y \phi(y') b(y, y') dy' - \phi(y) \int_0^y \frac{y'}{y} b(y, y') dy' \quad (3.11)$$

$$= \int_0^y b(y, y') \left( \phi(y') - \frac{y'}{y} \phi(y) \right) dy' \quad (3.12)$$

$$= \int_0^y y' b(y, y') \left( \frac{1}{y'} \phi(y') - \frac{1}{y} \phi(y) \right) dy'. \quad (3.13)$$

The aim of this section is to give conditions under which this fundamental identity holds and to state some properties of the operator  $F^*$ .

**Definition 3.4.1.** Assume (3.4). We define  $F^* \phi$  as the function

$$\begin{aligned} F^* \phi(y) &:= \int_0^y \phi(y') b(y, y') dy' - \phi(y) \int_0^y \frac{y'}{y} b(y, y') dy' \\ &=: F_1^* \phi(y) - F_2^* \phi(y) \end{aligned}$$

whenever these integrals are well-defined in the sense of Lebesgue.

**Lemma 3.4.2.** Let  $f : (0, +\infty) \rightarrow \mathbb{R}$  and  $b : \mathbb{T} \rightarrow [0, +\infty)$  be measurable. The following are equivalent:

- $F_1 f, F_2 f$  are well defined locally integrable functions.
- $F_1^* \phi, F_2^* \phi$  are well defined for all  $\phi \in \mathcal{C}_c(0, +\infty)$  and

$$\int_0^\infty |f(y) F_i^* \phi(y)| dy < +\infty, \quad i = 1, 2.$$

*Proof.* One can follow the derivation in (3.9), (3.10) with absolute values inside the integral; then, by Fubini's theorem for positive measurable functions, any side of the equality is finite if and only if the other side is.  $\square$

**Proposition 3.4.3 (Fundamental identity for the fragmentation operator).**

Let  $f, \psi : (0, +\infty) \rightarrow \mathbb{R}$  and  $b : \mathbb{T} \rightarrow [0, +\infty)$  be measurable functions such that both  $Ff$  and  $F^* \psi$  are well-defined and measurable. Then the following are equivalent:

- $\psi F_1 f, \psi F_2 f$  are integrable on  $(0, +\infty)$ .
- $f F_1^* \psi, f F_2^* \psi$  are integrable on  $(0, +\infty)$ .

And whenever the above holds,

$$\int_0^\infty Ff(y) \psi(y) dy = \int_0^\infty f(y) F^* \psi(y) dy.$$



*Proof.* One can prove the equivalence as in lemma 3.4.2. Then all the terms in the equality are well-defined, so we can carry out the derivation in (3.9), (3.10) without problems.  $\square$

**Corollary 3.4.4.** *If  $f$  and  $b$  are measurable functions such that  $F_1 f$ ,  $F_2 f$  are well defined and locally integrable, then for any  $\phi \in \mathcal{C}_c(0, +\infty)$ ,  $F^* \phi$  is well defined and*

$$\int_0^\infty \phi(y) F f(y) dy = \int_0^\infty f(y) F^* \phi(y) dy.$$

The next lemma gives weaker conditions under which  $F^* \phi$  is a well-defined measurable function, without mention of  $F$ :

**Lemma 3.4.5.** *Assume (3.4). Take any  $\phi : (0, +\infty) \rightarrow \mathbb{R}$  which is measurable and essentially bounded on compact sets of  $(0, +\infty)$ .*

*If for some  $\epsilon > 0$ ,  $|\phi(y)|/y$  is essentially bounded on  $(0, \epsilon)$ , then both  $F_1^* \phi$  and  $F_2^* \phi$  are well-defined measurable functions.*

*Additionally, suppose that (3.8) holds for some  $k \leq 1$ . Take  $m \geq k$ . If for some  $\epsilon > 0$ ,  $|\phi(y)|/y^m$  is essentially bounded on  $(0, \epsilon)$ , then both  $F_1^* \phi$  and  $F_2^* \phi$  are well-defined measurable functions.*

*Proof.* We only prove the second statement, as it includes the first one when  $k = m = 1$ . The second term in the definition of  $F^* \phi$  is clearly defined and measurable; for the first one, call

$$\begin{aligned} K &:= \operatorname{ess\,sup}_{0 < y < \epsilon} \frac{|\phi(y)|}{y^m} \\ x_y &:= \min\{\epsilon, y\} \quad \text{for } y > 0 \\ K_y &:= \operatorname{ess\,sup}_{y' \in (x_y, y)} |\phi(y')|. \end{aligned}$$

Then we have the following for almost all  $y > 0$ :

$$\begin{aligned} \int_0^y |\phi(y')| b(y, y') dy' &= \int_0^{x_y} |\phi(y')| b(y, y') dy' + \int_{x_y}^y |\phi(y')| b(y, y') dy' \\ &= y^k \int_0^{x_y} (y')^{m-k} \frac{|\phi(y')|}{(y')^m} \frac{(y')^k}{y^k} b(y, y') dy' + y \int_{x_y}^y \frac{|\phi(y')|}{y'} \frac{y'}{y} b(y, y') dy' \\ &\leq C \epsilon^{m-k} y^k K \beta(y) + y K_y \frac{1}{x_y} \beta(y). \end{aligned}$$

Hence, the integral in the first term is finite a.e., and by Fubini's theorem it is also measurable.  $\square$

**Lemma 3.4.6 (Some bounds for  $F^*$ ).** *Assume (3.4) and take any measurable  $\phi : (0, +\infty) \rightarrow \mathbb{R}$  such that  $y \mapsto \phi(y)/y$  is essentially bounded (this is,  $\phi \in L_{-1}^\infty$ ). Then  $F^*\phi$  is a well-defined measurable function and for  $K := \|\phi/y\|_\infty$  it holds that*

$$|F_i^*\phi| \leq K\beta(y)y, \quad i = 1, 2. \quad (3.14)$$

*Additionally, suppose that (3.8) holds for some  $k \leq 1$ . Take  $m \geq k$ . Then for any  $\phi \in L_{-m}^\infty$ ,  $F^*\phi$  is a well-defined measurable function and for  $A := \|\phi/y^m\|_\infty$  it holds that*

$$|F_i^*\phi| \leq AC\beta(y)y^m, \quad i = 1, 2.$$

where  $C$  is the constant in equation (3.8).

*Proof.* The conditions in the lemma imply those in lemma 3.4.5, so in both cases  $F^*\phi$  is well-defined and measurable. As for the bounds, we only need to prove the second one, as it includes the first one when  $k = m = 1$ .

For all  $y > 0$  we have:

$$\begin{aligned} |F^*\phi(y)| &\leq \int_0^y \frac{\phi(y')}{(y')^m} (y')^m b(y, y') dy' + \frac{\phi(y)}{y^m} y^{m-1} \int_0^y y' b(y, y') dy' \\ &\leq A \int_0^y (y')^m b(y, y') dy' + A y^{m-1} \int_0^y y' b(y, y') dy' \\ &\leq AC y^m \beta(y) + A y^m \beta(y) \leq 2AC y^m \beta(y). \end{aligned}$$

This proves the bound. □

**Lemma 3.4.7 (Support of  $F^*\phi$ ).** *Assume (3.4). If  $\phi : (0, +\infty) \rightarrow \mathbb{R}$  is any function with support contained in  $[\epsilon, +\infty)$  such that  $F^*\phi$  is well defined, then  $\text{supp } F^*\phi \subseteq [\epsilon, +\infty)$ .*

*Proof.* This is evident from the expression of  $F^*\phi$ . □

### 3.5. Definition in $\dot{L}_M^\infty$ spaces

**Lemma 3.5.1.** *Assume (3.4), suppose that  $\beta$  is bounded and that for some constant  $K \geq 0$ ,*

$$\int_y^\infty b(y', y) dy' < K \quad \text{for all } y > 0.$$

*Then  $F : L^\infty \rightarrow L^\infty$  is well defined and continuous.*

*Proof.* Take  $f \in L^\infty$ . It is easy to see that these hypotheses imply those in lemma 3.1.1, so  $Ff$  is well-defined. It is also clear that

$$\|F_2 f\|_\infty \leq \|f\|_\infty \|\beta\|_\infty,$$

and we also have that

$$\|F_1 f\|_\infty \leq \|f\|_\infty \sup_{y>0} \int_y^\infty b(y', y) dy' \leq K \|f\|_\infty.$$

This proves that  $F : L^\infty \rightarrow L^\infty$  is continuous.  $\square$

We can give different conditions that ensure  $y^k Ff(y)$  is bounded for some  $k \in \mathbb{R}$ :

**Lemma 3.5.2.** *Assume (3.4). Suppose that for some  $k \in \mathbb{R}$ ,*

$$(y')^{k+1} b(y, y') \leq C y^k \beta(y) \quad \text{a.e. } (y, y') \in \mathbb{T}. \quad (3.15)$$

*Suppose that for some  $m > 1 + k$ ,  $y^m \beta(y) |f(y)|$  is essentially bounded by a constant  $K \geq 0$ . Then,  $F$  is well defined and  $y^m |Ff(y)|$  is essentially bounded.*

*Proof.* For the term  $\beta(y)f(y)$  appearing in  $Ff$ , by hypothesis its absolute value is bounded when multiplied by  $y^m$ . For the other term, use that  $y^m \beta(y) |f(y)|$  is bounded and that (3.15) holds to get the following for almost all  $y > 0$ :

$$\begin{aligned} \int_y^\infty y^m b(y'', y) |f(y'')| dy'' &\leq C y^{m-k-1} \int_y^\infty (y'')^k \beta(y'') |f(y'')| dy'' \\ &\leq C K y^{m-k-1} \int_y^\infty (y'')^{k-m} dy'' = C K \frac{1}{k-m+1} y^{m-k-1} y^{k-m+1} = C'. \end{aligned}$$

This proves at once that  $Ff$  is well defined (as  $b(y'', y)f(y'')$  is integrable in  $y''$ ) and that  $y^m |Ff(y)|$  is bounded.  $\square$

**Corollary 3.5.3.** *Assume (3.4). Suppose that  $\beta(y)$  is in  $L^\infty$  and that for some  $k \in \mathbb{R}$ ,*

$$(y')^{k+1} b(y, y') \leq C \beta(y) y^k \quad \text{a.e. } (y, y') \in \mathbb{T}.$$

*Then  $F$  is a well defined operator*

$$F : \dot{L}_M^\infty \rightarrow \dot{L}_M^\infty$$

*for every  $M > k + 1$ .*

### 3.6. Definition in spaces of measures

The definition of  $Ff$  can be extended to the case in which  $f$  is only a measure on  $(0, +\infty)$ . This will be necessary to define and study measure solutions to the coagulation-fragmentation equation later. In this case,  $Ff$  will, in general, also be a measure on  $(0, +\infty)$ . However, it is enough to define the dual  $F^*$ , which is simpler and will suffice for our purposes. Another reason to restrict the study to  $F^*$  instead

of  $F$  is that, in order to give a definition for  $Ff$  as a measure, it is enough to define the quantities

$$\int_0^\infty Ff\phi$$

for each  $\phi$  continuous and of compact support on  $\mathcal{C}_c(0, +\infty)$ , in such a way that for each  $0 < \epsilon R$ , the functional

$$\begin{aligned} \mathcal{C}_c(\epsilon, R) &\rightarrow \mathbb{R} \\ \phi &\mapsto \int Ff\phi \end{aligned}$$

is continuous (when the uniform norm is considered on  $\mathcal{C}_c(\epsilon, R)$ ). Then, Riesz' representation theorem gives a unique measure  $Ff$  on  $(0, +\infty)$  which agrees with this. But of course the above quantities can be written in terms of  $F^*$  as

$$\int_0^\infty fF^*\phi,$$

so by studying  $F^*$  we are implicitly studying  $F$ .

*Remark 3.6.1.* The notation for integration with respect to a measure used here differs slightly from that used in other places; if  $\mu$  is a measure on some measurable space  $(\Omega, \mathcal{A})$  and  $f$  is a  $\mu$ -integrable function on  $\Omega$ , we write

$$\int_\Omega f\mu \quad \text{or} \quad \int_\Omega f(y)\mu(y) dy$$

to denote the integral of  $f$  with respect to  $\mu$ . At other places this is denoted as  $\int_\Omega f d\mu$  or  $\int_\Omega f(y)d\mu(y)$ , but here we denote it as above mainly for analogy with the case in which  $\mu$  can be identified with a function.

In the following we can weaken our conditions on the fragmentation coefficient  $b$ . We will assume that

$$\begin{aligned} b : (0, +\infty) &\rightarrow M_1 \quad \text{is a measurable function.} \\ \text{For all } y > 0, &b(y) \text{ is a positive measure} \\ \text{and its support is} &\text{ contained in } (0, y). \end{aligned} \tag{3.16}$$

(Recall that  $M_1$  is the space of measures  $\mu$  on  $(0, +\infty)$  such that  $y\mu(y)$  is a finite measure; see section 3.2.)

*Remark 3.6.2.* With the usual identification between integrable functions and measures, if we have a function  $b$  in the conditions (3.4), we can find a measure  $b$  in the conditions of (3.16) which coincides with it for almost all  $y > 0$ ; in this sense, these hypotheses are weaker than those in (3.4).

We call, as before,<sup>1</sup>

$$\beta(y) := \int_0^y \frac{y'}{y} b(y, y') dy' \quad \text{for } y > 0$$

The function  $\beta$  thus defined is measurable.

**Definition 3.6.3.** Assume (H2). For a function  $\phi \in \mathcal{C}_c(0, +\infty)$  we define  $F^*\phi$  as

$$F^*\phi(y) := \int_0^y \phi(y') b(y, y') dy' - \phi(y) \int_0^y \frac{y'}{y} b(y, y') dy'.$$

As  $b : (0, +\infty) \rightarrow M_1$  is measurable,  $F^*\phi$  defined as above is also measurable. Of course, if (3.4) holds, then  $F^*$  as defined here is the same as the  $F^*$  in 3.4.1 (see remark 3.6.2).

We have the following extension of lemma 3.4.6:

**Lemma 3.6.4.** *Assume (H2). Take any  $\phi \in \mathcal{C}_c^\infty(0, +\infty)$  and call  $\epsilon := \min \text{supp } \phi$ . Then  $\text{supp } F^*\phi \subseteq [\epsilon, +\infty)$  and for  $C := \|\phi/y\|_\infty$  it holds that*

$$|F^*\phi(y)| \leq 2C\beta(y)y.$$

The proof of this lemma is a repetition of the proof of lemma 3.4.6.

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<sup>1</sup>This is meant to denote the integral of the function  $y' \mapsto y'/y$  with respect to the measure  $b(y)$ ; see remark 3.6.1.

# Chapter 4

## The coagulation operator

### 4.1. Definition

As in the previous chapter, the ideas here are already known, but the results are included in order to have precise statements which do not appear in the literature in the form needed; again, see [33, 29, 86] and their references for related results. To our knowledge, the results on the weak definition of the coagulation operator appear only in [34], and we present them here in a slightly modified form.

Let us define the coagulation operator precisely. From here on, the coefficient  $a$  will always be a nonnegative Borel measurable function  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  which is symmetric (this is:  $a(y, y') = a(y', y)$  for all  $y, y' > 0$ ).

**Definition 4.1.1.** For a measurable function  $f : (0, +\infty) \rightarrow \mathbb{R}$ , we define  $C(f)$  (the *coagulation operator* acting on  $f$ ), as the function on  $(0, +\infty)$  defined for almost all  $y > 0$  as

$$\begin{aligned} C(f) &:= C_1(f) - C_2(f) \\ C_1(f)(y) &:= \frac{1}{2} \int_0^y a(y', y - y') f(y') f(y - y') dy' \\ C_2(f)(y) &:= f(y) \int_0^\infty a(y, y') f(y') dy', \end{aligned}$$

whenever all the Lebesgue integrals here make sense for almost all  $y > 0$ .

The above operator is quadratic, and sometimes its associated bilinear operator will be useful: for measurable functions  $f, g : (0, +\infty) \rightarrow \mathbb{R}$ , we define  $C(f, g)$  (the *coagulation operator* acting on  $f, g$ ), as the function on  $(0, +\infty)$  defined for almost all  $y > 0$  as

$$\begin{aligned} C(f, g) &:= C_1(f, g) - C_2(f, g) \\ C_1(f, g)(y) &:= \frac{1}{2} \int_0^y a(y', y - y') f(y') g(y - y') dy' \\ C_2(f, g)(y) &:= \frac{1}{2} f(y) \int_0^\infty a(y, y') g(y') dy' + \frac{1}{2} g(y) \int_0^\infty a(y, y') f(y') dy', \end{aligned}$$

whenever all the Lebesgue integrals here make sense for almost all  $y > 0$ .

*Remark 4.1.2.* Note that we use the same notation for both operators; they can be easily distinguished by the number of arguments they are used with. Of course,  $C(f, f) = C(f)$  whenever any of them makes sense.

As for the fragmentation, we look for conditions that ensure it is defined and has some additional regularity, in the sense that the integrals  $\int \phi C(f)$  make sense for certain functions  $\phi$ .

**Lemma 4.1.3 (Conditions for the definition of  $C$ ).** *Suppose that there are measurable functions  $A_1, A_2 : (0, +\infty) \rightarrow [0, +\infty)$  such that*

$$a(y, y') \leq A_1(y)A_2(y') + A_1(y')A_2(y). \quad (4.1)$$

*Take any measurable functions  $f, g : (0, +\infty) \rightarrow \mathbb{R}$  such that for  $i = 1, 2$*

$$\int_0^\infty A_i(y) |f(y)| dy < +\infty \quad (4.2)$$

$$\int_0^\infty A_i(y) |g(y)| dy < +\infty. \quad (4.3)$$

*Then  $C(f, g)$  is well defined. Furthermore, it is an integrable function on  $(0, +\infty)$  and*

$$\|C(f, g)\|_1 \leq \frac{3}{2} \int_0^\infty A_1 |f| \int_0^\infty A_2 |g| + \frac{3}{2} \int_0^\infty A_2 |f| \int_0^\infty A_1 |g|.$$

*Proof.* The integral in  $C_1$  is well-defined for almost all  $y > 0$ , and in fact it gives an integrable function of  $y$ :

$$\begin{aligned} & \int_0^\infty \int_0^y a(y', y - y') |f(y')| |g(y - y')| dy' dy \\ & \leq \int_0^\infty \int_0^y (A_1(y')A_2(y - y') + A_1(y - y')A_2(y')) |f(y')| |g(y - y')| dy' dy \\ & = \int_0^\infty \int_0^\infty (A_1(y')A_2(y) + A_1(y)A_2(y')) |f(y')| |g(y)| dy' dy \\ & = \int_0^\infty A_1(y') |f(y')| dy' \int_0^\infty A_2(y) |g(y)| dy \\ & \quad + \int_0^\infty A_2(y') |f(y')| dy' \int_0^\infty A_1(y) |g(y)| dy. \end{aligned}$$

These integrals are well-defined thanks to (4.2, 4.3). By Fubini's theorem, the integral in  $C_1(f, g)$  is well-defined for almost all  $y > 0$ .

Now, for  $C_2$  we can do something similar:

$$\begin{aligned} & \int_0^\infty a(y, y') |g(y')| dy' \\ & \leq A_1(y) \int_0^\infty A_2(y') |g(y')| dy' + A_2(y) \int_0^\infty A_1(y') |g(y')| dy', \end{aligned}$$

which is finite, so the first integral in  $C_2(f, g)$  is well-defined; the second integral is the same one, interchanging  $f$  and  $g$ . Let us see that  $C_2(f, g)$  is integrable:

$$\begin{aligned} \int_0^\infty |f(y)| \int_0^\infty a(y, y') |g(y')| dy' dy \\ \leq \int_0^\infty A_1(y) |f(y)| dy \int_0^\infty A_2(y') |g(y')| dy' \\ + \int_0^\infty A_2(y) |f(y)| dy \int_0^\infty A_1(y') |g(y')| dy' < +\infty. \end{aligned}$$

Again, the second term in  $C_2(f, g)$  can be treated in the same way. Finally, the bound is clear from the calculations above, as each term contributes with 1/2 of the same quantity.  $\square$

**Lemma 4.1.4 (Additional regularity of  $C(f, g)$ ).** *Let  $\phi : (0, +\infty) \rightarrow [0, +\infty)$  be a measurable function such that for some constant  $C > 0$*

$$\phi(y + y') \leq C(\phi(y) + \phi(y')).$$

*In addition to the hypotheses of lemma 4.1.3, suppose that for  $i = 1, 2$*

$$\int_0^\infty \phi(y) A_i(y) |f(y)| dy < +\infty \quad (4.4)$$

$$\int_0^\infty \phi(y) A_i(y) |g(y)| dy < +\infty \quad (4.5)$$

*Then  $C(f, g)$  (which is a well-defined integrable function thanks to lemma 4.1.3) is such that*

$$\begin{aligned} \int_0^\infty \phi(y) |C(f, g)(y)| dy \\ \leq \frac{(C+1)}{2} \left( \int_0^\infty \phi A_1 |f| \int_0^\infty A_2 |g| + \int_0^\infty \phi A_2 |f| \int_0^\infty A_1 |g| \right. \\ \left. + \int_0^\infty A_1 |f| \int_0^\infty \phi A_2 |g| + \int_0^\infty A_2 |f| \int_0^\infty \phi A_1 |g| \right). \end{aligned}$$

*Proof.* The proof follows the same line as that of lemma 4.1.3; the only difference is that this time we multiply by  $\phi$  before integrating. As the bound is straightforward we do not include the proof here.  $\square$

**Corollary 4.1.5.** *Let  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  be a symmetric measurable function essentially bounded above by a constant  $A > 0$ . Then for a function  $f \in L^1$  the integrals in the definition of  $C$  are defined for almost all  $y > 0$ . The function  $C(f)$  is in  $L^1$  and*

$$\|C(f)\|_1 \leq \frac{3}{2} A \|f\|_1^2.$$



In addition, if  $f \in \dot{L}_k^1$  for  $k > 0$ ,  $C(f)$  is in  $\dot{L}_k^1$  and

$$M_k(C(f)) \leq (C + 1)A M_k(f) \|f\|_1,$$

where  $C > 0$  is a constant such that  $(y + y')^k \leq C(y^k + (y')^k)$  for positive  $y, y'$ .

*Proof.* This is a particular case of lemma 4.1.4 when  $f = g$  and  $\phi(y) = y^k$ .  $\square$

## 4.2. Definition in $L^\infty$

**Lemma 4.2.1.** *As usual, assume that  $a : (0, +\infty) \times (0, +\infty) \rightarrow \mathbb{R}$  is a symmetric nonnegative measurable function. Suppose also that  $a$  is essentially bounded. Take  $f : (0, +\infty) \rightarrow \mathbb{R}$  which is in  $L^1 \cap L^\infty$ . Then  $C(f)$  is well defined and*

$$\|C(f)\|_\infty \leq \frac{3}{2} \|a\|_\infty \|f\|_\infty \|f\|_1.$$

*Proof.* The lemma follows from a direct estimate on the expression of  $C(f)$ .  $\square$

**Corollary 4.2.2.** *If  $a$  is a nonnegative bounded measurable function, then  $C$  is a continuous operator*

$$C : L^1 \cap L^\infty \rightarrow L^1 \cap L^\infty.$$

## 4.3. Weak form of the coagulation operator

**Definition 4.3.1.** Given  $f, g, \phi : (0, +\infty) \rightarrow \mathbb{R}$  measurable functions, we define the operator  $\mathcal{C}(f, g)$  acting on  $\phi$  as:

$$\langle \mathcal{C}(f, g), \phi \rangle := \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y') f(y) g(y') (\phi(y + y') - \phi(y) - \phi(y')) dy' dy \quad (4.6)$$

whenever the function under the integral is integrable in the sense of Lebesgue.

We will frequently denote  $\mathcal{C}(f, f)$  as  $\mathcal{C}(f)$ .

**Proposition 4.3.2 (Fundamental identity).** *Let  $f, g, \phi : (0, +\infty) \rightarrow \mathbb{R}$  be measurable functions, and assume that  $C(f, g)$  is well defined and  $C_1(f, g)\phi$ ,  $C_1(f, g)\phi$  are integrable. Then  $\langle \mathcal{C}(f, g), \phi \rangle$  is well-defined and*

$$\int_0^\infty \phi(y) C(f, g)(y) dy = \langle \mathcal{C}(f, g), \phi \rangle.$$

*Proof.* When the integrals below are well defined we can operate as follows:

$$\begin{aligned}
& \int_0^\infty \phi(y)C(f, g)(y) dy \\
&= \frac{1}{2} \int_0^\infty \int_0^y a(y', y - y')f(y')g(y - y')\phi(y) dy' dy \\
&+ \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y')f(y)g(y')\phi(y) dy' dy + \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y')f(y')g(y)\phi(y) dy' dy \\
&= \frac{1}{2} \int_0^\infty \int_0^\infty a(y', y)f(y')g(y)\phi(y + y') dy dy' \\
&+ \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y')f(y')g(y)(\phi(y') + \phi(y)) dy' dy \\
&= \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y')f(y)g(y')(\phi(y + y') - \phi(y) - \phi(y')) dy dy'.
\end{aligned}$$

Note that we have used the symmetry of  $a$ . This proves that  $\langle \mathcal{C}(f, g), \phi \rangle$  is also well-defined.  $\square$

**Corollary 4.3.3.** *Suppose that  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  is a measurable function which is essentially bounded.*

*Then  $\mathcal{C}(f, g)$  is well-defined on all integrable functions  $f, g : (0, +\infty) \rightarrow \mathbb{R}$  which are also integrable in some neighborhood of 0, and the integral in (4.6) makes sense for  $\phi \in \mathcal{C}_c(0, +\infty)$ .*

### 4.3.1. Weak conditions for the definition of $\mathcal{C}$

In certain cases it may happen that the weak form of the coagulation operator  $\mathcal{C}(f, g)$  makes sense while the coagulation operator  $C(f, g)$  does not. This is due to a cancellation between the positive and negative terms in  $\langle \mathcal{C}(f, g), \phi \rangle$  which does not take place directly in  $C(f, g)$ . What happens in these cases is that  $\mathcal{C}(f, g)$  can be defined as a distribution, but this distribution is not a function.

When the coagulation coefficient  $a$  is bounded near 0 we can show that  $\langle \mathcal{C}(f, g), \phi \rangle$  is well defined if  $\phi$  is  $\mathcal{C}^1$  and  $f, g$  are such that  $\int yf(y) dy$  and  $\int yg(y) dy$  are finite.

**Lemma 4.3.4.** *Let  $\phi : (0, +\infty) \rightarrow \mathbb{R}$  be a  $\mathcal{C}^1$  function with support contained in  $[\epsilon, \infty)$  for some  $\epsilon > 0$ . Then there is a constant  $C \geq 0$  which only depends on  $\epsilon$  such that*

$$|\phi(y + y') - \phi(y) - \phi(y')| \leq C y y' \|\phi\|_{\mathcal{C}^1} \quad \text{for all } y, y' > 0.$$

*Proof.* If  $y, y' \leq \epsilon/2$ , then the expression is zero. If both of them are  $\geq \epsilon/2$ , then

$$|\phi(y + y') - \phi(y) - \phi(y')| \leq 3 \|\phi\|_\infty \leq \frac{4}{\epsilon^2} 3 y y' \|\phi\|_\infty.$$

If  $y \leq \epsilon/2$  and  $y' \geq \epsilon/2$ ,

$$|\phi(y + y') - \phi(y) - \phi(y')| = |\phi(y + y') - \phi(y')| \leq y \|\phi\|_{C^1} \leq \frac{2}{\epsilon} y y' \|\phi\|_{C^1},$$

and the same bound is true if  $y' \leq \epsilon/2$  and  $y \geq \epsilon/2$ .  $\square$

**Lemma 4.3.5.** *Let  $\phi : (0, +\infty) \rightarrow \mathbb{R}$  be a  $C^1$  function of compact support, and let  $f, g \in \dot{L}_1^1$ . Suppose that the coagulation coefficient  $a$  is bounded on every set of the form  $[0, R]^2 \setminus [0, \epsilon]^2$  for  $R > \epsilon > 0$ .*

*Then  $\langle \mathcal{C}(f, g), \phi \rangle$  is well defined and there is a constant  $C \geq 0$  which depends only on the support of  $\phi$  and the local bound of  $a$ , such that*

$$|\langle \mathcal{C}(f, g), \phi \rangle| \leq C \|\phi\|_{C^1} M_1(f) M_1(g).$$

*Proof.* This is immediate using the previous lemma.  $\square$

The previous conditions will allow us later to consider a particle distribution  $f$  for which  $\int_0^\infty f$  is not necessarily finite.

Let us also give an example where we can consider some coagulation coefficients which are not bounded for  $y$  or  $y'$  near 0. Assume that  $a$  is of the following form:

$$\begin{aligned} a(y, y') &= y^\alpha (y')^\beta + (y')^\alpha y^\beta \quad \text{for all } y, y' > 0 \\ &\text{with } -1 \leq \alpha \leq \beta \leq 1 \text{ such that } \alpha + \beta \leq 1. \end{aligned} \quad (4.7)$$

(Note that this  $a$  does not satisfy the condition of lemma 4.3.5 when  $\alpha < 0$ ). If we suppose this special form of  $a$ , the conditions in the following lemma imply that  $\mathcal{C}(f)$  is well defined, but these are weaker than those in lemma 4.1.4, so again we cannot say that  $\mathcal{C}(f)$  is well defined.

For a measurable function  $f : (0, +\infty) \rightarrow (0, \infty)$  and  $\alpha, \beta \in \mathbb{R}$  we define the norm  $\|\cdot\|_{(\alpha, \beta)}$  as

$$\|f\|_{(\alpha, \beta)} := \int_0^1 y^\alpha |f(y)| dy + \int_1^\infty y^\beta |f(y)| dy.$$

**Lemma 4.3.6.** *Suppose that (4.7) holds, and let  $f, g \in \dot{L}_1^1$  be functions such that  $\|f\|_{(\alpha+1, \beta)}, \|g\|_{(\alpha+1, \beta)}$  are finite. Then  $\langle \mathcal{C}(f, g), \phi \rangle$  is well defined for all  $\phi \in \mathcal{C}_c^1(0, +\infty)$ .*

*There is a constant  $K_\epsilon > 0$  such that for all  $\phi \in \mathcal{C}_c^1(0, +\infty)$  with compact support contained in  $[\epsilon, +\infty)$*

$$|\langle \mathcal{C}(f, g), \phi \rangle| \leq K_\epsilon \|\phi\|_{C^1} \left( \|f\|_{(1,1)} \|g\|_{(\alpha+1, \beta)} + \|g\|_{(1,1)} \|f\|_{(\alpha+1, \beta)} \right).$$

*Proof.* We can bound the integrand  $I$  in (4.6) depending on the values of  $y, y'$ . Taking  $\delta := \min\{\epsilon/2, 1\}$  we have

- If  $y, y' < \delta$ , then the integrand is 0.
- If  $y < \delta$  and  $y' \geq \delta$ , then

$$|\phi(y + y') - \phi(y) - \phi(y')| = |\phi(y + y') - \phi(y')| \leq y \|\phi\|_{C^1},$$

so when we multiply by  $a(y, y')f(y)g(y')$  we get

$$I \leq \|\phi\|_{C^1} (y^{\alpha+1}(y')^\beta + y^{\beta+1}(y')^\alpha) f(y)g(y')$$

and finally

$$\begin{aligned} \int_0^\delta \int_\delta^\infty I \, dy \, dy' &\leq \|\phi\|_{C^1} \left( \int_0^\delta y^{\alpha+1} f(y) \, dy \int_\delta^\infty y^\beta g(y) \, dy \right. \\ &\quad \left. + \int_0^\delta y^{\beta+1} f(y) \, dy \int_\delta^\infty y^\alpha g(y) \, dy \right) \\ &\leq 2\delta^{\beta-1} \|\phi\|_{C^1} \left( \int_0^\delta y^{\alpha+1} f(y) \, dy \int_\delta^\infty y g(y) \, dy \right) \\ &\leq 2\delta^{\beta-1} \|\phi\|_{C^1} \|f\|_{(\alpha+1, \beta)} \|g\|_{(1,1)}. \end{aligned}$$

- If  $y' < \delta$  and  $y \geq \delta$ , we get an analogous estimate:

$$\int_0^\delta \int_\delta^\infty I \, dy' \, dy \leq 2\delta^{\beta-1} \|\phi\|_{C^1} \|g\|_{(\alpha+1, \beta)} \|f\|_{(1,1)}.$$

- Finally, if both  $y$  and  $y'$  are  $\geq \delta$ , then  $|\phi(y + y') - \phi(y) - \phi(y')|$  is bounded by  $\|\phi\|_\infty$  and

$$a(y, y') \leq \delta^{\alpha-\beta} (yy')^\beta \leq \delta^{\alpha-1} y^\beta y',$$

so we get:

$$\int_\delta^\infty \int_\delta^\infty I \, dy' \, dy \leq \delta^{\alpha-1} \|\phi\|_\infty \|f\|_{(\alpha+1, \beta)} \|g\|_{(1,1)}.$$

□

## 4.4. Definition in measures

In order to make sense of the coagulation-fragmentation equation in a space of measures, it is necessary to define the coagulation operator when  $f$  is a measure on  $(0, +\infty)$ , (as we did for the fragmentation operator). We will only need to use its weak form.

We take  $a$  as before: a nonnegative Borel measurable function  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  which is symmetric (this is:  $a(y, y') = a(y', y)$  for all  $y, y' > 0$ ).

**Definition 4.4.1.** Given  $f, g$  Borel measures on  $(0, +\infty)$  for which compact sets have finite measure, and  $\phi : (0, +\infty) \rightarrow \mathbb{R}$  continuous and of compact support, we define  $\langle \mathcal{C}(f, g), \phi \rangle$  as in equation (4.6), whenever the function  $(y, y') \mapsto a(y, y')(\phi(y+y') - \phi(y) - \phi(y'))$  is  $f \otimes g$ -integrable. As before, we will frequently denote  $\mathcal{C}(f, f)$  as  $\mathcal{C}(f)$ .

*Remark 4.4.2.* When  $f, g$  are measures, in equation (4.6) it is understood that the integration is with respect to the product measure  $f \otimes g$  (see also remark 3.6.1 about our notation for the integral with respect to a general measure). In general, if  $\mu, \nu$  are two measures, we will write their product with different variables (as in  $\mu(y)\nu(y')$ ) to imply the product measure  $(\mu \otimes \nu)$ .

# Chapter 5

## Existence of solutions

This chapter contains our main results on existence of solutions for the continuous coagulation-fragmentation equations. After proving the existence of regular solutions we develop the necessary estimates for the later proofs of the existence theorems. The estimates in section 5.4.1 are already known when one allows the constants to depend on the total number of particles (the integral of the solution  $f$ ), and the novelty here lies in obtaining bounds which do not depend on it. They are based on the estimates in [34], which do not take into account fragmentation effects. Section 5.4.2 contains estimates which were proved and used in [33, 35], and which stem from ideas in previous papers on existence theory; nevertheless, some of the proofs here differ from the existing ones in the technique used and we thought them to be of interest. On the other hand, estimates in section 5.4.4 deal with the interaction between coagulation and fragmentation for small particles and are new, to our knowledge.

The existence theorems in sections 5.5–5.7 are proved with the help of the estimates already mentioned. The new part of the theorem in section 5.5 is that it allows for the initial condition to be only in  $\dot{L}_1^1$  instead of  $\dot{L}_1^1 \cap L^1$ , together with less restrictions on the fragmentation coefficient. As a consequence, the solution may not satisfy that  $f(t) \in L^1$  for  $t > 0$ , and this opens the way for a study of solutions that behave in a singular way near  $y = 0$ . Section 5.6 contains a known result (stated in [33]) and is included for completeness, as the proof is short with the results in the rest of this work, and is presented in a different way from the existing literature. Results on the existence of measure solutions in section 5.7 are new and include an existence theorem for coagulation and fragmentation coefficients which are singular near  $y = 0$ .

## 5.1. Concept of solution

Let us recall the continuous coagulation-fragmentation equations from chapter 2:

$$\frac{\partial}{\partial t} f = C(f) + F(f), \quad t, y \in (0, +\infty) \quad (5.1)$$

$$f(0, y) = f^0(y), \quad y \in (0, +\infty). \quad (5.2)$$

We have included here the initial condition  $f(0, y) = f^0(y)$ ; the coagulation and fragmentation terms are given by

$$C(f) := C_1(f) - C_2(f) \quad (5.3)$$

$$F(f) := F_1(f) - F_2(f) \quad (5.4)$$

$$C_1(f)(y) := \frac{1}{2} \int_0^y a(y', y - y') f(y') f(y - y') dy' \quad (5.5)$$

$$C_2(f)(y) := f(y) \int_0^\infty a(y, y') f(y') dy' \quad (5.6)$$

$$F_1(f)(y) := \int_y^\infty b(y'', y) f(y'') dy'' \quad (5.7)$$

$$F_2(f)(y) := f(y) \int_0^y \frac{y'}{y} b(y, y') dy'. \quad (5.8)$$

(See 4.3.1 and 3.4.1 for their weak forms, respectively).

**Definition 5.1.1.** Let  $a, b$  be nonnegative measurable functions, with  $a$  defined on  $(0, +\infty) \times (0, +\infty)$  and symmetric, and  $b$  defined on  $\{(y, y') \in \mathbb{R}^2 \mid 0 < y' < y\}$ . Let  $f^0 : (0, +\infty) \rightarrow \mathbb{R}$  be a measurable function and  $T \in (0, +\infty]$ . We say that  $f : [0, T) \times (0, +\infty) \rightarrow \mathbb{R}$  is a solution to the coagulation-fragmentation equations (5.1), (5.2) if

- $f$  is locally integrable on  $[0, T) \times (0, +\infty)$ ,
- for almost all  $t \in (0, T)$ ,  $\langle \mathcal{C}(f(t, \cdot)), \phi \rangle$  is well-defined for all  $\phi \in \mathcal{D}([0, T))$  (as in definition 4.4.1),
- for all  $\phi \in \mathcal{D}([0, T) \times (0, +\infty))$ , the function

$$t \mapsto \langle \mathcal{C}(f(t)), \phi(t, \cdot) \rangle,$$

which is defined for almost all  $t \in [0, T)$ , is integrable on  $(0, T)$ ,

- For almost all  $t \in (0, T)$ ,  $F(f(t))$  is well-defined (as in definition 3.0.1), and  $Ff$  is locally integrable on  $[0, \infty) \times [0, T)$ .

- and the following holds for every  $\phi \in \mathcal{D}([0, T] \times (0, +\infty))$ :

$$\begin{aligned} - \int_0^T \int_0^\infty f(t, y) \partial_t \phi(t, y) dy dt &= \int_0^\infty f^0(y) \phi(0, y) dy \\ &+ \int_0^T \int_0^\infty F f(t, y) \phi(t, y) dy dt + \int_0^T \langle \mathcal{C}(f(t)), \phi(t, \cdot) \rangle dt. \end{aligned} \quad (5.9)$$

This definition essentially says that  $f$  is a solution if all terms are defined and the equation holds in a weak sense.

We can also give a definition of a *measure solution*, which generalizes the above to the case in which  $f(t)$  is a measure for each  $t$ :

**Definition 5.1.2.** Let  $a$  be a nonnegative symmetric Borel measurable function defined on  $(0, +\infty) \times (0, +\infty)$ , and  $b$  in the conditions (3.16). Let  $f^0$  be a measure in  $M_{\text{loc}}$  (this is, a Borel measure on  $(0, +\infty)$  which is finite on compact sets), and take  $T \in (0, +\infty]$ . We say that  $f : [0, T] \rightarrow M_{\text{loc}}$  is a *measure solution* to the coagulation-fragmentation equations (5.1), (5.2) if

- for all  $\phi \in \mathcal{D}([0, T] \times (0, +\infty))$ ,  $t \mapsto \int_0^\infty \phi(y) f(t, y) dy$  is  $t$ -integrable,
- for almost all  $t \in (0, T)$ ,  $\langle \mathcal{C}(f(t)), \phi \rangle$  is well-defined for all  $\phi \in \mathcal{D}([0, T])$  (as in definition 4.4.1),
- for all  $\phi \in \mathcal{D}([0, T] \times (0, +\infty))$ , the function

$$t \mapsto \langle \mathcal{C}(f(t)), \phi(t, \cdot) \rangle,$$

which is defined for almost all  $t \in [0, T]$ , is integrable on  $(0, T)$ ,

- for almost all  $t \in (0, T)$ ,  $F^* \phi$  is  $f(t)$ -integrable for all  $\phi \in \mathcal{D}([0, T])$ ,
- for all  $\phi \in \mathcal{D}([0, T] \times (0, +\infty))$ , the function

$$t \mapsto \int_0^\infty f(t, y) (F^* \phi(t))(y) dy,$$

which is defined for almost all  $t \in [0, T]$ , is integrable on  $(0, T)$ ,

- and the following holds for every  $\phi \in \mathcal{D}([0, T] \times (0, +\infty))$ :

$$\begin{aligned} - \int_0^T \int_0^\infty f(t, y) \partial_t \phi(t, y) dy dt &= \int_0^\infty f^0(y) \phi(0, y) dy \\ &+ \int_0^T \int_0^\infty f(t, y) F^* \phi(t, y) dy dt + \int_0^T \langle \mathcal{C}(f(t)), \phi(t, \cdot) \rangle dt. \end{aligned} \quad (5.10)$$



## 5.2. Existence of solutions for bounded coefficients

In certain cases, as shown in corollaries 3.3.2 and 3.5.3, the fragmentation operator  $F$  is a linear continuous operator in a certain space. Under certain conditions (as shown in corollary 4.1.5), the coagulation operator is continuous in  $L^1$ . Then we immediately have a solution that can be obtained as a limit of the Picard iterants associated to the equation by means of a standard process. The following is easily obtained:

**Theorem 5.2.1.** *Assume (3.4) and (3.8) for  $k = 0$ , and suppose that  $\beta$  is essentially bounded. Suppose that the coagulation coefficient  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  is an essentially bounded symmetric measurable function.*

*Let  $X$  be the Banach space  $\dot{L}_1^1 \cap L^1$  with the usual norm for the intersection of two spaces, and take  $f^0 \in X$ .*

*Then there is a solution  $f$  to the coagulation-fragmentation equation on  $(0, +\infty)$  with initial data  $f^0$  such that  $f \in C^1([0, +\infty), X)$  (with  $f(0) = f^0$ ),  $Lf(t)$  and  $C(f(t))$  are in  $X$  for all  $t \geq 0$  and*

$$\frac{d}{dt}f(t) = Lf(t) + C(f(t)) \quad t > 0,$$

*where the derivation in  $t$  is understood as that of a function in  $C^1([0, T], X)$ . The solution is the only one satisfying the above. This solution is also a solution in the sense of the definitions in chapter 10.*

*In addition, this solution conserves the mass, in the sense that*

$$\int_0^\infty y f(t, y) dy = \int_0^\infty y f^0(y) dy \quad \text{for all } t \in (0, T). \quad (5.11)$$

*Proof.* Thanks to lemma 3.3.1, under our hypotheses  $F$  is a continuous operator from  $L^1 \rightarrow L^1$  and from  $\dot{L}_1^1 \rightarrow \dot{L}_1^1$ , so it is also continuous as an operator  $F : X \rightarrow X$  (and hence Lipschitz, as it is linear).

For the coagulation term, corollary 4.1.5 ensures that for  $f \in X$ ,

$$\begin{aligned} \|C(f)\|_1 &\leq \text{const.} \|f\|_1^2 \\ M_1(C(f)) &\leq \text{const.} M_1(f) \|f\|_1, \end{aligned}$$

so  $C : X \rightarrow X$  is also a continuous operator, which must also be locally Lipschitz, as it is quadratic.

Then, solutions in the sense stated in the theorem can be found and are unique by a standard result (an argument on Picard iterants analogous to the one for ordinary differential equations can be carried out). We just need to prove that they are solutions in the sense of definition 5.1.1.

So, take a solution  $f$  in the sense of this theorem. All regularity requirements of definition 5.1.1 are satisfied. Also, the right hand side of the equation,  $Ff + C(f)$ , is

in  $L^1((0, T), X)$ , so this solution is a solution to the initial value problem (5.1), (5.2) in the sense of any of the definitions 10.1.10–10.1.16 (as it satisfies the requirement of being, for example, a mild solution). In particular, it is a weak solution to the initial value problem in the sense of definition 10.1.15, which implies the conditions in definition 5.1.1 (note that in our conditions  $\int_0^\infty \phi(y)C(f)(y) dy = \langle \mathcal{C}(f), \phi \rangle$  for all  $\phi \in \mathcal{D}(0, +\infty)$  thanks to lemma 4.3.2).

As proved in section 10.1, these solutions are solutions in the sense of the definitions in chapter 10, as in particular they are mild solutions in  $L^1$ .

Finally, mass is conserved because, as our solution is also a solution in the sense of moments (see definition 10.1.3) in the Banach space  $X$ , for  $\psi(y) = y$  we have

$$\begin{aligned} \int_0^\infty y f(t, y) dy &= \int_0^\infty y f^0(y) dy + \int_0^t \int_0^\infty y (F f(s, y) + C(f)(s, y)) dy ds \\ &= \int_0^\infty y f^0(y) dy + \int_0^t \int_0^\infty F^* \psi(y) f(s, y) dy ds + \int_0^t \langle \mathcal{C}(f(s)), \psi \rangle ds = \\ & \qquad \qquad \qquad \int_0^\infty y f^0(y) dy. \end{aligned}$$

Here we have used the fundamental identities in propositions 4.3.2 and 3.4.3 to change  $C$  by  $\mathcal{C}$  and interchange  $F$  and  $F^*$ .  $\square$

We can also find solutions in the space  $L^\infty$ :

**Theorem 5.2.2.** *In addition to the hypotheses of theorem 5.2.1, suppose that  $f^0$  is in  $L^\infty$  and write  $X := \dot{L}_1^1 \cap L^1 \cap L^\infty$ , with the usual norm for the intersection.*

*Then there is a solution  $f$  to the coagulation-fragmentation equation on  $(0, +\infty)$  with initial data  $f^0$  such that  $f \in \mathcal{C}^1([0, +\infty), X)$  (with  $f(0) = f^0$ ),  $Lf(t)$  and  $C(f(t))$  are in  $X$  for all  $t \geq 0$  and*

$$\frac{d}{dt} f(t) = Lf(t) + C(f(t)) \quad t > 0,$$

*where the derivation in  $t$  is understood as that of a function in  $\mathcal{C}^1([0, T], X)$ . The solution is the only one satisfying the above. This solution is also a solution in the sense of the definitions in chapter 10.*

*In addition, this solution conserves the mass, in the sense that*

$$\int_0^\infty y f(t, y) dy = \int_0^\infty y f^0(y) dy \quad \text{for all } t \in (0, T).$$

*Proof.* The same reasoning as in theorem 5.2.1, together with lemmas 3.5.1 and 4.2, proves that  $F : X \rightarrow X$  and  $C : X \rightarrow X$  are continuous. Then, the same argument as before gives the result.  $\square$

### 5.3. Positivity of the solution

**Lemma 5.3.1.** *Assume the hypotheses of theorem 5.2.1, and let  $f$  be the solution to the coagulation-fragmentation equations given by that theorem. If  $f^0$  is positive a.e., then  $f(t)$  is positive a.e. for all  $t \geq 0$ .*

*Proof.* Call  $f^-(t, y) := \max\{-f(t, y), 0\}$  and  $s(t, y) := -1$  if  $f(t, y) < 0$  and 0 otherwise, so that  $f^-(t, y) = s(t, y)f(t, y)$ . Then  $f^-(t, y)$  can be written as  $\beta(f(t, y))$ , with  $\beta(s) := \max\{-s, 0\}$ , and  $s(t, y) = \beta'(f(t, y))$  when  $f(t, y) \neq 0$ , so theorem 10.2.7 proves we can calculate as follows:

$$\frac{d}{dt} \|f^-(t)\|_1 = \frac{d}{dt} \int_0^\infty f^-(t, y) dy = \int_0^\infty s(t, y)(Ff(t, y) + C(f)(t, y)) dy.$$

**For the fragmentation part:**

$$\begin{aligned} & \int_0^\infty s(t, y)Ff(t, y) dy \\ &= \int_0^\infty \int_y^\infty s(t, y)b(y'', y)f(t, y'') dy'' dy - \int_0^\infty s(t, y)f(t, y)\beta(y) dy \\ &= \int_0^\infty \int_0^{y''} b(y'', y)s(t, y)f(t, y'') dy dy'' - \int_0^\infty y f^-(t, y)\beta(y) dy \\ &\leq \int_0^\infty f^-(t, y'') \int_0^{y''} b(y'', y) dy dy'' \\ &\leq \int_0^\infty f^-(t, y'')C_0\beta(y'') dy'' \leq B \|f^-(t)\|_1. \end{aligned}$$

Note that we have used that  $\beta$  is bounded by some positive constant and that (3.8) holds for  $k = 0$ , so for some constant  $C_0 > 0$  and all  $y'' > 0$  we have

$$\int_0^{y''} b(y'', y) dy \leq C_0\beta(y'') \leq B \quad \text{for some } B > 0.$$

We have also used that  $f(t, y'') \geq -f^-(t, y'')$  and  $s$  is nonpositive, so  $s(t, y)f(t, y'') \leq f^-(t, y'')$ .

**For the coagulation part:** use lemma 4.3.2 again to write:

$$\begin{aligned} & \int_0^\infty s(t, y)C(f(t))(y) dy = \langle \mathcal{C}(f(t)), s(t) \rangle \\ &= \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y')f(t, y')f(t, y)s(t, y + y') dy dy' \\ &\quad - \int_0^\infty \int_0^\infty a(y, y')f(t, y')f(t, y)s(t, y) dy dy'. \end{aligned}$$

For the last term we have:

$$\begin{aligned} \int_0^\infty \int_0^\infty a(y, y') f(t, y') f(t, y) s(t, y) dy dy' \\ = \int_0^\infty \int_0^\infty a(y, y') f(t, y') f^-(t, y) dy dy' \leq A \|f(t)\|_1 \|f^-(t)\|_1. \end{aligned}$$

For the first one, observe that

$$s(t, y + y') f(t, y) f(t, y') \leq \begin{cases} 0 & \text{if } f(t, y), f(t, y') \geq 0 \\ f^-(t, y) |f(t, y')| & \text{if } f(t, y) < 0, \quad f(t, y') \geq 0 \\ |f(t, y)| f^-(t, y') & \text{if } f(t, y) < 0, \quad f(t, y') < 0. \end{cases}$$

Hence

$$\begin{aligned} \int_0^\infty \int_0^\infty a(y, y') f(t, y') f(t, y) s(y + y') dy dy' \\ \leq 2A \int_0^\infty f^-(y) |f(y')| dy dy' \leq 2A \|f(t)\|_1 \|f^-(t)\|_1. \end{aligned}$$

Gronwall's lemma then proves that  $\|f^-(t)\|_1$  is always zero, as it is at  $t = 0$ , so  $f(t)$  is positive a.e. for all  $t \geq 0$ .  $\square$

## 5.4. Estimates for regular solutions

Let us give some estimates for the kind of solutions obtained in section 5.2. We are interested in obtaining information on the behavior of their moments and other properties by finding bounds which depend only on suitably weak requirements on the initial condition and the coefficients. One of the reasons for this is that these estimates will be used later in a limiting argument where we prove existence of solutions under various conditions, and there we will need them to be independent of the particular approximation we are using.

The results below are of the kind: "such quantity related to  $f$  is bounded by a constant which depends only on such and such quantity". What is meant by this is that if one has a different solution with different initial data and coefficients, the corresponding bound is still true with the same constant as long as the stated quantities on which it depends are the same for the new initial data and coefficients. It may seem odd to see these results phrased in a way that includes "constants" which depend on several other quantities, but this is reasonable in view of their intended application: later, for a given sequence of approximated solutions, these constants will really be fixed in the sense that they will be valid for every solution in the sequence.

In the following we will use  $C(t)$  or  $C$  to denote generic numbers that depend only on the quantities involved in the result being discussed at the moment; the number

denoted by them may change in the course of a proof, with the only requirement that they must depend only on the quantities of the result. To ease the language, we will refer to these as being *allowed constants* or constants that depend *only on the allowed quantities*. On some of the results we also specify whether the dependence of the constants on some quantities is increasing or decreasing; in these cases, the allowed constants are also required to have the same dependence on them.

Throughout this section  $f$  will be a solution to the coagulation-fragmentation equations on  $[0, +\infty)$  in the conditions of theorem 5.2.1 with an initial condition  $f^0$  which is a bounded function of compact support in  $(0, +\infty)$  and is positive almost everywhere. In order to carry out arguments involving various moments of  $f$ , we need to ensure in some way that they are finite for all times, so in addition we will suppose that the coagulation and fragmentation coefficients *also have compact support*. Then we know that  $f$  has compact support at all times. Let us gather all that for future reference:

**Hypothesis 5.4.1.** *Throughout this section we assume the following:*

- *The fragmentation coefficient  $b$  satisfies (3.4), and has compact support on  $\{(y, y') \in \mathbb{R}^2 \mid y > y' > 0\}$  (in particular, it satisfies (3.8) for any  $k \in \mathbb{R}$ ).*
- *The total fragmentation rate  $\beta$  (as defined in (3.5)) is essentially bounded.*
- *The coagulation coefficient  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  is a nonnegative symmetric measurable function with compact support on  $(0, +\infty) \times (0, +\infty)$ . There is some constant  $A \geq 0$  such that*

$$a(y, y') \leq A(1 + y + y'). \quad (5.12)$$

- *The initial data  $f^0$  is a bounded function with compact support on  $(0, +\infty)$ .*
- *$f$  is a solution to the coagulation-fragmentation equations on  $[0, +\infty)$  given by theorem 5.2.2 with coefficients  $a$ ,  $b$  and initial condition  $f^0$ .*

*Below we will call:*

$$\rho := \int_0^\infty y f^0(y) dy. \quad (5.13)$$

First of all, we know that the solution  $f$  is positive almost everywhere (lemma 5.3.1) and that mass is conserved (equation (5.11)); then  $\rho$ , the total mass of the initial condition, is also the mass of the solution at any later time:

$$\int_0^\infty y f(t, y) dy = \int_0^\infty y f^0(y) dy = \rho \quad \text{for all } t \geq 0. \quad (5.14)$$

In addition, we know that  $f(t)$  always has compact support on  $(0, +\infty)$ , thanks to the assumption that  $a$  and  $b$  have compact support: fragmentation never produces small clusters, and coagulation never produces large ones.

**Lemma 5.4.2.** *For all  $t \geq 0$ , the function  $f(t)$  has compact support on  $(0, +\infty)$ . To be more precise:*

- *If for some  $0 < R$   $f^0$  has support contained in  $(0, R)$  and  $a$  has support contained in  $\{(y, y') \mid y, y' > 0 \text{ and } \epsilon \leq y + y' \leq R\}$ , then  $f(t)$  has support contained in  $(0, R)$  for all  $t \geq 0$ .*
- *If for some  $0 < \epsilon$   $f^0$  has support contained in  $(\epsilon, +\infty)$  and  $b$  has support contained in  $\{(y, y') \mid \epsilon \leq y' < y\}$ , then  $f(t)$  has support contained in  $(\epsilon, +\infty)$  for all  $t \geq 0$ .*

*Proof.* For the first part, one can see directly that  $\frac{d}{dt} \int_R^\infty y f(t, y) dy \leq 0$ ; as  $f$  is nonnegative and  $\int_R^\infty y f^0(y) dy = 0$  the result follows. One can prove the second part analogously, considering  $\frac{d}{dt} \int_0^\epsilon y f(t, y) dy$ .  $\square$

In particular, this implies that all moments of the form  $\int_0^\infty f(t, y) \psi(y) dy$  for  $\psi$  locally bounded on  $(0, +\infty)$  are finite for all times  $t \geq 0$ .

### 5.4.1. Estimates independent of the number of particles

#### Superlinear moments of $f$

**Proposition 5.4.3 (Bound on superlinear moments of  $f$ ).** *Suppose that  $\Phi : [0, +\infty) \rightarrow \mathbb{R}$  is a nonnegative function such that  $y \mapsto \Phi(y)/y$  is concave and  $\lim_{y \rightarrow 0} \Phi(y)/y = 0$ . Call*

$$K_0 := \int_0^\infty \Phi(y) f^0(y) dy < +\infty.$$

*Then for all  $t > 0$  there is a constant  $C(t) > 0$  which depends (increasingly) only on  $\Phi$ ,  $t$ ,  $\rho$ ,  $A$  (see (5.12)) and  $K_0$  such that*

$$\int_0^\infty \Phi(y) f(t, y) dy \leq C(t).$$

*If in addition  $\Phi(y) \leq y^2$  for  $y > 0$ , then the following holds for some constant  $C(t)$  which depends only on  $t$ ,  $\rho$ ,  $A$  (see (5.12)) and  $K_0$ :*

$$\int_0^\infty C(f(t))(y) \Phi(y) dy \leq C(t) \quad \text{for all } t \geq 0.$$

Let us state some further results in order to prove this.

**Lemma 5.4.4.** *If  $\varphi : [0, +\infty) \rightarrow \mathbb{R}$  is a concave function with  $\varphi(0) = 0$ . Then  $y \mapsto \varphi(y)/y$  is decreasing and  $\varphi$  is sublinear; this is,*

$$\varphi(x + y) \leq \varphi(x) + \varphi(y) \quad \text{for all } x, y \geq 0.$$

*Proof.* If  $0 < x < y$ , writing  $x = \theta y + (1 - \theta)0$  with  $\theta = x/y$  gives

$$\varphi(x) \leq \frac{x}{y}\varphi(y),$$

which proves the first part. We use it to prove that  $\varphi$  is sublinear:

$$\frac{\varphi(x+y)}{x+y} \leq \frac{\varphi(x)}{x} \implies \varphi(x+y) \leq \varphi(x) + \frac{y}{x}\varphi(x) \leq \varphi(x) + \varphi(y).$$

□

**Lemma 5.4.5.** *Suppose that  $\varphi : [0, +\infty) \rightarrow \mathbb{R}$  is a concave function with  $\varphi(0) = 0$ . Then for all  $y, y' > 0$ ,*

$$(y+y')\varphi(y+y') - y\varphi(y) - y'\varphi(y') \leq 2\frac{yy'}{y+y'}\varphi(y+y').$$

*Proof.* As  $\varphi$  is concave, writing  $y = \frac{y'}{y+y'} \cdot 0 + \frac{y}{y+y'}(y+y')$  one has

$$\varphi(y) \geq \frac{y}{y+y'}\varphi(y+y').$$

Analogously,

$$\varphi(y') \geq \frac{y'}{y+y'}\varphi(y+y').$$

Substituting this on the left hand side of the inequality we have:

$$(y+y')\varphi(y+y') - y\varphi(y) - y'\varphi(y') \leq \varphi(y+y') \left( y+y' - \frac{y^2}{y+y'} - \frac{(y')^2}{y+y'} \right) = \varphi(y+y') \frac{2yy'}{y+y'}.$$

□

**Lemma 5.4.6.** *Suppose that  $\Phi : [0, +\infty) \rightarrow \mathbb{R}$  is such that  $y \mapsto \Phi(y)/y$  is concave and  $\lim_{y \rightarrow 0} \Phi(y)/y = 0$ . Then for all  $y, y' > 0$ ,*

$$\Phi(y+y') - \Phi(y) - \Phi(y') \leq 2\frac{(\Phi(y)y' + \Phi(y')y)}{y+y'}.$$

*Proof.* This is obtained applying the previous lemma to  $\varphi(y) := \Phi(y)/y$  for  $y > 0$ ,  $\varphi(0) = 0$ , and using that  $\varphi$  is sublinear (see lemma 5.4.4). □

**Lemma 5.4.7.** *Suppose that  $\Phi : [0, +\infty) \rightarrow \mathbb{R}$  is in the conditions of lemma 5.4.6, and that*

$$\Phi(y) \leq y^2 \quad \text{for all } y > 0.$$

*Then the following estimate holds for all  $y, y' > 0$ :*

$$a(y, y')(\Phi(y+y') - \Phi(y) - \Phi(y')) \leq 4A(\Phi(y)y' + \Phi(y')y + yy'), \quad (5.15)$$

*where  $A$  is the constant from (5.12).*

*Proof.* For  $y + y' \geq 1$  we use (5.12) and lemma 5.4.6:

$$\begin{aligned} a(y, y')(\Phi(y + y') - \Phi(y) - \Phi(y')) \\ \leq 2A(1 + y + y') \frac{\Phi(y)y' + \Phi(y')y}{y + y'} \leq 4A(\Phi(y)y' + \Phi(y')y). \end{aligned}$$

We also need an estimate for  $y + y' < 1$ . Call  $\varphi(y) := \Phi(y)/y$ ,  $\varphi(0) := 0$ . This is a concave function with  $\varphi(0) = 0$ , so in particular it is sublinear. Also, the bound on  $\Phi$  implies that  $\varphi(y) \leq y$  for  $y \geq 0$ . Then, for  $y, y' > 0$ ,

$$\begin{aligned} \Phi(y + y') - \Phi(y) - \Phi(y') &= (y + y')\varphi(y + y') - y\varphi(y) - y'\varphi(y') \\ &\leq (y + y')(\varphi(y) + \varphi(y')) - y\varphi(y) - y'\varphi(y') \\ &= y\varphi(y') + y'\varphi(y) \leq 2yy'. \end{aligned}$$

Hence, for  $y + y' \leq 1$ , using that  $a(y, y') < A(1 + y + y') < 2A$ ,

$$a(y, y')(\Phi(y + y') - \Phi(y) - \Phi(y')) \leq 4Ayy'.$$

Together with the bound for  $y + y' \geq 1$ , this proves the result.  $\square$

*Proof of proposition 5.4.3.* Let us estimate the time derivative of the  $\Phi$ -moment. Call  $\varphi(y) := \Phi(y)/y$  for  $y > 0$ , and  $\varphi(0) = 0$ . Then  $\varphi$  is nonnegative and concave, and in particular it must be increasing. Hence, we only need to worry about the coagulation term, as  $\int_0^\infty F(f)(y)\Phi(y) dy \leq 0$  due to proposition 3.4.3 (see expression (3.13)).

As a first step, suppose that  $\Phi(y) \leq y^2$  for all  $y > 0$ . Then we can estimate the coagulation part by using lemma 5.4.7:

$$\begin{aligned} \frac{d}{dt} \int_0^\infty f(y)\Phi(y) dy &\leq \int_0^\infty C(f)(y)\Phi(y) dy \\ &\leq \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y')f(y)f(y')(\Phi(y + y') - \Phi(y) - \Phi(y')) dy dy' \\ &\leq A \int_0^\infty \int_0^\infty f(y)f(y')(\Phi(y)y' + \Phi(y')y + 2yy') dy dy' \\ &\leq 2A\rho \int_0^\infty f(y)\Phi(y) dy + A\rho^2. \end{aligned}$$

By Gronwall's lemma,  $\int_0^\infty f(y)\Phi(y) dy$  is bounded on  $[0, t]$  for  $t > 0$ , with a bound  $C(t)$  that depends only on  $\rho$ ,  $A$  and  $K_0 = \int_0^\infty f^0(y)\Phi(y) dy$  (observe that this  $C(t)$  does not depend directly on  $\Phi$ ). This proves the last part of the proposition.

Now we drop the assumption that  $\Phi(y) \leq y^2$  for all  $y$ . Then, we can write  $\Phi = \Phi_1 + \Phi_2$ , with  $\Phi_1(y)$  smaller than a constant times  $y$  for all  $y$ , in such a way



that a multiple of  $\Phi_2$  satisfies the conditions of our first step. One way to do this is to define, for  $y \geq 0$ :

$$\Phi_2(y) := \begin{cases} \Phi(1)y^2 & \text{if } y < 1 \\ \Phi(y) & \text{if } y \geq 1 \end{cases}$$

$$\Phi_1(y) := \Phi(y) - \Phi_2(y).$$

Take  $C := \max\{1, \Phi(1)\}$ . Then,  $C^{-1}\Phi_2$  is in the conditions of our first step:  $y \mapsto \Phi_2(y)/y$  is still concave, nonnegative, has limit 0 when  $y \rightarrow 0$ ,  $\Phi_2(y) \leq Cy^2$  for  $y < 1$  and for  $y \geq 1$ ,

$$\Phi_2(y) = \Phi(y) = y\varphi(y) \leq y^2\varphi(1) = y^2\Phi(1) \leq Cy^2.$$

Also,  $\Phi_1(y)$  is zero for  $y > 1$ , and for  $0 < y \leq 1$  we have

$$\Phi_1(y) \leq \Phi(y) = y\varphi(y) \leq y\varphi(1) \leq Cy.$$

Hence,

$$\Phi_1(y) \leq Cy \quad \text{for } y \geq 0.$$

Finally, we can estimate the  $\Phi$ -moment as follows, using the constant  $C(t)$  from the previous step corresponding to  $C^{-1}\Phi_2$  (observe that this  $C(t)$  is allowed, as it can be bounded using only  $C, t, \rho, A$  and  $K_0$ ):

$$\int_0^\infty \Phi(y)f(y) dy = \int_0^\infty \Phi_1(y)f(y) dy + \int_0^\infty \Phi_2(y)f(y) dy \leq C\rho + CC(t).$$

This proves proposition 5.4.3. □

**Corollary 5.4.8.** *Suppose that  $\Phi : [0, +\infty) \rightarrow \mathbb{R}$  is a nonnegative function such that  $y \mapsto \Phi(y)/y$  is concave and  $\lim_{y \rightarrow 0} \Phi(y)/y = 0$ . Call*

$$K_0 := \int_0^\infty \Phi(y)f^0(y) dy < +\infty.$$

*Then for all  $t, S > 0$  there is a constant  $C(t) > 0$  which depends only on  $t, \Phi, S, \rho, A$  (see (5.12)) and  $K_0$  such that*

$$\int_S^\infty C(f(t))(y)\Phi(y) dy \leq C(t) \quad \text{for all } t \geq 0.$$

*This  $C(t)$  depends decreasingly on  $S$ , and increasingly on the rest of the involved quantities.*

*Proof.* If  $\Phi(S) = 0$  then  $\Phi \equiv 0$  and there is nothing to prove, so assume that  $\Phi(S) > 0$ . We can change  $\Phi$  on  $[0, S)$  and then apply proposition 5.4.3 in a very similar way as was done in its proof:

$$\tilde{\Phi}(y) := \begin{cases} \frac{\Phi(S)}{S^2}y^2 & \text{if } y \leq S \\ \Phi(y) & \text{if } y > S. \end{cases}$$

Call  $\tilde{\varphi}(y) := \tilde{\Phi}(y)/y$  for  $y > 0$ ,  $\tilde{\varphi}(0) = 0$ , which is concave. Then for  $y \geq S$ ,

$$\tilde{\Phi}(y) = y\tilde{\varphi}(y) \leq y^2 \frac{\tilde{\varphi}(S)}{S} = y^2 \frac{\tilde{\Phi}(S)}{S^2},$$

as  $y \mapsto \tilde{\varphi}(y)/y$  is decreasing (lemma 5.4.4). Hence,

$$\frac{S^2}{\tilde{\Phi}(S)} \tilde{\Phi}(y) \leq y^2 \quad \text{for all } y \geq 0.$$

Then  $\tilde{\Phi}S^2/\tilde{\Phi}(S)$  is in the conditions of proposition 5.4.3, so for some constant  $C(t)$  which depends on the allowed quantities (including  $\tilde{\Phi}(S)/S^2$ ), and knowing that the integrand below is nonnegative,

$$\int_S^\infty \tilde{\Phi}(y) f(t, y) dy \leq \int_0^\infty \tilde{\Phi}(y) f(t, y) dy \leq \frac{\tilde{\Phi}(S)}{S^2} C(t) \quad \text{for } t \geq 0.$$

This proves our result, noting that  $\tilde{\Phi}(S)/S^2$  is a decreasing function of  $S$ .  $\square$

Let us state a result on the behavior of the moments of  $f$  of order  $1 \leq k \leq 2$ , which is a direct consequence of proposition 5.4.3:

**Corollary 5.4.9.** *Take  $1 \leq k \leq 2$ . Call*

$$K_0 := \int_0^\infty y^k f^0(y) dy < +\infty.$$

*Then for all  $t > 0$  there is a constant  $C(t) > 0$  which depends only on  $t$ ,  $\rho$ ,  $A$  (see (5.12)) and  $K_0$  such that*

$$\int_0^\infty y^k f(t, y) dy \leq C(t).$$

*Proof.* Apply proposition 5.4.3 to

$$\Phi(y) := \begin{cases} y & \text{if } 0 < y < 1 \\ y^2 & \text{if } 1 \leq y. \end{cases}$$

Note that the resulting  $C(t)$  is independent of  $k$ .  $\square$

### A moment of $f$ related to the fragmentation coefficient

**Proposition 5.4.10.** *Suppose that  $\Phi : [0, +\infty) \rightarrow \mathbb{R}$  is such that  $y \mapsto \Phi(y)/y$  is concave and strictly increasing, and such that  $\lim_{y \rightarrow 0} \Phi(y)/y = 0$ . Call*

$$K_0 := \int_0^\infty \Phi(y) f^0(y) dy < +\infty. \quad (5.16)$$

Then for  $0 < R < S$  and all  $t \geq 0$  there is a constant  $C(t)$  which depends only on  $R, S, t, \rho, A$  (from (5.12)) and  $K_0$  such that

$$\int_0^t \int_S^\infty \frac{\Phi(y)}{y} f(s, y) \int_0^R y' b(y, y') dy' dy ds \leq C(t). \quad (5.17)$$

This  $C(t)$  depends decreasingly on  $S$  and increasingly on the other quantities.

*Proof.* Thanks to proposition 5.4.8 we know that there is a constant which depends only on the allowed quantities such that

$$\int_S^\infty C(f(t))(y) \Phi(y) dy \leq C(t) \quad \text{for all } t \geq 0.$$

Then, for  $t \geq 0$ ,

$$\begin{aligned} \frac{d}{dt} \int_S^\infty \Phi(y) f(t, y) dy &= \int_S^\infty F f(t, y) \Phi(y) dy + \int_S^\infty C(f(t))(y) \Phi(y) dy \\ &\leq \int_S^\infty F f(t, y) \Phi(y) dy + C(t), \end{aligned}$$

And we deduce that

$$- \int_0^t \int_S^\infty F f(s, y) \Phi(y) dy ds \leq t C(t) + \int_0^\infty \Phi(y) f^0(y) dy = t C(t) + K_0. \quad (5.18)$$

Now, for the left hand side we use that  $y \mapsto \Phi(y)/y$  is increasing:

$$\begin{aligned} - \int_0^\infty F f(y) \Phi(y) dy &= - \int_0^\infty f(y) F^* \Phi(y) dy \\ &= \int_0^\infty f(y) \int_0^y \left( \frac{\Phi(y)}{y} - \frac{\Phi(y')}{y'} \right) y' b(y, y') dy' dy \\ &\geq \int_S^\infty f(y) \int_0^R \left( \frac{\Phi(y)}{y} - \frac{\Phi(y')}{y'} \right) y' b(y, y') dy' dy \\ &\geq \int_S^\infty f(y) \int_0^R \left( \frac{\Phi(y)}{y} - \frac{\Phi(R)}{R} \right) y' b(y, y') dy' dy \quad (5.19) \end{aligned}$$

Then, using that for  $y \geq S$

$$\frac{\Phi(R)}{R} = \frac{\Phi(S)}{S} \frac{\Phi(R)}{\Phi(S)} \frac{S}{R} \leq \frac{\Phi(y)}{y} \frac{\Phi(R)}{\Phi(S)} \frac{S}{R} = C \frac{\Phi(y)}{y},$$

where

$$C := \frac{\Phi(R)}{\Phi(S)} \frac{S}{R} < 1,$$

as  $y \mapsto \Phi(y)/y$  is *strictly* increasing (note that  $C$  is increasing in  $R$  and decreasing in  $S$ ). Hence, from (5.19) we get:

$$-\int_0^\infty F f(y) \Phi(y) dy \geq (1 - C) \int_S^\infty \frac{\Phi(y)}{y} f(y) \int_0^R y' b(y, y') dy' dy.$$

Together with (5.18), we obtain the result in the proposition for some allowed constant  $C(t)$ :

$$\int_0^t \int_S^\infty \frac{\Phi(y)}{y} f(s, y) \int_0^R y' b(y, y') dy' dy ds \leq C(t) \quad \text{for } t \geq 0.$$

□

**Corollary 5.4.11.** *Assume the conditions of proposition 5.4.10, and take  $R > 0$ . Call*

$$B_0 := \sup_{0 < y < 2R} \beta(y). \quad (5.20)$$

*Then for any  $t > 0$  there is a constant  $C(t)$  which depends (increasingly) only on  $B_0$  and the quantities in proposition 5.4.10, such that*

$$\int_0^t \int_0^\infty \left(1 + \frac{\Phi(y)}{y}\right) f(s, y) \int_0^R y' b(y, y') dy' dy ds \leq C(t). \quad (5.21)$$

*(It is understood here that  $b(y, y') = 0$  when  $y \leq y'$ ).*

*Proof.* For  $y > 2R$ ,

$$1 + \frac{\Phi(y)}{y} \leq \left(\frac{2R}{\Phi(2R)} + 1\right) \frac{\Phi(y)}{y},$$

so we only need to estimate the integral when  $y < 2R$ , as the rest was bounded in proposition 5.4.10, applied for  $S := 2R$ . But  $1 + \Phi(y)/y$  is bounded when  $y \leq 2R$  by  $1 + \Phi(2R)/(2R)$ , so it is enough to estimate the following:

$$\begin{aligned} \int_0^t \int_0^{2R} f(s, y) \int_0^R y' b(y, y') dy' dy ds \\ \leq \int_0^t \int_0^{2R} f(s, y) \int_0^y y' b(y, y') dy' dy ds \\ = \int_0^t \int_0^{2R} y f(s, y) \beta(y) dy ds \leq B_0 t \rho. \end{aligned}$$

The bound we have found is increasing on all the quantities it depends on except for  $R$ , but it is clear that it can be taken to be increasing in  $R$  also, as the expression in the left hand side of (5.21) is itself increasing in  $R$ . □

**Corollary 5.4.12.** *For any  $t > 0$  there is a constant  $C(t) \geq 0$  which only depends on  $t, \rho, A$  such that*

$$\int_0^t \int_0^\infty f(s, y) \int_0^R y' b(y, y') dy' dy ds \leq C(t). \quad (5.22)$$

(It is understood here that  $b(y, y') = 0$  when  $y \leq y'$ ).

*Proof.* We can prove this by choosing a fixed  $\Phi$  such that  $\Phi(y) \leq 2y$  (for example) in corollary 5.4.11. Take, for example,

$$\Phi(y) := \begin{cases} y^2 & \text{if } 0 < y \leq 1 \\ 2y & \text{if } 1 < y. \end{cases}$$

Choosing any  $0 < R < S$ , corollary 5.4.11 gives a constant  $C(t)$  that satisfies the inequality (5.22); this constant depends on  $\rho, t, A$  and  $K_0$  (from (5.16)), but in our case

$$K_0 = \int_0^\infty \Phi(y) f^0(y) dy \leq 2 \int_0^\infty y f^0(y) dy = 2\rho,$$

so  $C(t)$  can be taken to be independent of  $K_0$ .  $\square$

### Local integrability estimates

Our bounds on local integrability below will depend on the following quantity:

$$b_x := \sup_{0 < y' < y < x} b(y, y') \quad \text{for } x > 0. \quad (5.23)$$

**Proposition 5.4.13 (Local estimate in  $\dot{L}_1^1$ ).** *Assume that the function  $z \mapsto z a(z, y')$  is increasing for all  $y' > 0$ . Take  $\Phi : [0, +\infty) \rightarrow \mathbb{R}$  such that  $y \mapsto \Phi(y)/y$  is concave and strictly increasing, and such that  $\lim_{y \rightarrow 0} \Phi(y)/y = 0$ . Suppose that  $\Lambda : [0, +\infty) \rightarrow [0, +\infty)$  is a  $C^1$  strictly convex function with  $\Lambda'$  concave and  $\Lambda(0) = \Lambda'(0) = 0$ , such that*

$$\Lambda'(b_y) \leq 1 + \frac{\Phi(y)}{y} \quad \text{for } y > 0.$$

Take  $R > 0$ . Define  $b_x$  as in (5.23), and

$$K_1 := \int_0^\infty y \Lambda(f^0(y)) dy \quad (5.24)$$

$$K_0 := \int_0^\infty \Phi(y) f^0(y) dy. \quad (5.25)$$

Then for all  $t \geq 0$  there is a constant  $C(t)$  which depends only on  $t, R, \rho, A$  (from (5.12)),  $b_y, B_1$  (with  $S := 2R$ ),  $K_1$  and  $K_0$ , such that

$$\int_0^R y \Lambda(f(t, y)) dy \leq C(t) \quad \text{for } t \geq 0.$$

*Proof.* Call  $\phi(y) := y\Lambda'(f(y))$  for  $0 < y < R$  and 0 otherwise, and write

$$\frac{d}{dt} \int_0^R y\Lambda(f(t, y)) dy = \int_0^\infty f(t, y)F^*\phi(y) dy + \langle C(f(t)), \phi \rangle.$$

**Step 1: bound for the fragmentation part.**

We have:

$$\int_0^\infty f(t, y)F^*\phi(y) dy \leq \int_0^\infty f(y)y \int_0^R y'\Lambda'(f(y'))\frac{1}{y}b(y, y') dy' dy$$

We estimate this integral on the regions with  $y < R$  and  $y \geq R$ : for  $y < R$ , use Young's inequality  $f(y)\Lambda'(f(y')) \leq \Lambda(f(y)) + \Lambda(f(y'))$  to write

$$\begin{aligned} & \int_0^R f(y)y \int_0^R \Lambda'(f(y'))\frac{y'}{y}b(y, y') dy' dy \\ & \leq \int_0^R \Lambda(f(y))y \int_0^R \frac{y'}{y}b(y, y') dy' dy + \int_0^R \int_0^R \Lambda(f(y'))y'b(y, y') dy' dy \\ & \leq R b_R \int_0^R \Lambda(f(y))y dy + R b_R \int_0^R \Lambda(f(y'))y' dy' \\ & = 2R b_R \int_0^R \Lambda(f(y'))y' dy'. \quad (5.26) \end{aligned}$$

For the part with  $y \geq R$ , use the following Young's inequality (see chapter 9.4):

$$\Lambda'(f(y'))b(y, y') \leq \Lambda^*(\Lambda'(f(y'))) + \Lambda(b(y, y')) \leq \Lambda(f(y')) + \Lambda(b(y, y'))$$

to write

$$\begin{aligned} & \int_R^\infty f(y) \int_0^R \Lambda'(f(y'))y'b(y, y') dy' dy \\ & \leq \int_R^\infty f(y) \int_0^R y'\Lambda(f(y')) dy' dy + \int_R^\infty f(y) \int_0^R y'\Lambda(b(y, y')) dy' dy \\ & =: I_1 + I_2. \end{aligned}$$

The first integral,  $I_1$ , is easy to estimate:

$$I_1 \leq \frac{1}{R} \rho \int_0^R y\Lambda(f(y)) dy. \quad (5.27)$$

For the second one,

$$\begin{aligned} I_2 & \leq \int_R^\infty f(y)\Lambda'(b_y) \int_0^R y'b(y, y') dy' dy \\ & \leq \int_R^\infty f(y) \left(1 + \frac{\Phi(y)}{y}\right) \int_0^R y'b(y, y') dy' dy =: u(t). \quad (5.28) \end{aligned}$$

Note that the integral of  $u$  on  $(0, t)$  for  $t > 0$  was bounded in corollary 5.4.11.

**Step 2: bound for the coagulation part.**

We also need to find a bound for the following:

$$\langle C(f(t)), \phi \rangle = \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y') f(y) f(y') (\phi(y + y') - \phi(y) - \phi(y')) dy dy'.$$

Let us rewrite  $\phi(y + y') - \phi(y) - \phi(y')$ : putting  $\varphi(y) := \chi(y)\Lambda'(f(y))$ ,

$$\begin{aligned} \phi(y + y') - \phi(y) - \phi(y') &= (y + y')\varphi(y + y') - y\varphi(y) - y'\varphi(y') \\ &= y(\varphi(y + y') - \varphi(y)) + y'(\varphi(y + y') - \varphi(y')). \end{aligned}$$

Thanks to the symmetry of the integral we have that

$$\langle C(f(t)), \phi \rangle = \int_0^\infty \int_0^\infty a(y, y') f(y) f(y') y (\varphi(y + y') - \varphi(y)) dy dy'.$$

Now use Young's inequality and the identity (9.5):

$$\begin{aligned} &f(y) (\varphi(y + y') - \varphi(y)) \\ &= f(y)\Lambda'(f(y + y'))\chi(y + y') - \chi(y)\Lambda(f(y)) - \chi(y)\Lambda^*(\Lambda'(f(y))) \\ &\leq \Lambda(f(y))\chi(y + y') + \Lambda^*(\Lambda'(f(y + y')))\chi(y + y') - \chi(y)\Lambda(f(y)) - \chi(y)\Lambda^*(\Lambda'(f(y))) \\ &\leq \Lambda^*(\Lambda'(f(y + y')))\chi(y + y') - \Lambda^*(\Lambda'(f(y)))\chi(y) \\ &=: \Sigma(y + y') - \Sigma(y), \end{aligned}$$

where we define  $\Sigma(y) := \Lambda^*(\Lambda'(f(y)))\chi(y)$ . Then,

$$\begin{aligned} \langle C(f(t)), \phi \rangle &\leq \int_0^\infty \int_0^\infty a(y, y') f(y') y (\Sigma(y + y') - \Sigma(y)) dy dy' \\ &= \int_0^\infty \int_0^\infty a(y, y') f(y') y \Sigma(y + y') dy dy' - \int_0^\infty \int_0^\infty a(y, y') f(y') y \Sigma(y) dy dy' \\ &= \int_0^\infty \int_{y'}^\infty a(y - y', y') f(y') (y - y') \Sigma(y) dy dy' - \int_0^\infty \int_0^\infty a(y, y') f(y') y \Sigma(y) dy dy' \\ &= \int_0^\infty \int_0^\infty ((y - y')a(y - y', y')\chi_{y > y'} - ya(y, y')) f(y') \Sigma(y) dy dy' \leq 0, \end{aligned}$$

the last inequality due to the fact that  $z \mapsto za(z, y')$  is increasing.

With this and (5.26), (5.27), (5.28) we finally get

$$\begin{aligned} &\int_0^R y\Lambda(f(t, y)) dy \\ &\leq \int_0^R y\Lambda(f^0(y)) dy + \int_0^t \left( C \int_0^R y\Lambda(f(s, y)) dy + u(s) \right) ds \end{aligned}$$

for some constant  $C \geq 0$  that depends only on the allowed quantities. The integral of  $u$  on  $(0, t)$  for  $t > 0$  is bounded by the constants in the statement, as proved in corollary 5.4.11. Thus, Gronwall's lemma proves that for some (other) constant  $C(t)$  we have

$$\int_0^R y \Lambda(f(t, y)) dy \leq C(t) \quad \text{for } t \geq 0.$$

□

### 5.4.2. Estimates which depend on the number of particles

#### $L^1$ estimate

To estimate the integral of  $f$ , which represents the total number of clusters, some control on the fragmentation coefficient is needed, as fragmentation produces an increase on their number. Take  $S > R > 0$  and  $B_1 \geq 0$  such that

$$\int_0^R b(y, y') dy' \leq B_1 \int_0^R y' b(y, y') dy' \quad \text{for all } y \geq S. \quad (5.29)$$

(This is also considered in [33]). Define

$$B_2 := \sup_{y \in (0, S)} \int_0^y b(y, y') dy'. \quad (5.30)$$

The estimates below will depend on  $B_1$  and  $B_2$ .

**Proposition 5.4.14.** *Take  $\Phi$  in the conditions of proposition 5.4.10, and define  $K_0$  as is done there. Choose  $S > R > 0$ . There is a constant  $C(t)$  which depends only on  $t \geq 0$ ,  $\Phi$ ,  $\rho$ ,  $A$  (from (5.12)),  $K_0$ ,  $R$ ,  $S$ ,  $B_1$  and  $B_2$  (from (5.29) and (5.30)) such that*

$$\|f(t)\|_1 \leq C(t) \quad \text{for all } t \geq 0.$$

*This constant  $C(t)$  is decreasing in  $S$  and increasing in  $t$ ,  $\Phi$ ,  $\rho$ ,  $A$ ,  $K_0$ ,  $B_1$  and  $B_2$  (note that nothing is said about  $R$ ).*

*Proof.* To find a bound for  $\|f(t)\|_1$  we only need to control the behavior of  $f$  near 0, as we know that the total mass is finite and for all times  $t \geq 0$

$$\int_R^\infty f(t, y) dy \leq \int_R^\infty y f(t, y) dy \leq \rho/R.$$

Near 0 we can calculate as follows: call  $\chi := \chi_{(0, R)}$ , and note that  $\chi(y + y') - \chi(y) -$



$\chi(y') \leq 0$  for  $y, y' > 0$ , so  $\langle C(f), \chi \rangle \leq 0$ . Hence we have:

$$\begin{aligned}
\frac{d}{dt} \int_0^R f(y) &= \int_0^R F f(y) dy + \langle C(f), \chi \rangle \leq \int_0^R F f(y) dy \\
&\leq \int_0^R \int_y^\infty f(y') b(y', y) dy' dy = \int_0^\infty f(y') \int_0^{y'} b(y', y) \chi(y) dy dy' \\
&\leq \int_0^S f(y') \int_0^{y'} b(y', y) dy dy' + \int_S^\infty f(y') \int_0^R b(y', y) dy dy' \\
&\leq B_2 \int_0^S f(y') dy' + B_1 \int_S^\infty f(y') \int_0^R y b(y', y) dy dy' \\
&\leq B_2 \int_0^R f(y') dy' + B_2 \frac{\rho}{R} + B_1 \int_S^\infty f(y') \int_0^R y b(y', y) dy dy'.
\end{aligned}$$

Integrating in time we have:

$$\int_0^R f(t, y) \leq \int_0^R f^0(y) dy + \int_0^t \left( B_2 \int_0^R f(s, y) dy + h(s) \right) ds,$$

where we have called

$$h(s) := B_2 \frac{\rho}{R} + B_1 \int_S^\infty f(s, y') \int_0^R y b(y', y) dy dy'.$$

Now, using proposition 5.4.10 for our  $R, S$ , there is some constant  $C(t)$  depending on the allowed quantities such that

$$\int_0^t h(s) ds \leq C(t) \quad \text{for all } t \geq 0.$$

Gronwall's lemma then finishes the proof.  $\square$

### Local integrability estimates

Our bounds on local integrability below will depend on the following quantity:

$$b_x := \sup_{0 < y' < y < x} b(y, y') \quad \text{for } x > 0. \tag{5.31}$$

**Lemma 5.4.15.** *Suppose that  $\Lambda : [0, +\infty) \rightarrow [0, +\infty)$  is a  $C^1$  strictly convex function with  $\Lambda'$  concave and  $\Lambda(0) = \Lambda'(0) = 0$ . Then,*

$$x\Lambda'(y) \leq \Lambda(x) + \Lambda(y) \quad \text{for all } x, y \geq 0.$$

*Proof.* Young's inequality from theorem 9.4.3 gives that

$$x\Lambda'(y) \leq \Lambda(x) + \Lambda^*(\Lambda'(y)). \tag{5.32}$$

But, as  $\Lambda'$  is concave,

$$\Lambda(y) = \int_0^y \Lambda'(s) ds \geq \int_0^y s \frac{\Lambda'(s)}{s} ds \geq \frac{\Lambda'(y)}{y} \int_0^y s ds = \frac{1}{2} y \Lambda'(y).$$

Hence,  $y\Lambda'(y) \leq 2\Lambda(y)$ . Use this in (9.5) to obtain

$$\Lambda^*(\Lambda'(y)) = y\Lambda'(y) - \Lambda(y) \leq \Lambda(y).$$

Putting this into (5.32) proves the lemma.  $\square$

**Proposition 5.4.16 (Local estimate in  $L^1$ ).** *Suppose that  $\Phi : [0, +\infty) \rightarrow \mathbb{R}$  is such that  $y \mapsto \Phi(y)/y$  is concave and strictly increasing, and such that  $\lim_{y \rightarrow 0} \Phi(y)/y = 0$ . Suppose that  $\Lambda : [0, +\infty) \rightarrow [0, +\infty)$  is a  $C^1$  strictly convex function with  $\Lambda'$  concave and  $\Lambda(0) = \Lambda'(0) = 0$ , such that*

$$\Lambda'(b_y) \leq 1 + \frac{\Phi(y)}{y} \quad \text{for } y > 0.$$

Take  $R > 0$ . Define  $b_x$  as in (5.31),  $B_1$  as in (5.29) and

$$K_1 := \int_0^\infty \Lambda(f^0(y)) dy \tag{5.33}$$

$$K_0 := \int_0^\infty \Phi(y) f^0(y) dy. \tag{5.34}$$

Then for all  $t \geq 0$  there is a constant  $C(t)$  which depends only on  $t$ ,  $R$ ,  $\rho$ ,  $A$  (from (5.12)),  $b_y$ ,  $B_1$  (with  $S := 2R$ ),  $K_1$  and  $K_0$ , such that

$$\int_0^R \Lambda(f(t, y)) dy \leq C(t) \quad \text{for } t \geq 0.$$

*Proof of proposition 5.4.16.* Call  $\phi(y) := \Lambda'(f(y))$  for  $0 < y < R$  and 0 otherwise, and write

$$\frac{d}{dt} \int_0^R \Lambda(f(t, y)) dy = \int_0^\infty f(t, y) F^* \phi(y) dy + \langle C(f(t)), \phi \rangle.$$

**Step 1: bound for the fragmentation part.**

We have:

$$\int_0^\infty f(t, y) F^* \phi(y) dy \leq \int_0^\infty f(y) \int_0^R \Lambda'(f(y')) b(y, y') dy' dy$$

Thanks to the previous lemma

$$\Lambda'(f(y')) b(y, y') \leq \Lambda(f(y')) + \Lambda(b(y, y')),$$

so we can write

$$\begin{aligned} & \int_0^\infty f(y) \int_0^R \Lambda'(f(y')) b(y, y') dy' dy \\ & \leq \int_0^\infty f(y) \int_0^R \Lambda(f(y')) dy' dy + \int_0^\infty f(y) \int_0^R \Lambda(b(y, y')) dy' dy \\ & =: I_1 + I_2. \end{aligned}$$

The first integral,  $I_1$ , is easy to estimate:

$$I_1 \leq \|f\|_1 \int_0^R \Lambda(f(y)) dy. \quad (5.35)$$

For the second one, use that  $\Lambda(x) \leq x\Lambda'(x)$  for all  $x \geq 0$ :

$$\begin{aligned} I_2 & \leq \int_0^\infty f(y) \Lambda'(b_y) \int_0^R b(y, y') dy' dy \\ & \leq B_1 \int_0^\infty f(y) \left(1 + \frac{\Phi(y)}{y}\right) \int_0^R y' b(y, y') dy' dy =: u(t). \end{aligned} \quad (5.36)$$

Note that the integral of  $u$  on  $(0, t)$  for  $t > 0$  was bounded in corollary 5.4.11, and that the bound is allowed here (in particular,  $B_0 \leq 2R b_{2R}$ ).

**Step 2: bound for the coagulation part.**

For the coagulation part we can keep only the positive term. Calling  $\chi := \chi_{(0, R)}$ ,

$$\begin{aligned} & \langle C(f(t)), \phi \rangle \\ & \leq \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y') f(y) f(y') \chi(y + y') \Lambda'(f(y + y')) dy dy' \\ & \leq \frac{1}{2} A(1 + 2R) \int_0^R \int_0^R f(y) f(y') \Lambda'(f(y + y')) \chi(y + y') dy dy' \end{aligned}$$

Using lemma 5.4.15 we have that  $f(y) \Lambda'(f(y + y')) \leq \Lambda(f(y)) + \Lambda(f(y + y'))$ , so

$$\begin{aligned} \langle C(f(t)), \phi \rangle & \leq \frac{1}{2} A(1 + 2R) \int_0^R \int_0^R \Lambda(f(y)) f(y') dy dy' \\ & \quad + \frac{1}{2} A(1 + 2R) \int_0^R \int_0^R f(y') \Lambda(f(y + y')) \chi(y + y') dy dy'. \end{aligned} \quad (5.37)$$

For the first integral we can write

$$\begin{aligned} \int_0^R \int_0^R \Lambda(f(y)) f(y') dy dy' & = \int_0^R f(y) dy \int_0^R \Lambda(f(y)) dy \\ & \leq \|f\|_1 \int_0^R \Lambda(f(y)) dy, \end{aligned}$$

and for the second one,

$$\begin{aligned} \int_0^R \int_0^R f(y') \Lambda(f(y+y')) \chi(y+y') dy dy' \\ = \int_0^R f(y') \int_{y'}^{R+y'} \Lambda(f(y)) \chi(y) dy dy' \\ \leq \int_0^R f(y') dy' \int_0^R \Lambda(f(y)) dy \leq \|f\|_1 \int_0^R \Lambda(f(y)) dy. \end{aligned}$$

So from (5.37) we have

$$\langle C(f(t)), \phi \rangle \leq A(1+2R) \|f(t)\|_1 \int_0^R \Lambda(f(y)) dy.$$

Thanks to proposition 5.4.14 (taking  $S := 2R$ ), there is an allowed constant  $C(t)$  such that

$$\|f(t)\|_1 \leq C(t) \quad \text{for } t \geq 0$$

(note that the constant  $B_2$  from (5.30) is bounded by  $2Rb_{2R}$ ). With this and (5.35), (5.36) we finally get

$$\begin{aligned} \int_0^R y \Lambda(f(t, y)) dy \\ \leq \int_0^R y \Lambda(f^0(y)) dy + \int_0^t \left( C(s) \int_0^R y \Lambda(f(s, y)) dy + u(s) \right) ds \end{aligned}$$

for some constant  $C(t) \geq 0$  that depends only on the allowed quantities. Also, the integral of  $u$  on  $(0, t)$  for  $t > 0$  is bounded by the constants in the statement, as proved in corollary 5.4.11. Thus, Gronwall's lemma proves that for some (other) allowed constant  $C(t)$  we have

$$\int_0^R \Lambda(f(t, y)) dy \leq C(t) \quad \text{for } t \geq 0.$$

□

### 5.4.3. Weak continuity estimates

Take a continuous positive function  $\Phi : (0, +\infty) \rightarrow (0, +\infty)$  such that  $\lim_{y \rightarrow \infty} \Phi(y) = +\infty$ , and take  $T, R_0 > 0$ . Call

$$C_F(R) := \int_0^T \int_R^\infty \Phi(y) f(t, y) \int_0^R y' b(y, y') dy' dy dt \quad \text{for } R > 0. \quad (5.38)$$

Also, call

$$B(\delta, R) := \sup_{y \in (\delta, R)} \beta(y) \quad \text{for } 0 < \delta < R.$$

Take constants  $\alpha < \beta$  with  $\beta > 0$ , and  $A_0 > 0$  such that

$$a(y, y') \leq A_0(y^\alpha(y')^\beta + y^\beta(y')^\alpha) \quad \text{for } y, y' > 0, \quad (5.39)$$

Take a number  $m < 0$  and call

$$C_C := \int_0^T \int_0^1 \int_0^1 y^m a(y, y') f(t, y) f(t, y') y y' dy dy' dt. \quad (5.40)$$

**Proposition 5.4.17.** *Assume the conditions above, and take  $\phi \in \mathcal{C}_c$ . Then the function*

$$G(t) := \int_0^\infty \phi(y) f(t, y) dy \quad \text{for } t \in [0, T)$$

*is continuous, with a modulus of continuity which depends only on  $\phi$ ,  $C_F$ ,  $C_C$ ,  $A_0$ ,  $B$  and  $\rho$ . This is: for each  $t \in [0, T)$  and  $\epsilon > 0$  there is a  $\delta > 0$  which depends only on  $t, \epsilon$  and the above quantities, such that if  $|h| \leq \delta$  and  $t + h \in [0, T)$ , then*

$$|G(t) - G(t + h)| \leq \epsilon.$$

*Proof.* Equivalently, we will prove that for given  $t, \epsilon$  we can find  $\delta > 0$  such that if  $|h| \leq \delta$ ,

$$\left| \int_t^{t+h} \frac{d}{ds} G(s) ds \right| \leq \epsilon. \quad (5.41)$$

The time derivative of  $G$  is:

$$\begin{aligned} \frac{d}{dt} \int_0^\infty \phi(y) f(y) dy = & \\ & \int_0^\infty f(y) \int_0^y \phi(y') b(y, y') dy' dy - \int_0^\infty f(y) \phi(y) \beta(y) dy \\ & + \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y') f(y) f(y') (\phi(y + y') - \phi(y) - \phi(y')) dy dy'. \end{aligned}$$

Take  $r, R > 0$  so that the support of  $\phi$  is contained on  $(r, R)$ . We can bound uniformly the absolute value of the second term:

$$\int_0^\infty f(y) \phi(y) \beta(y) dy \leq \frac{1}{r} \|\phi\|_\infty \rho B(r, R),$$

For the first term, fix  $t \in [0, T)$  and  $\epsilon > 0$ , and let us find  $\delta$  such that (5.41) holds. As  $\lim_{y \rightarrow \infty} \Phi(y) = +\infty$  (see (5.38)), we can choose  $S > R > 0$  which only depends on  $\epsilon$  and  $C_F$  such that

$$\int_0^T \int_S^\infty f(y) \int_0^R y' b(y, y') dy' dy \leq \epsilon.$$

Then, taking  $\delta \leq \epsilon/B(r, S)$  and  $h$  such that  $|h| \leq \delta$  and  $t + h \in [0, T)$ ,

$$\begin{aligned} & \left| \int_t^{t+h} \int_0^\infty f(s, y) \int_0^y y' \phi(y') b(y, y') dy' dy ds \right| \\ & \leq \|\phi\|_\infty \left| \int_t^{t+h} \int_r^S y f(s, y) \beta(y) dy ds \right| + \|\phi\|_\infty \left| \int_t^{t+h} \int_S^\infty f(s, y) \int_0^R y' b(y, y') dy' ds \right| \\ & \leq \|\phi\|_\infty \delta \rho B(r, S) + \|\phi\|_\infty \epsilon \leq \|\phi\|_\infty (\rho + 1) \epsilon, \end{aligned}$$

which can be made as small as desired by choosing  $\epsilon$  correctly.

For the third term we can do something similar: fix  $t \in [0, T)$  and  $\epsilon > 0$ . Thanks to (5.40), we can find  $\tau > 0$  which depends only on  $\epsilon$ ,  $R$  and  $C_C$  such that

$$\int_0^T \int_0^\tau \int_0^R a(y, y') f(t, y) f(t, y') y y' dy dy' dt \leq \epsilon.$$

Also, note that the integrand of the third term is 0 when  $y \geq R$ . Take  $\delta > 0$  such that

$$\int_\tau^R f(s, y) y^{\alpha+1} dy \leq \epsilon/\delta \quad \text{for all } s \in [0, T)$$

(such a  $\delta$  depends only on  $\alpha$ ,  $\tau$ ,  $R$  and  $\rho$ , thanks to the uniform bound on the mass) and take any  $0 < h < \delta$  with  $t + h \in [0, T)$ . Then, using lemma 4.3.4 and (5.39),

$$\begin{aligned} & \left| \int_t^{t+h} \int_0^\infty \int_0^\infty a(y, y') f(s, y) f(s, y') (\phi(y + y') - \phi(y) - \phi(y')) dy dy' ds \right| \\ & \leq C \int_t^{t+h} \int_0^\tau \int_0^R a(y, y') f(t, y) f(t, y') y y' dy dy' dt \\ & \quad + C A_0 \int_t^{t+h} \int_\tau^R \int_\tau^R f(s, y) f(s, y') y^{\alpha+1} (y')^{\beta+1} dy dy' ds \\ & \leq C\epsilon + C \int_t^{t+h} \int_\tau^R f(s, y) y^{\alpha+1} dy ds \\ & \leq C\epsilon + C\delta \sup_{s \in [0, T)} \int_\tau^R f(s, y) y^{\alpha+1} dy \leq 2C\epsilon. \end{aligned}$$

One can follow the same argument, with the obvious modifications, for  $h < 0$ .  $\square$

#### 5.4.4. Regularization of moments of order less than 1 near $y = 0$

In order to study the regularity of solutions near  $y = 0$  one needs to estimate the behavior of moments less than 1, as we already know that the first moment, which represents the total mass, is constant in time and depends only on the first moment of the initial data (at least for the regular solutions used in this section).

The bounds below apply to a solution in the conditions of hypotheses 5.4.1 (at the beginning of section 5.4), with the following additional requirements on the form of the coagulation and fragmentation coefficients:

**Hypothesis 5.4.18.** ■ *There are  $0 < \epsilon_a < 1 < R_a$ ,  $0 < \epsilon_b < 1 < R_b$  such that*

$$\begin{aligned} a & \text{ has support contained in } \{(y, y') \mid \epsilon_a \leq y, y'\} \\ b & \text{ has support contained in } \{(y, y') \mid \epsilon_b \leq y' < y - \epsilon_b\}. \end{aligned}$$

■ *There are constants  $K'_a > 0$  and  $\alpha < \beta \leq 1 \in \mathbb{R}$  such that*

$$a(y, y') \leq K'_a (y^\alpha (y')^\beta + (y')^\alpha y^\beta)$$

*for all  $y, y' > 0$ . We always denote  $\lambda := \alpha + \beta$ .*

■ *There are  $\gamma \in \mathbb{R}$ ,  $0 < k_0 < 1$ , and  $K_b, K'_b > 0$  such that the fragmentation coefficient  $b$  satisfies*

$$b(y, y') \leq K'_b \phi_\gamma(y) \frac{1}{y} \left( \frac{y'}{y} \right)^{-1-k_0} \quad (5.42)$$

*for all  $0 < y' < y$ , where for  $y > 0$  we set*

$$\begin{aligned} \phi_\gamma(y) &= y^\gamma && \text{if } \gamma \leq 0, \\ \phi_\gamma(y) &= \min\{y^\gamma, 1\} && \text{if } \gamma > 0. \end{aligned}$$

■ *We assume that the initial data  $f^0$  has support contained in  $[\epsilon_b, +\infty)$ . As a consequence (see lemma 5.4.2), the support of  $f(t)$  is contained in  $[\epsilon_b, +\infty)$  for all  $t \geq 0$ .*

*Remark 5.4.19.* Observe that the hypotheses on  $b$  imply that for each  $0 < R_0 < S_0$  and  $k > k_0$  there is some constant  $B_k > 0$  which depends on  $k$ ,  $R_0$ ,  $S_0$  and  $K'_b$  such that

$$\int_0^y (y')^k b(y, y') dy' \leq B_k y^k \beta(y) \quad \text{for all } y \leq S_0. \quad (5.43)$$

$$\int_0^{R_0} (y')^k b(y, y') dy' \leq B_k \int_0^{R_0} y' b(y, y') dy' \quad \text{for all } y \geq S_0. \quad (5.44)$$

These bounds will be useful below.

### Coagulation is stronger near $y = 0$

In order to prove a regularizing effect on moments less than 1 when coagulation is stronger than fragmentation near  $y = 0$  we need some further assumptions:

**Hypothesis 5.4.20.** *In addition to 5.4.18 and 5.4.1, we assume that  $\epsilon_a \leq \epsilon_b$  and that there are constants  $K_a > 0$  and  $R_a > 1$  such that*

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

for all  $\epsilon_b < y, y' < R_a$ .

We also assume that  $\beta - \alpha < 1$ .

Take  $0 < k < 1$  and a function  $\psi$  which behaves as  $y^k$  near 0. We want to estimate  $\int_0^\infty \psi(y)f(y) dy$ . Let us calculate its time derivative:

$$\begin{aligned} \frac{d}{dt} \int_0^\infty \psi(y)f(y) dy = & \\ & \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y')f(y)f(y')(\psi(y + y') - \psi(y) - \psi(y')) dy dy' \\ & + \int_0^\infty f(y)F^*\psi(y) dy. \end{aligned} \quad (5.45)$$

To find a good bound for the coagulation part (the first on the right hand side), we use a technique very similar to that in lemma 3.1 of [34]: we write  $(\psi(y + y') - \psi(y) - \psi(y'))$  as a sum (actually an integral) of other functions, interchange the integrals, and finally use the Cauchy-Schwartz inequality on the resulting expression; this gives a bound which does *not* seem to follow from an inequality of the kind  $\psi(y + y') - \psi(y) - \psi(y') < h(y, y')$  for any  $h$ . Let us write, for a suitable function  $\phi$ ,

$$\psi(y) = \int_0^\infty \phi(A)\phi_y(A) dA, \quad (5.46)$$

where

$$\phi_y(A) := \begin{cases} y^m & \text{if } y < A \leq 1 \\ A^m & \text{if } A < y \leq 1 \\ 0 & \text{if } 1 < y, \end{cases}$$

for some  $m \in \mathbb{R}$ . A formal calculation, having in mind that we want to use a function  $\psi$  that behaves as  $y^k$  near  $y = 0$ , suggests that we take

$$\phi(y) := \begin{cases} y^{k-m-1} & \text{if } y \leq 1 \\ 0 & \text{if } y > 1. \end{cases}$$

Choose any  $m > k$ ; then we can calculate  $\psi$  from (5.46): for  $y \leq 1$ ,

$$\begin{aligned} \psi(y) &= \int_0^\infty \phi(A)\phi_y(A) dA = \int_0^y A^{k-1} dA + y^m \int_y^1 A^{k-m-1} dA \\ &= \frac{1}{k}y^k + \frac{1}{k-m}y^m(1 - y^{k-m}) = \left(\frac{1}{k} + \frac{1}{m-k}\right)y^k - \frac{1}{m-k}y^m, \end{aligned}$$



while  $\psi(y) = 0$  for  $y > 1$ . One can see then that for  $y < 1$ ,

$$C_1 y^k \leq \psi(y) \leq C_2 y^k,$$

with  $C_1 := \frac{1}{k}$  and  $C_2 := \left(\frac{1}{k} + \frac{1}{m-k}\right)$ , which are positive finite constants.

Note that,

$$\phi_{y+y'}(A) - \phi_y(A) - \phi_{y'}(A) \leq \begin{cases} -A^m & \text{if } 1 \geq y, y' \geq A \\ 0 & \text{otherwise.} \end{cases}$$

With this we can estimate the coagulation part from (5.45):

$$\begin{aligned} & \int_0^\infty \int_0^\infty a(y, y') f(y) f(y') (\psi(y + y') - \psi(y) - \psi(y')) dy dy' \\ &= \int_0^1 \phi(A) \int_0^\infty \int_0^\infty a(y, y') f(y) f(y') (\phi_{y+y'}(A) - \phi_y(A) - \phi_{y'}(A)) dy dy' dA \\ &\leq - \int_0^A \phi(A) A^m \int_A^1 \int_A^1 a(y, y') f(y) f(y') dy dy' dA \\ &\leq -K_a \int_0^1 \phi(A) A^m \left( \int_A^1 f(y) y^{\lambda/2} dy dA \right)^2 \quad (5.47) \end{aligned}$$

Here we have used that  $a(y, y') \geq K_a (yy')^{\lambda/2}$  for  $\epsilon \leq y, y' \leq R$  and that

$$a(y, y') f(y) f(y') \geq K_a (yy')^{\lambda/2} f(y) f(y') \quad \text{for all } y, y' \leq 1.$$

Note that  $\epsilon_b$  does not appear here, as the support of  $f$  is contained in  $[\epsilon_b, +\infty)$ .

Take two functions  $g_1, g_2$  to be chosen later; the Cauchy-Schwartz inequality implies that:

$$\begin{aligned} & \int_0^1 g_1(A) g_2(A) \int_A^1 f(y) y^{\lambda/2} dy dA \leq \\ & \left( \int_0^1 g_1^2(A) dA \right)^{1/2} \left( \int_0^1 g_2^2(A) \left( \int_A^1 f(y) y^{\lambda/2} dy \right)^2 dA \right)^{1/2}. \end{aligned}$$

If we want to compare this to our previous equation, one must take  $g_2^2(A) = \phi(A) A^m$ , or

$$g_2(A) := A^{\frac{k-1}{2}} \chi_{[A < 1]}.$$

If we choose  $g_1$  to be a power near 0, it must have an exponent greater than  $-1/2$ , as we need it to be square-integrable. Then, take any  $\delta > 0$  and  $g_1(A) := A^{-\frac{1}{2} + \delta} \chi_{[A < 1]}$ .

Then we can continue from 5.47 and write

$$\begin{aligned} & \int_0^\infty \int_0^\infty a(y, y') f(y) f(y') (\psi(y + y') - \psi(y) - \psi(y')) dy dy' \\ & \leq K_a \left( \int_0^1 g_1^2(A) dA \right)^{-1} \left( \int_0^1 g_1(A) g_2(A) \int_A^1 f(y) y^{\lambda/2} dy dA \right)^2 \\ & =: K_a C_3 \left( \int_0^1 g_1(A) g_2(A) \int_A^1 f(y) y^{\lambda/2} dy dA \right)^2. \end{aligned} \quad (5.48)$$

The latter part is

$$\int_0^1 g_1(A) g_2(A) \int_A^1 f(y) y^{\lambda/2} dy dA = \int_0^1 f(y) y^{\lambda/2} \int_0^y g_1(A) g_2(A) dA dy, \quad (5.49)$$

and, for  $y < 1$ ,

$$\int_0^y g_1(A) g_2(A) dA = \int_0^y A^{\frac{k}{2}-1+\delta} dA = \frac{2}{k+2\delta} y^{\frac{k}{2}+\delta} =: C_4 y^{\frac{k}{2}+\delta}. \quad (5.50)$$

Then, from (5.48) and using (5.49)–(5.50) we have

$$\begin{aligned} & \int_0^\infty \int_0^\infty a(y, y') f(y) f(y') (\psi(y + y') - \psi(y) - \psi(y')) dy dy' \\ & \leq -K_a C_3 C_4^2 \left( \int_0^1 f(y) y^{\frac{\lambda+k}{2}+\delta} dy \right)^2. \end{aligned} \quad (5.51)$$

Now, let us estimate the fragmentation part from (5.45). In addition to  $0 < k < 1$ , we suppose that  $k \geq k_0$  and calculate as follows:

$$\begin{aligned} & \int_0^\infty f(y) F^* \psi(y) dy \leq \int_0^\infty f(y) \int_0^y \psi(y') b(y, y') dy' dy \\ & \leq C_2 \int_0^S f(y) \int_0^y (y')^k b(y, y') dy' dy + C_2 \int_S^\infty f(y) \int_0^1 (y')^k b(y, y') dy' dy, \end{aligned} \quad (5.52)$$

where  $S > 1$  is some number. The second part can be bounded thanks to our bound on the fragmentation coefficient in eq. (5.42) and (5.44) for  $R_0 = 1$ ,  $S_0 = S$ :

$$\begin{aligned} & \int_S^\infty f(y) \int_0^1 (y')^k b(y, y') dy' dy \leq B_k \int_S^\infty f(y) \int_0^1 y' b(y, y') dy' dy \\ & \leq C B_k \int_S^\infty f(y) dy \leq C \rho. \end{aligned} \quad (5.53)$$

for some constant  $C > 0$  which depends only on the constants in the bound (5.42). As for the first part, we can use (5.43) (again for  $S_0 = S$ ) to obtain

$$\begin{aligned} \int_0^S f(y) \int_0^1 (y')^k b(y, y') dy' dy \\ \leq B_k \int_0^S f(y) y^k \beta(y) dy \leq B_k K'_b \int_0^S f(y) y^{k+\gamma} dy \\ \leq B_k K'_b \int_0^1 f(y) y^{k+\gamma} dy + B_k K'_b C \rho, \end{aligned} \quad (5.54)$$

where  $C = \max\{1, S^{k+\gamma-1}\}$ . Gathering the latter estimates one has

$$\int_0^\infty f(y) F^* \psi(y) dy \leq C_2 B_k K'_b \int_0^1 f(y) y^{k+\gamma} dy + C_2 B_k K'_b C \rho + C.$$

With this and (5.45), (5.51) we finally obtain

$$\frac{d}{dt} \int_0^\infty \psi(y) f(y) dy \leq -K_C \left( \int_0^1 f(y) y^{\frac{\lambda+k}{2}+\delta} dy \right)^2 + K_F \int_0^1 f(y) y^{k+\gamma} dy + K,$$

where  $K_C > 0$ ,  $K_F, K \geq 0$  are the quantities obtained in the previous estimates.

**Proposition 5.4.21.** *Assume that  $a, b, f$  satisfy the conditions in hypothesis 5.4.18 (in addition to hypothesis 5.4.1, which is assumed to hold in all of our estimates). Take  $k_0 \leq k < 1$  and  $\delta > 0$  ( $k_0$  appears in hypotheses 5.4.18).*

*Then, there is a function  $\psi : (0, +\infty) \rightarrow (0, +\infty)$  such that  $\psi(y) = 0$  when  $y \geq 1$  and*

$$C_1 y^k \leq \psi(y) \leq C_2 y^k \quad \text{for all } 0 < y < 1$$

*for some constants  $C_1, C_2 > 0$  which depend on  $k$ , and there are constants  $K_C > 0$ ,  $K, K_F \geq 0$  which depend only on  $k, \delta, \rho, K_a, K'_b, \lambda$  and  $\gamma$  (from hypothesis 5.4.18), such that*

$$\frac{d}{dt} \int_0^\infty \psi(y) f(y) dy \leq -K_C \left( \int_0^1 f(y) y^{\frac{\lambda+k}{2}+\delta} dy \right)^2 + K_F \int_0^1 f(y) y^{k+\gamma} dy + K,$$

*for almost all  $t > 0$ .*

**Proposition 5.4.22.** *Assume 5.4.1, 5.4.18 and 5.4.20, and suppose that*

$$\gamma > \frac{\lambda - 1}{2}.$$

*Then there exist  $k < 1, \theta < \alpha + 1$  and constants  $C, C(t) > 0$  that depend only on  $\rho, K_a, K'_b, \lambda, \gamma$  and  $k_0$ , such that*

$$\begin{aligned} \int_0^1 f(s, y) y^k dy &\leq \max \left\{ \frac{C}{t}, C \right\} \\ \int_0^t \left( \int_0^1 f(s, y) y^\theta dy \right)^2 ds &\leq C(t) \end{aligned}$$

*for all  $t > 0$ .*

*Proof.* We can take  $\delta > 0$  and  $k_0 < k < 1$  such that  $k > \lambda$  and

$$\frac{\lambda + k}{2} + \delta < k + \gamma.$$

Actually, we can choose  $k$  such that, additionally,

$$\frac{\lambda + k}{2} + \delta < \alpha + 1,$$

as

$$\frac{\lambda + 1}{2} < \alpha + 1 \quad \Leftrightarrow \quad \alpha + \beta + 1 < 2\alpha + 2 \quad \Leftrightarrow \quad \beta - \alpha < 1,$$

which holds by hypothesis.

Call

$$\theta := \frac{\lambda + k}{2} + \delta.$$

Then, as  $\theta < k + \gamma$ , we use the previous proposition to obtain that

$$\frac{d}{dt} \int_0^\infty \psi(y) f(y) dy \leq -K_C \left( \int_0^1 f(y) y^\theta dy \right)^2 + K_F \int_0^1 f(y) y^\theta dy + K,$$

where  $\psi$  is the function given there. Now, suppose that the following holds:

$$\int_0^1 f(y) y^\theta dy > \max \left\{ \frac{4K_F}{K_C}, \sqrt{\frac{4K_F}{K_C} K} \right\}.$$

Then we have

$$\begin{aligned} \int_0^1 f(y) y^\theta dy &\leq \frac{K_C}{4K_F} \left( \int_0^1 f(y) y^\theta dy \right)^2 \\ K &\leq \frac{K_C}{4K_F} \left( \int_0^1 f(y) y^\theta dy \right)^2, \end{aligned}$$

so, when  $\int_0^1 f(y) y^\theta dy > \frac{4K_F}{K_C}$ , our differential inequality implies that

$$\frac{d}{dt} \int_0^\infty \psi(y) f(y) dy \leq -\frac{K_C}{2} \left( \int_0^1 f(y) y^\theta dy \right)^2 \leq -C \left( \int_0^1 f(y) \psi(y) dy \right)^2. \quad (5.55)$$

(Note that  $\theta < k$ , as  $k > \lambda$ .) In particular, knowing that for some allowed constant  $C > 0$  one has that  $\int_0^\infty \psi(y) f(y) dy \leq C \int_0^1 f(y) y^\theta dy$ , we see that the above equation holds when  $\int_0^\infty \psi(y) f(y) dy > \frac{K_C}{4CK_F}$ . By a Gronwall-type estimate, for some (other) allowed constant  $C > 0$ , we have

$$\int_0^\infty \psi(y) f(t, y) dy \leq \max \left\{ \frac{C}{t}, C \right\} \quad \text{for } t \geq 0.$$

Now take  $k'$  with  $k < k' < 1$ . By interpolation with the moment of order one, we know that the moment of order  $k'$  is integrable on  $(0, t)$  for any  $t > 0$ , and its integral is bounded above by some allowed constant. So, from equation (5.55) we obtain that

$$\int_0^t \left( \int_0^1 f(s, y) y^\theta dy \right)^2 ds \leq C(t)$$

for some allowed constant  $C(t)$ . □

### Fragmentation is stronger near $y = 0$

There is also a regularization near zero when the fragmentation is strong enough, which can be seen by studying the behavior of moments greater than 1. For this, we assume the following:

**Hypothesis 5.4.23.** *In addition to 5.4.18 and 5.4.1, we assume that  $2\epsilon_b < \epsilon_a$  and that there are constants  $K_b > 0$  and  $R_b > 1$  such that*

$$K_b \phi_\gamma(y) \frac{1}{y} \left( \frac{y'}{y} \right)^{-1-k_0} \leq b(y, y')$$

for all  $\epsilon_a < y' < y - \epsilon_a < R_b$ .

We will use the following lemma, which is a direct consequence of the inequalities in proposition 11.1.2:

**Lemma 5.4.24.** *Suppose that  $\alpha \leq \beta \in \mathbb{R}$  such that  $\beta - \alpha < 1$ , and take  $1 < k < 2 - (\beta - \alpha)$ . Call  $\lambda := \alpha + \beta$ . Then, there is a constant  $C > 0$  such that*

$$(y^\alpha (y')^\beta + (y')^\alpha y^\beta) ((y + y')^k - y^k - (y')^k) \leq C (yy')^{\frac{\lambda+k}{2}} \quad \text{for all } y, y' \leq 1.$$

With this we can estimate the behavior of the moment of order  $k$  of a solution to the coagulation-fragmentation equations. Take  $\psi(y) := y^k$  for  $\epsilon_a < y < 1$  and  $\psi(y) = 0$  otherwise; then,

$$\begin{aligned} \frac{d}{dt} \int_0^1 \psi(y) f(y) dy \leq & \\ & \frac{1}{2} \int_0^1 \int_0^1 a(y, y') f(y) f(y') (\psi(y + y') - \psi(y) - \psi(y')) dy dy' \\ & + \int_0^\infty f(y) F^* \psi(y) dy. \end{aligned} \quad (5.56)$$

We can estimate the coagulation part as follows, using the previous lemma:

$$\begin{aligned}
& \int_0^1 \int_0^1 a(y, y') f(y) f(y') (\psi(y + y') - \psi(y) - \psi(y')) dy dy' \\
& \leq K'_a \int_{\epsilon_a}^1 \int_{\epsilon_a}^1 f(y) f(y') (y^\alpha (y')^\beta + (y')^\alpha y^\beta) ((y + y')^k - y^k - (y')^k) dy dy' \\
& \leq C \int_{\epsilon_a}^1 \int_{\epsilon_a}^1 f(y) f(y') (yy')^{\frac{\lambda+k}{2}} dy dy' = C \left( \int_{\epsilon_a}^1 f(y) y^{\frac{\lambda+k}{2}} dy \right)^2, \quad (5.57)
\end{aligned}$$

where  $C$  depends only on  $K'_a$ ,  $\alpha$ ,  $\beta$  and  $k$ . For the fragmentation part we have:

$$\begin{aligned}
& \int_0^\infty f(y) F^* \psi(y) dy = \int_1^\infty f(y) \int_0^1 \psi(y') b(y, y') dy' dy \\
& + \int_0^1 f(y) \int_0^y \psi(y') b(y, y') dy' dy - \int_0^1 f(y) \psi(y) \int_0^y \frac{y'}{y} b(y, y') dy' dy. \quad (5.58)
\end{aligned}$$

For the first term we can use an estimate similar to that in (5.52)–(5.53) to obtain

$$\int_1^\infty f(y) \int_0^1 \psi(y') b(y, y') dy' dy \leq C \rho, \quad (5.59)$$

and for the last two terms in the sum in (5.58), we have:

$$\begin{aligned}
& \int_0^1 f(y) \int_0^y \psi(y') b(y, y') dy' dy - \int_0^1 f(y) \psi(y) \int_0^y \frac{y'}{y} b(y, y') dy' dy \\
& \leq \int_{\epsilon_a}^1 f(y) \int_{\epsilon_b}^{y-\epsilon_b} (y')^k b(y, y') dy' dy - \int_{\epsilon_a}^1 f(y) y^k \int_{\epsilon_b}^{y-\epsilon_b} \frac{y'}{y} b(y, y') dy' dy \\
& = - \int_{\epsilon_a}^1 f(y) y^k \int_{\epsilon_b}^{y-\epsilon_b} \left( \frac{y'}{y} - \frac{(y')^k}{y^k} \right) b(y, y') dy' dy \\
& \leq -K_b \int_{\epsilon_a}^1 f(y) y^{k+\gamma} \int_{\epsilon_b/y}^{(y-\epsilon_b)/y} (z - z^k) z^{-1-k_0} dz dy \\
& \leq -K_b \int_{\epsilon_a}^1 f(y) y^{k+\gamma} \int_{\epsilon_b}^{(\epsilon_a - \epsilon_b)/\epsilon_a} (z - z^k) z^{-1-k_0} dz dy = -K_b C \int_{\epsilon_a}^1 f(y) y^{k+\gamma} dy \quad (5.60)
\end{aligned}$$

for some constant  $C > 0$  that depends only on  $\epsilon_a$ ,  $\epsilon_b$ ,  $k$  and  $k_0$ . Finally we obtain from (5.56) and (5.57)–(5.60):

$$\frac{d}{dt} \int_{\epsilon_a}^1 y^k f(y) dy \leq C \left( \int_{\epsilon_a}^1 f(y) y^{\frac{\lambda+k}{2}} dy \right)^2 - C' \int_{\epsilon_a}^1 f(y) y^{k+\gamma} dy + C''.$$

**Proposition 5.4.25.** *Assume hypotheses 5.4.1, 5.4.18 and 5.4.23. Then there are constants  $k > 1$ ,  $C' > 0$  and  $C, C'' \geq 0$  that depend only on  $K'_a, K_b, \alpha, \beta, \gamma, k_0$  and  $\rho$ , such that*

$$\frac{d}{dt} \int_{\epsilon_a}^1 y^k f(y) dy \leq C \left( \int_{\epsilon_a}^1 f(y) y^{\frac{\lambda+k}{2}} dy \right)^2 - C' \int_{\epsilon_a}^1 f(y) y^{k+\gamma} dy + C''.$$

**Proposition 5.4.26.** *Assume hypotheses 5.4.1, 5.4.18 and 5.4.23, and suppose that  $\gamma < \lambda - 1$ . There is  $m < \alpha + 1$  and a constant  $C(t)$  that depends only on  $K'_a, K_b, \lambda, \gamma$  and  $\rho$ , such that*

$$\int_0^t \int_{\epsilon_a}^1 f(s, y) y^m dy ds \leq C(t) \quad \text{for all } t > 0.$$

*Proof.* By interpolation in the previous proposition, there are allowed constants  $C' > 0$  and  $C, C'' \geq 0$  such that

$$\frac{d}{dt} \int_{\epsilon_a}^1 y^k f(y) dy \leq C \int_{\epsilon_a}^1 f(y) y^{\lambda+k-1} dy - C' \int_{\epsilon_a}^1 f(y) y^{k+\gamma} dy + C''.$$

As  $\gamma < \lambda - 1$ , again by interpolation we have

$$\frac{d}{dt} \int_{\epsilon_a}^1 y^k f(y) dy \leq C \int_{\epsilon_a}^1 f(y) y^{\lambda+k-1} dy - C' \left( \int_{\epsilon_a}^1 f(y) y^{\lambda+k-1} dy \right)^\theta + C'',$$

for some  $\theta > 1$ . Reasoning as in the previous section, there are allowed constants  $C_1, C'_1 \geq 0$  such that

$$\frac{d}{dt} \int_{\epsilon_a}^1 y^k f(y) dy \leq -C_1 \left( \int_{\epsilon_a}^1 f(y) y^{\lambda+k-1} dy \right)^\theta \quad \text{when } \int_{\epsilon_a}^1 f(y) y^{\lambda+k-1} dy \geq C'_1.$$

In particular, as  $\lambda + k - 1 < k$  and hence  $\int_{\epsilon_a}^1 f(y) y^{\lambda+k-1} dy \geq \int_{\epsilon_a}^1 f(y) y^k dy$ ,

$$\int_{\epsilon_a}^1 y^k f(t, y) dy \leq \max \left\{ \int_{\epsilon_a}^1 y^k f^0(y) dy, C'_1 \right\} \quad \text{for all } t > 0$$

and, for some allowed constant  $C \geq 0$ ,

$$\int_0^t \left( \int_{\epsilon_a}^1 f(s, y) y^{\lambda+k-1} dy \right)^\theta ds \leq C + Ct \quad \text{for all } t > 0.$$

Choosing  $k$  so that  $\lambda + k - 1 < \alpha + 1$  (which can always be done, as we assume  $\beta < 1$ ), we obtain the result.  $\square$

## 5.5. Solutions with finite mass

In this section we want to prove existence of solutions for the coagulation-fragmentation equation when the total mass  $\int_0^\infty y f(y) dy$  is finite, relaxing the usual assumption that the number of clusters  $\int_0^\infty f(y) dy$  is bounded.

We gather our hypotheses below, which include the assumption that  $z \mapsto z a(z, y')$  is increasing for all  $y' > 0$ .

**Hypothesis 5.5.1.** *Throughout this section we assume the coefficients  $a, b$  satisfy the following:*

- *The fragmentation coefficient  $b$  satisfies (3.4), and is bounded on  $\{(y, y') \mid 0 < y' < y < R\}$  for all  $R > 0$ .*
- *The coagulation coefficient  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  is a measurable symmetric function such that  $a(y, y') \leq A(1 + y + y')$  for some constant  $A > 0$ , and*

$$z \mapsto z a(z, y') \quad \text{is increasing for all } y' > 0.$$

We also assume that the initial condition  $f^0 : (0, +\infty) \rightarrow \mathbb{R}$  is a nonnegative function in  $\dot{L}_1^1$ .

Below we will write

$$\rho := \int_0^\infty y f^0(y) dy \tag{5.61}$$

$$b_x := \sup_{0 < y' < y < x} b(y, y') \quad \text{for } x > 0, \quad b_0 := 0 \tag{5.62}$$

We will prove the following theorem:

**Theorem 5.5.2.** *Assume the above hypotheses on the coefficients  $a, b$ , and take a nonnegative function  $f^0 \in \dot{L}_1^1$ . Then for all  $0 < T \leq +\infty$  there is a solution  $f$  to the coagulation-fragmentation equations (5.1)–(5.2) with initial data  $f^0$  (in the sense of definition 5.1.1), and such that  $f \in L^\infty([0, T], \dot{L}_1^1)$ . In addition, this solution conserves the mass.*

The strategy goes as usual: we will prove that a solution can be obtained as a certain limit of solutions to a regularized problem. The solutions to this simpler problem are of the kind obtained in section 5.2, and we will need some estimates on their behavior in order to be able to pass to the limit in (5.9). These estimates should depend only on the properties of the coefficients or the initial condition we want to use, and in particular should not depend on the regularization used.



### 5.5.1. Passing to the limit

We define a sequence of approximations as follows: for  $y > y' > 0$  we set

$$b_n(y, y') := \begin{cases} b(y, y') & \text{if } \frac{1}{n} < y' < y - \frac{1}{n} < n \\ 0 & \text{otherwise.} \end{cases}$$

In the same way, we set for  $y, y' > 0$ :

$$a_n(y, y') := \begin{cases} a(y, y') & \text{if } \frac{1}{n} < y, y' < n \\ 0 & \text{otherwise.} \end{cases}$$

We also define a regularization of the initial condition: for  $y > 0$ ,

$$f_n^0(y) := \begin{cases} \min\{f^0(y), n\} & \text{if } \frac{1}{n} < y < n \\ 0 & \text{otherwise.} \end{cases}$$

Observe that the coefficients  $a_n, b_n$  satisfy the hypotheses in theorem 5.2.1 and also the stronger hypothesis 5.4.1 from section 5.4; in particular, all estimates from this section apply to the regularized solution defined below.

**Lemma 5.5.3.** *For any  $\psi : (0, +\infty) \times (0, +\infty) \rightarrow \mathbb{R}$  which is in  $L^\infty$  and any compact set  $K \subseteq [0, +\infty)$ ,*

$$\int_0^y \psi(y') b_n(y, y') dy' \rightarrow \int_0^y \psi(y') b(y, y') dy' \quad \text{uniformly for } y \in K.$$

*In particular, if  $\beta_n$  is the total fragmentation rate associated to the fragmentation coefficient  $b_n$ , then applying the above for  $\psi(y, y') := y'/y$  whenever  $0 < y' < y \in K$  and  $\psi \equiv 0$  otherwise,*

$$\beta_n \rightarrow \beta \quad \text{uniformly in } K.$$

*Proof.* As  $b$  is bounded in  $K \times K$  by some constant  $C$ , we have the following for a large enough  $n$  and any  $y \in K$ :

$$\begin{aligned} & \left| \int_0^y \psi(y') b(y, y') dy' - \int_0^y \psi(y') b_n(y, y') dy' \right| \\ &= \left| \int_0^y \psi(y') (b(y, y') - b_n(y, y')) dy' \right| \\ &\leq \|\psi\|_\infty \int_0^{1/n} b(y, y') dy' \leq \|\psi\|_\infty C \frac{1}{n} \rightarrow 0 \quad \text{as } n \rightarrow \infty. \end{aligned}$$

□

Call  $F_n, C_n$  the fragmentation and coagulation operators associated to  $b_n, a_n$ , respectively. We know from theorem 5.2 that there is a solution  $f_n$  of the coagulation-fragmentation equations with coefficients  $a_n, b_n$  and initial condition  $f_n^0$ , in the sense stated there. We intend to prove that the sequence  $\{f_n\}$  converges in a certain sense to a solution of the coagulation-fragmentation equations with coefficients  $a$  and  $b$  and initial data  $f^0$ . For this we will prove that, given a number  $0 < T < +\infty$ , the conditions of the Dunford-Pettis theorem (more precisely, the version in theorem 9.2.3) hold for this sequence with the measure  $\lambda \otimes (y dy)$  on  $[0, T] \times (0, +\infty)$ , where  $\lambda$  is the Lebesgue measure on  $[0, T]$ . For this we have to show that:

- The sequence  $\{f_n\}$  is bounded in this space; this is,

$$\int_0^T \int_0^\infty y f_n(t, y) dy dt \quad \text{is uniformly bounded in } n \quad (5.63)$$

(recall that the  $f_n$  are nonnegative).

- The integral of  $y f_n(y)$  on small sets contained in a given compact set tends to zero uniformly in  $n$ ,
- and the integral of  $y f_n(t, y)$  on sets of the form  $[0, T] \times (N, +\infty)$  tends to zero when  $N \rightarrow \infty$  uniformly in  $n$ .

Equation (5.63) holds because of mass conservation: we know that for all  $n \geq 1$ ,

$$\int_0^T \int_0^\infty y f_n(t, y) dy dt = T \int_0^\infty y f_n^0(y) dy \leq T\rho. \quad (5.64)$$

Below we prove the remaining points.

**Lemma 5.5.4.** *There is a  $C^\infty$  function  $\Phi : [0, +\infty) \rightarrow [0, +\infty)$  such that  $y \mapsto \Phi(y)/y$  is concave,  $\lim_{y \rightarrow 0} \Phi(y)/y = 0$ ,  $\Phi(y) \leq y^2$  for  $y \geq 0$ ,  $\Phi(0) = 0$ ,  $\lim_{y \rightarrow \infty} \Phi(y)/y = +\infty$  and*

$$\int_0^\infty \Phi(y) f^0(y) dy < +\infty.$$

*Proof.* This is just proposition 9.1.1 applied to  $f^0$  and the measure  $y dy$ . □

**Lemma 5.5.5.** *Let  $\Phi$  be the function from lemma 5.5.4. For all  $T > 0$  the integral*

$$\int_0^T \int_0^\infty f_n(t, y) \Phi(y) dy dt$$

*is uniformly bounded in  $n$ .*

*Proof.* Proposition 5.4.3 gives a bound for this moment, which depends only on  $\int_0^\infty \Phi(y) f^0(y) dy$  (which is finite, as  $\Phi$  was chosen as satisfying this), and quantities which are uniformly bounded independently of  $n$ . □

**Lemma 5.5.6.** *There is a  $C^\infty$  function  $\Lambda : [0, +\infty) \rightarrow [0, +\infty)$  which is strictly convex, such that  $\Lambda'$  is concave,  $\Lambda(0) = \Lambda'(0) = 0$ ,  $\lim_{y \rightarrow \infty} \Lambda(y)/y = +\infty$ , for which*

$$\int_0^\infty y \Lambda(f^0(y)) dy < +\infty$$

and such that

$$\Lambda'(b_y) \leq 1 + \frac{\Phi(y)}{y} \quad \text{for all } y > 0.$$

*Proof.* This  $\Lambda$  is given by proposition 9.1.2. The bound on  $\Lambda'$  can be written as

$$\Lambda'(y) \leq 1 + \frac{\Phi(h(y))}{h(y)} \quad \text{for all } y > 0, \quad (5.65)$$

where  $h$  is the “inverse” of  $y \mapsto b_y$ , defined as  $h(0) := 0$  and

$$h(y) := \sup\{x \geq 0 \mid b_x < y\} \quad \text{for } y > 0.$$

Note that  $h$  is increasing, and that it becomes  $+\infty$  at some point if  $b$  is bounded. This  $h$  satisfies that  $h(b_y) = y$  for all  $y \geq 0$ , so (5.65) implies the bound in the statement. In turn, we can satisfy (5.65) thanks to proposition 9.1.2 (see also the conditions in proposition 9.1.1), as  $h(y) \rightarrow \infty$  when  $y \rightarrow \infty$  and hence  $\Phi(h(y))/h(y) \rightarrow \infty$  when  $y \rightarrow \infty$ .  $\square$

**Lemma 5.5.7.** *For all  $t, R > 0$  there is a constant  $C(t)$ , which depends on them increasingly, such that*

$$\int_0^R y \Lambda(f_n(t, y)) dy \leq C(t) \quad \text{for all } n \geq 1.$$

*Proof.* This is given by proposition 5.4.13.  $\square$

**Lemma 5.5.8.** *There is a nonnegative function  $f : [0, +\infty) \times (0, +\infty)$  with*

$$f \in L^\infty([0, +\infty), \dot{L}_1^1)$$

and a subsequence of  $\{f_n\}$  (which we denote also as  $\{f_n\}$ ) such that for every  $T > 0$ ,

$$f_n \rightharpoonup f \text{ in } L^1([0, T], \dot{L}_1^1) \text{ weakly.}$$

In addition this function  $f$  conserves the mass:  $\int_0^\infty y f(t, y) dy = \int_0^\infty y f^0(y) dy$  for almost all  $t > 0$ .

*Proof.* Take  $T > 0$ . Let us first find a subsequence of  $\{f_n\}$  which converges weakly in  $L^1([0, T], \dot{L}_1^1)$ . This space is canonically identified with the space of integrable functions on  $X := [0, T] \times [0, +\infty)$  with the measure  $\mu := \lambda \otimes y dy$ , where  $\lambda$  is the usual Lebesgue measure on  $[0, T]$  (see theorem 10.2.1), so we can find such a

subsequence by proving that  $\{f_n\}$  satisfies the hypotheses of Dunford-Pettis' theorem 9.2.3 in  $L^1(X, \mu)$ :  $\{f_n\}$  is bounded in this space, which is a consequence of mass conservation (see (5.64)); by a standard argument, uniform local integrability is given by lemma 5.5.7 and a uniform bound for the integral outside a compact set is given by lemma 5.5.5. Hence, there is a subsequence of  $\{f_n\}$  which converges weakly to an  $f \in L^1(X, \mu)$ . Then, repeating the argument for each  $T$  in a diverging sequence and applying a usual diagonal argument we can find a subsequence of  $\{f_n\}$  (still denoted  $\{f_n\}$ ) and a function  $f : [0, +\infty) \rightarrow \dot{L}_1^1$  such that  $f_n$  converges to  $f$  weakly in  $L^1([0, T], \dot{L}_1^1)$  for all  $T > 0$ .

To show that  $f \in L^\infty([0, \infty), \dot{L}_1^1)$ , note that for any compact  $K$  in  $[0, +\infty)$  we have, thanks to the weak convergence we have already proved, that

$$\int_K \int_0^\infty y f(t, y) dy dt = \lim \int_K \int_0^\infty y f_n(t, y) dy dt = \rho |K|.$$

This proves that  $f \in L^\infty([0, \infty), \dot{L}_1^1)$ , and also mass conservation.  $\square$

**Lemma 5.5.9.** *The function  $f$  from lemma 5.5.8 is in  $\mathcal{C}([0, T], \dot{L}_1^1 - \text{weak})$  for all  $T > 0$  and*

$$f_n \rightarrow f \text{ in } \mathcal{C}([0, T], \dot{L}_1^1 - \text{weak}).$$

*Proof.* We eventually want to apply proposition 9.3.1. For that, let us first prove that for every  $\phi \in \mathcal{C}_c^1[0, +\infty)$  the sequence of functions given by

$$G_n(t) := \int_0^\infty \phi(y) y f_n(t, y) dy$$

is equicontinuous on  $[0, T]$ . Their time derivative is:

$$\begin{aligned} \frac{d}{dt} \int_0^\infty \phi(y) y f_n(y) dy = & \\ & \int_0^\infty f_n(y) \int_0^y y' \phi(y') b(y, y') dy' dy - \int_0^\infty f_n(y) y \phi(y) \beta(y) dy \\ & + \int_0^\infty \int_0^\infty a(y, y') f_n(y) f_n(y') y (\phi(y + y') - \phi(y)) dy dy'. \end{aligned}$$

Take  $R > 0$  so that the support of  $\phi$  is contained on  $(0, R)$ . We can bound uniformly the absolute value of the last two terms:

$$\int_0^\infty f_n(y) y \phi(y) \beta(y) dy \leq \|\phi\|_\infty \rho B,$$

where  $B$  is an upper bound of  $\beta$  on  $(0, R)$ . For the third term, note that the

integrand is 0 when  $y \geq R$ , so

$$\begin{aligned}
& \left| \int_0^\infty \int_0^\infty a(y, y') f_n(y) f_n(y') y (\phi(y + y') - \phi(y)) \, dy \, dy' \right| \\
& \leq \int_R^\infty \int_0^R a(y, y') f_n(y) f_n(y') y \phi(y) \, dy \, dy' + \\
& \quad \int_0^R \int_0^R a(y, y') f_n(y) f_n(y') y |\phi(y + y') - \phi(y)| \, dy \, dy' \\
& \leq \|\phi\|_\infty A \int_R^\infty (1 + R + y') f_n(y') \int_0^R y f_n(y) \, dy \, dy' + (1 + 2R) A \|\phi\|_{C^1} \rho^2 \\
& \leq \|\phi\|_\infty A \rho \left( \frac{1}{R} \rho + 2\rho \right) + A \|\phi\|_{C^1} (1 + 2R) \rho^2 \\
& \leq A \|\phi\|_{C^1} \rho^2 \left( \frac{1}{R} + 3 + 2R \right).
\end{aligned}$$

For the first term we can prove that for  $t \in [0, T]$ ,

$$\int_t^{t+h} \int_0^\infty f_n(y) \int_0^y y' \phi(y') b(y, y') \, dy' \, dy \rightarrow 0 \quad \text{when } h \rightarrow 0^+$$

uniformly in  $n$ , and this would finally prove that the sequence of functions  $G_n$  defined at the beginning of the proof is equicontinuous on  $[0, T]$ . So take any  $\epsilon > 0$  and choose  $S > R > 0$  such that

$$\int_0^{T+1} \int_S^\infty f(y) \int_0^S y' b(y, y') \, dy' \, dy \leq \epsilon.$$

(This can be done thanks to lemma 5.5.5.) Then, taking  $0 \leq h \leq \epsilon/B$ , where  $B$  is an upper bound of  $\beta$  on  $(0, S)$ ,

$$\begin{aligned}
& \int_t^{t+h} \int_0^\infty f_n(y) \int_0^y y' \phi(y') b(y, y') \, dy' \, dy \\
& \leq \|\phi\|_\infty \int_t^{t+h} \int_0^S y f_n(y) \beta(y) \, dy + \|\phi\|_\infty \int_t^{t+h} \int_S^\infty f_n(y) \int_0^S y' b(y, y') \, dy' \, dy \\
& \leq \|\phi\|_\infty h \rho B + \|\phi\|_\infty \epsilon \\
& \leq \|\phi\|_\infty (\rho + 1) \epsilon,
\end{aligned}$$

which can be made as small as desired by choosing  $\epsilon$  correctly.

Now we can apply Ascoli-Arzelà's theorem and conclude that there is a subsequence of  $G_n$  which converges uniformly on  $[0, T]$  (note that the sequence is obviously uniformly bounded by  $\|\phi\|_\infty \rho$ ). However, we already knew that  $\{f_n\}$  converges weakly in  $L^1([0, T], \dot{L}_1^1)$ ; this implies that for all  $\psi \in L^\infty(0, T)$ ,

$$\int_0^T \psi(t) \int_0^\infty \phi(y) y f_n(y) \, dy \, dt \rightarrow \int_0^T \psi(t) \int_0^\infty \phi(y) y f(y) \, dy \, dt.$$

This means that if we define

$$G(t) := \int_0^\infty \phi(y) y f(t, y) dy$$

then

$$G_n \rightarrow G \quad \text{weakly in } L^1(0, T).$$

Then the above subsequence of  $G_n$ , which is known to converge uniformly, must converge to  $G$ . An extension of the above reasoning proves that every subsequence of  $G_n$  has a subsequence which converges uniformly to  $G$ ; this implies that

$$G_n \rightarrow G \quad \text{uniformly on } (0, T).$$

Then the sequence  $f_n$  and the function  $f$  are in the conditions of proposition 9.3.1 (lemma 5.5.7 ensures that  $f_n(t)$  is in a fixed weakly compact set of  $\dot{L}_1^1$  for all  $n$  and  $t$ ). Hence we can finally conclude that  $f \in \mathcal{C}([0, T], \dot{L}_1^1 - \text{weak})$  and

$$f_n \rightarrow f \text{ in } \mathcal{C}([0, T], \dot{L}_1^1 - \text{weak}).$$

□

### Convergence of the fragmentation term

Let us first show that for almost all  $t \geq 0$ ,  $Ff(t)$  makes sense.

**Lemma 5.5.10.** *For all  $S > R > 0$  and  $T > 0$  there is some constant  $C = C(T, R, S)$  such that*

$$\int_0^T \int_S^\infty \frac{\Phi(y)}{y} f_n(t, y) \int_0^R y' b_n(y, y') dy' dy dt \leq C \quad \text{for all } n \geq 1.$$

*Proof.* This is proposition 5.4.10 applied for these  $R, S, \Phi$ , and  $t := T$ . □

**Lemma 5.5.11.** *For all  $S > R > 0$  and  $T > 0$  there is some constant  $C = C(T, R, S)$  such that the function  $f$  from lemma 5.5.8 satisfies*

$$\int_0^T \int_S^\infty \frac{\Phi(y)}{y} f(t, y) \int_0^R y' b(y, y') dy' dy dt \leq C.$$

*Proof.* The last lemma proves in particular that for some constant  $C = C(T, R, S)$ ,

$$\int_0^T \int_S^\infty \frac{\Phi(y)}{y} f_n(t, y) \int_0^R y' b_n(y, y') dy' dy dt \leq C \quad \text{for all } n \geq 1.$$

Now, for any  $M > S$  we know from lemma 5.5.3 that

$$\int_0^R y' b_n(y, y') dy' \rightarrow \int_0^R y' b(y, y') dy' \quad \text{uniformly for } y \in [S, M],$$

so, thanks to the weak convergence of  $\{f_n\}$ ,

$$\begin{aligned} C &\geq \int_0^T \int_S^M \frac{\Phi(y)}{y} f_n(t, y) \int_0^R y' b_n(y, y') dy' dy dt \\ &\rightarrow \int_0^T \int_S^M \frac{\Phi(y)}{y} f(t, y) \int_0^R y' b(y, y') dy' dy dt \quad \text{as } n \rightarrow \infty. \end{aligned}$$

This is true for any  $M > S$ , so

$$\int_0^T \int_S^\infty \frac{\Phi(y)}{y} f(t, y) \int_0^R y' b(y, y') dy' dy dt \leq C,$$

which proves the lemma.  $\square$

Now the following is a consequence of our last result and lemma 3.1.1:

**Lemma 5.5.12.**  *$Ff(t)$  is well defined for almost all  $t \in [0, T)$ , and for  $\phi \in \mathcal{C}_c([0, T) \times (0, +\infty))$  the fundamental identity in proposition 3.4.3 holds:*

$$\int_0^T \int_0^\infty Ff(t)(y)\phi(t, y) dy dt = \int_0^T \int_0^\infty f(t, y)F^*\phi(t)(y) dy dt.$$

**Lemma 5.5.13.** *For each  $\phi \in \mathcal{C}_c([0, T) \times (0, +\infty))$ ,*

$$\int_0^T \int_0^\infty F_n f_n(t)(y)\phi(t, y) dy dt \rightarrow \int_0^T \int_0^\infty Ff(t)(y)\phi(t, y) dy dt.$$

*Proof.* Using the fundamental identity, what we have to prove is that

$$\int_0^T \int_0^\infty f_n(t, y)F_n^*\phi(t)(y) dy dt \rightarrow \int_0^T \int_0^\infty f(t, y)F^*\phi(t)(y) dy dt. \quad (5.66)$$

Note that, as the expression of the adjoint of the fragmentation operator is linear in  $\beta$ ,  $F_n^*\phi(t) - F^*\phi(t) = \tilde{F}^*\phi(t)$ , where  $\tilde{F}$  is the fragmentation operator associated to the fragmentation coefficient  $\tilde{b} := b - b_n \geq 0$ . As we know that  $\beta_n \rightarrow \beta$  uniformly on bounded sets of  $[0, +\infty)$ , lemma (3.14) proves that

$$F_n^*\phi \rightarrow F^*\phi \quad \text{uniformly on bounded sets of } [0, T) \times (0, +\infty).$$

Hence, as we know  $f_n \rightarrow f$  weakly in  $L^1$  on compact sets of  $[0, T) \times (0, +\infty)$ , we know that for any  $S > 0$

$$\int_0^T \int_0^S f_n(t, y)F_n^*\phi(t)(y) dy dt \rightarrow \int_0^T \int_0^S f(t, y)F^*\phi(t)(y) dy dt.$$

Hence, we only need to prove the convergence of the remaining part for large enough  $S$ . Take  $R > 0$  such that  $\text{supp } \phi \subseteq (0, R)$ ,  $S \geq 2R$  and calculate as follows:

$$\begin{aligned} & \left| \int_0^T \int_S^\infty f_n(t, y) F_n^* \phi(t)(y) dy dt \right| \\ &= \int_0^T \int_S^\infty f_n(t, y) \int_0^y \phi(y') b_n(y, y') dy' dy dt. \\ &\leq \frac{S}{\Phi(S)} \|\phi\|_\infty \int_0^T \int_S^\infty \frac{\Phi(y)}{y} f_n(t, y) \int_0^R b_n(y, y') dy' dy dt \\ &\leq \frac{S}{\Phi(S)} \|\phi\|_\infty C \end{aligned}$$

for some constant  $C$  independent of  $n$ , given by lemma 5.5.10. This converges to 0 as  $S \rightarrow \infty$ , and the same bound applies to  $f, b$  instead of  $f_n, b_n$  thanks to lemma 5.5.11. This proves the stated convergence.  $\square$

### Convergence of the coagulation term

**Lemma 5.5.14.** *For each  $\phi \in \mathcal{C}_c([0, \infty) \times (0, +\infty))$ ,*

$$\int_0^\infty \int_0^\infty C_n(f_n(t))(y) \phi(t, y) dy dt \rightarrow \int_0^\infty \int_0^\infty C(f(t))(y) \phi(t, y) dy dt.$$

*Proof.* Take  $\phi \in \mathcal{C}_c([0, \infty) \times (0, +\infty))$  and  $T, R > 0$  such that the support of  $\phi$  is contained in  $[0, T) \times (0, R)$ . Write  $\Delta\phi(t, y, y') := \phi(t, y+y') - \phi(t, y) - \phi(t, y')$ . Using the weak form of the operator  $C$ , what we want to prove is that, when  $n \rightarrow \infty$ ,

$$\begin{aligned} & \int_0^T \int_0^R f_n(t, y) \int_0^R a_n(y, y') f_n(t, y') \Delta\phi(t, y, y') dy' dy dt \\ &\longrightarrow \int_0^T \int_0^R f(t, y) \int_0^R a(y, y') f(t, y') \Delta\phi(t, y, y') dy' dy dt. \end{aligned}$$

We know that  $f_n \rightharpoonup f$  weakly in  $L^1((0, T), \dot{L}_1^1)$ . Thanks to lemma 9.2.4, we only need to show that the sequence of functions on  $(0, T) \times (0, R)$  given by

$$(t, y) \mapsto \frac{1}{y} \int_0^R a_n(y, y') f_n(t, y') \Delta\phi(t, y, y') dy'$$

is uniformly bounded and converges pointwise a.e. to

$$\frac{1}{y} \int_0^R a(y, y') f(t, y') \Delta\phi(t, y, y') dy'.$$

Note that lemma 4.3.4 implies that for some constant  $C \geq 0$ ,

$$\frac{1}{y} |\phi(y+y') - \phi(y) - \phi(y')| \leq C y' \|\phi\|_{C^1} \quad \text{for all } y, y' > 0,$$



so for each  $y$ , the function  $(t, y') \mapsto \Delta\phi(t, y, y')$  is in the dual of  $L^1([0, T], \dot{L}_1^1)$ . Then the uniform boundedness is clear, as

$$\left| \frac{1}{y} \int_0^R a_n(y, y') f_n(t, y') \Delta\phi(t, y, y') dy' \right| \leq 3A(1 + 2R)C \|\phi\|_{C^1} \rho.$$

Let us prove the pointwise convergence. As  $f_n \rightarrow f$  in  $\mathcal{C}([0, T], \dot{L}_1^1 - \text{weak})$ , we know that

$$f_n(t, \cdot) \rightharpoonup f(t, \cdot) \text{ weakly in } \dot{L}_1^1 \quad \text{for all } t \in (0, T)$$

and also that for all  $y, y' > 0$ ,

$$\begin{aligned} a_n(y, y') &< A(1 + 2R) \\ a_n(y, y') &\rightarrow a(y, y'). \end{aligned}$$

Hence, using lemma 9.2.4 again shows that for all  $(t, y) \in (0, T) \times (0, R)$

$$\int_0^R a_n(y, y') f_n(t, y') \Delta\phi(t, y, y') dy' \rightarrow \int_0^R a(y, y') f(t, y') \Delta\phi(t, y, y') dy'.$$

This proves the lemma.  $\square$

## 5.6. Existence of solutions with finite mass and finite number of particles

We want to prove existence of solutions for the coagulation-fragmentation equation (in the sense of definition 5.1.1) when both the total mass  $\int_0^\infty yf(y) dy$  and the number of clusters  $\int_0^\infty f(y) dy$  are finite. Except for the assumption on the coagulation coefficient  $a$ , the hypotheses in this section include those in the previous one.

**Hypothesis 5.6.1.** *Throughout this section we assume the coefficients  $a, b$  satisfy the following:*

- *The fragmentation coefficient  $b$  satisfies (3.4), and is bounded on  $\{(y, y') \mid 0 < y' < y < R\}$  for all  $R > 0$ .*
- *There are constants  $R_0 > 0$  and  $B_1 \geq 0$  such that*

$$\int_0^{R_0} b(y, y') dy' \leq B_1 \int_0^{R_0} y' b(y, y') dy' \quad \text{for all } y \geq 2R_0. \quad (5.67)$$

- *The coagulation coefficient  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  is a measurable symmetric function such that  $a(y, y') \leq A(1 + y + y')$  for some constant  $A > 0$ .*

We also assume that the initial condition  $f^0 : (0, +\infty) \rightarrow \mathbb{R}$  is a nonnegative function in  $L^1 \cap \dot{L}^1_1$ .

Below we will write

$$\rho := \int_0^\infty y f^0(y) dy \quad (5.68)$$

$$b_x := \sup_{0 < y' < y < x} b(y, y') \quad \text{for } x > 0, \quad b_0 := 0 \quad (5.69)$$

We will prove the following theorem:

**Theorem 5.6.2.** *Assume the above hypotheses on the coefficients  $a, b$ , and take a nonnegative function  $f^0 \in \dot{L}^1_1 \cap L^1$ . Then for all  $0 < T \leq +\infty$  there is a solution  $f$  to the coagulation-fragmentation equations (5.1)–(5.2) with initial data  $f^0$  (in the sense of definition 5.1.1), and such that  $f \in L^1([0, T) \times (0, +\infty)) \cap L^\infty([0, T), \dot{L}^1_1)$ . In addition, this solution conserves the mass.*

To prove this we will follow the same approach as before. In fact, we can use many of the results from the previous section, as the only hypothesis we are missing here is that, for  $y > 0$ ,  $z \mapsto a(z, y)$  is an increasing function of  $z$ .

Define the approximations  $a_n, b_n, f_n, f_n$  as in the previous section. Then, results 5.5.3–5.5.5 are still valid here, as they do not make use of the hypothesis on  $a$ . Let us prove the additional ones which are needed to pass to the limit in this case.

**Lemma 5.6.3.** *There is a  $C^\infty$  function  $\Lambda : [0, +\infty) \rightarrow [0, +\infty)$  which is strictly convex, such that  $\Lambda'$  is concave,  $\Lambda(0) = \Lambda'(0) = 0$ ,  $\lim_{y \rightarrow \infty} \Lambda(y)/y = +\infty$ , for which*

$$\int_0^\infty \Lambda(f^0(y)) dy < +\infty$$

and such that

$$\Lambda'(b_y) \leq 1 + \frac{\Phi(y)}{y} \quad \text{for all } y > 0.$$

*Proof.* This  $\Lambda$  is given by proposition 9.1.2; one can find  $\Lambda$  additionally satisfying the bound for the same reason as in lemma 5.5.6.  $\square$

In order to use some of the results from section 5.4 we will need to prove that the constants used there are uniformly bounded for the sequence of coefficients  $b_n$  and  $a_n$  (this is, a fixed constant can be used for all  $n$ ). This is the aim of the following lemma:

**Lemma 5.6.4.** *For all large enough integers  $n \geq B_1$  it holds that*

$$\int_0^{R_0} b_n(y, y') dy' \leq B_1 \int_0^{R_0} y' b_n(y, y') dy' \quad \text{for all } y \geq 2R_0.$$

*Remark 5.6.5.* We can take a subsequence of the approximated solutions and say that this inequality is satisfied *for all integers  $n$* ; we will frequently omit the fact that a suitable subsequence must be taken, and it should be understood that the sequence of solutions is not necessarily the full sequence we defined initially.

*Proof.* Take  $n \geq \max\{B_1, 1/R_0\}$  and  $y \geq 2R_0$ . Then,

$$\int_0^{R_0} b_n(y, y') dy' = \int_0^{R_0} b(y, y') dy' - \int_0^{R_0} (b(y, y') - b_n(y, y')) dy'.$$

For the first term, use (5.67):

$$\int_0^{R_0} b(y, y') dy' \leq B_1 \int_0^{R_0} y' b(y, y') dy'.$$

For the second one, as  $n \geq 1/R_0$  and hence  $b(y, y')$  is the same as  $b_n(y, y')$  for  $1/n < y' < R_0 < 2R_0 < y$ ,

$$\begin{aligned} \int_0^{R_0} (b(y, y') - b_n(y, y')) dy' &= \int_0^{1/n} (b(y, y') - b_n(y, y')) dy' \\ &\geq n \int_0^{1/n} y' (b(y, y') - b_n(y, y')) dy' \geq B_1 \int_0^{R_0} y' (b(y, y') - b_n(y, y')) dy'. \end{aligned}$$

Putting the last three equations together proves the lemma.  $\square$

**Lemma 5.6.6.** *For all  $t \geq 0$  there is a constant  $C(t)$  which is increasing in  $t$  and such that*

$$\|f_n(t)\|_1 \leq C(t) \quad \text{for all } n \geq 1.$$

*Proof.* Apply proposition 5.4.14 for  $R := R_0$ ,  $S := 2R_0$ . Note that all constants that appear there can be bounded independently of  $n$ ; in particular, the constant  $B_1$  there can be taken to be independent of  $n$  thanks to lemma 5.6.4, and  $B_2$  is bounded by  $2R_0 b_{2R_0}$ .  $\square$

**Lemma 5.6.7.** *For all  $t, R > 0$  there is a constant  $C(t)$ , which depends on them increasingly, such that*

$$\int_0^R \Lambda(f_n(t, y)) dy \leq C(t) \quad \text{for all } n \geq 1.$$

*Proof.* This is given by proposition 5.4.16, but a remark is needed: note that the quantity  $B_1$  that appears there depends on  $R$  and is not exactly the  $B_1$  in this section, so we need to prove that for each fixed  $R > 0$ , the  $B_1$  in the proposition can be bounded independently of  $n$ . Actually, it is enough to prove this for each  $R \geq R_0$ , as it is clearly enough to prove the lemma for  $R \geq R_0$ .

For  $R = R_0$  this is given by lemma 5.6.4. For  $R > R_0$  and  $y > 2R$  note that

$$\begin{aligned} \int_0^R b_n(y, y') dy' &= \int_0^{R_0} b_n(y, y') dy' + \int_{R_0}^R b_n(y, y') dy' \\ &\leq B_1 \int_0^{R_0} y' b_n(y, y') dy' + \frac{1}{R_0} \int_{R_0}^R y' b_n(y, y') dy' \\ &\leq \left( B_1 + \frac{1}{R_0} \right) \int_0^R y' b_n(y, y') dy'. \end{aligned}$$

Then, the number  $B_1$  corresponding to  $R$  in proposition 5.4.16 is bounded by a constant, and the proposition can be applied also for  $R > R_0$ , finishing the proof.  $\square$

**Lemma 5.6.8.** *There is a nonnegative function  $f : [0, +\infty) \times (0, +\infty)$  with*

$$\begin{aligned} f &\in L^\infty([0, +\infty), \dot{L}_1^1) \\ f &\in L^1([0, T] \times (0, +\infty)) \\ f &\in \mathcal{C}([0, T], L^1 - \text{weak}) \quad \text{for all } T > 0, \end{aligned}$$

and a subsequence of  $\{f_n\}$  (which we denote also as  $\{f_n\}$ ) such that for every  $T > 0$ ,

$$\begin{aligned} f_n &\rightharpoonup f \text{ in } L^1([0, T] \times (0, +\infty)) \text{ weakly} \\ f_n &\rightharpoonup f \text{ in } L^1([0, T], \dot{L}_1^1) \text{ weakly} \\ f_n &\rightarrow f \text{ in } \mathcal{C}([0, T], L^1 - \text{weak}), \end{aligned}$$

and such that  $\int_0^\infty y f(t, y) dy = \rho$  for all  $t \geq 0$ .

*Proof.* Lemma 5.5.8 applies here, as we have proved lemma 5.6.7, which can be used instead of 5.5.7. Hence, there is a subsequence of  $\{f_n\}$  which converges weakly to a function  $f$  in  $L^1([0, T], \dot{L}_1^1)$  for all  $T > 0$ . Additionally  $f \in L^\infty([0, \infty), \dot{L}_1^1)$ .

To find a further subsequence that converges weakly also in  $L^1([0, T] \times (0, +\infty))$  for every  $T > 0$  we can apply theorem 9.2.3 again, now for the usual Lebesgue measure on  $[0, T] \times [0, +\infty)$ : uniform local integrability is given by lemma 5.5.7; a uniform bound for the integral outside sets of the form  $[0, T] \times [0, R]$  which tends uniformly to 0 as  $R \rightarrow \infty$  is given by mass conservation; and lemma 5.6.6 proves that  $\{f_n\}$  is uniformly bounded in this space. The same argument used above gives a subsequence which converges weakly on  $L^1([0, T] \times (0, +\infty))$  and proves that  $f \in L^1([0, T] \times (0, +\infty))$  for all  $T > 0$ .

To show that  $f \in \mathcal{C}([0, T], L^1 - \text{weak})$  and that  $\{f_n\}$  converges to  $f$  in this space one can apply the arguments in [52, lemma 2.7, proposition 2.8].  $\square$

### Convergence of the fragmentation term

As the conditions on the fragmentation term include those in the previous section, we already have the following:

**Lemma 5.6.9.** *For each  $\phi \in \mathcal{C}_c([0, T] \times (0, +\infty))$ ,*

$$\int_0^T \int_0^\infty F_n f_n(t)(y) \phi(t, y) dy dt \rightarrow \int_0^T \int_0^\infty F f(t)(y) \phi(t, y) dy dt.$$

### Convergence of the coagulation term

The proof of convergence of the coagulation term in section 5.5 only uses hypotheses included here, so we directly have the following:

**Lemma 5.6.10.** *For each  $\phi \in \mathcal{C}_c([0, \infty) \times (0, +\infty))$ ,*

$$\int_0^\infty \int_0^\infty C_n(f_n(t))(y) \phi(t, y) dy dt \rightarrow \int_0^\infty \int_0^\infty C(f(t))(y) \phi(t, y) dy dt.$$

## 5.7. Existence of measure solutions

We would like to prove that there exist measure solutions to the coagulation-fragmentation equations (see definition 5.1.2)) when the coefficients are less regular than in previous sections, so that we allow for a singular behavior of the small-size particles and possible loss of mass due to the creation of dust or “shattering”. In particular, we want to allow for  $\beta(y)$  not to be bounded near  $y = 0$ .

### 5.7.1. Stability result

**Theorem 5.7.1.** *Take  $T > 0$ . Suppose that for each  $n \in \mathbb{N}$  we have a function  $f_n$  which is a measure solution to the coagulation-fragmentation equations on  $[0, T]$  (see definition 5.1.2) with coagulation coefficient  $a_n$ , fragmentation coefficient  $b_n$  and initial data  $f_n^0$ . We assume that  $a_n$ ,  $b_n$  and  $f_n^0$  satisfy the conditions on the coefficients from definition 5.1.2. Additionally, we suppose that for all continuous  $\phi$ ,*

$$\int_0^y y' \phi(y') b_n(y, y') dy' \quad \text{is continuous in } y, \quad (5.70)$$

*that each  $a_n$  is a continuous function and there are some  $\alpha \leq \beta \in \mathbb{R}$  and  $C > 0$  such that*

$$a_n(y, y') \leq C(y^\alpha (y')^\beta + y^\beta (y')^\alpha) \quad \text{for } y, y' > 0, \quad n \in \mathbb{N}. \quad (5.71)$$

*Suppose also that*

1. *For each  $n \in \mathbb{N}$  and  $t \in [0, T)$ ,  $f_n(t)$  is a nonnegative measure.*
2. *There is a constant  $\rho > 0$  such that*

$$\int_0^\infty y f_n(t, y) dy < \rho \quad \text{for all } n \in \mathbb{N}, t \in [0, T).$$

3. For each  $\phi \in \mathcal{C}_c$ , the sequence  $\{F_n\}$ , defined by  $F_n(t) := \int_0^\infty \phi(y) f_n(t, y) dy$  ( $t \in [0, T]$ ), is equicontinuous.
4. There is a positive increasing continuous function  $\Psi : (0, +\infty) \rightarrow (0, +\infty)$  such that  $\lim_{y \rightarrow \infty} \Psi(y) = +\infty$  and for all  $R, \epsilon > 0$  there is a constant  $C_{\epsilon, R} > 0$  such that,

$$\int_0^T \int_\epsilon^\infty \Psi(y) f_n(t, y) \int_0^R y' b_n(y, y') dy' dy \leq C_{\epsilon, R} \quad \text{for all } n \in \mathbb{N}.$$

5. There is a function  $b$  in the conditions (3.16) such that for all continuous  $\phi : [0, +\infty) \rightarrow \mathbb{R}$  it holds that

$$\int_0^\infty y' \phi(y') b_n(y, y') dy' \rightarrow \int_0^\infty y' \phi(y') b(y, y') dy'$$

uniformly for  $y$  in compact sets of  $(0, +\infty)$ .

6. There is a function  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  such that  $a_n$  tends to  $a$  uniformly in compact sets of  $(0, +\infty) \times (0, +\infty)$ .

7. There are constants  $C > 0$  and  $m < 0$  such that

$$\int_0^T \int_0^1 \int_0^1 a(y, y') f_n(t, y) f_n(t, y') y y' dy dy' dt \leq C \quad \text{for } n \in \mathbb{N}.$$

Then, there is a measure  $f^0 \in M_1$  and a function  $f \in \mathcal{C}([0, T]; M_1\text{-weak-}^*)$  which is a solution to the coagulation-fragmentation equations on  $[0, T]$  with coefficients  $a, b$  and initial condition  $f^0$ , and there is a subsequence of  $\{f_n\}$  (which we still refer to as  $\{f_n\}$ ) such that

$$f_n \rightarrow f \text{ in } \mathcal{C}([0, T]; M_1\text{-weak-}^*).$$

In the rest of this section we will prove this result.

*Remark 5.7.2.* A function  $f : [0, T] \rightarrow M_1$  is in  $\mathcal{C}([0, T], M_1\text{-weak-}^*)$  if it is continuous in the weak- $*$  topology<sup>1</sup> of  $M_1$ . In the space  $\mathcal{C}([0, T], M_1\text{-weak-}^*)$  we consider the topology for which a fundamental system of neighborhoods of a point  $f$  is formed by the sets  $\{W_j\}_{j \in J}$  given by

$$W_j := \{g \in \mathcal{C}([0, T], M_1\text{-weak-}^*) \mid (f - g)([0, T]) \subseteq V_j\},$$

where  $\{V_j\}_{j \in J}$  is a fundamental system of neighborhoods of 0 in the weak- $*$  topology of  $M_1$ . A sequence  $\{f_n\}$  converges to a function  $f$  in this space if and only if for each  $\phi \in \mathcal{C}_c(0, +\infty)$

$$\int_0^\infty \phi(y) f_n(t, y) dy \rightarrow \int_0^\infty \phi(y) f(t, y) dy$$

uniformly for  $t \in [0, T]$ .

---

<sup>1</sup> $M_1$  is seen as the dual space of  $\mathcal{C}_c$  with the norm of  $\dot{L}^\infty_1$ ; see section 3.2 for the notation.

### Convergence of $f_n$

Each  $f_n$  can be naturally identified with a positive measure on  $[0, T) \times (0, +\infty)$ , thanks to the regularity assumptions in definition 5.1.2. Point 2 in our hypotheses ensures that the sequence of measures  $(t, y) \mapsto y f_n(t, y)$  is uniformly bounded when they are considered as measures on  $[0, T) \times (0, +\infty)$ . This implies that there is a subsequence of  $f_n$  (still referred to as  $\{f_n\}$ ) and a positive measure  $f$  on  $[0, T) \times (0, +\infty)$  such that  $y f_n(t, y)$  converges to  $y f(t, y)$  in the weak-\* topology of the space of finite measures on  $[0, T) \times (0, +\infty)$ . In other words, there is a subsequence of  $f_n$  such that

$$\int_0^T \int_0^\infty \phi(t, y) f_n(t, y) dy dt \rightarrow \int_0^T \int_0^\infty \phi(t, y) f(t, y) dy dt$$

for all  $\phi \in \mathcal{C}_c([0, T) \times (0, +\infty))$ .

In particular, this shows that we can pass to the limit in the first term of equation (5.10). Now, point 3 and Ascoli-Arzelà's theorem allow us to say that, for each  $\phi \in \mathcal{C}_c$ , there is a further subsequence of  $\{f_n\}$  such that  $t \mapsto F_n(t) := \int_0^\infty \phi(y) f_n(t, y) dy$  converges uniformly in compact sets of  $[0, T)$  to some function; the above weak convergence proves that this function must in fact be equal to  $t \mapsto \int_0^\infty \phi(y) f(t, y) dy$ , and in turn that the latter must be continuous. Actually, the same argument proves that *any subsequence* of  $\{f_n\}$  has a further subsequence that satisfies this; this implies that

$$\int_0^\infty \phi(y) f_n(t, y) dy \rightarrow \int_0^\infty \phi(y) f(t, y) dy \quad \text{for all } \phi \in \mathcal{C}_c,$$

or, equivalently, that  $f_n \rightarrow f$  in  $\mathcal{C}([0, T); M_1\text{-weak-}^*)$ . With this, if we define  $f^0 := f(0)$ , we have

$$\int_0^\infty f_n^0(y) \phi(y) dy \rightarrow \int_0^\infty f^0(y) \phi(y) dy \quad \text{for } \phi \in \mathcal{C}_c,$$

so we can pass to the limit in the term with the initial condition of equation (5.10).

### Convergence of the fragmentation term

To complete the proof of the stability result we need to show that it is possible to pass to the limit in both the coagulation and fragmentation terms (and on the way, prove that the function  $f$  does satisfy the conditions in definition 5.1.2, so that the equation makes sense for  $f$ ).

To prove the convergence of the fragmentation term we need a previous result:

**Lemma 5.7.3.** *In the above hypotheses, it holds that*

$$\int_0^T \int_\epsilon^\infty \Psi(y) f(t, y) \int_0^R y' b(y, y') dy' dy \leq +\infty \quad \text{for all } \epsilon, R > 0.$$

*Proof.* Take  $\epsilon, R > 0$ . Choose a continuous function  $\phi$  which is equal to 1 on  $(0, R)$ , is always less than 1 and is zero on  $(2R, +\infty)$ ; take also  $S > 0$  and another continuous function  $\varphi$  which is less than 1, is equal to 1 on  $(\epsilon, S)$ , and has compact support contained in  $(\epsilon/2, 2S)$ . Then, for  $n \in \mathbb{N}$ ,

$$\begin{aligned} \int_0^T \int_\epsilon^\infty \Psi(y) f_n(t, y) \int_0^R y' b_n(y, y') dy' dy \\ \leq \int_0^T \int_{\epsilon/2}^\infty \varphi(y) \Psi(y) f_n(t, y) \int_0^{2R} \phi(y') y' b_n(y, y') dy' dy \leq C_{\epsilon/2, 2R}. \end{aligned}$$

The uniform convergence of  $y \mapsto \int_0^{2R} \phi(y') y' b_n(y, y') dy'$  (point 5) and the weak-\* convergence of  $f_n$  prove the result.  $\square$

We need to show that for all  $\phi \in \mathcal{C}_c^\infty([0, T] \times (0, +\infty))$ ,

$$\int_0^T \int_0^\infty f_n(t, y) F_n^* \phi(t, y) dy dt \rightarrow \int_0^T \int_0^\infty f(t, y) F^* \phi(t, y) dy dt,$$

where  $F_n^*, F^*$  are the adjoint fragmentation operators associated to  $b_n$  and  $b$ , respectively (see definition 3.6.3). Point 4 and the previous lemma prove that these integrals are finite.

Our hypotheses on the continuity of integrals of  $b_n$  (eq. (5.70)) ensures that  $F_n^* \phi$  is continuous on  $[0, T] \times (0, +\infty)$ , and it is easy to see, in the same way as in the proof of lemma 3.6.4, that there is a constant  $C > 0$  such that

$$|F_n^* \phi(t, y) - F^* \phi(t, y)| \leq C |\beta(y) - \beta_n(y)| \quad \text{for } (t, y) \in [0, T] \times (0, +\infty), \quad n \in \mathbb{N},$$

where  $\beta$  and  $\beta_n$  are the total fragmentation rates associated to  $b$  and  $b_n$ , respectively. As point 5 implies (choosing  $\phi(y) = y$ ) that  $\beta_n \rightarrow \beta$  uniformly in compact sets of  $(0, +\infty)$ , we see that for each  $K \subseteq (0, +\infty)$  compact,

$$F_n^* \phi \rightarrow F^* \phi \quad \text{uniformly in } [0, T] \times K.$$

Hence, thanks to the weak-\* convergence of  $\{f_n\}$ , we can say that for each  $\varphi \in \mathcal{C}_c$ ,

$$\int_0^T \int_0^\infty \varphi(y) f_n(t, y) F_n^* \phi(t, y) dy dt \rightarrow \int_0^T \int_0^\infty \varphi(y) f(t, y) F^* \phi(t, y) dy dt.$$

Take  $\delta, R > 0$  such that  $\phi$  has support contained in  $[0, T] \times (\delta, R)$ . Then, take  $S > R$  and choose a continuous function  $\varphi \in \mathcal{C}_c$  which is always less than 1 and equal to 1 on  $(\delta, S)$ ; notice that  $F_n^* \phi$  and  $F^* \phi$  have support contained in  $[0, T] \times (\delta, +\infty)$  (see lemma 3.6.4). To prove the expected convergence we can now follow a standard



argument (below omit the variables  $(t, y)$  for simplicity):

$$\begin{aligned} & \left| \int_0^T \int_0^\infty f_n F_n^* \phi \, dy \, dt - \int_0^T \int_0^\infty f F^* \phi \, dy \, dt \right| \\ & \leq \left| \int_0^T \int_0^\infty \varphi f_n F_n^* \phi \, dy \, dt - \int_0^T \int_0^\infty \varphi f F^* \phi \, dy \, dt \right| \\ & \quad + \left| \int_0^T \int_0^\infty (1 - \varphi) f_n F_n^* \phi \, dy \, dt \right| + \left| \int_0^T \int_0^\infty (1 - \varphi) f F^* \phi \, dy \, dt \right| \\ & =: S_1 + S_2 + S_3. \end{aligned}$$

The first part ( $S_1$ ), converges to zero as  $n \rightarrow \infty$  as proved above. When  $y > R$ , only the positive part of  $F_n^* \phi(t, y)$ ,  $F^* \phi(t, y)$  is nonzero (see the expression in 3.6.3); then we can find a bound for  $S_2$  and  $S_3$  using lemma 5.7.3:

$$\begin{aligned} S_3 & \leq \left| \int_0^T \int_S^\infty f(t, y) \int_0^R \phi(t, y') b(y, y') \, dy \, dt \right| \\ & \leq \frac{1}{\Psi(S)} \left| \int_0^T \int_S^\infty \Psi(y) f(t, y) \int_0^R \phi(t, y') b(y, y') \, dy \, dt \right| \leq \frac{C}{\Psi(S)}, \end{aligned}$$

where  $C > 0$  is a constant that only depends on  $R$  and  $\phi$ ; the latter bound is given by lemma 5.7.3, and the same can be done for  $S_2$  by using the bound in point 4. Then, if  $\epsilon > 0$  is any number, we can find  $S$  such that  $C/\Psi(S) \leq \epsilon/4$  (as  $\lim_{y \rightarrow \infty} \Psi(y) = +\infty$ ), and then take  $n$  large enough for  $S_1$  to be less than  $\epsilon/2$ . This proves the convergence of the fragmentation term.

### Convergence of the coagulation term

For the coagulation part we need to prove that, for each  $\phi \in \mathcal{C}_c^\infty$ ,

$$\int_0^T \int_0^\infty \int_0^\infty a_n(y, y') f_n(t, y) f_n(t, y') (\phi(t, y + y') - \phi(t, y) - \phi(t, y')) \, dy \, dy' \, dt$$

converges to the corresponding expression with  $a, f$  instead of  $a_n, f_n$ . We will denote

$$\Delta\phi(t, y, y') := \phi(t, y + y') - \phi(t, y) - \phi(t, y')$$

to make expressions shorter. Take  $R > 0$  such that the support of  $\phi$  is contained in  $[0, T) \times (0, R)$ ; then, note that the support of  $\Delta\phi$  is contained in  $[0, T) \times (0, R) \times (0, R)$ .

To prove the convergence we will break the  $y, y'$  integral into two parts: one for  $(y, y')$  in a compact set of  $(0, +\infty) \times (0, +\infty)$ , and the remaining one which includes the “borders” where  $y, y'$  are small (this is enough, as  $\Delta\phi$  has support contained in  $[0, T) \times (0, R) \times (0, R)$ ). For the first part we can use the convergence of  $\{a_n\}$  from point 6, and for the latter part one needs the bound in point 7.

In order to do this, take a function  $\varphi \in \mathcal{C}_c$ . Then,

$$\begin{aligned} & \int_0^T \int_0^\infty \int_0^\infty a_n(y, y') f_n(t, y) f_n(t, y') \Delta\phi(t, y, y') dy dy' dt \\ &= \int_0^T \int_0^\infty \int_0^\infty \varphi(y) \varphi(y') a_n(y, y') f_n(t, y) f_n(t, y') \Delta\phi(t, y, y') dy dy' dt \\ &+ \int_0^T \int_0^\infty \int_0^\infty (1 - \varphi(y) \varphi(y')) a_n(y, y') f_n(t, y) f_n(t, y') \Delta\phi(t, y, y') dy dy' dt =: I_1 + I_2. \end{aligned}$$

Let us rewrite  $I_1$  as

$$\begin{aligned} & \int_0^T \int_0^\infty f_n(t, y) \varphi(y) \int_0^\infty \varphi(y') a_n(y, y') f_n(t, y') \Delta\phi(t, y, y') dy' dy dt \\ &=: \int_0^T F_n(t) dt. \end{aligned}$$

To prove that this converges to the expected limit it is enough to show that  $F_n$  converges pointwise on  $[0, T)$ , as then we can apply the dominated convergence theorem, knowing that

$$F_n(t) \leq C \int_\epsilon^R y^\beta f_n(t, y) dy \int_\epsilon^R y^\alpha f_n(t, y) dy \leq C',$$

thanks to (5.71), where  $\epsilon > 0$  is such that the support of  $\varphi$  is contained in  $(\epsilon, +\infty)$  and  $C, C' > 0$  are constants independent of  $n$ . This bound is a consequence of the uniform bound on  $\int_0^\infty y f_n(t, y) dy$  in point 2. In turn, as  $f_n$  converges to  $f$  in  $\mathcal{C}([0, T]; M_1\text{-weak-}^*)$ , to prove that  $F_n$  converges pointwise it is enough to see that, for each  $t \in [0, T)$ ,

$$\int_0^\infty \varphi(y') a_n(y, y') f_n(t, y') \Delta\phi(t, y, y') dy' \quad \text{converges uniformly for } y \in (0, \infty). \quad (5.72)$$

(Of course, we must prove it converges to the right limit). To see this, fix  $t \in [0, T)$  and write:

$$\begin{aligned} & \int_0^\infty \varphi(y') a_n(y, y') f_n(t, y') \Delta\phi(t, y, y') dy' = \\ & \int_0^\infty \varphi(y') (a_n(y, y') - a(y, y')) f_n(t, y') \Delta\phi(t, y, y') dy' \\ & \quad + \int_0^\infty \varphi(y') a(y, y') f_n(t, y') \Delta\phi(t, y, y') dy'. \end{aligned}$$

Here, the first term converges uniformly to 0 thanks to the uniform convergence of  $a_n$  on compact sets and the uniform bound on  $\int_0^\infty y f_n(y) dy$  (point 2); the second term

converges pointwise for  $y \in (0, +\infty)$  to the same expression with  $f$  instead of  $f_n$  thanks to the weak-\* convergence of  $\{f_n\}$ ; it is equicontinuous in  $y$  and uniformly bounded again due to point 2, so by Ascoli-Arzelà's theorem it has a uniformly convergent subsequence. As the same argument can be applied to any subsequence of the second term, we can say that the whole sequence converges to the expected limit. Hence, we have proved (5.72). As explained above, this implies that  $I_1$  converges to the right limit.

As for  $I_2$ , by choosing a suitable  $\varphi$  we can make it small enough and carry out an argument analogous to the one for the convergence of the fragmentation term. If we take  $\varphi \leq 1$  such that  $\varphi(y) = 1$  for  $y \in (\delta, 2R)$ , then

$$\begin{aligned} |I_2| &\leq \int_0^T \int_0^\delta \int_0^\delta a_n(y, y') f_n(t, y) f_n(t, y') |\Delta\phi(t, y, y')| dt dy dy' \\ &\leq C \int_0^T \int_0^\delta \int_0^\delta a_n(y, y') f_n(t, y) f_n(t, y') y y' dt dy dy' \leq C' \delta^{-m} \end{aligned}$$

where we have used lemma 4.3.4 and point 7. As  $m < 0$ , this expression tends to 0 as  $\delta \rightarrow 0$ , and the proof can be finished in a way analogous to the proof of convergence of the fragmentation part.

This proves the stability result in theorem 5.7.1.

### 5.7.2. Measure solutions for nonsingular coagulation

In this section we will prove existence of measure solutions to the coagulation-fragmentation equations under the following conditions:

**Hypothesis 5.7.4.** *We will assume the following:*

- *The fragmentation coefficient  $b$  is in the conditions in (3.4). For each continuous function  $\phi$ ,*

$$\int_0^y y' \phi(y') b(y, y') dy' \quad \text{is continuous in } y.$$

- *The coagulation coefficient  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  is a continuous symmetric function such that for some numbers  $0 < \alpha \leq \beta \leq 1$  and some constant  $C > 0$ ,*

$$a(y, y') \leq C(y^\alpha (y')^\beta + y^\beta (y')^\alpha) \quad \text{for } y, y' > 0.$$

We will prove the following theorem:

**Theorem 5.7.5.** *Assume the above hypotheses on the coefficients  $a, b$ , and take a positive measure  $f^0 \in M_1$ . Then for all  $0 < T \leq +\infty$  there is a measure solution  $f$  to the coagulation-fragmentation equations (5.1)–(5.2) with initial data  $f^0$  (in the sense of definition 5.1.2), and such that  $f \in L^\infty([0, T], M_1)$ .*

The general method of proof will be similar to the one used in previous sections: we will construct a sequence of approximated solutions for which the conditions of the stability theorem 5.7.1 hold.

### Approximated solutions

We define a sequence of approximations to the coagulation and fragmentation coefficients as follows: take a continuous function  $\varphi_n^b : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  which is less than 1, is equal to 1 on the set  $\{(y, y') \mid 1/n < y' < y - 1/n < n - 1/n\}$ , and has compact support contained in the set  $\{(y, y') \mid 1/(2n) < y' < y - 1/(2n) < 2n - 1/(2n)\}$ . Set

$$\tilde{b}_n(y, y') := \varphi_n^b(y, y')b(y, y') \quad \text{for } y > y' > 0.$$

Then, take a regularizing sequence  $\{\rho_n\}$  such that the support of  $\rho_n$  is contained in  $(-1/(4n), 1/(4n))^2$  and set, for  $y > y' > 0$ ,

$$b_n(y, y') := \int_0^y \rho_n(y' - z)\tilde{b}_n(y, z) dz,$$

We also regularize the coagulation coefficient: take a continuous function  $\varphi_n^a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  which is less than 1, is equal to 1 on the set  $\{(y, y') \mid 1/n < y, y' < n\}$ , and has compact support contained in the set  $\{(y, y') \mid 1/(2n) < y, y' < 2n\}$ . Set

$$a_n(y, y') := \varphi_n^a(y, y')a(y, y') \quad \text{for } y, y' > 0.$$

In a similar way, we define a regularization of the initial condition: for a continuous function  $\varphi_n^0 : (0, +\infty) \rightarrow [0, +\infty)$  which is less than 1, is equal to 1 on  $(1/n, n)$  and has compact support contained in  $(1/(2n), 2n)$ ,

$$\tilde{f}_n^0(y) := f^0(y)\varphi_n^0(y),$$

and

$$f_n^0(y) := \frac{1}{y} \int_0^\infty \rho_n(y - y')y'\tilde{f}_n^0(y') dy'.$$

The coefficients  $a_n, b_n$  satisfy the hypotheses in theorem 5.2.1 and also the stronger hypothesis 5.4.1 from section 5.4; in particular, all estimates from this section apply to the regularized solutions defined below.

Call  $F_n, C_n$  the fragmentation and coagulation operators associated to  $b_n, a_n$ , respectively. We know from theorem 5.2 that there is a solution  $f_n$  of the coagulation-fragmentation equations with coefficients  $a_n, b_n$  and initial condition  $f_n^0$ , in the sense stated there.

---

<sup>2</sup>A sequence of nonnegative  $C^\infty$  functions with integral equal to 1 and supports that converge to 0.

### Uniform estimates

We need to prove that all of the conditions in the stability theorem 5.7.1 hold for the sequence just defined. First,  $a_n$  is a continuous function and the continuity condition (5.70) on  $b_n$  is also satisfied, as well as the bound (5.71). Points 1 and 2 are satisfied thanks to the conservation of positivity (lemma 5.3.1) and mass (see theorem 5.2.1). Observe that with this regularization we still have the usual bounds for the mass of the initial condition  $f_n^0$ : namely,

$$\begin{aligned} \int_0^\infty y f_n^0(y) dy &\leq \int_0^\infty y \frac{1}{y} \int_0^\infty \rho_n(y-y') y' f^0(y') dy' dy \\ &= \int_0^\infty y' f^0(y') \int_0^\infty \rho_n(y-y') dy dy' = \int_0^\infty y' f^0(y') dy' = \rho. \end{aligned}$$

Lemmas 5.5.4 and 5.5.5 are still true in the present case (one can apply 9.1.1 to the measure  $f^0$  to prove the first one and prove the second one just as before, using that the mass of  $f_n^0$  is uniformly bounded and that  $a_n(y, y') \leq A(1 + y + y')$ ), so point 4 of theorem 5.7.1 also holds. The convergence conditions in points 5 and 6 are satisfied thanks to the way of regularizing the coefficients  $a$  and  $b$ , and point 7 is trivially satisfied, as in our case  $\alpha > 0$  and the uniform bound on the mass proves it. Hence, the only remaining point is 3: this is proved by proposition 5.4.17, (observe that all the quantities that appear there can be bounded independently of  $n$ , using the function  $\Phi$  and the uniform bounds found above).

With these uniform bounds, the stability theorem 5.7.1 proves theorem 5.7.5.

### 5.7.3. Measure solutions for singular coagulation

Now we will study the case in which the coagulation coefficient may not be bounded near  $y = 0$  or  $y' = 0$ . For this, we assume a special form of the coagulation and fragmentation coefficients. The following hypotheses are stronger than 5.7.4 except in the fact that they allow  $\alpha < 0$  in the bounds of the coagulation coefficient:

**Hypothesis 5.7.6.** *We will assume the following:*

1. *The fragmentation coefficient  $b$  is in the conditions in (3.16). For each continuous function  $\phi$ ,*

$$\int_0^y y' \phi(y') b(y, y') dy' \quad \text{is continuous in } y.$$

2. *There are  $\gamma \in \mathbb{R}$ ,  $0 < k_0 < 1$ , and  $K_b, K'_b > 0$  such that the fragmentation coefficient  $b$  satisfies the following:*

$$K_b \phi_\gamma(y) \frac{1}{y} \left( \frac{y'}{y} \right)^{-1-k_0} \leq b(y, y') \leq K'_b \phi_\gamma(y) \frac{1}{y} \left( \frac{y'}{y} \right)^{-1-k_0}$$

for all  $0 < y' < y$ , where for  $y > 0$  we set

$$\begin{aligned}\phi_\gamma(y) &= y^\gamma && \text{if } \gamma \leq 0, \\ \phi_\gamma(y) &= \min\{y^\gamma, y^{-l}\} && \text{if } \gamma > 0,\end{aligned}$$

for some number  $l > 0$ .

3. The coagulation coefficient  $a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  is a continuous symmetric function. There are constants  $K_a, K'_a > 0$  and  $\alpha < \beta \in \mathbb{R}$  such that

$$K_a(y^\alpha(y')^\beta + (y')^\alpha y^\beta) \leq a(y, y') \leq K'_a(y^\alpha(y')^\beta + (y')^\alpha y^\beta)$$

for all  $y, y' > 0$ . We assume that

$$\begin{aligned}\alpha &< \beta < 1 \\ 0 &< \lambda := \alpha + \beta < 1 \\ \beta - \alpha &< 1.\end{aligned}$$

*Remark 5.7.7.* We impose that the total fragmentation rate be bounded on  $(1, +\infty)$  to avoid difficulties when estimating the total fragmentation rate for large particles, as proposition 5.4.10 is not applicable here. This is not a fundamental restriction, as we are interested in the interplay between coagulation and fragmentation for small particles.

We will prove the following theorem:

**Theorem 5.7.8.** *Assume the above hypotheses on the coefficients  $a, b$ , and take a positive measure  $f^0 \in M_1$ . Suppose that*

$$\gamma < \lambda - 1 \quad \text{or} \quad \frac{\lambda - 1}{2} < \gamma.$$

*Then for all  $0 < T \leq +\infty$  there is a measure solution  $f$  to the coagulation-fragmentation equations (5.1)–(5.2) with initial data  $f^0$  (in the sense of definition 5.1.2), and such that  $f \in L^\infty([0, T], M_1)$ .*

*In addition, when  $\frac{\lambda-1}{2} < \gamma$  and  $f^0 \in M_1 \cap M_m$  for some  $m < 1$ , this solution conserves the mass.*

We will follow the same strategy as before: construct a sequence of approximations, prove the necessary estimates and then pass to the limit using theorem 5.7.1.

### Approximated solutions

We define an approximation to the coefficients in a very similar way to that in the previous section, with the advantage that we do not need to regularize the

fragmentation coefficient by convolution, as now it is already a function (not only a measure).

Take a continuous function  $\varphi_n^b : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  which is less than 1, is equal to 1 on the set  $\{(y, y') \mid 1/n < y' < y - 1/n < n - 1/n\}$ , and has compact support contained in the set  $\{(y, y') \mid 1/(2n) < y' < y - 1/(2n) < 2n - 1/(2n)\}$ . Set

$$b_n(y, y') := \varphi_n^b(y, y')b(y, y') \quad \text{for } y > y' > 0.$$

We regularize the coagulation coefficient as in section 5.7.2: take  $m \in \mathbb{N}$ , and a continuous function  $\varphi_m^a : (0, +\infty) \times (0, +\infty) \rightarrow [0, +\infty)$  which is less than 1, is equal to 1 on the set  $\{(y, y') \mid 1/m < y, y' < m\}$ , and has compact support contained in the set  $\{(y, y') \mid 1/(2m) < y, y' < 2m\}$ . Set

$$a_m(y, y') := \varphi_m^a(y, y')a(y, y') \quad \text{for } y, y' > 0.$$

We use the same regularization of the initial condition as in section 5.7.2.

As before, these coefficients satisfy the hypotheses in theorem 5.2.1 and also hypothesis 5.4.1, so there exist solutions, in the strong sense stated in that theorem, of the coagulation-fragmentation equations with coefficients  $a_n$ ,  $b_n$ , to which the estimates in section 5.4 apply.

For  $n, m \in \mathbb{N}$ , we define  $f_{n,m}$  as the solution (in the sense of theorem 5.2.1) to the coagulation-fragmentation equations with coefficients  $b_n$ ,  $a_m$ .

### Uniform estimates

Point 4 in theorem 5.7.1 holds for the sequence just constructed, as by hypothesis, for all  $0 < \epsilon < R$ ,  $\int_\epsilon^R f_n(t, y)y\beta_n(y) dy$  is uniformly bounded and for  $1 < R < S$  we have

$$\int_S^\infty y^l f_n(y) \int_0^R y' b_n(y, y') dy' dy \leq \int_S^\infty y^l f_n(y) y \beta(y) dy \leq \int_S^\infty f_n(y) y dy \leq \rho,$$

thanks to point 2 in hypothesis 5.7.6.

The rest of the uniform bounds needed to apply theorem 5.7.1 can be seen to hold in the same way as in section 5.7.2, except for point 7. Estimating the moments near  $y = 0$  is the difficulty in this case. We can do this depending on the relative values of  $\lambda$  and  $\gamma$ : when  $\gamma > \frac{\lambda-1}{2}$ , we can pass to the limit in the sequence  $\{f_{n,2n}\}$  and the estimate in proposition 5.4.22 proves point 7; when  $\gamma < \lambda - 1$ , we can pass to the limit in the sequence  $\{f_{4n,n}\}$  and the estimate in proposition 5.4.26 proves it. The particular sequence used to take the limit is chosen so that the hypotheses on the supports of the coagulation and fragmentation coefficients in propositions 5.4.22 and 5.4.26 hold.

As for mass conservation, observe that proposition 5.4.22 (applied when  $\gamma > (\lambda - 1)/2$ ) proves that for some  $k < 1$  and some bounded function  $C$ ,

$$\int_0^1 y^k f(t, y) dy \leq C(T)$$
$$\int_0^1 y^k f_{n,2n}(t, y) dy \leq C(T)$$

for all  $T > 0$  and all  $t \in [0, T)$ . A usual argument then proves that

$$\lim \int_0^\infty y f_{n,2n}(t, y) dy = \int_0^\infty y f(t, y) dy,$$

so the limit  $f$  is a mass-conserving solution.





# Chapter 6

## Asymptotic behavior of solutions to the generalized Becker-Döring cluster equations

The results in this chapter were obtained under the supervision and help of Stéphane Mischler, and were published in [14].

### 6.1. Introduction

Coagulation-fragmentation equations are useful as models that describe the dynamics of many physical phenomena in which a large number of particles or units can stick together to form groups of particles, or clusters. A first version of them was initially proposed by Becker and Döring [6], and a variant by Penrose and Lebowitz [79]; these relatively simple models take into account only processes in which a cluster gains or loses one particle, and describe only the concentration of clusters of a given size at a certain moment, omitting also a description of their spatial distribution. Since then a number of generalizations have been studied which also allow reactions between clusters of more than one particle, the main examples of this being the discrete coagulation-fragmentation equations (see for example [4, 15, 16]), their continuous version [52, 53, 84, 86, 87, 35, 33, 71] and the respective versions including a spatial description by means of diffusion [57, 54]. An introduction to these equations can be found in chapters 1 and 2, and a recent review can be found in [58].

The generalized Becker-Döring equations are an intermediate step between the Becker-Döring system and the full discrete coagulation-fragmentation equations in which we allow reactions between clusters of at most a given finite size  $N$  and other

clusters. The system of equations is the following:

$$\begin{aligned}
 \dot{c}_1 &= - \sum_{k=1}^{\infty} W_{1,k} & (6.1) \\
 \dot{c}_j &= \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k} - \sum_{k=1}^{\infty} W_{j,k}, & 2 \leq j \leq N \\
 \dot{c}_j &= \frac{1}{2} \sum_{k=1}^{j-1} W_{j-k,k} - \sum_{k=1}^N W_{j,k}, & N+1 \leq j \leq 2N \\
 \dot{c}_j &= \sum_{k=1}^N W_{j-k,k} - \sum_{k=1}^N W_{j,k}, & j \geq 2N+1
 \end{aligned}$$

Here the unknowns are  $c_j = c_j(t)$  for  $j = 1, \dots$ , positive functions depending on the time  $t$  which are intended to represent the density of clusters of size  $j$  (those formed by  $j$  elementary particles). The quantities  $W_{jk}$ , which depend on the  $c_j$ , are given by

$$W_{jk} := a_{jk}c_jc_k - b_{jk}c_{j+k} \quad (j, k \geq 1),$$

where the numbers  $a_{jk}, b_{jk}$  for  $j, k \geq 1$  with  $\min\{j, k\} \leq N$  are the coagulation and fragmentation coefficients, respectively, which are symmetric in  $j, k$ . As can be seen, this system is a particular case of the coagulation-fragmentation equations when  $a_{jk} = b_{jk} = 0$  if  $\min\{j, k\} > N$ .

The study of the long-time behavior of solutions to these equations is expected to be a model of physical processes such as phase transition. Call  $\sum_{j=1}^{\infty} jc_j$  the *density* of a solution  $\{c_j\}_{j \geq 1}$ . For the Becker-Döring equations it was proved in [5] and [3] that, under certain general conditions which include a detailed balance (see below), there is a critical density  $\rho_s \in [0, \infty]$  such that any solution that initially has density  $\rho_0 \leq \rho_s$  ( $\rho_0 < \infty$  if  $\rho_s = \infty$ ) will converge for large times, in a certain strong sense, to an equilibrium solution with density  $\rho_0$ , while any solution with density above  $\rho_s$  will converge (in a weak sense) to the only equilibrium with density  $\rho_s$ . The rate of convergence to equilibrium was studied in [47]. The mentioned weak convergence can then be interpreted as a phase transition in the physical process modelled by the equation (see below for a precise statement). It is an interesting problem to extend this result to more general models; this has been done for the generalized Becker-Döring equations in [16] under some conditions on the decay of the initial data and in [20] for suitably small initial data. The aim of this chapter is to prove that this result about the generalized Becker-Döring system is true for general initial data. The corresponding result is expected to hold for the full coagulation-fragmentation equations, but finding a proof of this is still an open problem.

## 6.2. Statement of the main result

Let us recall some usual definitions and notation from previous works on the coagulation-fragmentation equations. We will make use of the vector space

$$X := \left\{ \{c_j\}_{j \geq 1} \mid \sum_{j=1}^{\infty} j |c_j| < \infty \right\}$$

with norm

$$\|c\| := \sum_{j=1}^{\infty} j |c_j| \quad \forall c = \{c_j\}_{j \geq 1} \in X.$$

The space  $X$  is clearly a Banach space (actually, this space is isometric to the space of absolutely summable sequences under the map  $\{c_j\} \mapsto \{j c_j\}$ ). In it we will make use of the notion of convergence associated to the norm  $\|\cdot\|$ , which we will call “strong convergence” following common usage. We will also say that a sequence  $\{c^i\}_{i \geq 1}$  of elements of  $X$  converges weak-\* to an element  $c \in X$ , and will denote it by  $c^i \xrightarrow{*} c$ , if

1. there exists  $M \geq 0$  such that  $\|c^i\| \leq M$  for all  $i \geq 1$  and
2.  $c_j^i \rightarrow c_j$  when  $i \rightarrow \infty$ , for all  $j \geq 1$  (where  $c^i = \{c_j^i\}_{j \geq 1}$  and  $c = \{c_j\}_{j \geq 1}$ ).

This is just the usual weak-\* convergence in the space  $X$  when it is regarded as the dual space of the space of sequences  $\{c_k\}_{k \geq 1}$  such that  $\lim_{k \rightarrow \infty} k^{-1} c_k = 0$ , with norm given by  $\|\{c_k\}\| := \max \{k^{-1} |c_k| \mid k \geq 1\}$  (see [5], p. 672). We also cite a result from [5]:

**Lemma 6.2.1** ([5], Lemma 3.3). *If  $\{c^n\}$  is a sequence in  $X$  such that  $c^n \xrightarrow{*} c \in X$  and  $\|c^n\| \rightarrow \|c\|$ , then  $c^n \rightarrow c$  strongly in  $X$ .*

The subset of  $X$  formed by the sequences of nonnegative terms will be referred to as  $X^+$ :

$$X^+ := \{\{c_j\}_{j \geq 1} \in X \mid c_j \geq 0 \ \forall j \geq 1\}.$$

We will ask for any solution  $\{c_j(t)\}_{j \geq 1}$  to be, for each fixed time  $t$ , in  $X^+$ ; this is natural, given that densities should be positive and that the sum  $\sum_{j=1}^{\infty} j c_j(t)$  represents the total density of particles at time  $t$  (or total mass, depending on the interpretation given to the  $c_j$ 's). More precisely, we will use the following concept of solution from [4], section 2:

**Definition 6.2.2.** A solution on the interval  $[0, T[$  (for a given  $T > 0$  or  $T = \infty$ ) of (6.1) is a function  $c : [0, T[ \rightarrow X^+$  such that, if we put  $c(t) = \{c_j(t)\}_{j \geq 1}$  for  $t \in [0, T[$ ,

1.  $c_j : [0, T[ \rightarrow \mathbb{R}$  is absolutely continuous for all  $j \geq 1$  and  $\|c(t)\|$  is bounded on  $[0, T[$ ,

2. for all  $j = 1, 2, \dots$ , the sums  $\sum_{k=1}^{\infty} a_{j,k}c_k(t)$  and  $\sum_{k=1}^{\infty} b_{j,k}c_{j+k}(t)$  are finite for almost all  $t \in [0, T[$ ,
3. and equations (6.1) hold for almost all  $t \in [0, T[$ .

*Remark 6.2.3.* For convenience, this definition has been slightly changed with respect to that in [4]: it has been stated for the generalized Becker-Döring system instead of the full coagulation equations, and conditions have been phrased in different terms, but it can easily be checked that if the coefficients  $a_{jk}, b_{jk}$  satisfy hypothesis 6.2.6 below then this concept of solution is equivalent to that in [4]. Hence, results from [4] are also applicable in our case, a fact that we will use later.

As we do not know of a uniqueness result that can be applied under the above hypotheses we need to define a concept of admissibility to precise which solutions our result applies to. In [16] this is done by choosing solutions which are limits of solutions to the finite set of equations obtained by truncating system (6.1). We will call these solutions *Carr–da Costa admissible*. Here we will define a slight modification of this concept: an admissible solution will be one which is the limit of Carr–da Costa admissible solutions with truncated initial data. The concept must of course be the same under any set of conditions that ensure uniqueness, but we have not found a sufficiently general uniqueness result and thus the following will be needed:

**Definition 6.2.4.** Take  $T > 0$  or  $T = +\infty$ . An admissible solution of the generalized Becker-Döring equations (6.1) on  $[0, T[$  with initial data  $c^0 = \{c_j^0\}_{j \geq 1} \in X^+$  is a solution  $c$  which is a limit in  $L_{\text{loc}}^{\infty}([0, T[, X)$  of Carr–da Costa admissible solutions  $c_n = \{c_n^j\}_{j \geq 1}$  of (6.1) with truncated initial data  $c^{0,n}$  given by

$$\begin{aligned} c_j^{0,n} &:= c_j^0 \text{ for } j \leq n \\ c_j^{0,n} &:= 0 \text{ for } j > n. \end{aligned}$$

*Remark 6.2.5.* The above convergence is uniform in compact subsets of  $[0, T[$ , in the sense of the norm  $\|\cdot\|$  in  $X$ ; in particular, the functions  $c_j^n$  in the definition converge uniformly when  $n \rightarrow \infty$  in compact subsets of  $[0, T[$  to  $c_j$ .

Below we state the conditions on the coefficients under which we will prove our result. Though in the equations only the coefficients  $a_{jk}, b_{jk}$  with  $\min\{j, k\} \leq N$  appear, for convenience we will use coefficients  $a_{jk}, b_{jk}$  defined for all  $j, k \geq 1$  and simply set  $a_{jk} = b_{jk} = 0$  if  $\min\{j, k\} > N$ . Thus we have hypothesis 6.2.6:

**Hypothesis 6.2.6 (Generalized Becker-Döring).** *There exists an  $N \geq 2$  such that  $a_{jk} = b_{jk} = 0$  if  $\min\{j, k\} > N$ , and  $a_{jk}, b_{jk} > 0$  otherwise.*

Detailed balance is a physical assumption also used, for example, in [5, 16], which expresses the principle of microscopic reversibility from chemical kinetics; essentially, it states that equilibria of a certain form exist (see theorem 6.2.19 below):

**Hypothesis 6.2.7 (Detailed Balance).** *There exists a positive sequence  $\{Q_j\}_{j \geq 1}$  with  $Q_1 = 1$  such that for all  $j, k \geq 1$ ,*

$$a_{jk}Q_jQ_k = b_{jk}Q_{j+k}. \quad (6.2)$$

A certain bound on the growth rate of coefficients is known to be necessary to ensure the existence of density-conserving solutions [4, 33] (in other situations density is only conserved for a finite time after which density decreases, a phenomenon known as gelation); for our main result to be true (theorem 6.2.20) it is evidently necessary that density is conserved, so we impose a condition ensuring this.

**Hypothesis 6.2.8 (Growth of coefficients).** *For some constants  $K > 0$  and  $0 \leq \alpha < 1$ ,*

$$\begin{aligned} a_{jk} &\leq K(j^\alpha + k^\alpha), \\ b_{jk} &\leq K(j^\alpha + k^\alpha). \end{aligned}$$

In the next hypothesis, (6.3) is a physical condition that asserts that any cluster has a lower free energy than its pieces taken separately (see [16], Remark 5.1); (6.4) will be seen to imply the existence of a critical density  $\rho_s$  (the relationship between the following  $z_s$  and this critical density is given below in 6.2.19):

**Hypothesis 6.2.9.** *The sequence  $Q_j$  satisfies:*

$$\log Q_j + \log Q_k \leq \log Q_{j+k} \quad \text{for all } j, k \geq 1, \quad (6.3)$$

$$0 < \lim_{j \rightarrow \infty} \frac{Q_j}{Q_{j+1}} := z_s < \infty. \quad (6.4)$$

*Remark 6.2.10.* This implies that  $\lim_{j \rightarrow \infty} \frac{Q_j}{Q_{j+m}} = z_s^m$  for  $m \geq 1$  and that

$$\lim_{j \rightarrow \infty} Q_j^{1/j} = \frac{1}{z_s}.$$

We also need to assume, as new hypotheses, a certain regularity of the coefficients:

**Hypothesis 6.2.11.** *For  $j, m = 1, \dots, N$ ,*

$$\frac{a_{jk}}{a_{j,k+m}} \rightarrow 1 \quad \text{when } k \rightarrow \infty$$

**Hypothesis 6.2.12.** *For some constant  $K_a$ ,  $j, m = 1, \dots, N$  and  $k \geq 1$ ,*

$$|a_{jk} - a_{j,k+m}| \leq K_a.$$

Observe that hypotheses 6.2.11 and 6.2.12 are independent; for example, for  $j = 1, \dots, N$  and  $k \geq 1$ ,  $a_{jk} = \exp(-j - k)$  satisfies the second one but not the first; and  $a_{jk} = [\log(j + k)]\sqrt{j + k}$  (with  $[x]$  being the integer part of  $x$ ) satisfies the first but not the second.

*Remark 6.2.13.* The kind of coefficients allowed by the previous hypotheses are, for example,  $a_{jk} \leq C(j^\alpha + k^\alpha)$  for  $j = 1, \dots, N$  and  $k \geq 1$ , sufficiently regular to fulfill hypotheses 6.2.11 and 6.2.12, and  $b_{jk}$  given by hypothesis 6.2.7 with any choice of  $Q_j$  satisfying (6.3) and (6.4). Note that (6.3) implies that  $b_{jk} \leq a_{jk}$ , so  $b_{jk} \leq C(j^\alpha + k^\alpha)$  also. For a concrete example, pick  $C_1, C_2 > 0$  and  $\alpha, \delta \in [0, 1[$  and define the following coefficients for  $\min\{j, k\} \leq N$ :

$$\begin{aligned} a_{jk} &:= C_1(j^\alpha + k^\alpha) \\ b_{jk} &:= C_1(j^\alpha + k^\alpha) \exp(C_2((j+k)^\delta - j^\delta - k^\delta)). \end{aligned}$$

The coefficients are taken to be zero when  $\min\{j, k\} > N$ . These correspond to  $Q_j = \exp(C_2(j - j^\delta))$  and have  $z_s = e^{-C_2}$ .

We borrow known existence results for the kind of admissible solutions of definition 6.2.4 from [4]:

**Theorem 6.2.14** ([4], **Theorems 2.4, 3.6 and 5.4**). *Assume hypotheses 6.2.6 and 6.2.8, and take  $c^0 \in X^+$ . Then there exists an admissible solution  $c$  to (6.1) on  $[0, +\infty[$  with  $c(0) = c^0$ . Furthermore, under hypothesis 6.2.6 all solutions to (6.1) are density-conserving.*

*Remark 6.2.15.* Theorem 2.4 in [4] gives the existence of a solution (in fact, a Carr–da Costa admissible solution by the method of construction). Theorem 3.6 from [4] proves this solution conserves density. Finally, Theorem 5.4 in the same paper gives the existence of a solution that can be obtained as the uniform limit in compact sets of  $[0, T[$  of Carr–da Costa admissible solutions with truncated initial data, thus giving the existence of an admissible solution in the sense used here.

**Lemma 6.2.16.** *Assume hypotheses 6.2.6 and 6.2.8. Take  $\mu > 1$  and suppose that  $c = \{c_j\}_{j \geq 1}$  is an admissible solution to (6.1) on  $[0, T[$  for some  $T > 0$  with initial data  $c(0) = c^0$  such that  $\sum_{j=1}^{\infty} j^\mu c_j^0 < +\infty$ . Then  $\sum_{j=1}^{\infty} j^\mu c_j(t)$  is finite for all  $0 \leq t < T$ .*

*Proof.* This is just Theorem 3.3 in [16], stated for admissible solutions in the sense we use here. As Carr–da Costa admissible solutions satisfy the estimate given in the proof of the above theorem in [16] (which depends only on  $\sum_{j=1}^{\infty} j^\mu c_j^0$ ), we can pass to the limit and thus prove that our admissible solutions also satisfy it.  $\square$

Hypotheses 6.2.6–6.2.9 imply those of Theorems 5.1 and 5.2 in [16]: (1.7) and **(H2)** in [16] are always fulfilled if we assume hypothesis 6.2.6; **(H1)** is our 6.2.8 and **(H3)**, **(H4)** from [16] are contained in hypotheses 6.2.6 and 6.2.9 here, respectively. This enables us to use these theorems here (recall remark 6.2.3); we will need the following one about the equilibrium solutions of (6.1).

**Definition 6.2.17.** An equilibrium of (6.1) is a solution of (6.1) that does not depend on time. The density of an equilibrium  $c$  is the norm of  $c$  in  $X$ ,  $\sum_{j=1}^{\infty} j c_j$ .

**Definition 6.2.18.** The critical density  $\rho_s$  is defined to be

$$\rho_s := \sum_{j=1}^{\infty} Q_j z_s^j, \quad (0 < \rho_s \leq \infty).$$

**Theorem 6.2.19** ([16], **Theorem 5.2**). *Assume hypotheses 6.2.6–6.2.9.*

1. For  $0 \leq \rho \leq \rho_s$  (and also  $\rho < +\infty$  if  $\rho_s = +\infty$ ), there exists exactly one equilibrium  $\{c_j^\rho\}$  of (6.1) with density  $\rho$ , which is given by

$$c_j^\rho = Q_j z^j \quad \forall j \geq 1,$$

where  $z$  is the only positive number such that  $\sum_{j=1}^{\infty} j Q_j z^j = \rho$ .

2. For  $\rho_s < \rho < +\infty$  there is no equilibrium of (6.1) with density  $\rho$ .

Observe that when  $\rho_s$  is finite and  $\{c_j^{\rho_s}\}_{j \geq 1}$  represents the critical equilibrium (the one with density  $\rho_s$ ),  $z_s$  is the single particle density  $c_1^{\rho_s}$  of this equilibrium.

The main result in this chapter is the following:

**Theorem 6.2.20.** *Assume hypotheses 6.2.6–6.2.12, and let  $c = \{c_j\}_{j \geq 1}$  be an admissible solution of the generalized Becker–Döring equations (6.1) (whose existence is given by theorem 6.2.14). Call  $\rho_0 := \sum_{j=1}^{\infty} j c_j(0)$ , the initial density.*

1. If  $0 \leq \rho_0 \leq \rho_s$  then  $c$  converges strongly in  $X$  to the equilibrium with density  $\rho_0$ .
2. If  $\rho_s < \rho_0$  then  $c$  converges in the weak-\* topology to the equilibrium with density  $\rho_s$ .

## 6.3. Proofs

The following result from [16] already gives part of Theorem 6.2.20. Again, note that the hypotheses in [16] are contained in those here:

**Theorem 6.3.1** ([16], **Theorem 6.1**). *Assume hypotheses 6.2.6–6.2.9. Let  $c = \{c_j\}$  be a solution of (6.1) on  $[0, \infty[$ , and call  $\rho_0 := \sum_{j=1}^{\infty} j c_j$ .*

*Then there exists  $0 \leq \rho \leq \min\{\rho_0, \rho_s\}$  such that  $c \xrightarrow{*} c^\rho$ , where  $c^\rho$  is the only equilibrium of (6.1) with density  $\rho$  (given by Theorem 6.2.19).*

With Theorem 6.3.1, the next result will be enough to complete a proof of Theorem 6.2.20:

**Theorem 6.3.2.** *Assume hypotheses 6.2.6–6.2.12 hold. Suppose that  $c$  is an admissible solution to the generalized Becker–Döring equations (6.1) with initial data  $c^0 \in X_+$  such that  $c$  converges weak-\* to an equilibrium with density  $\rho < \rho_s$ . Then,  $c$  converges strongly to this equilibrium (and in particular,  $\rho$  is the density of the solution  $c$ , i.e.  $\rho = \rho_0$ ).*



Hence, the aim of the rest of this section will be to prove Theorem 6.3.2. The following key result gives a bound on the solutions that will easily imply the pre-compactness of the orbits, which in turn implies Theorem 6.3.2. Call, for  $i \geq 1$ ,

$$G_i(t) \equiv \sum_{j=i}^{\infty} j c_j(t).$$

**Proposition 6.3.3.** *Let  $c = \{c_j\}_{j \geq 1}$  be an admissible solution of the generalized Becker-Döring equations (6.1). Assume hypotheses 6.2.6-6.2.12.*

*Suppose that for some  $z < z_s$*

$$c_j(t) \leq z_j := z^j Q_j \quad \text{for all } j = 1, \dots, N \text{ and all } t \geq 0.$$

*Suppose that  $\{r_i\}_{i \geq 1}$  is a strictly decreasing sequence of positive numbers that satisfy, for some  $\lambda$  with  $1 < \lambda < z_s/z$ :*

$$\frac{r_{k-1} - r_k}{r_k - r_{k+1}} < \lambda \quad \text{for all } k$$

*and such that  $G_i(0) \leq r_i$  for all  $i$ .*

*Then there exist a positive integer  $k_0$  and a constant  $C > 0$  such that  $G_i(t) \leq Cr_i$  for all  $i \geq k_0$  and all positive times.*

The proof of proposition 6.3.3, which contains the core of the argument, is a generalization of a method used in unpublished notes by Ph. Laurençot and S. Mischler [80]. This method is inspired by the proof of uniqueness of solutions to the Becker-Döring equation in [55]. The use of this kind of argument can be traced back to [3].

Note that the condition on  $\{r_k\}$  in proposition 6.3.3 is not very stringent as the following lemma states:

**Lemma 6.3.4.** *Given  $\lambda > 1$  and a positive sequence  $\{g_k\}_{k \geq 1}$  which tends to zero as  $k$  tends to infinity, there exists a strictly decreasing positive sequence  $\{r_k\}_{k \geq 1}$  which converges to zero, such that  $g_k \leq r_k$  and*

$$\frac{r_{k-1} - r_k}{r_k - r_{k+1}} \leq \lambda \quad \text{for all } k$$

*Proof.* Define

$$\begin{aligned} \bar{g}_1 &:= \sup_{j \geq 1} \{g_j\} + 1 \\ \bar{g}_k &:= \sup_{j \geq k} \{g_j\}, \quad \text{for } k \geq 2 \\ h_k &:= \bar{g}_k - \bar{g}_{k+1}, \quad \text{for } k \geq 1. \end{aligned}$$

Then  $\bar{g}_k$  is decreasing, tends to zero and for all  $k$  we have  $\bar{g}_k = \sum_{j=k}^{\infty} h_j$ . Define  $s_k$  recursively as:

$$s_1 := h_1$$

$$s_{k+1} := \max \left\{ \frac{s_k}{\lambda}, h_{k+1} \right\}.$$

Then  $s_k > 0$  for all  $k$  (it is to ensure this that we added 1 to  $\bar{g}_1$ ) and we can see that  $\sum_{k \geq 1} s_k$  converges. For this, note that  $s_{k+1} \leq (s_k/\lambda) + h_{k+1}$  and write for  $m \geq 2$ :

$$\sum_{k=1}^{m+1} s_k = s_1 + \sum_{k=1}^m s_{k+1} \leq h_1 + \sum_{k=1}^m h_{k+1} + \frac{1}{\lambda} \sum_{k=1}^m s_k \leq \bar{g}_1 - \bar{g}_{m+2} + \frac{1}{\lambda} \sum_{k=1}^m s_k,$$

so we have that

$$\left(1 - \frac{1}{\lambda}\right) \sum_{k=1}^m s_k \leq \bar{g}_1,$$

which proves the summability of  $\{s_k\}$  since  $\lambda > 1$ . (I thank the referees for suggesting a simpler version of this proof).

Clearly,  $s_k \geq h_k$ . Let us finally define

$$r_k := \sum_{j=k}^{\infty} s_j \geq \sum_{j=k}^{\infty} h_j = \bar{g}_k \geq g_k,$$

which is positive, greater than  $g_k$ , strictly decreasing, tends to zero as  $k \rightarrow \infty$  and

$$\frac{r_{k-1} - r_k}{r_k - r_{k+1}} = \frac{s_{k-1}}{s_k} \leq \lambda.$$

□

### 6.3.1. Proof of the proposition

We will prove the proposition for solutions whose initial data is a truncation at a sufficiently large finite size of  $\{c_i(0)\}_{i \geq 1}$ , with constants  $C$  and  $k_0$  that do not depend on the size of this truncation; then the proposition follows for general initial data by a standard approximation argument using definition 6.2.4 of an admissible solution.

Take an  $L \geq 1$  and consider a solution  $\{c_i^L\}_{i \geq 1}$  with initial data  $c_i^L(0) = c_i(0)$  for  $i = 1, \dots, L$  and  $c_i^L(0) = 0$  for  $i > L$ . It is again enough to prove the bound in the result up to a finite time  $T > 0$ , with a constant that does not depend on  $T$ . So fix  $T > 0$ , and let us find  $C$  and  $k_0$  (independent of  $L$  and  $T$ ) such that

$$c_i^L(t) \leq Cr_i \quad \text{for all } i \geq k_0, \quad t \in [0, T] \text{ and } L \text{ sufficiently large.}$$

By the admissibility of  $c$  we know that the functions  $c_j^L$  converge uniformly in  $[0, T]$  to  $c_j$  as  $L \rightarrow \infty$  (see remark 6.2.5), so the hypotheses of the proposition imply that for sufficiently large  $L$

$$c_j^L(t) < z^j Q_j \text{ for } j = 1, \dots, N, t \in [0, T].$$

In the following  $L$  will always be large enough for this to hold (note that the choice of  $L$  depends also on  $T$ ).

Furthermore,  $G_i^L(0) \leq G_i(0) \leq r_i$  for all  $i$  (where we have denoted  $G_i^L = \sum_{j=1}^{\infty} j c_j^L$ , the corresponding to  $G_i$  for the solution  $\{c_j^L\}$ ).

From now, to simplify the notation a bit, we will omit the  $L$  in both  $c_j^L$  and  $G_j^L$ , as the full  $c_j$  and  $G_j$  will not be mentioned anymore.  $W_{jk}$  will be used to denote  $a_{jk} c_j^L c_k^L - b_{jk} c_{j+k}^L$ .

For any sequence  $\{\Psi_j\}_{j \geq 1}$  it holds formally that:

$$\frac{d}{dt} \sum_{j=1}^{\infty} \Psi_j c_j = \frac{1}{2} \sum_{j,k=1}^{\infty} (\Psi_{j+k} - \Psi_j - \Psi_k) W_{jk}$$

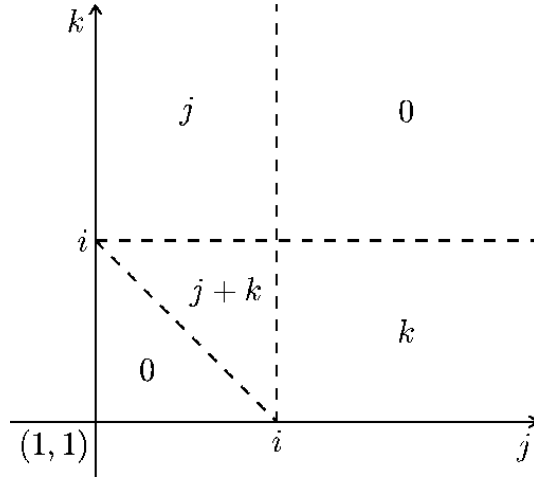


Figure 6.1: Values of  $\Psi_{j+k} - \Psi_j - \Psi_k$

In particular we can apply the previous relation to  $\Psi_j = j \cdot \chi_{j \geq i}$  ( $i \geq 1$ ) to get:

$$\frac{d}{dt} \sum_{j=i}^{\infty} j c_j = \frac{1}{2} \sum_{j=1}^{i-1} \sum_{k=i-j}^{i-1} (j+k) W_{jk} + \sum_{j=1}^{i-1} \sum_{k=i}^{\infty} j W_{jk}, \quad (6.5)$$

and this equality is rigorously justified because the solution  $\{c_i\}$  has finite moments  $\sum_{j=1}^{\infty} j^\mu c_j^L(t)$  of every order  $\mu \in \mathbb{R}$  for every positive time  $t$  (see lemma 6.2.16), so the sums on both sides of the previous equality converge uniformly and we can obtain the equation by means of standard results on differentiation of uniformly convergent

series of functions. One way to obtain the expression on the right hand side is to write the sum over  $j, k$  as a sum over the regions depicted in figure 6.1, where the value of  $\Psi_{j+k} - \Psi_j - \Psi_k$  is indicated in each of them.

Due to hypothesis 6.2.6,  $W_{jk} = 0$  if  $\min\{j, k\} > N$ . Hence, for  $i > 2N$  the first sum in (6.5) (which comprises all pairs  $j, k < i$  such that  $j + k \geq i$ ) can be broken into those terms where  $j \leq N$  and those where  $k \leq N$ :

$$\begin{aligned} \frac{1}{2} \sum_{j=1}^{i-1} \sum_{k=i-j}^{i-1} (j+k)W_{jk} &= \frac{1}{2} \sum_{j=1}^N \sum_{k=i-j}^{i-1} (j+k)W_{jk} + \frac{1}{2} \sum_{j=i-N}^{i-1} \sum_{k=i-j}^{i-1} (j+k)W_{jk} \\ &= \frac{1}{2} \sum_{j=1}^N \sum_{k=i-j}^{i-1} (j+k)W_{jk} + \frac{1}{2} \sum_{k=1}^N \sum_{j=i-k}^{i-1} (j+k)W_{jk} \\ &= \sum_{j=1}^N \sum_{k=i-j}^{i-1} (j+k)W_{jk}, \end{aligned}$$

where we have changed the order of the double sum and used the symmetry of  $(j+k)W_{jk}$ . If  $i > N$ , the second sum in (6.5) is nonzero only if  $j \leq N$ , so for  $i > 2N$  we have

$$\frac{d}{dt} \sum_{j=i}^{\infty} j c_j = \sum_{j=1}^N \sum_{k=i-j}^{i-1} (j+k)W_{jk} + \sum_{j=1}^N \sum_{k=i}^{\infty} j W_{jk}. \quad (6.6)$$

We rewrite the latter double sum:

$$\begin{aligned} \sum_{j=1}^N \sum_{k=i}^{\infty} j W_{jk} &= \sum_{j=1}^N \sum_{k=i}^{\infty} j (a_{jk} c_j c_k - b_{jk} c_{j+k}) \\ &= \sum_{j=1}^N \sum_{k=i-j}^{\infty} j a_{j,j+k} c_j c_{j+k} - \sum_{j=1}^N \sum_{k=i}^{\infty} j b_{jk} c_{j+k} \\ &= \sum_{j=1}^N \sum_{k=i-j}^{i-1} j a_{j,j+k} c_j c_{j+k} + \sum_{j=1}^N \sum_{k=i}^{\infty} j c_{j+k} (a_{j,j+k} c_j - b_{jk}) \\ &=: S_1 + S_2 \quad (6.7) \end{aligned}$$

where we have denoted the two double sums as  $S_1, S_2$  to mention them later.

We know that

$$c_j(t) \leq Q_j z^j \quad \text{for all } j = 1, \dots, N \text{ and } t \in [0, T].$$

Hence, as  $z < z_s$ , we see that thanks to hypothesis 6.2.7 and for  $j \in \{1, \dots, N\}$ ,

$$\begin{aligned} a_{j,j+k} c_j - b_{jk} &\leq a_{j,j+k} Q_j z^j - a_{jk} Q_j \frac{Q_k}{Q_{j+k}} \\ &= Q_j a_{j,j+k} \left( z^j - \frac{a_{jk}}{a_{j,j+k}} \frac{Q_k}{Q_{j+k}} \right). \end{aligned}$$

Note that the term in parenthesis tends to  $z^j - z_s^j$  as  $k \rightarrow \infty$  (thanks to hypotheses 6.2.11 and 6.2.9), so  $S_2 \leq 0$  for  $t \in [0, T]$  and  $i$  sufficiently large. Then, continuing from (6.6), using (6.7) and omitting  $S_2$ , we have for  $i$  large that

$$\frac{d}{dt} \sum_{j=i}^{\infty} j c_j \leq \sum_{j=1}^N \sum_{k=i-j}^{i-1} (j+k) W_{jk} + \sum_{j=1}^N \sum_{k=i-j}^{i-1} j a_{j,j+k} c_j c_{j+k} \quad (6.8)$$

Using again  $c_j \leq z_j := z^j Q_j$  for  $j = 1, \dots, N$  and

$$c_k = \frac{1}{k} (G_k - G_{k+1}) \quad \text{for all } k,$$

rewrite (6.8) as:

$$\begin{aligned} & \frac{d}{dt} G_i(t) \\ & \leq \sum_{j=1}^N \sum_{k=i-j}^{i-1} (j+k) \left( a_{jk} c_j \frac{G_k - G_{k+1}}{k} - b_{jk} \frac{G_{j+k} - G_{j+k+1}}{j+k} \right) \\ & \quad + \sum_{j=1}^N \sum_{k=i-j}^{i-1} j a_{j,j+k} c_j \frac{1}{j+k} (G_{j+k} - G_{j+k+1}) \\ & \leq \sum_{j=1}^N \sum_{k=i-j}^{i-1} (j+k) \left( a_{jk} z_j \frac{G_k - G_{k+1}}{k} - b_{jk} \frac{G_{j+k} - G_{j+k+1}}{j+k} \right) \\ & \quad + \sum_{j=1}^N \sum_{k=i-j}^{i-1} j a_{j,j+k} z_j \frac{1}{j+k} (G_{j+k} - G_{j+k+1}) \\ & = \sum_{j=1}^N \sum_{k=i-j}^{i-1} (A_{jk} (G_k - G_{k+1}) - B_{jk} (G_{j+k} - G_{j+k+1})) \quad (6.9) \end{aligned}$$

Where

$$\begin{aligned} A_{jk} &:= \frac{(j+k) a_{jk} z_j}{k} \\ B_{jk} &:= \frac{(j+k) b_{jk} - j a_{j,j+k} z_j}{j+k}. \end{aligned}$$

Now we take any  $\lambda < \bar{\lambda} < \frac{z_s}{z}$  (recall  $\lambda$  appears in the condition on  $r_i$ ), and note that the following holds for  $k$  large enough:

$$B_{jk} \geq \bar{\lambda}^j A_{jk} \quad \text{for } j = 1, \dots, N. \quad (6.10)$$

The proof of this is easy, as (note that we can divide by  $a_{jk}$  by hypothesis 6.2.6):

$$\begin{aligned} \frac{B_{jk}}{A_{jk}} &= \frac{kb_{jk}}{(j+k)a_{jk}z_j} - \frac{jka_{j,j+k}z_j}{(j+k)^2a_{jk}z_j} \\ &= \frac{ka_{jk}Q_jQ_k}{(j+k)a_{jk}Q_{j+k}Q_jz^j} - \frac{jka_{j,j+k}}{(j+k)^2a_{jk}} \\ &= \frac{k}{j+k} \frac{Q_k}{Q_{j+k}} \frac{1}{z^j} - \frac{jka_{j,j+k}}{(j+k)^2a_{jk}}, \end{aligned} \quad (6.11)$$

where the detailed balance hypothesis 6.2.7 has been used to pass to the second line. Now observe that the term with the negative sign converges to 0 thanks to hypothesis 6.2.11, and that the other term

$$\lim_{k \rightarrow \infty} \frac{k}{j+k} \frac{Q_k}{Q_{j+k}} \frac{1}{z^j} = \left(\frac{z_s}{z}\right)^j > \bar{\lambda}^j \quad (6.12)$$

because of hypothesis 6.2.9. Hence we have (6.10).

So, thanks to (6.10), we can continue from (6.9) and get, for  $i$  large enough:

$$\frac{d}{dt}G_i \leq \sum_{j=1}^N \sum_{k=i-j}^{i-1} A_{jk} (G_k - G_{k+1} - \bar{\lambda}^j(G_{j+k} - G_{j+k+1})) \quad (6.13)$$

It is easy to see from hypothesis 6.2.11 that for  $j, m = 1, \dots, N$ ,

$$\frac{A_{jk}}{A_{j,k+m}} \rightarrow 1 \quad \text{as } k \rightarrow \infty.$$

This means that for small variations of  $k$ ,  $A_{jk}$  changes little when  $k$  is large. Take  $\epsilon$  such that

$$\frac{1-\epsilon}{1+\epsilon} \geq \frac{\lambda}{\bar{\lambda}}. \quad (6.14)$$

We can then find an  $i_0 > 2N$  such that (6.13) holds for  $i \geq i_0$  and we have, also for  $i \geq i_0$ :

$$(1-\epsilon)A_{j,i-j} \leq A_{jk} \leq (1+\epsilon)A_{j,i-j} \quad \text{for } j = 1, \dots, N, \quad k = i-j, \dots, i-1 \quad (6.15)$$

So for  $i \geq i_0$  we can write from (6.13):

$$\begin{aligned} &\frac{d}{dt}G_i \\ &\leq \sum_{j=1}^N A_{j,i-j} \sum_{k=i-j}^{i-1} ((1+\epsilon)(G_k - G_{k+1}) - (1-\epsilon)\bar{\lambda}^j(G_{j+k} - G_{j+k+1})) \\ &= \sum_{j=1}^N A_{j,i-j} [(1+\epsilon)(G_{i-j} - G_i) - (1-\epsilon)\bar{\lambda}^j(G_i - G_{i+j})] \end{aligned} \quad (6.16)$$

From the hypothesis on  $r_i$ , for  $j = 1, \dots, N$  and  $i > j$ ,

$$\begin{aligned} r_{i-j} - r_i &= \sum_{k=1}^j (r_{i-k} - r_{i-k+1}) \\ &\leq \sum_{k=1}^j \lambda(r_{i-k+1} - r_{i-k+2}) = \lambda(r_{i-j+1} - r_{i+1}) \end{aligned}$$

Apply this  $j$  times to get:

$$r_{i-j} - r_i \leq \lambda^j (r_i - r_{i+j}) \leq \bar{\lambda}^j \frac{1-\epsilon}{1+\epsilon} (r_i - r_{i+j}), \quad (6.17)$$

where we used (6.14) together with  $\lambda/\bar{\lambda} < 1$  to say that

$$\frac{1-\epsilon}{1+\epsilon} \geq \left(\frac{\lambda}{\bar{\lambda}}\right)^j.$$

If the sequence  $\{r_i\}$  satisfies (6.17) then  $\{Cr_i\}$  also satisfies it, for any positive  $C$ . Take  $C > 1$  sufficiently large so that

$$Cr_i > M_0 \geq G_i(t) \quad \text{for } i < i_0 \text{ and } t \leq T, \quad (6.18)$$

where by  $M_0$  we mean the density of the full initial data with no truncation. Now define

$$M_i := G_i - Cr_i, \quad (6.19)$$

$$H_i := (G_i - Cr_i)_+ \quad (6.20)$$

We know  $H_i(t) = 0$  for  $i < i_0$  and  $t < T$  because of (6.18).

As the  $Cr_i$  satisfy (6.17) we can write, continuing from (6.16), for  $i \geq i_0$ :

$$\frac{d}{dt} M_i \leq \sum_{j=1}^N A_{j,i-j} [(1+\epsilon)(M_{i-j} - M_i) - (1-\epsilon)\bar{\lambda}^j (M_i - M_{i+j})] \quad (6.21)$$

Then, the same inequality holds for  $H_i$ : note that most of the previous reorganization was done in order to have the term in  $M_i$  as *the only term with negative sign* in (6.21). Otherwise we cannot justify writing the inequality in terms of  $H_i$  as is done next:

$$\begin{aligned} \frac{d}{dt} H_i &= \chi_{M_i > 0} \frac{d}{dt} M_i \leq \\ &\leq \chi_{M_i > 0} \sum_{j=1}^N A_{j,i-j} [(1+\epsilon)(M_{i-j} - M_i) - (1-\epsilon)\bar{\lambda}^j (M_i - M_{i+j})] \\ &\leq \sum_{j=1}^N A_{j,i-j} [(1+\epsilon)(H_{i-j} - H_i) - (1-\epsilon)\bar{\lambda}^j (H_i - H_{i+j})]. \end{aligned} \quad (6.22)$$

(We have used  $\chi_{M_i > 0} M_i = H_i$  and  $\chi_{M_i > 0} M_k \leq H_k$  for any  $i, k$ ). Now we can sum this from  $i = i_0$  to infinity (note again that the sums are all convergent, as the solution  $\{c_j\}$  with truncated initial data has finite moments of all orders) and reorganize the terms:

$$\begin{aligned}
\frac{d}{dt} \sum_{i=i_0}^{\infty} H_i &\leq \sum_{i=i_0}^{\infty} \sum_{j=1}^N A_{j,i-j} [(1+\epsilon)(H_{i-j} - H_i) - (1-\epsilon)\bar{\lambda}^j(H_i - H_{i+j})] \\
&= \sum_{j=1}^N \sum_{i=i_0-j}^{\infty} H_i ((1+\epsilon)A_{ji} - (1-\epsilon)\bar{\lambda}^j A_{j,i-j}) - \sum_{j=1}^N \sum_{i=i_0}^{\infty} H_i (1+\epsilon)A_{j,i-j} \\
&\quad + \sum_{j=1}^N \sum_{i=i_0+j}^{\infty} H_i (1-\epsilon)\bar{\lambda}^j A_{j,i-2j} \\
&= \sum_{j=1}^N \sum_{i=i_0-j}^{i_0-1} A_{ji} (1+\epsilon)H_i + \sum_{i=i_0}^{\infty} H_i (1+\epsilon) \sum_{j=1}^N [A_{ji} - A_{j,i-j}] \\
&\quad + \sum_{i=i_0}^{\infty} H_i (1-\epsilon) \sum_{j=1}^N \bar{\lambda}^j [A_{j,i-2j} - A_{j,i-j}] - \sum_{j=1}^N \sum_{i=i_0}^{i_0+j-1} H_i A_{j,i-2j} \bar{\lambda}^j (1-\epsilon) \\
&=: T_1 + T_2 + T_3 + T_4, \quad (6.23)
\end{aligned}$$

where the  $T_i$  ( $i=1,2,3,4$ ) are the sums above. Observe that  $T_4$  is negative and  $T_1$  only contains terms in  $H_i$  for  $i < i_0$ , so it is directly zero (recall (6.18)). Also, note that for  $j = 1, \dots, N$  and  $i \geq i_0$  we have, by using hypothesis 6.2.12, that

$$\begin{aligned}
|A_{ji} - A_{j,i-j}| &= \left| \frac{j+i}{i} a_{ji} z_j - \frac{i}{i-j} a_{j,i-j} z_j \right| \\
&\leq z_j a_{ji} \left| \frac{j+i}{i} - \frac{i}{i-j} \right| + z_j \frac{i}{i-j} |a_{ji} - a_{j,i-j}| \\
&\leq z_j K(i+j) \frac{j^2}{i(i-j)} + z_j \frac{i}{i-j} K_a,
\end{aligned}$$

which is easily seen to be bounded by a certain constant  $A'$  for  $j = 1, \dots, N$  and  $i > N$ . Hence, the coefficient of  $H_i$  in  $T_2$  and  $T_3$  is bounded by a certain constant  $A$  independent of  $j$  and  $i$  and then

$$\frac{d}{dt} \sum_{i=i_0}^{\infty} H_i \leq A \sum_{i=i_0}^{\infty} H_i.$$

Gronwall's lemma then shows that  $H_i(t) = 0$  for  $i \geq i_0$  and  $t \in [0, T]$ ; that is to say  $G_i(t) \leq Cr_i$ . This proves our claim.



### 6.3.2. Proof of the main theorem

Finally, we arrive at the proof of theorems 6.3.2 and 6.2.20, which is not difficult once the proposition of the previous section has been established.

*Proof of Theorem 6.3.2.* Let  $c$  be an admissible solution that converges weak-\* in  $X$  to an equilibrium of mass  $\rho < \rho_s$ , which must be given by  $\{Q_j \bar{z}^j\}_{j \geq 1}$  for some  $0 \leq \bar{z} < z_s$  (see theorem 6.2.19). We will prove that the orbit of any such solution must be relatively compact in  $X$  and hence the convergence must be strong.

Pick  $z \in ]\bar{z}, z_s[$ . As we know that  $c_j \rightarrow Q_j \bar{z}^j$  when  $t \rightarrow \infty$  for all  $j$ , we can find a  $t_0 > 0$  so that

$$c_j(t) \leq Q_j z^j \quad \text{for all } j = 1, \dots, N \text{ and } t \geq t_0.$$

As Lemma 6.3.4 ensures, we can always find a sequence  $\{r_i\}$  tending to zero as  $i \rightarrow \infty$  that satisfies the conditions in Proposition 6.3.3 with  $G_i(t_0)$  instead of  $G_i(0)$ . We can apply the proposition, with the  $z$  we have chosen, to  $\{c_j(t + t_0)\}_{j \geq 1}$  (which is a translation in time of the solution  $c$  and thus is a solution itself) and deduce that for some  $C > 0$ ,  $k_0 \geq 1$  and all  $t > t_0$ ,

$$G_i(t) \leq Cr_i \quad \text{for } i \geq k_0.$$

As  $\{r_i\}$  tends to zero, this bound says that the solution  $c$  is relatively compact in  $X_+$ , and we have finished.  $\square$

*Proof of Theorem 6.2.20.* Suppose that  $c$  is an admissible solution of (6.1) in  $[0, +\infty[$  with initial data  $c(0) = c^0 \in X_+$ . Theorem 6.3.1 shows that  $c$  converges weak-\* in  $X$  to an equilibrium of mass  $\rho$  for some  $0 \leq \rho \leq \rho_0$ .

If  $\rho_0 < \rho_s$ , then this convergence is also strong (by theorem 6.3.2) and hence  $\rho = \rho_0$ .

If  $\rho_0 = \rho_s$  (with  $\rho_s < \infty$ ), then  $\rho \leq \rho_s$ . But if  $\rho < \rho_s$  then again the convergence must be strong and  $\rho = \rho_s$ , which is a contradiction. Hence,  $\rho = \rho_0 = \rho_s$  and we see the convergence is strong because of lemma 6.2.1.

Finally, if  $\rho_0 > \rho_s$ , then  $\rho \leq \rho_s$  and it must be  $\rho = \rho_s$  or otherwise the convergence is strong, which is not possible given that  $\rho_0 > \rho$ .  $\square$

# Chapter 7

## Asymptotic analysis and numerical simulation of a simple case

This chapter presents the results obtained together with Luis Bonilla and John Neu, which were published in [73].

### 7.1. Description of the equations

Finding a manageable approximation to the behavior of the coagulation-fragmentation equations is both a very interesting and very challenging task. Here we present such an approximation by means of an asymptotic analysis in a case which is simple enough to be studied but still realistic enough to be a good candidate as a model for certain physical processes. Results will be checked against numerical solutions to the equations. We will deal with the Becker-Döring equations when the binding energy depends linearly on the cluster size; this is,

$$\epsilon_k = (k - 1)\alpha kT, \quad (7.1)$$

where  $\alpha kT$  is the monomer-monomer binding energy ( $k$  is Boltzmann's constant and  $T$  the temperature). As we are considering the Becker-Döring model, we are taking into account only reactions between monomers (individual particles) and other clusters. This expression for the binding energy is suitable for aggregates of certain kinds of lipids when these form rodlike clusters. The molecules of these lipids typically have a hydrophilic head and a hydrophobic tail, so in aqueous solution they spontaneously arrange themselves so that tails are away from the surrounding water and heads are in contact with it. Depending on the shape of the particular molecule, they can form spherical aggregates with tails pointing inwards and heads pointing outwards, or form lipid bilayers such as those found in cell membranes, where lipid molecules form a double layer with heads on the external surface and tails on the inside. Clusters formed by lipids in aqueous solution are called *micelles*, and the process by which they form is called *micellization*.

In order to model the kinetics of the system with the Becker-Döring equations we need to give the value of the coagulation and fragmentation coefficients. We will assume that the detailed balance hypotheses holds (cf. hypotheses 6.2.7). Under this condition, recall the relationship between the binding energy and the coagulation and fragmentation coefficients given in (2.18):

$$Q_i = e^{-\frac{\epsilon_i}{kT}}.$$

Here  $\epsilon_i$  is the binding energy of an  $i$ -cluster and the  $Q_i$  are the coefficients in the detailed balance condition, so that coagulation coefficients  $a_i$  and fragmentation coefficients  $b_i$  are related by

$$Q_i a_i = Q_{i+1} b_i.$$

The Becker-Döring equations (eqs. (1.1)) take the following form when the above is taken into account:

$$\frac{d}{dt} \rho_k = j_{k-1} - j_k, \quad k \geq 2, \quad (7.2)$$

$$j_k := b_k \left( e^{\frac{\epsilon_{k+1} - \epsilon_k}{kT}} \rho_1 \rho_k - \rho_{k+1} \right), \quad k \geq 1, \quad (7.3)$$

and  $c_1$  evolves so that the total density remains constant. Note that we write  $\rho_k$  here instead of  $c_k$  in (1.1).

To completely specify the equations we need to give the fragmentation coefficient  $b_k$  (or, equivalently, the coagulation coefficient, as they are related by the detailed balance hypothesis). The simplest possible model is obtained by setting  $b_k = 1$  for all  $k$  (actually, we could set  $b_k$  to some other constant, but a time rescaling leaves the same equations as for  $b_k = 1$ ). Hence we will set  $b_k = 1$  for simplicity and rewrite equations (7.2), (7.3) using (7.1) as

$$\frac{d}{dt} \rho_k + (e^\alpha \rho_1 - 1)(\rho_k - \rho_{k-1}) = \rho_{k+1} - 2\rho_k + \rho_{k-1} \quad k \geq 2. \quad (7.4)$$

At an initial condition at time  $t = 0$  we will assume that there are only monomers:  $\rho_1(0) = \rho > 0$  and  $\rho_k(0) = 0$  for all  $k \geq 2$ .

For the asymptotic analysis we will consider the limit in which  $\rho \gg e^{-\alpha}$ , where the initial concentration is much larger than the critical monomer concentration. The parameters  $\rho$  and  $\alpha$  are not really independent. If we rescale the cluster densities with  $\rho$  so that

$$\rho_k = \rho r_k,$$

and define a scaled time

$$\tau \equiv e^\alpha \rho t \equiv \frac{t}{\epsilon},$$

then the rescaled problem contains the single parameter

$$\epsilon \equiv \frac{e^{-\alpha}}{\rho} \ll 1.$$

Equations (7.4) become then

$$\frac{dr_k}{d\tau} + (r_1 - \epsilon)(r_k - r_{k-1}) = \epsilon(r_{k+1} - 2r_k + r_{k-1}), \quad k \geq 2 \quad (7.5)$$

while the density conservation condition becomes

$$\sum_{k=1}^{\infty} k r_k = 1 \quad (7.6)$$

and our initial conditions are, in terms of the  $r_k$ ,

$$r_1(0) = 1, \quad r_k(0) = 0 \quad \text{for } k \geq 2. \quad (7.7)$$

Finally, let us define the *total density of clusters* as

$$r_c := \sum_{k=1}^{\infty} r_k. \quad (7.8)$$

Then, two identities are easily derived from (7.5) and (7.6):

$$\frac{dr_1}{d\tau} + r_1(r_1 + r_c) + \epsilon(r_1 - r_2 - r_c) = 0, \quad (7.9)$$

$$\frac{dr_c}{d\tau} + r_1 r_c + \epsilon(r_1 - r_c) = 0. \quad (7.10)$$

## 7.2. Numerical results

The numerical solution of the initial value problem given by equations (7.5)–(7.7) clearly expresses the phenomenology of micellization, and backs up the singular perturbation analysis carried out in section 7.3. Figures 7.1 (a) and 7.2–7.4 are histograms of  $r_k$  as a function of  $k$  at different times, and figure 7.5 records the time-dependent behavior of the average cluster size  $\langle k \rangle$ .

Figure 7.1 (a) depicts an early stage of the kinetics. The sequences of small dots at each  $k$  record the values of  $r_k$  at times between  $\tau = 0$  and  $\tau = 2$ , in increments of  $\Delta\tau = 0.2$ , and the larger dots joined by straight lines record the values of  $r_k$  at  $\tau = 10$ . The direction of increasing time is generally clear. As indicated in figure 7.1 (b), the monomer concentration rapidly decreases to a small fraction of its initial value  $r_1 = 1$ , so that the time orientation on the line  $k = 1$  is downward. Many small clusters of sizes  $2 \leq k \leq 5$  are simultaneously created, so the time orientation on the lines of these  $k$  is generally upwards. Notice that  $\rho_2$  reaches a maximum and then decreases to a constant value, as can be seen in figure 7.1 (c). By the end of the initial stage at time  $\tau = 10$ , the creation of smaller clusters (with  $2 \leq k \leq 5$ ) has slowed down greatly relative to the initial rate for times  $0 < \tau < 2$ . Furthermore, the number of clusters with more than five monomers is negligible. At  $\tau = 10$ ,

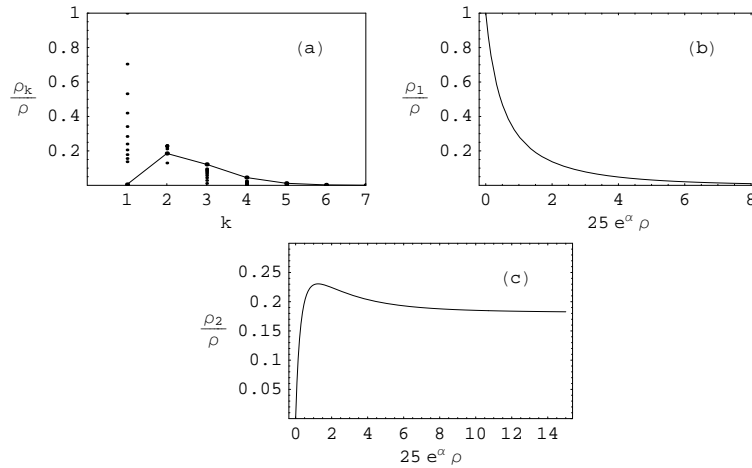


Figure 7.1: (a) Scaled cluster size distribution  $\rho_k/\rho$  as a function of  $k$  for  $0 \leq \tau \leq 10$ . At time  $\tau = 10$ , the values of  $\rho_1/\rho$ ,  $\rho_2/\rho$ , etc., have been joined by straight lines as a guide to the eye. (b) Evolution of the scaled monomer concentration  $\rho_1/\rho$ . (c) Evolution of the scaled dimer concentration  $\rho_2/\rho$ . Parameter values are  $\alpha = 10$  and  $\rho = 0.1$ .

$\langle k \rangle \approx 2.69$ , much smaller than the equilibrium value  $\langle k \rangle \approx \sqrt{\rho e^\alpha} = \epsilon^{-1/2} \approx 46.9$ . To determine the time scales appropriate for exploring the subsequent kinetics, it is highly instructive to plot the average cluster size  $\langle k \rangle$  as a function of time, based on the numerical solution. Figure 7.5 is a log-log plot of  $\langle k \rangle / e$  as a function of  $\tau$ . It reveals an initial rapid growth of  $\langle k \rangle$  to a “plateau value” close to  $e$ , roughly located in the interval  $10 < \tau < 100$ . In the subsequent growth after the plateau, large clusters with  $k \gg 1$  eventually appear. Figure 7.5 indicates that by time  $\tau = 5 \times 10^4$ ,  $k$  clusters having  $\langle k \rangle = 10$  are prevalent.

Figure 7.2 shows frames at times  $\tau = 20, 10^4$  and  $2 \times 10^4$ , thereby continuing those in figure 7.1. The heavy dots correspond to  $\tau = 20$ , which is well inside the plateau phase. The histograms at  $\tau = 10^4$  and  $2 \times 10^4$  indicate the clear emergence of a continuum limit of the kinetics.

In the time interval  $2 \times 10^4 < \tau < 5 \times 10^5$ , the log-log plot of  $\langle k \rangle / e$  as a function of  $\tau$  in figure 7.5 is close to a straight line of slope  $1/2$ . This strongly supports the existence of a self-similar stage of the kinetics. The line graphs in figure 7.4 depict  $\langle k \rangle^2 r_k$  as a function of  $x = k / \langle k \rangle$  for the times  $\tau = 0.5 \times 10^5, 10^5$  and  $1.5 \times 10^5$ . They are nearly superimposed on top of each other. The heavy dots correspond to the plateau time  $\tau = 20$ , so the change in the distribution shape over the whole time span  $20 < \tau < 1.5 \times 10^5$  is not very great.

The self-similar stage is not the final chapter of the kinetics story either. By  $\tau = 10^6$ , the linear dependence of  $\log(\langle k \rangle / e)$  with  $\log \tau$  breaks down. In fact, at  $\tau = 10^6$ ,  $\langle k \rangle \approx 31.1$ , which is comparable to the equilibrium value of 46.9 mentioned before. Evidently, there is a final stage of kinetics in which the size distribution asymptotes to its equilibrium form. Figure 7.3 is the final era of cluster aggregation, continued from figure 7.2, in which the snapshots of the size distribution are taken

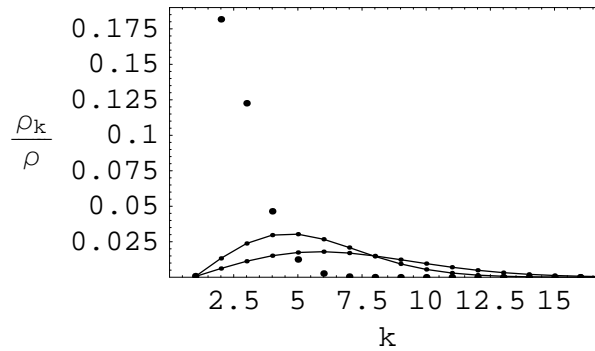


Figure 7.2: Same as figure 7.1 (a), for the times  $\tau = 20$ ,  $10^4$  and  $2 \times 10^4$ . At the two later times, we have joined values of  $\rho_k/\rho$  corresponding to neighboring  $k$ 's by straight lines as a guide to the eye.

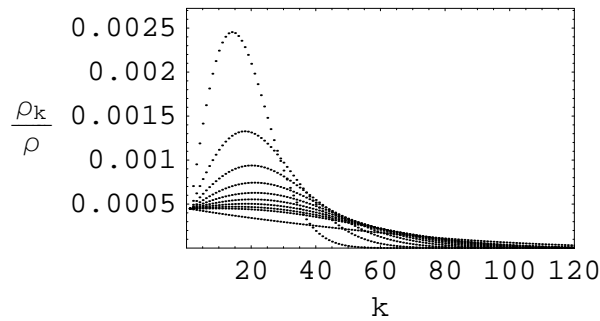


Figure 7.3: Same as figure 7.1 (a), starting at  $\tau = 2 \times 10^5$ . Snapshots of the size distribution have been taken at time intervals of  $\tau = 2 \times 10^5$ , until a time  $\tau = 16 \times 10^5$ . The last snapshot corresponds to  $\tau = 40 \times 10^5$ .

at  $\tau$  increments of  $0.2 \times 10^6$ , from  $0.2 \times 10^6$  to  $4 \times 10^6$ . Convergence to an exponential distribution with  $\langle k \rangle$  equal to the equilibrium value is clear.

## 7.3. Asymptotic approximation

In this section we will interpret the numerical results shown in section 7.2 by using singular perturbation methods.

### 7.3.1. Initial transient

Initially,  $r_1(0) = 1$ , and there are no multiparticle aggregates. As we have seen in section 7.2, the numerical solution of the complete model shows that there is an initial transient stage during which dimers, trimers, etc. form at the expense of

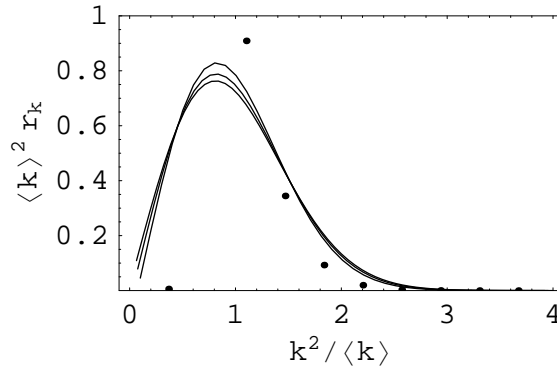


Figure 7.4: Approximate self-similar behavior of the size distribution at times  $\tau = 50000, 100000$ , and  $150000$  (solid lines). Notice that  $\langle k \rangle^2 r_k$  is approximated by the same function of  $k/\langle k \rangle$  at different times. The dots correspond to  $\tau = 20$ .

th monomers, and that  $r_k \approx 0$  for sufficiently large  $k$ . Taking the  $\epsilon \rightarrow 0$  limit of equations (7.9) and (7.10) yields the following planar dynamical system:

$$\frac{dr_1}{ds} = -(r_1 + r_c) \quad (7.11)$$

$$\frac{dr_c}{ds} = -r_c \quad (7.12)$$

$$\frac{ds}{d\tau} = r_1 \quad (7.13)$$

in the *adaptive time*  $s = \int_0^\tau \rho_1 d\tau$ . The general solution of the linear system (7.11)–(7.12) is

$$r_1 = (a - bs)e^{-s}, \quad r_c = be^{-s},$$

where  $a$  and  $b$  are arbitrary constants. Our initial condition yields  $a = b = 1$ , so that

$$r_1 = (1 - s)e^{-s}, \quad r_c = e^{-s}, \quad (7.14)$$

and from equation (7.13),

$$\tau = \int_0^s \frac{e^s}{1 - s} ds. \quad (7.15)$$

Clearly,  $\tau \rightarrow \infty$  corresponds to  $s \rightarrow 1^-$ . At  $s = 1$ , equation (7.14) yields  $r_1 = 0$ ,  $r_c = e^{-1}$ , which are the limiting values of the variables  $r_1$  and  $r_c$  at the end of the initial stage. Equation (7.5) with  $\epsilon = 0$  becomes  $d(r_k e^s)/ds = r_{k-1} e^s$ , which can be solved recursively to yield

$$r_k = \left( \frac{s^{k-1}}{(k-1)!} - \frac{s^k}{k!} \right) e^{-s}. \quad (7.16)$$

As  $\tau \rightarrow \infty$ ,  $r_k \rightarrow (k-1)e^{-1}/k!$ . Since  $r_6(1) = 0.00255$ , after the initial transient stage there are insignificant numbers of aggregates with more than five monomers.

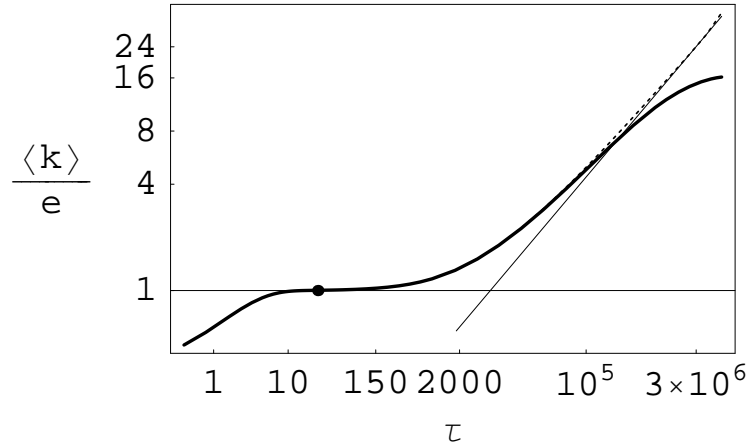


Figure 7.5: Evolution of the average cluster size  $\langle k \rangle / e$  as a function of the scaled time  $\tau$  (thick solid line). The dotted line corresponds to the solution of the system 7.21 below with an initial condition corresponding to the dot. The straight line of slope 1/2 corresponds to the self-similar continuum size distribution given by 7.29.

In fact, the average aggregate cluster size is  $\langle k \rangle = 1/r_c = e$ ; whereas at equilibrium,  $\langle k \rangle \sim \sqrt{\rho e^\alpha} \gg 1$ . We therefore conclude that there must be successive transients on time scales much larger than  $t = O(\epsilon)$ .

### 7.3.2. Intermediate transient

Examination of the exact equation (7.5) shows that when  $r_1$  decreases to size  $O(\epsilon)$ , but  $r_2, r_3, \dots$  are of order 1, all terms in its right hand side are  $O(\epsilon)$ . This suggests rescaling  $r_1 = \epsilon R_1$ , so that  $\rho_1 = e^{-\alpha R_1}$ , and using the original time  $t = \epsilon \tau$ . Equation (7.5) becomes

$$\frac{dr_2}{dt} = -(R_1 - 1)(r_2 - \epsilon R_1) + r_3 - 2r_2 + \epsilon R_1, \quad (7.17)$$

$$\frac{dr_k}{dt} = -(R_1 - 1)(r_k - r_{k-1}) + r_{k+1} - 2r_k + r_{k-1}, \quad k \geq 2. \quad (7.18)$$

The global identities (7.9) and (7.10) become

$$(R_1 - 1)r_c - r_2 + \epsilon \left( \frac{dR_1}{dt} + R_1^2 + R_1 \right) = 0, \quad (7.19)$$

$$\frac{dr_c}{dt} + (R_1 - 1)r_c + \epsilon R_1 = 0, \quad (7.20)$$

where now  $r_c = \epsilon R_1 + \sum_{k=2}^{\infty} r_k \approx \sum_{k=2}^{\infty} r_k$ , as  $\epsilon \rightarrow 0$ . In the limit  $\epsilon \rightarrow 0$ ,  $R_1 - 1 = r_2/r_c$  and equation (7.18) becomes

$$\frac{dr_k}{dt} = -\frac{r_2(r_k - r_{k-1})}{r_c} + r_{k+1} - 2r_k + r_{k-1}, \quad k \geq 2. \quad (7.21)$$



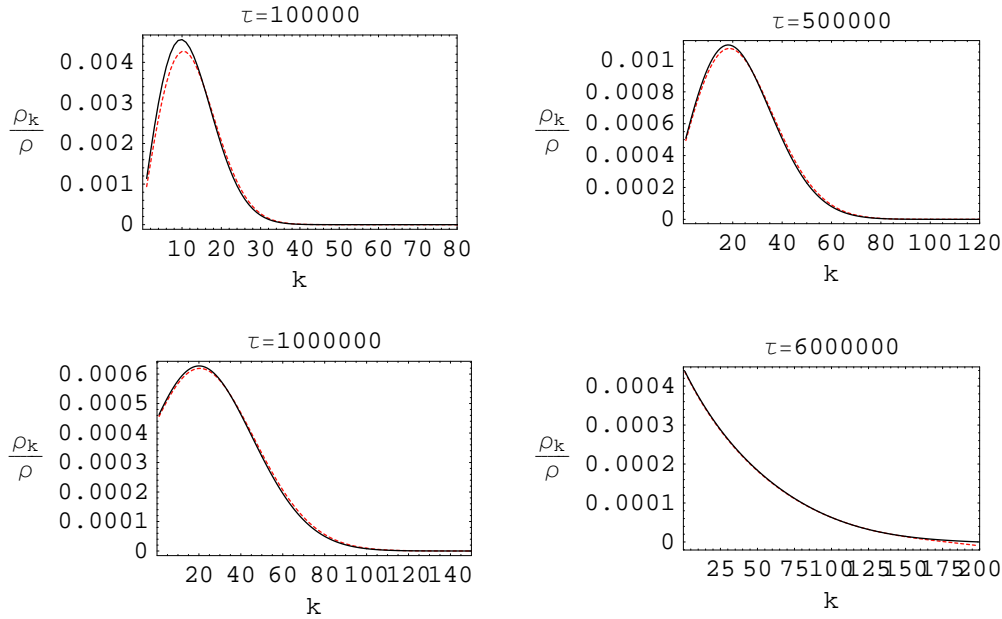


Figure 7.6: Comparison of the approximation 7.49 (dashed line) to the numerical solution of the full kinetic model (solid line) for four different times  $\tau$ : (a) 100 000, (b) 500 000, (c) 1 000 000, (d) 3 000 000. Notice that the agreement improves as the equilibrium distribution is approached.

This is a closed system of equations for  $r_2, r_3, \dots$ , to be solved with the asymptotic values  $r_k = (k-1)e^{-1}/k!$  as initial conditions. It can be shown that the reduced versions of equation (7.20) ( $\dot{r}_c = -(R_1 - 1)r_c$ ) and the conservation condition  $\sum_{k=2}^{\infty} kr_k = 1$ , are upheld automatically by the solution of equation (7.21), so that they are redundant for this stage.

The numerical solution of the reduced system of equations (7.21) for  $r_k$ ,  $k \geq 2$  closely approximates that of the full system of kinetic equations at this stage. It can be seen that more and more of the  $r_k$  become different from zero as  $t$  increases, and that  $r_k - r_{k-1}$  becomes small. This strongly suggests that  $r_k$  can be approximated by a continuum limit for long times. To find the continuum limit, we set

$$r_k(t) \approx \delta^a r(x, T), \quad x = \delta k, \quad T = \delta^b t. \quad (7.22)$$

Here  $\delta \rightarrow 0$  fixes the scale of  $k = O(1/\delta)$ , so that  $x$  is fixed at some value of order 1;  $a$  and  $b$  are positive exponents to be determined. To find  $a$ , we use the conservation condition  $\sum_{k=2}^{\infty} kr_k = 1$ :

$$1 = \delta^{a-2} \sum_{k=2}^{\infty} (k\delta) r(k\delta, T = \delta) \sim \int_0^{\infty} xr(x, T) dx,$$

provided  $a = 2$ . The limiting form of the particle conservation is thus

$$\int_0^\infty x r(x, T) dx = 1. \quad (7.23)$$

A similar calculation for the total number of clusters yields  $r_c \sim \delta \int_0^\infty r(x, T) dx$ , which suggests the definition

$$r_c \sim \delta R_c, \quad R_c \equiv \int_0^\infty r(x, T) dx. \quad (7.24)$$

We now substitute equation (7.22) in (7.21) and use (7.24) instead of  $r_c$ . The result is

$$\delta^b \frac{\partial r}{\partial T} \sim -\frac{\delta^2 r(2\delta, T)(r(x, T) - r(x - \delta, T))}{\delta R_c} + r(x + \delta, T) - 2r(x, T) + r(x - \delta, T).$$

The right hand side of this expression is of order  $O(\delta^2)$ , so that the following distinguished limit is obtained if we set  $b = 2$  and take  $\delta \rightarrow 0$ :

$$\frac{\partial r(x, T)}{\partial T} = -\frac{r(0, T)}{R_c(T)} \frac{\partial r(x, T)}{\partial x} + \frac{\partial^2 r(x, T)}{\partial x^2}. \quad (7.25)$$

For  $k =$ , equation (7.21) and the scaling (7.22) with  $a = b = 2$  imply that  $r(0, T) = 0$ . Therefore equation (7.25) becomes the simple diffusion equation

$$\frac{\partial r}{\partial T} = \frac{\partial^2 r}{\partial x^2}, \quad (7.26)$$

for  $x > 0, t > 0$  to be solved with boundary condition  $r(0, T) = 0$ .

The numerical solution of the discrete equations (7.21) show that large aggregates do not emerge until  $t \gg 1$ . This suggests that the appropriate solution of (7.26) should be concentrated around  $x = 0$  as  $T \rightarrow 0+$ . That solution is proportional to the  $x$  derivative of the diffusion kernel,

$$r(x, T) = -\frac{\partial}{\partial x} \left( \frac{e^{-x^2/4T}}{\sqrt{\pi T}} \right) \frac{x}{2\sqrt{\pi T^{3/2}}} e^{-x^2/4T}. \quad (7.27)$$

The numerical factor is chosen so that particle conservation, given by equation (7.23), holds. It follows from equation (7.24) that  $R_c = (\pi T)^{-1/2}$ . Hence the average aggregate size is

$$\langle k \rangle = \frac{1}{\delta R_c} = \frac{\sqrt{\pi T}}{\delta}. \quad (7.28)$$

In terms of the original variables  $k, t$  and  $r_k$ , the previous expressions are

$$r_k(t) \sim \frac{k}{2\sqrt{\pi t^{3/2}}} e^{-k^2/4t}, \quad (7.29)$$

$$\langle k \rangle \sim \sqrt{\pi t}, \quad (7.30)$$

as  $t \rightarrow \infty$ . These two equations yield

$$\langle k \rangle^2 r_k \sim \frac{\pi k}{2 \langle k \rangle} \exp\left(-\frac{\pi}{4} \left(\frac{k}{\langle k \rangle}\right)^2\right), \quad (7.31)$$

which resembles the behavior of the numerical solution of the full kinetic model as indicated in figure 7.4. Notice that the average cluster size  $\langle k \rangle$  corresponding to the solution of equations (7.21) (dotted line in figure 7.5) approaches the value (7.30) (straight line of slope 1/2 in figure 7.5).

### 7.3.3. Equilibrium transient

The large time limit of equation (7.29) does not match the equilibrium size distribution, which is  $r_k \sim \epsilon e^{-k\sqrt{\epsilon}}$  in the same scaled units; see section 2.5. Thus the limit given by equation (7.29) is expected to break down when it predicts an average  $\langle k \rangle$  of the order of the equilibrium length  $1/\sqrt{\epsilon}$ . According to equation (7.30), this occurs at a time  $\sqrt{t} = O(\epsilon^{-1/2})$ , this is,  $t = O(\epsilon^{-1})$ . In this third and final transient towards equilibrium, we set

$$r_k(t) = \epsilon r(x, t), \quad x = \sqrt{\epsilon} k, \quad T = \epsilon t. \quad (7.32)$$

This is the same scaling as in equation (7.22) with  $a = b = 2$  and  $\delta = \sqrt{\epsilon}$ , and therefore we use here the same notation for the variables. With this scaling, the scaled particle conservation is

$$1 = \sum_{k=1}^{\infty} k r_k = \epsilon^{1/2} \sum_{k=1}^{\infty} \epsilon^{1/2} k r(x, T),$$

and the limit  $\epsilon \rightarrow 0$  yields

$$\int_0^{\infty} x r(x, T) dx = 1. \quad (7.33)$$

Similarly,

$$r_c \sim \epsilon^{1/2} \int_0^{\infty} r(x, T) dx \equiv \epsilon^{1/2} R_c. \quad (7.34)$$

The scaled version of the global identity (7.8) is

$$R_c(R_1 - 1) + \epsilon^{1/2} R_1 + \epsilon \frac{dR_c}{dT} = 0. \quad (7.35)$$

Here  $r_1 0 \epsilon R_1 = \epsilon r(\epsilon^{1/2}, T)$ . It follows from (7.35) that

$$R_1 - 1 = -\frac{\epsilon^{1/2}}{R_c} + O(\epsilon). \quad (7.36)$$

The scaled kinetic equation (7.5) is

$$\begin{aligned} \epsilon^3 \frac{\partial r}{\partial T} = & -\epsilon^2 (R_1 - 1) (r(x, T) - r(x - \epsilon^{1/2}, T)) \\ & + \epsilon^2 (r(x + \epsilon^{1/2}, T) - 2r(x, T) + r(x - \epsilon^{1/2}, T)). \end{aligned}$$

We now substitute equation (7.36) in this expression, divide it by  $\epsilon^3$ , and take the limit  $\epsilon \rightarrow 0$ . The result is

$$\frac{\partial r}{\partial T} = \frac{1}{R_c(T)} \frac{\partial r}{\partial x} + \frac{\partial^2 r}{\partial x^2}.$$

In these units, the average aggregate length is  $\langle x \rangle = 1/R_c$ , and the last equation can be rewritten as

$$\frac{\partial r}{\partial T} = \langle x \rangle \frac{\partial r}{\partial x} + \frac{\partial^2 r}{\partial x^2}, \quad (7.37)$$

to be solved with the boundary condition

$$r(0, T) = 1, \quad (7.38)$$

which follows from equation (7.36) with  $\epsilon \rightarrow 0$ . It can be readily checked that  $(d/dT) \int_0^\infty x r(x, T) dx = 0$ , and therefore  $\int_0^\infty x r(x, T) dx = 1$ , provided  $r(x, 0)$  satisfies this particle conservation condition.

We now have to show two things:

1. As  $T \rightarrow 0+$ , the solution of equations (7.37) and (7.38) is asymptotic to the right hand side of equation (7.27), the self-similar limiting solution of the intermediate transient stage.
2. The solution of equations (7.37) and (7.38) tends to the equilibrium size distribution as  $T \rightarrow \infty$ .

This completes the description of the dynamics of the aggregate size distribution.

### Matching with the intermediate transient stage

We represent  $r(x, T)$  as

$$r(x, T) = \frac{1}{T} h(\zeta, T), \quad \zeta = \frac{x}{\sqrt{T}}. \quad (7.39)$$

With the factor  $1/T$ , the particle conservation equation (7.6) and the total cluster density adopt the invariant forms

$$\int_0^\infty \zeta h(\zeta, T) d\zeta = 1, \quad (7.40)$$

$$R_c(T) = \int_0^\infty r(x, T) dx = \frac{1}{\sqrt{T}} \int_0^\infty h(\zeta, T) d\zeta = \frac{h_c(T)}{\sqrt{T}}. \quad (7.41)$$

Then

$$\langle x \rangle = \sqrt{\frac{T}{h_c(T)}}. \quad (7.42)$$

Inserting this equation together with equation (7.39) in equation (7.37) we obtain

$$\frac{\partial^2 h}{\partial \zeta^2} + h + \frac{1}{2} \zeta \frac{\partial h}{\partial \zeta} = T \left( \frac{\partial h}{\partial T} + \frac{\zeta h}{h_c} \right), \quad (7.43)$$

to be solved with the boundary condition indicated by equations (7.38) and (7.39),

$$h(0, T) = T. \quad (7.44)$$

Asymptotic similarity as  $T \rightarrow 0$  means that  $h(\zeta, T)$  in equation (7.39) has a limit  $H(\zeta)$  as  $T \rightarrow 0$ . The limit equations obtained from equations (7.40)–(7.44) are

$$\begin{aligned} \frac{\partial^2 H}{\partial \zeta^2} + H + \frac{1}{2} \zeta \frac{\partial H}{\partial \zeta} &= 0 \quad \text{for } \zeta > 0, \\ H(0) &= 0, \\ \int_0^\infty \zeta H(\zeta) d\zeta &= 1. \end{aligned}$$

The unique solution of these equations is

$$H(\zeta) = \zeta \frac{e^{-\zeta^2/4}}{2\sqrt{\pi}},$$

which is the right hand side of equation (7.27).

### Trend towards equilibrium

The stationary solution of equation (7.37) with the condition (7.38) is  $r_e = e^{-x\langle x \rangle}$ , and the particle conservation condition gives  $\langle x \rangle^2 = 1$ , so that  $\langle x \rangle = 1$ . Then the stationary solution of equation (7.37) is  $r_e = e^{-x}$ , which is the sought equilibrium solution. To show that  $r(x, T) \rightarrow r_e(x)$  as  $T \rightarrow \infty$ , we define the associated free energy

$$f[r] = \int_0^\infty \left( -r + r \log \left( \frac{r}{r_0} \right) \right) dx - 1 \quad (7.45)$$

$$r_0 = e^{-x}, \quad (7.46)$$

and show that it is a Lyapunov functional for equation (7.37). Notice that we have  $\int_0^\infty r \log r_0 dx = -\int_0^\infty xr dx = -1$ , and therefore  $f[r]$  is the usual free energy,

$$f[r] = \int_0^\infty (r \log r - r) dx.$$

First, the standard inequality  $x \log x \geq x - 1$  for positive  $x = r/r_0$  yields  $f \geq -\int_0^\infty e^{-x} dx - 1 = -2$ , and therefore  $f$  is bounded below. Notice that  $f[r_0] = -2$  at equilibrium.

Second, time differentiation of equation (7.46) yields

$$\frac{df}{dT} = \int_0^\infty \frac{\partial r}{\partial T} \log \left( \frac{r}{r_0} \right) dx.$$

If we now substitute equation (7.37), integrate by parts, and use  $r(0, T) = r_0(0) = 1$  and  $\int_0^\infty r dx = \frac{1}{\langle x \rangle}$ , we obtain

$$\frac{df}{dT} = \langle x \rangle - \int_0^\infty \frac{1}{r} \left( \frac{\partial r}{\partial T} \right)^2 dx = \langle x \rangle \left( 1 - \int_0^\infty r dx \int_0^\infty \frac{1}{r} \left( \frac{\partial r}{\partial T} \right)^2 dx \right). \quad (7.47)$$

The right hand side of this equation is less than or equal to zero because of the Cauchy-Schwarz inequality

$$\begin{aligned} 1 = r(0, T)^2 &= \left( \int_0^\infty \frac{\partial r}{\partial x} dx \right)^2 \leq \left( \int_0^\infty \left| \frac{\partial r}{\partial x} \right| dx \right)^2 \\ &\leq \int_0^\infty r dx \int_0^\infty \frac{1}{r} \left( \frac{\partial r}{\partial x} \right)^2 dx. \end{aligned}$$

Therefore, we have proved that the free energy is a Lyapunov functional. We can rewrite equation (7.47) in an equivalent form by defining  $\tilde{r}_0 = \exp -x \langle x \rangle$ , and using the identities

$$\begin{aligned} \langle x \rangle &= \langle x \rangle^2 \int_0^\infty r dx = \int_0^\infty r \left( \frac{\partial \log \tilde{r}_0}{\partial x} \right)^2 dx, \\ \langle x \rangle &= -\langle x \rangle \int_0^\infty \frac{\partial r}{\partial x} dx = \int_0^\infty r \frac{\partial \log r}{\partial x} \frac{\partial \log \tilde{r}_0}{\partial x} dx, \end{aligned}$$

to obtain

$$\frac{df}{dT} = - \int_0^\infty r \left( \frac{\partial}{\partial x} \log \left( \frac{r}{\tilde{r}_0} \right) \right)^2 dx \leq 0. \quad (7.48)$$

This equation shows that  $r \rightarrow \tilde{r}_0$  as  $T \rightarrow \infty$ . The particle conservation condition  $\int_0^\infty x \tilde{r}_0 dx = 1$  yields  $\langle x \rangle^2 = 1$ , and therefore  $\tilde{r}_0 = e^{-x}$ .

### 7.3.4. Approximation of the size distribution function by matched asymptotic expansions

An uniformly valid approximation to the size distribution function can be easily formed from

- $r_k^{(1)}(\tau)$ , given by equations (7.15) and (7.16),
- $r_k^{(2)}(\tau)$ , which solves the approximate system of equations (7.21), and  $r_c = \sum_{k=2}^{\infty} r_k$  with the initial conditions  $r_k(0) = (k-1)e^{-1}/k!$ ,
- and  $r(x, T)$ , which solves the nonlinear Fokker-Planck equation (7.37) with the condition (7.38), and matches equation (7.26) as  $T \rightarrow 0+$ .

The result is

$$r_k^{(\text{unif})} = r_k^{(1)}(\tau) + r_k^{(2)}(\epsilon\tau) + \epsilon r(\sqrt{\epsilon}k, \epsilon^2\tau) - \frac{k-1}{k!e} - \frac{k}{2\sqrt{\pi}(\epsilon\tau)^{3/2}} \exp\left(-\frac{k^2}{4\epsilon\tau}\right). \quad (7.49)$$

Figure 7.6 compares the distribution function given by equation (7.49) to the numerical solution of the complete model equations in times corresponding to the end of the intermediate stage and the beginning of the equilibration stage. We observe a good agreement between approximate and numerical solutions, which improves as the time elapses and the equilibrium distribution is approached.

## 7.4. Conclusions

On the basis of a simple kinetic model and starting from the initial state of pure monomers, we have shown that the process of micellization of rodlike aggregates at high critical micelle concentration occurs in three separated stages or eras. In the first era, many clusters of small size are produced while the number of monomers decreases sharply. During the second era, aggregates are increasing steadily in size and their distribution approaches a self-similar solution of the diffusion equation. Before the continuum limit can be realized, the average size of the nuclei becomes comparable to its equilibrium value, and a simple mean-field Fokker-Planck equation describes the final era until the equilibrium distribution is reached. A continuum size distribution does not describe micellization until the third era has started; during the first two eras the effects of discreteness dominate the dynamics.

In order to validate our theory by an experiment, it would be important to measure the average cluster size as a function of time, as in figure 7.5; the multiscale behavior is more clearly seen in this figure. To determine the time scale, we need a measure of the cluster diffusion coefficient  $d$  that was set equal to 1 in section 7.1. A convenient relation could be equation (7.30), which in dimensional units is  $\langle k \rangle \approx$

$\sqrt{d\pi t}$ . In case the self-similar size distribution is not reached during the intermediate phase, another way to determine  $d$  is to study the equilibration era and compare the experimentally obtained size distribution with the numerical solution of the model. At equilibrium,  $\langle k \rangle^2 \approx \rho e^\alpha$ , and this relation determines the dimensionless binding energy  $\alpha$ .





# Chapter 8

## Existence theory in $L^1$ for the Wigner-Poisson-Fokker-Planck system

In this chapter we present the results obtained in collaboration with Juan José Nieto and José Luis López, published in [13].

### 8.1. Introduction and main result

As explained in section 1.2 of the introduction, we are interested in the following initial value problem for the function  $W(t, x, \xi)$  with  $x, \xi \in \mathbb{R}^3$  and  $t \geq 0$ :

$$\frac{\partial W}{\partial t} + (\xi \cdot \nabla_x)W + \Theta[V]W = \frac{D_{pp}}{m^2} \Delta_\xi W + 2\lambda \operatorname{div}_\xi(\xi W) + D_{qq} \Delta_x W \quad (8.1)$$

$$W(x, \xi, 0) = W_0(x, \xi), \quad (8.2)$$

where the self-consistent electrostatic potential  $V$  is given by the Poisson equation:

$$V(x, t) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{n(y, t)}{|x - y|} dy, \quad (8.3)$$

with

$$n(x, t) = \int_{\mathbb{R}^3} W(x, \xi, t) d\xi. \quad (8.4)$$

Here,  $\Theta[V]$  stands for the pseudo-differential operator

$$\begin{aligned} \Theta[V]W(x, \xi, t) &= \frac{i}{(2\pi)^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{V(x + \frac{\hbar}{2m}\eta, t) - V(x - \frac{\hbar}{2m}\eta, t)}{\hbar} \\ &\quad \times W(x, \xi', t) e^{-i(\xi - \xi') \cdot \eta} d\xi' d\eta, \end{aligned} \quad (8.5)$$

with  $\hbar$  denoting the reduced Planck constant and  $m$  the effective mass of the particles, while  $\lambda, D_{pp}, D_{qq}$  are positive constants related to the interactions between the particles and the reservoir (cf. [24]):

$$\lambda = \frac{\eta}{2m}, \quad D_{pp} = \eta k_B T, \quad D_{qq} = \frac{\eta \hbar^2}{12m^2 k_B T}, \quad (8.6)$$

where  $\eta > 0$  is the coupling (damping) constant of the bath,  $k_B$  the Boltzmann constant and  $T$  the temperature of the bath.

We prove the following new result:

**Theorem 8.1.1.** *Let  $W_0 \in L^1(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3) \cap L^1(\mathbb{R}_\xi^3; L^2(\mathbb{R}_x^3))$  be such that*

$$\int_{\mathbb{R}_x^3} \int_{\mathbb{R}_\xi^3} |\xi|^2 W_0(x, \xi) d\xi dx < \infty.$$

*Then, the Wigner–Poisson–Fokker–Planck equation (8.1)–(8.6) admits a unique global mild solution*

$$W \in C([0, \infty); L^1(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)) \cap C([0, \infty); L^1(\mathbb{R}_\xi^3; L^2(\mathbb{R}_x^3))).$$

Moreover,

$$W \in C((0, \infty); W^{1,1} \cap W^{1,\infty}(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)).$$

*Also, the charge density (8.4) and the electric potential (8.3) satisfy the following Hölder–regularity properties: for all  $t > 0$ ,*

$$n(\cdot, t) \in C^{0,\alpha}(\mathbb{R}_x^3) \text{ with } 0 < \alpha < \frac{1}{2}, \quad V(\cdot, t) \in C^{1,\beta}(\mathbb{R}_x^3) \text{ with } 0 < \beta < \frac{1}{3}.$$

This chapter is structured as follows: in Section 2 we construct the fundamental solution of the linear kinetic Fokker–Planck operator and establish its main properties. Section 3 concerns the local existence and uniqueness of solutions to the 3D WFPF system with nonvanishing friction. In Section 4 we show some regularization effects of the Fokker–Planck kernel on the Wigner function, the charge density and the electric potential. Finally, Section 5 is devoted to prove that the solution found in Section 3 exists globally in time.

## 8.2. On the fundamental solution

This section is devoted to the description of the fundamental solution of the quantum Fokker–Planck model (8.1)–(8.5) and the derivation of some of its main properties. The Green function  $G$  associated with the linear kinetic Wigner–Fokker–Planck equation under study is the fundamental solution of

$$L[W] := \frac{\partial W}{\partial t} + (\xi \cdot \nabla_x)W - \frac{D_{pp}}{m^2} \Delta_\xi W - 2\lambda \operatorname{div}_\xi(\xi W) - D_{qq} \Delta_x W = 0. \quad (8.7)$$

**Lemma 8.2.1.** *The fundamental solution of the linear operator (8.7) is given by*

$$G(x, \xi, z, v, t) = G_0\left(x - z - \left(\frac{1 - e^{-2\lambda t}}{2\lambda}\right)v, \xi - e^{-2\lambda t}v, t\right), \quad (8.8)$$

where

$$G_0(x, \xi, t) = d(t) \exp\{-a(t)|x|^2 + b(t)(x \cdot \xi) - c(t)|\xi|^2\} \quad (8.9)$$

with coefficients

$$a(t) = \frac{m^2 \lambda^3}{D_{pp}} \frac{(1 - e^{-4\lambda t})}{D(t)}, \quad (8.10)$$

$$b(t) = \frac{m^2 \lambda^2}{D_{pp}} \frac{(1 - e^{-2\lambda t})^2}{D(t)}, \quad (8.11)$$

$$c(t) = \frac{m^2 \lambda}{4D_{pp}} \frac{\left(4\lambda t \left(1 + 4\lambda^2 m^2 \frac{D_{qq}}{D_{pp}}\right) - (1 - e^{-2\lambda t})(3 - e^{-2\lambda t})\right)}{D(t)}, \quad (8.12)$$

$$d(t) = \left(\frac{\sqrt{4a(t)c(t) - b(t)^2}}{2\pi}\right)^3 = \left(\frac{m^2 \lambda^2}{\pi D_{pp} \sqrt{D(t)}}\right)^3, \quad (8.13)$$

and where

$$D(t) = \lambda \left(1 + 4\lambda^2 m^2 \frac{D_{qq}}{D_{pp}}\right) t (1 - e^{-4\lambda t}) - (1 - e^{-2\lambda t})^2. \quad (8.14)$$

Notice that  $D(t)$  and  $4a(t)c(t) - b(t)^2$  are positive functions for all positive times.

The proof is based on the Fourier transformation of Eq. (8.7) with respect to the  $(x, \xi)$ -variables and then integration of the resulting linear first order hyperbolic problem for  $\hat{G}(y, \eta, t)$

$$\begin{aligned} \frac{\partial \hat{G}}{\partial t} - (y \cdot \nabla_\eta) \hat{G} + 2\lambda(\eta \cdot \nabla_\eta) \hat{G} + \frac{D_{pp}}{m^2} \eta^2 \hat{G} + D_{qq} y^2 \hat{G} &= 0, \\ \hat{G}(y, \eta, 0) &= 1, \end{aligned}$$

along the characteristics  $\eta \mapsto e^{2\lambda t} \eta + \frac{1}{2\lambda}(1 - e^{2\lambda t})y$ , where we denoted

$$\hat{G}(y, \eta, t) = \mathcal{F}_{x \mapsto y, \xi \mapsto \eta} G(y, \eta, t) = \int_{\mathbb{R}_x^3} \int_{\mathbb{R}_\xi^3} G(x, \xi, t) e^{i(x \cdot y + \xi \cdot \eta)} d\xi dx.$$

From now on, when there is no possible confusion we shall denote

$$L^p = L^p(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3), \quad L^{q,p} = L^q(\mathbb{R}_\xi^3; L^p(\mathbb{R}_x^3)).$$

In the following result we list some of the properties of  $G$  that will be useful in the sequel to deal with mild solutions of the system (8.1)–(8.5). We have

**Lemma 8.2.2.** *The fundamental solution  $G$  of the linear kinetic Fokker–Planck equation (8.7), given by formulae (8.8)–(8.14), satisfies the following properties for any  $t \geq 0$ :*

$$(i) \int_{\mathbb{R}_x^3} \int_{\mathbb{R}_\xi^3} G(x, \xi, z, v, t) d\xi dx = 1 \quad \text{for all } z, v \in \mathbb{R}^3.$$

$$(ii) \|G_0(t)\|_{L^{q,p}} \leq C(q, p) a(t)^{\frac{3}{2}(\frac{1}{q}-\frac{1}{p})} d(t)^{1-\frac{1}{q}} \quad \text{for all } 1 \leq q, p < \infty.$$

(iii) For all  $1 \leq q \leq p < \infty$ , we have

$$\begin{aligned} \|\nabla_{(x,\xi)} G_0(t)\|_{L^p(\mathbb{R}_x^3; L^q(\mathbb{R}_\xi^3))} &\leq C(p, q) \left[ \left(2a(t) + b(t)\right) d(t)^{\frac{2}{3}-\frac{1}{p}} c(t)^{\frac{1}{2}(1+\frac{3}{p}-\frac{3}{q})} \right. \\ &\quad \left. + \left(2c(t) + b(t)\right) d(t)^{\frac{2}{3}-\frac{1}{q}} a(t)^{\frac{1}{2}(1+\frac{3}{q}-\frac{3}{p})} \right]. \end{aligned}$$

In particular, for  $q = p$  we have

$$\|\nabla_{(x,\xi)} G_0(t)\|_{L^p} \leq C(p) d(t)^{\frac{2}{3}-\frac{1}{p}} \left[ \left(2a(t) + b(t)\right) \sqrt{c(t)} + \left(2c(t) + b(t)\right) \sqrt{a(t)} \right].$$

*Proof.* The proof follows from elementary computations. We just make a few remarks on the proof of (iii). First we observe that

$$|\nabla_{(x,\xi)} G_0(x, \xi, t)| \leq \left[ \left(2a(t) + b(t)\right) |x| + \left(2c(t) + b(t)\right) |\xi| \right] G_0(x, \xi, t).$$

Then, we can estimate

$$\begin{aligned} \|\nabla_{(x,\xi)} G_0(t)\|_{L^p(\mathbb{R}_x^3; L^q(\mathbb{R}_\xi^3))} &\leq \left(2a(t) + b(t)\right) \| |x| G_0(t) \|_{L^p(\mathbb{R}_x^3; L^q(\mathbb{R}_\xi^3))} \\ &\quad + \left(2c(t) + b(t)\right) \| |\xi| G_0(t) \|_{L^{q,p}}, \end{aligned}$$

where we have used Minkowski's inequality to reverse the order of the norms acting on  $|\xi|G_0$ .

### 8.3. Existence of local–in–time mild solutions

In this section we prove the existence and uniqueness of local–in–time mild solutions to the 3D WFPF system (8.1)–(8.6) by application of a fixed–point argument of contractive type. Local existence was also dealt with in [2] for the simplest frictionless Wigner–Fokker–Planck model (1.7). By a mild solution  $W(x, \xi, t)$  of the WFPF system (8.1)–(8.2) we understand that satisfying the following integral equation:

$$\begin{aligned} W(x, \xi, t) &= \int_{\mathbb{R}_v^3} \int_{\mathbb{R}_z^3} G(x, \xi, z, v, t) W_0(z, v) dz dv \\ &\quad - \int_0^t \int_{\mathbb{R}_v^3} \int_{\mathbb{R}_z^3} G(x, \xi, z, v, t-s) \Theta[V] W(z, v, s) dz dv ds. \end{aligned} \quad (8.15)$$

Clearly, from the concept of mild solution we may consider  $W$  to be split into two parts: the linear part, only depending on the initial data  $W_0$ , and the nonlinear part depending upon the potential  $V$  through the pseudo-differential operator  $\Theta[V]W$ . Also, we observe that the first term in the above decomposition actually solves the linear Wigner–Fokker–Planck problem (8.7) with initial data  $W_0$ .

Henceforth in the paper the following identity for the nonlinear term constitutes a crucial ingredient (see [2]):

$$\Theta[V]W = H *_{\xi} W,$$

where

$$\begin{aligned} H(x, \xi, t) &= \frac{i}{(2\pi)^3} \int_{\mathbb{R}_\eta^3} \frac{V(x + \frac{\hbar}{2m}\eta, t) - V(x - \frac{\hbar}{2m}\eta, t)}{\hbar} e^{-i\xi \cdot \eta} d\eta \\ &= 16 \left(\frac{m}{\hbar}\right)^3 \operatorname{Re} \left\{ i e^{i\frac{2m}{\hbar}x \cdot \xi} \mathcal{F}_{x \rightarrow \xi}^{-1} V\left(\frac{2m}{\hbar}\xi, t\right) \right\}. \end{aligned}$$

In fact, it is a simple matter to conclude that

$$|H(x, \xi, t)| \leq 16 \left(\frac{m}{\hbar}\right)^3 \left| \mathcal{F}_{x \rightarrow \xi}^{-1} V\left(\frac{2m}{\hbar}\xi, t\right) \right|, \tag{8.16}$$

where we denoted  $\mathcal{F}_{x \rightarrow y}^{-1} f = \frac{1}{(2\pi)^3} \int_{\mathbb{R}_x^3} f(x) e^{-ix \cdot y} dx$  the inverse Fourier transform of  $f$ . We also introduce the following notation for convenience: given  $f \in L^1$ , define the uniparametric semigroup  $G(t)$  acting on  $f$  as the integral operator

$$G(t)[f] = \int_{\mathbb{R}_v^3} \int_{\mathbb{R}_z^3} G(x, \xi, z, v, t) f(z, v) dz dv.$$

Now, the mild WFPF equation (8.15) may be rewritten as

$$W(t) = G(t)[W_0] - \int_0^t G(t-s)[(H *_{\xi} W)(s)] ds. \tag{8.17}$$

We first proceed to derive *a priori* bounds on  $W$ . In the sequel we shall denote by  $C$  various positive constants. We have the following

**Lemma 8.3.1.** *Let  $G(t)$  denote the Green function operator. Let also  $1 \leq p, q < \infty$  and  $1 + \frac{1}{p} = \frac{1}{r} + \frac{1}{l}, 1 + \frac{1}{q} = \frac{1}{s} + \frac{1}{m}$ , with  $m \leq l$ . Then, the following estimates*

- (i)  $\|G(t)[f]\|_{L^{q,p}} \leq e^{6\lambda(1-\frac{1}{m})t} \|G_0\|_{L^{s,r}} \|f\|_{L^{m,l}},$
- (ii)  $\|\nabla(G(t)[f])\|_{L^p(\mathbb{R}_x^3; L^q(\mathbb{R}_\xi^3))} \leq e^{6\lambda(1-\frac{1}{m})t} \|\nabla G_0\|_{L^r(\mathbb{R}_x^3; L^s(\mathbb{R}_\xi^3))} \|f\|_{L^{m,l}},$
- (iii)  $\|H\|_{L^1(\mathbb{R}_\xi^3)} \leq C(\|n\|_{L^1(\mathbb{R}^3)} + \|n\|_{L^2(\mathbb{R}^3)}) \leq C(\|W\|_{L^1} + \|W\|_{L^{1,2}}),$

hold true. Here, the symbol  $\nabla$  denotes any first order derivative. Furthermore, in the particular case  $p = q = 1$  in (i) we have

$$\|G(t)[f]\|_{L^1} \leq \|f\|_{L^1}.$$

*Proof.* (i) follows from the change of variables  $z + \left(\frac{1-e^{-2\lambda t}}{2\lambda}\right)v \mapsto z$ , then  $e^{-2\lambda t}v \mapsto v$ . The proof concludes after application of Young's inequality for the resulting convolution and Minkowski's inequality for the norm of  $f$ . The particular case  $p = q = 1$  is a direct consequence of Lemma 8.2.2 (i). The calculations leading to (ii) are analogous to those of (i). Finally, (iii) follows from (8.16) by the identity (see [2])

$$\begin{aligned} \|\mathcal{F}_{x \rightarrow y}^{-1}V(\cdot, t)\|_{L^1(\mathbb{R}^3)} &= \frac{1}{4\pi} \left\| \mathcal{F}_{x \rightarrow y}^{-1} \left( \frac{1}{|x|} * n \right) (\cdot, t) \right\|_{L^1(\mathbb{R}^3)} \\ &= \left\| \frac{1}{|\cdot|^2} (\mathcal{F}_{x \rightarrow y}^{-1}n)(\cdot, t) \right\|_{L^1(\mathbb{R}^3)}. \end{aligned}$$

Indeed, we first estimate the  $L^1$  norm of  $|\cdot|^{-2}(\mathcal{F}_{x \rightarrow y}^{-1}n)(\cdot, t)$  outside and inside the 3D unit ball  $B$ . We have

$$\left\| \frac{1}{|\cdot|^2} (\mathcal{F}_{x \rightarrow y}^{-1}n)(\cdot, t) \right\|_{L^1(\mathbb{R}^3 \setminus B)} \leq C \|\mathcal{F}_{x \rightarrow y}^{-1}n(\cdot, t)\|_{L^2(\mathbb{R}^3)} \leq C \|n(\cdot, t)\|_{L^2(\mathbb{R}^3)}.$$

Likewise, inside  $B$  we get

$$\left\| \frac{1}{|\cdot|^2} (\mathcal{F}_{x \rightarrow y}^{-1}n)(\cdot, t) \right\|_{L^1(B)} \leq C \|\mathcal{F}_{x \rightarrow y}^{-1}n(\cdot, t)\|_{L^\infty(\mathbb{R}^3)} \leq C \|n(\cdot, t)\|_{L^1(\mathbb{R}^3)}.$$

Finally, bounding the norms of  $n$  by those of  $W$

$$\|n(\cdot, t)\|_{L^1(\mathbb{R}^3)} \leq \|W(t)\|_{L^1}, \quad \|n(\cdot, t)\|_{L^2(\mathbb{R}^3)} \leq \|W(t)\|_{L^{1,2}},$$

we conclude (iii).

Let  $T > 0$ . In the sequel we shall manipulate functions  $W(x, \xi, t)$  defined on the Banach space  $C([0, T]; L^1 \cap L^{1,2})$ , endowed with the norm

$$\|W\| := \sup_{0 \leq t \leq T} \left( \|W(t)\|_{L^1} + \|W(t)\|_{L^{1,2}} \right).$$

More precisely, we shall restrict ourselves to the following closed, bounded subset of  $C([0, T]; L^1 \cap L^{1,2})$ :

$$X_K^T = \{W \in C([0, T]; L^1 \cap L^{1,2}) : W(t=0) = W_0; \|W\| \leq K\}$$

and define the map  $\Gamma : X_K^T \rightarrow C([0, T]; L^1 \cap L^{1,2})$  by

$$\Gamma(W)(t) = G(t)[W_0] - \int_0^t G(t-s)[(H *_{\xi} W)(s)] ds.$$

We first notice that  $\Gamma$  is well-defined. Indeed, from Lemma 8.3.1 (i) and (iii) we have

$$\begin{aligned} \|G(t)[W_0]\|_{L^1} &\leq \|W_0\|_{L^1}, \\ \|G(t-s)[(H *_{\xi} W)(s)]\|_{L^1} &\leq C \|W\| \|W(s)\|_{L^1}, \end{aligned} \quad (8.18)$$

where we estimated

$$\|H *_{\xi} W\|_{L^1} \leq \|H\|_{L^1(\mathbb{R}_x^3)} \|W\|_{L^1}$$

by Young's inequality. On the other hand, the same type of estimates are also true for the  $L^{1,2}$  norm. Again from Lemma 8.3.1 (i) and (iii) we have

$$\begin{aligned} \|G(t)[W_0]\|_{L^{1,2}} &\leq \|W_0\|_{L^{1,2}}, \\ \|G(t-s)[(H *_{\xi} W)(s)]\|_{L^{1,2}} &\leq C \|W\| \|W(s)\|_{L^{1,2}}. \end{aligned} \quad (8.19)$$

Now, having chosen  $K = 2\|W_0\|_T$  and  $T \leq \frac{1}{4CK}$ , it is clear that  $\Gamma$  maps  $X_K^T$  onto itself and

$$\|\Gamma(W_1) - \Gamma(W_2)\|_T \leq \frac{1}{2} \|W_1 - W_2\|_T \quad \forall W_1, W_2 \in X_K^T.$$

Hence  $\Gamma : X_K^T \rightarrow X_K^T$  is a contractive map, so it has a unique fixed point  $W \in X_K^T$ . This is equivalent to saying that there exists a unique solution  $W(t) \in L^1 \cap L^{1,2}$  of the WFPF system (8.1)–(8.2) defined on  $[0, T]$ , for sufficiently small  $T > 0$  only depending on  $W_0$ . Actually (see [77]), there is a maximum time of existence  $T_{max}$  which is either  $T_{max} = \infty$  or  $T_{max} < \infty$  and  $\|W\| \rightarrow \infty$  when  $T \rightarrow T_{max}$ . In the last section we shall prove that the second possibility cannot occur, hence global existence is attained.

## 8.4. Smoothing effects and regularity of the Wigner function

The purpose of this section is to take advantage of the regularization properties of the Fokker–Planck operator in order to derive some smoothing effects on the (Wigner function) solution under the only assumption that the initial data is in  $L^1 \cap L^{1,2}$ .

We first introduce some useful notations and results.

**Definition 8.4.1.** Let  $T > 0$  and  $f, g$  be continuous functions in  $(0, T)$ . We will say that  $f(t)$  is equivalent to  $g(t)$  at  $t = 0$  (and denote it by  $f(t) \stackrel{t=0}{\sim} g(t)$ ) if there exist three positive constants  $c_1, c_2$  and  $t_0$  such that

$$c_1 f(t) \leq g(t) \leq c_2 f(t), \quad \text{for all } 0 < t \leq t_0.$$



This concept allows to easily identify the rates of time growth/decay near  $t = 0$  of the coefficients of the fundamental solution  $G_0$ . We have the following

**Lemma 8.4.2.** *Let  $a(t)$ ,  $b(t)$ ,  $c(t)$ ,  $d(t)$  and  $D(t)$  be given by formulae (8.13)–(8.14). Then*

$$D(t) \stackrel{t=0}{\sim} t^2, \quad a(t) \stackrel{t=0}{\sim} c(t) \stackrel{t=0}{\sim} \frac{1}{t}, \quad d(t) \stackrel{t=0}{\sim} \frac{1}{t^3}, \quad b(t) \stackrel{t=0}{\sim} 1.$$

*Proof.* For  $a(t)$  we observe that  $(1/a)(0) = 0$  and  $(1/a)'(0) = 4D_{qq}$ . Then, a simple integration allows to deduce that

$$\frac{1}{6D_{qq}t} \leq a(t) \leq \frac{1}{2D_{qq}t}$$

is satisfied in  $(0, t_0)$ , for some  $t_0 > 0$ . Analogously, we observe that the first nonvanishing derivative of  $1/c$  at  $t = 0$  is  $(1/c)'(0)$  and that of  $1/d$  is  $(1/d)'''(0)$ . For  $b(t)$  we directly check that  $0 < b(0) < \infty$ . Finally,  $D''(0)$  is the first nonvanishing derivative of  $D(t)$  at  $t = 0$ . The proof concludes after integration.

We summarize the main regularity properties of  $W(x, \xi, t)$ ,  $n(x, t)$  and  $V(x, t)$  in the following

**Proposition 8.4.3.** *Let  $0 < T < T_{max}$  and let also  $W(x, \xi, t)$  be the solution of (8.1)–(8.2) given by (8.15). Then,*

- (i)  $W \in C((0, T); L^\infty(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3))$ ,
- (ii)  $W \in C((0, T); W^{1,1} \cap W^{1,\infty}(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3))$ .

*Also, the following Hölder regularity is achieved for the density and the potential:*

- (iii)  $n(t) \in C^{0,\alpha}(\mathbb{R}_x^3)$ , for all  $t \in (0, T)$  and  $0 < \alpha < \frac{1}{2}$ ,
- (iv)  $V(t) \in C^{1,\beta}(\mathbb{R}_x^3)$ , for all  $t \in (0, T)$  and  $0 < \beta < \frac{1}{3}$ .

*Besides,*

- (v)  $\nabla_x V \in L^2 \cap L^\infty(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)$ ,
- (vi)  $\nabla_x n \in L^2(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)$ ,
- (vii)  $\xi W \in L^1(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)^3$  for all  $t \in (0, T)$ . *Actually,*

$$\|\xi W\|_{L^1(\mathbb{R}_x^3 \times \mathbb{R}_\xi^3)^3} \leq K e^{Ct}, \quad 0 < t < T, \quad (8.20)$$

*where  $K$  and  $C$  are positive constants depending on  $\|W\|_T$ .*

*Proof.* The first result is reached as a consequence of Lemmata 8.2.2 and 8.3.1 by using that  $d(t) \stackrel{t=0}{\sim} t^{-3}$ , then  $d(t)^{\frac{1}{p'}} \in L^1(0, T)$  for  $1 \leq p < \frac{3}{2}$ . We prove (i) in four steps. The *first step* consists of estimating

$$\begin{aligned} \|W(t)\|_{L^p} &\leq \|G(t)[W_0]\|_{L^p} + \int_0^t \|G(t-s)[(H * W)(s)]\|_{L^p} ds \\ &\leq C\|W_0\|_{L^1} d(t)^{\frac{1}{p'}} + C\|W\|^2 \int_0^t d(s)^{\frac{1}{p'}} ds. \end{aligned}$$

Then, we deduce that  $W \in C((0, T_{max}); L^p)$  for all  $1 \leq p < \frac{3}{2}$ . In the *second step* we start from an arbitrarily small time  $\epsilon > 0$ , that is, rewrite  $W(t)$  for  $t > \epsilon$  as

$$W(t) = G(t - \epsilon)[W(\epsilon)] - \int_{\epsilon}^t G(t - s)[(H * W)(s)] ds,$$

then we estimate  $\|W(t)\|_{L^q}$  with  $q < 3$  as

$$\|W(t)\|_{L^q} \leq C d(t - \epsilon)^{\frac{1}{p'}} \|W(\epsilon)\|_{L^p} + C \|W\| \int_{\epsilon}^t d(t - s)^{\frac{1}{p'}} \|W(s)\|_{L^p} ds.$$

The *third step* is analogous. Indeed, for  $r < \infty$  and  $t > 2\epsilon$  we can now estimate  $\|W(t)\|_{L^r}$  as

$$\|W(t)\|_{L^r} \leq C d(t - 2\epsilon)^{\frac{1}{p'}} \|W(2\epsilon)\|_{L^q} + C \|W\| \int_{2\epsilon}^t d(t - s)^{\frac{1}{p'}} \|W(s)\|_{L^q} ds.$$

Finally, in a *fourth step* we obtain a uniform bound for  $W$  by writing

$$\|W(t)\|_{L^\infty} \leq C d(t - 3\epsilon)^{\frac{1}{p'}} \|W(3\epsilon)\|_{L^r} + C \|W\| \int_{3\epsilon}^t d(t - s)^{\frac{1}{p'}} \|W(s)\|_{L^r} ds$$

for any  $t > 3\epsilon$ . Notice that  $p$ ,  $q$  and  $r$  are linked by Young's relations at every step. The arbitrariness of  $\epsilon$  allows us to conclude. Also note that we have repeatedly used the property  $G(t)[G(s)[f]] = G(t + s)[f]$  of evolution semigroups. Finally, Pazy's results (see § 6 of [77]) ensure the continuity of the Green function operator  $G(t)$ , thus of the Wigner function.

To prove (ii), we first take gradients in the mild equation (8.17) and obtain

$$\nabla_{(x,\xi)} W(t) = \nabla_{(x,\xi)} G(t)[W_0] - \int_0^t \nabla_{(x,\xi)} G(t-s)[H * W(s)] ds.$$

As for (i) we can prove (ii) in several steps, depending on the time integrability of  $\|\nabla_{(x,\xi)} G(x, \xi, z, v, t)\|_{L^p} = \|\nabla_{(x,\xi)} G_0(x, \xi, t)\|_{L^p}$ . Using Lemma 8.2.2 (iii) with  $q = p$  and Lemma 8.4.2 we conclude that

$$\|\nabla_{(x,\xi)} G_0(x, \xi, t)\|_{L^p} \leq C t^{\frac{3}{p} - \frac{7}{2}}.$$

Therefore,  $\|\nabla_{(x,\xi)}G_0(x,\xi,t)\|_{L^p} \in L^1(0,T)$  for  $1 \leq p < \frac{6}{5}$ . Using now the same ideas than before, (ii) can be reached in seven steps. The time continuity is deduced as before.

To prove (iii) we first observe that Morrey's Theorem (see for example [10]) yields

$$|n(x,t) - n(y,t)| \leq \|\nabla_x n(\cdot,t)\|_{L^p(\mathbb{R}^3)} |x-y|^{1-\frac{3}{p}}, \quad \text{for } p > 3.$$

Then, it suffices to control  $\|\nabla_x n(\cdot,t)\|_{L^p(\mathbb{R}^3)}$  for some  $p > 3$ . To this aim, we shall show that  $\|\nabla_x W(t)\|_{L^p(\mathbb{R}_x^3; L^1(\mathbb{R}_\xi^3))}$  is bounded. By using Lemmata 8.2.2 (iii) and 8.3.1, we have

$$\begin{aligned} \|\nabla_x W(t)\|_{L^p(\mathbb{R}_x^3; L^1(\mathbb{R}_\xi^3))} &\leq \|\nabla_x G_0(t)\|_{L^q(\mathbb{R}_x^3; L^1(\mathbb{R}_\xi^3))} \|W_0\|_{L^{1,2}} \\ &\quad + \|W\|^2 \int_0^t \|\nabla_x G_0(s)\|_{L^q(\mathbb{R}_x^3; L^1(\mathbb{R}_\xi^3))} ds \\ &\leq \|W_0\|_{L^{1,2}} t^{\frac{3}{2q}-2} + C \|W\|^2 t^{\frac{3}{2q}-1} \end{aligned}$$

with  $1 + \frac{1}{p} = \frac{1}{q} + \frac{1}{2}$ . Now, choosing  $\frac{6}{5} < q < \frac{3}{2}$  and then  $3 < p < 6$  we get the desired bound with  $\alpha = 1 - \frac{3}{p}$ . We notice that the above inequality is still valid for  $p = 2$  ( $q = 1$ ), then assertion (vi) holds.

We prove (iv) by using the convolution form (8.3) of  $V$  and splitting the integral into two parts:

$$\begin{aligned} |V(x,t) - V(z,t)| &\leq C \int_{\mathbb{R}^3} \frac{|n(x-y,t) - n(z-y,t)|}{|y|} dy \leq \int_{|y| < R} + \int_{|y| \geq R} \\ &\leq C \|\nabla_x n(\cdot,t)\|_{L^p} |x-z|^{1-\frac{3}{p}} \int_{|y| < R} \frac{1}{|y|} dy \\ &\quad + \frac{1}{R} \int_{\mathbb{R}^3} |n(x-y,t) + n(z-y,t)| dy \\ &\leq CR^2 \|\nabla_x n(\cdot,t)\|_{L^p} |x-z|^{1-\frac{3}{p}} + \frac{2Q}{R}. \end{aligned}$$

Then, optimizing over  $R$  we get

$$|V(x,t) - V(z,t)| \leq CQ^{\frac{2}{3}} \|\nabla_x n(\cdot,t)\|_{L^p}^{\frac{1}{3}} |x-z|^{\frac{1}{3}-\frac{1}{p}},$$

thus the continuity of  $V$ . For the first order derivative we may analogously write

$$\begin{aligned} |\nabla_x V(x,t) - \nabla_x V(z,t)| &\leq C \int_{\mathbb{R}^3} \frac{|n(x-y,t) - n(z-y,t)|}{|y|^2} dy \\ &\leq CQ^{\frac{1}{3}} \|\nabla_x n(\cdot,t)\|_{L^p}^{\frac{2}{3}} |x-z|^{\frac{2}{3}-\frac{2}{p}}, \end{aligned}$$

which yields the Hölder continuity of  $\nabla_x V$ . This concludes the proof of (iv) with  $\beta = \frac{2}{3} - \frac{2}{p}$ .

To prove (v), we first notice that

$$\|\nabla_x V\|_{L^2} \leq C \left( \|n\|_{L^1} + \|n\|_{L^2} \right).$$

Also, the boundedness of  $\nabla_x V$  is a straightforward consequence of  $\nabla_x V \in L^2$  and the Hölder regularity  $\nabla_x V \in C^{0,\beta}$ .

Finally, (vii) follows by multiplying Eq. (8.15) against  $\xi$  and taking  $L^1$  norms. Then, using (vi), Lemma 8.4.2 and the fact that  $\|\xi H\|_{L^1} \leq C \left( \|W\|_T + \|\nabla_x n\|_{L^2} \right)$  we get

$$\|\xi W(\cdot, \cdot, t)\|_{L^1} \leq \sup_{0 < t < T} F(t) + C \|W\|_T \int_0^t e^{-2\lambda(t-s)} \|\xi W(\cdot, \cdot, s)\|_{L^1} ds,$$

with

$$\begin{aligned} F(t) &= C \|W_0\|_{L^1} \sqrt{t} + e^{-2\lambda t} \|\xi W_0\|_{L^1} + C \|W\|_T^2 t^{\frac{3}{2}} \\ &\quad + C \|W\|_T^2 t + \int_0^t e^{-2\lambda(t-s)} \|\nabla_x n(\cdot, s)\|_{L^2} ds. \end{aligned}$$

Now, Gronwall's inequality applies to yield (8.20).

## 8.5. Existence of global solutions

This section is devoted to prove that the solution obtained in Section 3 is actually defined in  $[0, \infty)$ , that is,  $T_{max} = \infty$ . To this aim, we shall equivalently show that the norm in  $L^1 \cap L^{1,2}$  cannot blow up in finite time.

We start with some considerations concerning the kinetic energy of the system.

**Lemma 8.5.1.** *Consider the electron kinetic energy associated with  $f(x, \xi, t)$  to be defined by*

$$E[f](t) = \int_{\mathbb{R}_x^3} \int_{\mathbb{R}_\xi^3} \frac{|\xi|^2}{2} f(x, \xi, t) d\xi dx.$$

Let  $W$  and  $W^H$  be the solution of the WFPF system (8.1)–(8.5) and its corresponding Hussimi transform (cf. (1.14)), respectively. The following assertions hold true:

(i)  $E[W](t) < +\infty$  for all  $0 < t < T$ .

(ii)  $E[W]$  solves

$$\begin{aligned} \frac{d}{dt} \left( E[W](t) + \frac{1}{2m} \|\nabla_x V(\cdot, t)\|_{L^2(\mathbb{R}^3)}^2 \right) \\ = 3 \frac{D_{pp}}{m^2} Q - 4\lambda E[W](t) - \frac{D_{qq}}{m} \|n(\cdot, t)\|_{L^2(\mathbb{R}^3)}^2. \end{aligned}$$

(iii) The Husimi kinetic energy  $E[W^H]$  is connected to  $E[W]$  through the following relation

$$E[W^H](t) = E[W](t) + \frac{3\hbar}{2m}Q.$$

(iv)  $E[W]$  is bounded from below. In fact,

$$E[W](t) \geq -\frac{3\hbar}{2m}Q, \quad \forall t > 0.$$

*Proof.* (i) follows from Eq. (8.15) by integrating against  $|\xi|^2$  and estimating

$$\begin{aligned} E[W](t) &\leq e^{-4\lambda t} E[W](0) + \| |\xi|^2 G_0(t) \|_{L^1} \|n\|_{L^1} \\ &\quad + \int_0^t \| |\xi|^2 G_0(t-s) \|_{L^1} \| (H *_{\xi} W)(s) \|_{L^1} ds \\ &\quad + \int_0^t e^{-4\lambda(t-s)} \int_{\mathbb{R}_x^3} \int_{\mathbb{R}_{\xi}^3} |\xi|^2 (H *_{\xi} W) d\xi dx ds \\ &\leq E[W](0) + C t \|n\|_{L^1} + C t^2 \|W\|_T^2 \\ &\quad + \int_0^t \int_{\mathbb{R}_x^3} \int_{\mathbb{R}_{\xi}^3} |\xi|^2 (H *_{\xi} W) d\xi dx ds \\ &\leq C(T) + \int_0^t \left( \int_{\mathbb{R}_x^3} J \cdot \nabla_x V dx \right) ds, \end{aligned}$$

where we have used again Lemma 8.4.2. Then, Proposition 8.4.3 (v) and (vii) allows to conclude.

Multiplying Eq. (8.1) by  $|\xi|^2$ , integrating against  $x$  and  $\xi$  and using the Poisson equation  $\Delta_x V = n$  leads to (ii). (iii) follows from a straightforward calculation. (iv) is a simple consequence of (iii) given that the Husimi function  $W^H$  is positive.

We first remark that the density function  $n(x, t)$  is nonnegative (see for example [2, 62]). Then, integrating Eq. (8.15) in  $x$  and  $\xi$  shows that the total charge of the system

$$Q = \int_{\mathbb{R}_x^3} n(x, t) dx = \int_{\mathbb{R}_x^3} \int_{\mathbb{R}_{\xi}^3} W(x, \xi, t) d\xi dx$$

is preserved along the time evolution.

Now we are ready to finish the proof of Theorem 8.1.1. We only need to show the existence of a solution as stated in the theorem. To this aim, estimating as in (8.18) and (8.19) and using Lemma 8.3.1 (iii), we find

$$\begin{aligned} \|W(t)\|_{L^1} + \|W(t)\|_{L^{1,2}} &\leq \|W_0\|_{L^1} + \|W_0\|_{L^{1,2}} \\ &\quad + C \int_0^t \left( \|n(s)\|_{L^1(\mathbb{R}^3)} + \|n(s)\|_{L^2(\mathbb{R}^3)} \right) \left( \|W(s)\|_{L^1} + \|W(s)\|_{L^{1,2}} \right) ds. \end{aligned}$$

Now it is enough to prove that

$$\int_0^t \left( \|n(s)\|_{L^1(\mathbb{R}^3)} + \|n(s)\|_{L^2(\mathbb{R}^3)} \right) ds$$

is finite for finite time, as in that case we finish by using Gronwall's lemma. As  $\|n(t)\|_{L^1(\mathbb{R}^3)} = Q$  is constant in time, the problem is reduced to showing that  $\int_0^t \|n(s)\|_{L^2(\mathbb{R}^3)} ds$  remains bounded on bounded time intervals.

Now, integrating (i) in Lemma 8.5.1 between 0 and  $t$  and using the lower bound for the kinetic energy given in Lemma 8.5.1 (iii), we get

$$\int_0^t \|n(s)\|_{L^2(\mathbb{R}^3)} ds \leq t + \int_0^t \|n(s)\|_{L^2(\mathbb{R}^3)}^2 ds \leq C(W_0) + C(\lambda, D_{pp}, D_{qq}) t$$

after some simple estimates. This implies that  $\int_0^t \|n(s)\|_{L^2(\mathbb{R}^3)} ds$  cannot blow up at finite time. Now we are done with the proof of Theorem 8.1.1.

*Remark 8.5.2.* Notice that the same proof applies to the general WFPF equation with nonvanishing friction (1.6), with inessential modifications (in the sense of estimates and time integrability) in the expression for the fundamental solution due to the additional term  $\frac{2D_{pq}}{m} \operatorname{div}_x(\nabla_\xi W)$ . In fact, we find again

$$G(x, \xi, z, v, t) = G_0\left(x - z - \left(\frac{1 - e^{-2\lambda t}}{2\lambda}\right)v, \xi - e^{-2\lambda t}v, t\right),$$

where now

$$G_0(x, \xi, t) = \delta(t) \exp \left\{ -\alpha(t)|x|^2 + \beta(t)(x \cdot \xi) - \gamma(t)|\xi|^2 \right\}$$

with

$$\begin{aligned} \alpha(t) &= m^2 \lambda^3 D_{pp} \frac{(1 - e^{-4\lambda t})}{\Delta(t)}, \\ \beta(t) &= m^2 \lambda^2 \frac{\left( D_{pp}(1 - e^{-2\lambda t})^2 + 8m\lambda^2 D_{pq}t \right)}{\Delta(t)}, \\ \gamma(t) &= \frac{m^2 \lambda D_{pp}}{4} \frac{\left( 4\lambda t \left( 1 + 4\lambda^2 m^2 \frac{D_{qq}}{D_{pp}} \right) - (1 - e^{-2\lambda t})(3 - e^{-2\lambda t}) \right)}{\Delta(t)}, \\ \delta(t) &= \left( \frac{m^2 \lambda^2}{\pi D_{pp} \sqrt{\Delta(t)}} \right)^3, \\ \Delta(t) &= D_{pp}^2 D(t) - 4m\lambda^2 D_{pq}t \left( D_{pp}(1 - e^{-2\lambda t})^2 + m\lambda^2 D_{pq} \right). \end{aligned}$$

On the contrary, the ideas employed in the proof of Theorem 8.1.1 cannot be extended to the frictionless WFPF system (1.7) because of the lack of elliptic regularization in the  $x$ -direction. This problem will be tackled by the authors in a forthcoming paper.

*Remark 8.5.3.* The regularity properties proved in Theorem 8.1.1 allow to rigorously justify all the *a priori* estimates derived on the Wigner function, the density and the potential. In particular, the energy equation established in Lemma 8.5.1 (i) makes full sense. Indeed, it is clear that

$$\|n(t)\|_{L^2(\mathbb{R}^3)} \leq \|W(t)\|_{L^{1,2}}.$$

Also, from standard elliptic estimates we have

$$\|\nabla_x V(t)\|_{L^2(\mathbb{R}^3)} \leq C \|n(t)\|_{L^{\frac{6}{5}}(\mathbb{R}^3)} \leq C Q^{\frac{2}{3}} \|n(t)\|_{L^2(\mathbb{R}^3)}^{\frac{1}{3}}.$$

*Remark 8.5.4.* Some (exponential) control of the growth in time of the kinetic energy is also possible. Indeed, one can easily deduce from the energy equation stated in Lemma 8.5.1 (i) the following bound

$$E[W](t) \leq C(W_0) + 3\frac{D_{pp}}{m^2}Qt + 4\lambda \int_0^t |E[W](s)| ds.$$

Then, once we know from Lemma 8.5.1 (iii) that  $E[W]$  cannot be "very negative", it is clear that a (sufficiently large) positive constant (denoted again by  $C(W_0)$  for simplicity) must exist such that the above inequality is still valid for  $|E[W](t)|$ . Consequently, Gronwall's lemma applies to give

$$E[W](t) \leq C(W_0, \lambda, D_{pp}) \left(1 + t e^{4\lambda t}\right).$$

# Chapter 9

## Appendix A: Some results from functional analysis

In this chapter we gather some results used in the proofs of the main results in this thesis. All of them are known, but either they are difficult to find, or they are not common, or they cannot be found in the particular form we need, so they are included here for the convenience of the reader. In each of them we indicate other sources where one can obtain more complete information.

### 9.1. Integrable majorants of integrable functions

We present here a version of the classical lemma of de la Vallée-Poussin; a similar one can be found in [22].

**Proposition 9.1.1.** *Let  $\mu$  be a positive Borel measure on  $(0, +\infty)$ , and  $f : (0, +\infty) \rightarrow \mathbb{R}$  a nonnegative  $\mu$ -integrable function. Then there is a measurable function  $\Phi : [0, +\infty) \rightarrow [0, +\infty)$  which is increasing, such that  $\lim_{y \rightarrow \infty} \Phi(y) = \infty$ , and*

$$\int_0^{\infty} \Phi f \mu < +\infty.$$

*In addition, the function  $\Phi$  can be chosen so that it is strictly increasing,  $\Phi(0) = 0$ ,  $\Phi$  is  $C^\infty$ , concave, and such that  $\Phi(y) \leq y$  for all  $y \geq 0$ .*

*If  $G : [0, +\infty) \rightarrow \mathbb{R}$  is a nonnegative function such that  $\lim_{y \rightarrow \infty} G(y) = +\infty$  and, for some  $\epsilon > 0$  and all  $y \in [0, \epsilon]$ ,  $G(y) \geq \epsilon y$ , then  $\Phi$  can be also chosen to be less than  $G$ .*

*Proof.* Define

$$F(x) := \int_x^{\infty} f \mu$$

which is a decreasing function and tends to zero as  $x \rightarrow \infty$  (as  $f$  is integrable). Define

$$a_n := \inf\{x > 0 \mid F(x) < 1/n^2\} \in \mathbb{R}, \quad n \geq 1,$$



and consider the increasing sequence  $\{x_n\}_{n \geq 0}$  given by

$$\begin{aligned} x_0 &:= 0 \\ x_{n+1} &:= \max\{x_n + 1, a_{n+1} + 1\}. \end{aligned}$$

The point of this sequence is that  $x_n \rightarrow \infty$  when  $n \rightarrow \infty$  (which is not necessarily true of  $a_n$ ) and that

$$F(x_n) \leq \frac{1}{n^2}.$$

Finally, we can define  $\phi$ :

$$\begin{aligned} \chi_n &:= \chi_{[x_n, \infty)} \quad \text{for } n \geq 0 \\ \phi &:= \sum_{n=0}^{\infty} \chi_n. \end{aligned}$$

The function  $\phi$  is well defined because for every  $x > 0$ ,  $\phi(x)$  is given by a finite sum. Actually, we could define  $\phi$  equivalently as

$$\phi(x) = n + 1 \quad \text{for } x \in [x_n, x_{n+1}), \quad n \geq 0.$$

It is clear that  $\lim_{x \rightarrow \infty} \phi(x) = \infty$ , as  $\phi(x) > n + 1$  for  $x > x_n$ . Also, the integral of  $\phi f$  is finite because

$$\int_0^{\infty} \phi f \mu = \int_0^{\infty} \left( \sum_{n=0}^{\infty} \chi_n \right) f \mu = \sum_{n=0}^{\infty} \int_0^{\infty} \chi_n f \mu = \sum_{n=0}^{\infty} F(x_n) \leq \sum_{n=0}^{\infty} \frac{1}{n^2} < +\infty.$$

(The monotone convergence theorem justifies the interchange of sums and integral here.)

Now, let us find a function  $\Phi$  in these conditions, which is also concave and strictly increasing, with  $\Phi(0) = 0$  and  $\Phi(y) \leq y$  for  $y \geq 0$ . With the help of  $\phi$  and the above sequence  $\{x_n\}$ , we will define  $\Phi$  recursively as follows:

$$\begin{aligned} d_0 &:= 1; \\ \Phi(0) &= 0; \\ d_{n+1} &:= \min \left\{ d_n, \frac{n + 1 - \Phi(x_n)}{x_{n+1} - x_n} \right\} \quad \text{for } n \geq 0 \\ \Phi(x) &:= \Phi(x_n) + d_{n+1}(x - x_n) \quad \text{for } n \geq 0, \quad x \in [x_n, x_{n+1}]. \end{aligned}$$

First, note that  $\Phi$  is continuous and  $\Phi(0) = 0$  by definition. Its derivative on the interval  $(x_n, x_{n+1})$  is  $d_{n+1}$ ; as  $\{d_n\}$  is decreasing and positive,  $\Phi$  is concave and strictly increasing, and as  $d_0 = 1$ , we have  $\Phi(y) \leq y$  for  $y \geq 0$ . Also,  $\Phi(x)$  is smaller than  $\phi(x)$ , as for  $x$  on the interval  $[x_n, x_{n+1})$  ( $n \geq 0$ ) one has

$$\begin{aligned} \Phi(x) &= \Phi(x_n) + d_{n+1}(x - x_n) \\ &\leq \Phi(x_n) + \frac{n + 1 - \Phi(x_n)}{x_{n+1} - x_n}(x_{n+1} - x_n) = n + 1 = \phi(x). \end{aligned}$$

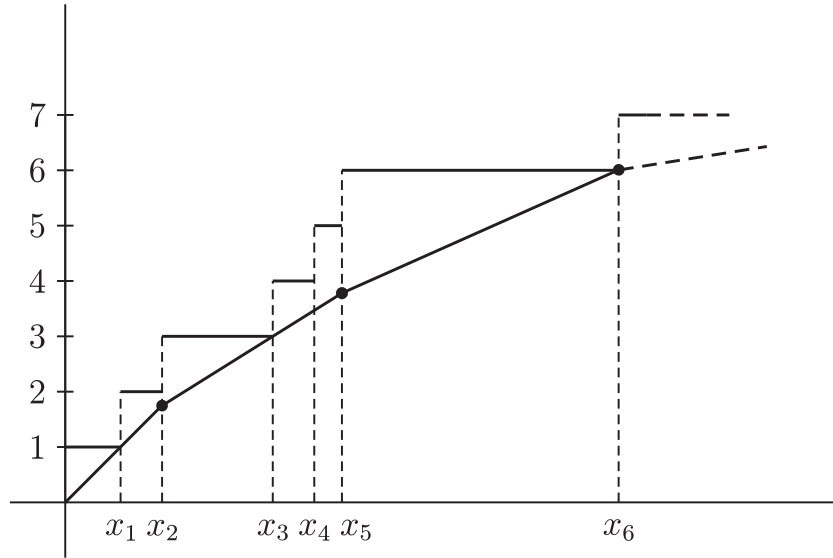


Figure 9.1: Definition of  $\Phi$ . The step function is  $\phi$ , and the piecewise linear one is  $\Phi$ . The scales on the axes are not the same.

So the function  $\Phi f$  is still  $\mu$ -integrable (as  $\phi f$  is). Note that the latter inequality, written for  $x = x_{n+1}$ , also proves that  $\Phi(x_n) \leq n$  for  $n \geq 0$ . Also,  $\lim_{x \rightarrow \infty} \Phi(x) = \infty$ . To prove this, observe that  $d_n$  is always positive (as  $\Phi(x_n) \leq n < n + 1$ ), so  $\Phi$  is strictly increasing. Consider the set of the  $n$  such that  $d_{n+1}$  is different from  $d_n$ ; if it is finite, then from some point on  $\Phi$  has a constant positive slope and hence it tends to  $\infty$ ; if it is infinite, then for all such  $n$  one has

$$\begin{aligned} \Phi(x_{n+1}) &= \Phi(x_n) + d_{n+1}(x_{n+1} - x_n) \\ &= \Phi(x_n) + \frac{n + 1 - \Phi(x_n)}{x_{n+1} - x_n}(x_{n+1} - x_n) = n + 1. \end{aligned}$$

(The equality holds because  $d_{n+1}$  is not  $d_n$ , so it must be the other quantity in the minimum). So  $\lim_{x \rightarrow \infty} \Phi(x) = \infty$ .

Now we can find a function  $\Psi$  with the same properties as  $\Phi$ , and which is also  $\mathcal{C}^\infty$ : extend  $\Phi$  to all of  $\mathbb{R}$  as

$$\Phi(x) := d_1 x \quad \text{for } x \leq 0.$$

Take a ‘‘bump function’’  $\rho : \mathbb{R} \rightarrow \mathbb{R}$  which is  $\mathcal{C}^\infty$ , nonnegative, with integral 1, symmetric about the  $x = 0$  axis and with support contained in  $[-1/2, 1/2]$ . The function

$$\Psi(x) := (\Phi * \rho)(x) = \int_{-\infty}^{\infty} \Phi(x - y)\rho(y) dy = \int_{-\infty}^{\infty} \Phi(y)\rho(x - y) dy$$

is the one we are looking for:  $\Psi(0) = 0$ , as  $\Phi$  is equal to  $d_1 y$  on the interval  $[-1/2, 1/2]$

(recall that  $x_1 \geq 1$ ) and  $\rho$  is symmetric, so

$$\Psi(0) = \int_{-\infty}^{\infty} \Phi(y)\rho(-y) dy = d_1 \int_{-1/2}^{1/2} y\rho(-y) dy = 0.$$

$\Psi$  is  $\mathcal{C}^\infty$ , being a regularization of  $\Phi$  by a  $\mathcal{C}^\infty$  function; it is less than  $x$ , as for  $0 \leq x \leq 1/2$  we know that  $\Psi(x) = d_1 x \leq x$ , and for  $x \geq 1/2$  we have, using the symmetry of  $\rho$  and the bound for  $\Phi$ ,

$$\begin{aligned} \Psi(x) &= \int_{-\infty}^{\infty} \rho(y)\Phi(x-y) dy \leq \int_{-\infty}^{\infty} \rho(y)(x-y) dy \\ &= x \int_{-\infty}^{\infty} \rho(y) dy - \int_{-\infty}^{\infty} \rho(y)y dy = x. \end{aligned}$$

(Note that  $\Phi(x)$  is *not* less than  $x$  for  $x < 0$ , so this calculation does not work for  $0 \leq x < 1/2$ ).  $\Psi$  is concave and strictly increasing because  $\Phi$  is, and convolution with a positive function preserves this;  $\Psi(x)$  tends to  $\infty$  when  $x \rightarrow \infty$ , and if we observe that for  $x \geq 0$

$$\Psi(x) = \int_{-\infty}^{\infty} \Phi(y)\rho(x-y) dy \leq \|\rho\|_\infty \Phi(x+1/2) \leq \|\rho\|_\infty (\Phi(x) + \Phi(1/2)), \quad (9.1)$$

(note that  $\Psi$  is sublinear, as it is concave and  $\Psi(0) = 0$ , so  $\Psi(x+y) \leq \Psi(x) + \Psi(y)$  for  $x, y \geq 0$ ), then it is clear that  $\Psi f$  is integrable on  $(0, +\infty)$ .

Finally, let us see that  $\Psi$  can be chosen to be less than a  $G$  in the conditions of the statement. Call

$$b_n := \inf\{x \in [0, +\infty) \mid G(x) > n + 1\} < +\infty.$$

In the definition at the beginning of the proof, put  $y_n := \max x_n, b_n + 1$ , and define  $\phi$  using  $y_n$  instead of  $x_n$ . Then,

$$\phi(x) \leq G(x) + 1 \quad \text{for } x \geq x_1.$$

Define  $\Phi$  accordingly (so  $\Phi(x) \leq G(x) + 1$  for  $x \geq x_1$ ), and choose  $\delta > 0$  such that

$$\delta \leq \min\{1, 1/\|\rho\|_\infty, 1/(\|\rho\|_\infty \Phi(1/2))\}.$$

Then define  $\Psi$  as the convolution above, times  $\delta$ :

$$\Psi := \delta\Phi * \rho.$$

The bound in (9.1) proves that  $\Psi(y) \leq G(y)$  for  $y \geq x_1$ , and this  $\Psi$  still satisfies all the other properties of the proposition. Now we only have to choose another  $\delta > 0$  such that

$$\begin{aligned} \delta\Psi'(0) &\leq \epsilon \\ \delta\Psi(x) &\leq G(x) \quad \text{for } \epsilon \leq x \leq x_1, \end{aligned}$$

and then  $\delta\Psi$  is less than  $G$  (recall that  $G(x) \geq \epsilon x$  for  $x \in [0, \epsilon]$  and  $\Psi$  is concave) and satisfies all the other properties.  $\square$

In the rest of this section,  $S$  will be a set,  $\mathcal{A}$  will be a  $\sigma$ -algebra of subsets of  $S$  and  $\mu$  be a positive measure on  $\mathcal{A}$ .

**Proposition 9.1.2.** *Consider the positive measure space  $(S, \mathcal{A}, \mu)$ . If  $f : S \rightarrow \mathbb{R}$  is a nonnegative  $\mu$ -integrable function, then there is a continuous function  $\Lambda : [0, +\infty) \rightarrow [0, +\infty)$  which is increasing, such that  $\lim_{y \rightarrow \infty} \Lambda(y)/y = \infty$ , and*

$$\int_0^\infty \Lambda(f(y))\mu(y) < +\infty.$$

The function  $\Lambda$  can be chosen so that  $\Lambda(0) = 0$ ,  $\Lambda$  is  $\mathcal{C}^\infty$ , and strictly convex.

If  $H : [0, +\infty) \rightarrow \mathbb{R}$  is an absolutely continuous function so that  $G = H'$  is in the conditions of  $G$  in proposition 9.1.1, then  $\Lambda$  can be chosen to be less than  $H$ .

This result is a corollary of the previous proposition if one uses the concept of the *distribution function* of a given function  $f$ :

**Definition 9.1.3.** If  $f : S \rightarrow \mathbb{R}$  is a nonnegative  $\mu$ -integrable function, then its *distribution function* is the function  $F_f : (0, +\infty) \rightarrow [0, +\infty)$  given by

$$F_f(\lambda) := \mu\{y \in X \mid f(y) > \lambda\} \quad \text{for } \lambda > 0.$$

Note that the set  $\{y \in X \mid f(y) > \lambda\}$  is measurable, as  $f$  is. It is clear that  $F_f$  is decreasing, so in particular it is Borel measurable. The following lemma gives a way to calculate the integral of  $\varphi(f)$  for suitable functions  $\phi$  knowing only the distribution function  $F_f$ .

**Lemma 9.1.4.** *Let  $\varphi : [0, +\infty) \rightarrow [0, +\infty)$  be a nonnegative  $\mathcal{C}^1$  function such that  $\varphi(0) = 0$ , and  $f : S \rightarrow \mathbb{R}$  a nonnegative  $\mu$ -integrable function. Then*

$$\int_S \varphi(f(x))\mu(x) = \int_0^\infty F_f(\lambda)\varphi'(\lambda) d\lambda.$$

*Proof.* To prove this, note first that the function

$$\begin{aligned} G : S \times [0, +\infty) &\rightarrow \mathbb{R} \\ (x, t) &\mapsto f(x) - t \end{aligned}$$

is measurable for the product  $\sigma$ -algebra  $\mathcal{A} \otimes \mathcal{B}$ , as it is a sum of two measurable functions. Hence, the set  $\{(x, t) \in S \times [0, +\infty) \mid f(x) < t\}$  is measurable, and therefore the function

$$\begin{aligned} \chi : S \times [0, +\infty) &\rightarrow \mathbb{R} \\ (x, t) &\mapsto \begin{cases} 1 & \text{if } f(x) < t \\ 0 & \text{if } f(x) \geq t \end{cases} \end{aligned}$$

is measurable. Observe that

$$F_f(\lambda) = \int_S \chi(x, \lambda) \mu(x) \quad \text{for } \lambda > 0.$$

Hence we can apply Fubini's theorem and write

$$\begin{aligned} \int_0^\infty F_f(\lambda) \varphi'(\lambda) d\lambda &= \int_0^\infty \int_S \chi(x, \lambda) \mu(x) \varphi'(\lambda) d\lambda \\ &= \int_S \int_0^\infty \chi(x, \lambda) \varphi'(\lambda) d\lambda \mu(x) = \int_S \int_0^{f(x)} \varphi'(\lambda) d\lambda \mu(x) = \int_S \varphi(f(x)) \mu(x). \end{aligned}$$

This proves the lemma.  $\square$

Now we can prove proposition 9.1.2:

*Proof of proposition 9.1.2.* The previous lemma proves that  $\int_S f \mu = \int_0^\infty F_f(\lambda) d\lambda$ , so  $F_f$  is integrable. Proposition 9.1.1 then shows that there is a  $\mathcal{C}^\infty$  nonnegative concave function on  $[0, +\infty)$ , which we call  $\Lambda'$ , such that  $\Lambda'(0) = 0$ ,  $\lim_{\lambda \rightarrow \infty} \Lambda'(\lambda) = +\infty$  and

$$\int_0^\infty F_f(\lambda) \Lambda'(\lambda) d\lambda < +\infty.$$

We define  $\Lambda$  as its primitive:

$$\Lambda(\lambda) := \int_0^\lambda \Lambda'(y) dy.$$

Then  $\Lambda$  clearly fulfills the requirements of the proposition; in particular,

$$\int_S \Lambda(f(x)) \mu(x) = \int_0^\infty F_f(\lambda) \Lambda'(\lambda) d\lambda < +\infty,$$

and also, using l'Hôpital's rule,

$$\lim_{\lambda \rightarrow \infty} \Lambda(\lambda)/\lambda = \lim_{\lambda \rightarrow \infty} \Lambda'(\lambda) = +\infty.$$

Finally, if  $H$  is in the conditions of the proposition, we may choose  $\Lambda'$  less than  $H'$  and the result follows.  $\square$

## 9.2. Weak compactness in $L^1$

The following characterizations of weak compactness are needed in the proofs of chapter 5. First we give a general theorem on weak compactness for sets of integrable functions in a general measure space, and then a more concrete one which is more convenient for our aims.

**Theorem 9.2.1 (Dunford-Pettis).** *Let  $(S, \mathcal{A}, \mu)$  be a positive measure space. A subset  $K$  of  $L^1(S, \mu)$  is weakly sequentially compact if and only if it is bounded and for each decreasing sequence  $\{E_n\} \subseteq \mathcal{A}$  with empty intersection the limit*

$$\lim_n \int_{E_n} f \mu = 0 \quad \text{uniformly for } f \in K.$$

An easy consequence is the following:

**Theorem 9.2.2.** *Let  $(S, \mathcal{A}, \mu)$  be a positive measure space. A set  $K \subseteq L^1(S, \mu)$  is weakly sequentially compact if and only if it is bounded and*

$$\lim_{\mu(E) \rightarrow 0} \int_E f \mu = 0 \quad \text{uniformly for } f \in K$$

and there exists a sequence  $\{A_n\}$  of measurable sets of finite measure such that

$$\lim_{n \rightarrow \infty} \int_{S \setminus A_n} f \mu = 0 \quad \text{uniformly for } f \in K.$$

Under stronger conditions on the measure space we have a more direct result:

**Theorem 9.2.3.** *Let  $X$  be a locally compact topological space, and  $\mu$  a regular positive measure on  $\mathcal{B}$ , the Borel sets of  $X$ . Then a subset  $K \subseteq L^1(X, \mu)$  is weakly compact if and only if*

1.  $K$  is bounded,
2. for any compact set  $C \subseteq X$  and any  $\epsilon > 0$  there is a  $\delta > 0$  such that if  $E \in \mathcal{B}$  with  $E \subseteq C$  and  $\mu(E) < \delta$ , then

$$\int_E |f| \mu < \epsilon \quad \text{for all } f \in K,$$

3. for any  $\epsilon > 0$  there is a compact set  $C \subseteq X$  such that

$$\int_{X \setminus C} |f| \mu < \epsilon \quad \text{for all } f \in K.$$

The first of these results and its proof can be found in [32, IV.8.9]; it was first proved by Dunford [30, p. 643] for a finite measure, and by Dunford and Pettis [31, p. 376] for a  $\sigma$ -finite measure. The second is stated as an exercise in [32, IV.13.54], and the third one was proved by Dieudonné [23, p. 93].

When proving the convergence of nonlinear expressions of a sequence  $\{f_n\}$  in a certain Banach space  $X$ , one frequently uses the following result: if  $\{f_n\} \rightharpoonup f$  weakly in  $X$  and  $\phi_n \rightarrow \phi$  in its dual  $X'$ , then  $\phi_n(f_n) \rightarrow \phi(f)$ . For the space  $L^1(U)$ ,

with  $U$  an open bounded subset of  $\mathbb{R}^N$ , this means that when  $f_n \rightharpoonup f$  weakly in  $L^1(U)$  and  $\phi_n \rightarrow \phi \in L^\infty(U)$  uniformly, then

$$\int_U f_n \phi_n \rightarrow \int_U f \phi.$$

In this case, the conditions for this to hold can be weakened, as stated by the following lemma. Its proof can be found in [54, Lemma A.2].

**Lemma 9.2.4.** *Let  $U$  be an open bounded subset of  $\mathbb{R}^N$ ,  $N \geq 1$ . Suppose that  $v_n, v$  are functions in  $L^1(U)$  and  $w_n, w$  are in  $L^\infty(U)$  for  $n \geq 1$ , such that*

$$\begin{aligned} v_n &\rightharpoonup v && \text{weakly in } L^1(U) \\ \{w_n\} &&& \text{is uniformly bounded in } L^\infty(U) \\ w_n(x) &\rightarrow w(x) && \text{a.e. in } U. \end{aligned}$$

Then,

$$\int_U |v_n| |w_n - w| \rightarrow 0$$

and in particular,  $v_n w_n \rightharpoonup v w$  weakly in  $L^1(U)$ .

### 9.3. Compactness in $\mathcal{C}([0, T], L^1 - \text{weak})$

In nonlinear evolution equations it is often useful to obtain a certain time regularity of solutions. The following result gives a way of proving that a sequence of solutions converges in the space  $\mathcal{C}([0, T], L^1(\mu) - \text{weak})$ , where  $\mu$  is a positive Borel measure on an open set  $\Omega \subseteq \mathbb{R}^N$ . The conditions in it are not optimal, but are easy to prove in some interesting cases. A more complete treatment of similar results can be found in [88].

If  $\Omega \subseteq \mathbb{R}^N$  is an open set and  $\mu$  is a positive Borel measure on  $\Omega$ , the space  $\mathcal{C}([0, T], L^1(\mu) - \text{weak})$  is the set of functions  $f : [0, T] \rightarrow L^1(\mu)$  which are continuous when one considers the weak topology on  $L^1(\mu)$  (we call them *weakly continuous functions*). That  $f$  is weakly continuous is equivalent to saying that for all  $\Psi \in L^\infty(\mu)$ ,

$$t \mapsto \int f(t) \Psi \, d\mu \text{ is continuous on } [0, T].$$

Take  $\{V_i\}_{i \in I}$  a fundamental system of neighborhoods of 0 in  $L^1(\mu)$  for the weak topology. We consider the topology on  $\mathcal{C}([0, T], L^1(\mu) - \text{weak})$  for which a fundamental system of neighborhoods of 0 is formed by the sets  $\mathcal{C}([0, T], V_i - \text{weak})$ , for  $i \in I$ , and a fundamental system of neighborhoods of other points is obtained by translation. It can be shown that a sequence of functions  $\{f_n\}$  in  $\mathcal{C}([0, T], L^1(\mu) - \text{weak})$  converges to a function  $f$  in this space if and only if for all  $\Psi \in L^\infty(\mu)$ ,

$$\int f_n(t) \Psi \, d\mu \rightarrow \int f(t) \Psi \, d\mu \quad \text{uniformly for } t \in [0, T].$$

**Proposition 9.3.1.** *Let  $(X, \mathcal{A}, \mu)$  be a positive measure space and  $\{f_n\}$  a sequence of functions in  $\mathcal{C}([0, T], L^1(\mu) - \text{weak})$ . Suppose that there is a set  $K \subseteq L^1(\mu)$  which is weakly compact and such that*

$$f_n(t) \in K \quad \text{for all } t \in [0, T] \text{ and all } n.$$

*Suppose also that there is a function  $f : [0, T] \rightarrow L^1$  such that for all  $\phi \in \mathcal{C}_c^\infty(\Omega)$ ,*

$$\int f_n(t)\phi \, d\mu \rightarrow \int f(t)\phi \, d\mu \quad \text{uniformly in } [0, T].$$

*Then  $f$  is weakly continuous from  $[0, T]$  to  $L^1$  and  $f_n \rightarrow f$  in  $\mathcal{C}([0, T], L^1(\mu) - \text{weak})$ .*

*Proof.* We need to prove that for all  $\Psi \in L^\infty(\mu)$ ,

$$\int f_n(t)\Psi \, d\mu \rightarrow \int f(t)\Psi \, d\mu \quad \text{uniformly in } [0, T].$$

Then, as the convergence is uniform and each function is continuous on  $[0, T]$ , we have that  $t \mapsto \int f(t)\Psi \, d\mu$  is continuous on  $[0, T]$ , so  $f$  is weakly continuous. This same convergence proves that  $f_n \rightarrow f$  in  $\mathcal{C}([0, T], L^1(\mu) - \text{weak})$ .

First, suppose that  $\Psi$  has support contained in a set  $A$  of finite measure. Then  $\Psi$  is integrable and, as  $\mathcal{C}_c^\infty$  is dense in  $L^1(\mu)$ , given a  $\delta > 0$  we can find a function  $\phi \in D$  and a set  $E \subseteq A$  such that

$$\begin{aligned} \mu(E) &\leq \delta \\ |\Psi(y) - \phi(y)| &\leq \delta \quad \text{for all } y \in A \setminus E \\ \|\phi\|_\infty &\leq \|\Psi\|_\infty. \end{aligned}$$

(Thanks to Egorov's theorem, as  $A$  has finite measure; such a  $\phi$  can be found by convolution with a regularizing sequence of functions, and then the last condition also holds.) Now, as  $f_n(t) \in K$  for all  $n$  and  $t$ , Dunford-Pettis' theorem 9.2.2 proves that for any  $\epsilon > 0$  we can choose  $\delta < \epsilon$  such that for all sets  $F \subseteq A$  with  $\mu(F) \leq \delta$  we have

$$\begin{aligned} \int_F |f_n| \, d\mu &\leq \epsilon \quad \text{for all } n \\ \int_F |f| \, d\mu &\leq \epsilon. \end{aligned}$$

So take any  $\epsilon > 0$ ; we choose  $\delta < \epsilon$  such that the latter is satisfied, and then choose  $\phi \in D$  so that the previous equations are also satisfied. Then, for  $t \in [0, T]$ ,

$$\begin{aligned} &\left| \int \Psi f_n(t) \, d\mu - \int \Psi f(t) \, d\mu \right| \\ &\leq \int_A |\Psi - \phi| |f_n(t)| \, d\mu + \left| \int \phi (f_n(t) - f(t)) \, d\mu \right| + \int_A |\phi - \Psi| |f(t)| \, d\mu. \end{aligned}$$



Choose  $n$  so that the middle term is less than  $\epsilon$  for all  $t \in [0, T]$ . The other two terms can be bounded as follows:

$$\begin{aligned} \int_A |\Psi - \phi| |f_n(t)| \, d\mu &\leq \int_{A \setminus E} |\Psi - \phi| |f_n| \, d\mu + \int_E |\Psi| |f_n| \, d\mu + \int_E |\phi| |f_n| \, d\mu \\ &\leq \delta \|f_n\|_1 + \|\Psi\|_\infty \epsilon + \|\phi\|_\infty \epsilon \leq \epsilon(\|f_n\|_1 + 2\|\Psi\|_\infty). \end{aligned}$$

As  $K$  is weakly compact, it is bounded in  $L^1(\mu)$ , so  $\|f_n\|_1 \leq C$  for some  $C > 0$  and all  $n$ . Hence, the previous quantity tends to 0 uniformly in  $n$  when  $\epsilon \rightarrow 0$  and we have proved that for all functions  $\Psi \in L^\infty(\mu)$  with support of finite measure,

$$\int f_n(t) \Psi \, d\mu \rightarrow \int f(t) \Psi \, d\mu \quad \text{uniformly in } [0, T].$$

Now take any function  $\Psi \in L^\infty(\mu)$ . For any  $\epsilon > 0$ , using again Dunford-Pettis' theorem we can find a compact set  $A \subseteq \Omega$  such that for all  $t \in [0, T]$ ,

$$\begin{aligned} \int_{\Omega \setminus A} |f_n(t)| \, d\mu &\leq \epsilon \quad \text{for all } n \\ \int_{\Omega \setminus A} |f(t)| \, d\mu &\leq \epsilon. \end{aligned}$$

Then,

$$\begin{aligned} \left| \int \Psi f_n(t) \, d\mu - \int \Psi f(t) \, d\mu \right| &\leq \left| \int_A \Psi f_n(t) \, d\mu - \int_A \Psi f(t) \, d\mu \right| + \int_{\Omega \setminus A} |\Psi| |f_n| \, d\mu + \int_{\Omega \setminus A} |\Psi| |f| \, d\mu \\ &\leq \left| \int_A \Psi f_n(t) \, d\mu - \int_A \Psi f(t) \, d\mu \right| + 2\epsilon. \end{aligned}$$

Now by choosing  $n$  large enough so that the first term is smaller than  $\epsilon$  we can see that we have the same convergence as before for a general  $\Psi \in L^\infty$ . This proves the result.  $\square$

## 9.4. Young's inequality for real numbers

Here we give a summary of the statement and results related to the well-known Young's inequality, used in the proofs in chapter 5. Proofs and sharper statements can be found in [50].

The most familiar form of Young's inequality, which is frequently used to prove the well-known Hölder inequality for  $L^p$  functions, is the following:

**Theorem 9.4.1 (Young's inequality).** For  $a, b \geq 0$  and  $p, q \geq 1$  such that  $\frac{1}{p} + \frac{1}{q} = 1$  one has

$$ab \leq \frac{1}{p}a^p + \frac{1}{q}b^q.$$

The next theorem is a generalization:

**Theorem 9.4.2 (General Young's inequality).** Let  $c > 0$  and  $f : [0, c] \rightarrow \mathbb{R}$  be a strictly increasing continuous function such that  $f(0) = 0$ . Let  $a \in [0, c]$  and  $b \in [0, f(c)]$ . Then,

$$ab \leq \int_0^a f(x) dx + \int_0^b f^{-1}(x) dx \quad (9.2)$$

Note that we obtain the previous inequality taking  $f(x) := x^{p-1}$ .

In these conditions, if we call

$$\begin{aligned} \Lambda(x) &:= \int_0^x f(y) dy \\ \Lambda^*(x) &:= \int_0^x f^{-1}(y) dy \end{aligned}$$

then another way to state the same result is to say that:

$$ab \leq \Lambda(a) + \Lambda^*(b).$$

As  $\Lambda^*$  can be obtained from  $\Lambda$ , we can rewrite theorem 9.4.2 as follows:

**Theorem 9.4.3 (General Young's inequality, second form).** Take  $c > 0$  and let  $\Lambda : [0, c] \rightarrow \mathbb{R}$  be  $\mathcal{C}^1$  and strictly convex with  $\Lambda(0) = \Lambda'(0) = 0$ . Then for any  $a \in [0, c]$  and  $b \in [0, \Lambda'(c)]$  it holds that

$$ab \leq \Lambda(a) + \Lambda^*(b) \quad (9.3)$$

where

$$\Lambda^*(x) := \int_0^x (\Lambda')^{-1}(y) dy \quad \text{for } x \in \Lambda([0, c]). \quad (9.4)$$

The following is a useful identity relating  $\Lambda$  and  $\Lambda^*$ :

**Lemma 9.4.4.** Let  $c > 0$  and  $\Lambda : [0, c] \rightarrow \mathbb{R}$  be a  $\mathcal{C}^1$  and strictly convex with  $\Lambda(0) = \Lambda'(0) = 0$ . Define  $\Lambda^*$  by (9.4). Then,

$$x\Lambda'(x) = \Lambda(x) + \Lambda^*(\Lambda'(x)). \quad (9.5)$$



# Chapter 10

## Appendix B: Evolution equations in a Banach space

This chapter contains well-known results on evolution equations which are used elsewhere in this thesis. They are mainly based on personal notes by Stéphane Mischler [70].

### 10.1. Solutions of an evolution equation in an abstract separable Banach space

We are interested in defining the concept of solution to the following evolution equation in a certain complete separable normed space  $X$ :

$$\frac{d}{dt}f = F, \tag{10.1}$$

where  $F : (0, T) \rightarrow X$  (for some  $0 < T \leq +\infty$ ). We also want to define a solution of the initial value problem

$$\frac{d}{dt}f = F \tag{10.2}$$

$$f(0) = f^0 \tag{10.3}$$

for some  $f^0 \in X$ .<sup>1</sup>

There are many concepts of solution that occur naturally, and in many situations one cannot just stick to one of them and study solutions in that sense. It is good to be able to find solutions with strong differentiability, but it might be difficult to prove their existence, so one usually needs to find solutions in a weaker sense first. Actually, it may happen that some problems have solutions in a weak sense but not

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<sup>1</sup>The theory developed here is valid for a general interval  $I \subseteq \mathbb{R}$  instead of  $(0, T)$  and a point  $x_0 \in \bar{I}$  instead of 0, with minor modifications.

strong solutions, so some of the properties and behavior of the equation is lost if we only look at strong solutions.

Here we will always suppose that  $F : (0, T) \rightarrow X$  is integrable. Under this regularity requirement we will be able to prove that all the concepts or solution of equation (10.1) or the initial value problem (10.2) defined below are indeed the same one. We will make use of the theory of integration of functions with values on a Banach space; for an introduction see [32].

Let us first state the different definitions of solution we will consider. In the following,  $X$  is a complete separable normed space,  $T \in (0, +\infty]$ ,  $f$  is a function  $f : (0, T) \rightarrow X$  (with no particular regularity assumed) and  $F : (0, T) \rightarrow X$  is in  $L^1((0, T), X)$ . Here we mean a concrete function  $F$  and not a class of functions in  $L^1((0, T), X)$ , though the following definitions are the same if  $F$  is changed in a set of measure zero. We will denote the norm of  $X$  by  $\|\cdot\|$ .

Some of the definitions below have a distinctive name (such as “mild solution” or “weak solution”) and others are stated simply as “solutions”. We will always make clear which definition we are talking about when referring to these.

### 10.1.1. Definitions of solution to the equation

**Definition 10.1.1 (Mild solution).** We say that  $f : (0, T) \rightarrow X$  is a *mild solution* (or *solution in the sense of semigroups*) to equation (10.1) if  $f$  is continuous in the norm topology and

$$f(t_2) = f(t_1) + \int_{t_1}^{t_2} F(s) ds \quad \text{for all } t_1, t_2 \in (0, T). \quad (10.4)$$

**Definition 10.1.2 (Mild solution, no regularity).** We say that  $f : (0, T) \rightarrow X$  is a solution to equation (10.1) if

$$f(t_2) = f(t_1) + \int_{t_1}^{t_2} F(s) ds \quad \text{for almost all } (t_1, t_2) \in (0, T)^2. \quad (10.5)$$

**Definition 10.1.3 (Solution in the sense of moments).** We say that  $f : (0, T) \rightarrow X$  is a *solution in the sense of moments* to equation (10.1) if  $f$  is weakly continuous and

$$\langle f(t_2), \phi \rangle = \langle f(t_1), \phi \rangle + \int_{t_1}^{t_2} \langle F(s), \phi \rangle ds \quad \text{for all } t_1, t_2 \in (0, T), \quad \phi \in X'. \quad (10.6)$$

*Remark 10.1.4.* By *weakly continuous* we mean that  $f : (0, T) \rightarrow X$  is continuous when the weak topology in  $X$  is considered (and the usual one in  $(0, T)$ ). This is equivalent to the statement that  $t \mapsto \langle f(t), \phi \rangle$  is continuous for all  $\phi \in X'$ .

*Remark 10.1.5.* Note that, for all  $\phi \in X'$ ,  $s \mapsto \langle F(s), \phi \rangle$  is integrable in  $(0, T)$ , since  $F : (0, T) \rightarrow X$  is integrable (see [32], part I, III.2.19 (c)).

**Definition 10.1.6 (Solution in the sense of moments, no regularity).** We say that  $f : (0, T) \rightarrow X$  is a solution to equation (10.1) if for all  $\phi \in X'$  it holds that

$$\langle f(t_2), \phi \rangle = \langle f(t_1), \phi \rangle + \int_{t_1}^{t_2} \langle F(s), \phi \rangle ds \quad \text{for almost all } (t_1, t_2) \in (0, T)^2. \quad (10.7)$$

**Definition 10.1.7.** Let  $D \subseteq X'$  be dense in the weak-\* topology. We say that  $f : (0, T) \rightarrow X$  is a solution to equation (10.1) if the conditions in definition 10.1.6 hold for for all  $\phi \in D$  (instead of all  $\phi \in X'$ ).

**Definition 10.1.8 (Weak solution).** We say that  $f : (0, T) \rightarrow X$  is a *weak solution* to equation (10.1) if for all  $\phi \in X'$  we have that  $t \mapsto \langle f(t), \phi \rangle$  is locally integrable in  $(0, T)$  and

$$\int_0^T \langle f(s), \phi \rangle \frac{d}{ds} \psi(s) ds = - \int_0^T \langle F(s), \phi \rangle \psi(s) ds \quad \text{for all } \phi \in X' \quad \psi \in \mathcal{C}_c^\infty(0, T). \quad (10.8)$$

**Definition 10.1.9.** Let  $D \subseteq X'$  be dense in the weak-\* topology. We say that  $f : (0, T) \rightarrow X$  is a solution to equation (10.1) if the conditions in definition 10.1.8 hold for for all  $\phi \in D$  (instead of all  $\phi \in X'$ ).

### 10.1.2. Definitions of solution to the initial value problem

The previous definitions can be easily modified to give definitions of solution to the initial value problem (10.2); we state them here in the same order as before; note that the conditions in the definitions below clearly include those in the corresponding definition from the previous section.

**Definition 10.1.10 (Mild solution).** We say that  $f : (0, T) \rightarrow X$  is a *mild solution* (or *solution in the sense of semigroups*) to the initial value problem (10.2) if  $f$  is continuous in the norm topology and

$$f(t) = f^0 + \int_0^t F(s) ds \quad \text{for all } t \in (0, T). \quad (10.9)$$

**Definition 10.1.11 (Mild solution, no regularity).** We say that  $f : (0, T) \rightarrow X$  is a solution to the initial value problem (10.2) if

$$f(t) = f^0 + \int_0^t F(s) ds \quad \text{for almost all } t \in (0, T). \quad (10.10)$$

**Definition 10.1.12 (Solution in the sense of moments).** We say that  $f : (0, T) \rightarrow X$  is a *solution in the sense of moments* to the initial value problem (10.2) if  $f$  is weakly continuous and

$$\langle f(t), \phi \rangle = \langle f^0, \phi \rangle + \int_0^t \langle F(s), \phi \rangle ds \quad \text{for all } t \in (0, T), \quad \phi \in X'. \quad (10.11)$$

**Definition 10.1.13 (Solution in the sense of moments, no regularity).** We say that  $f : (0, T) \rightarrow X$  is a solution to the initial value problem (10.2) if for all  $\phi \in X'$  it holds that

$$\langle f(t), \phi \rangle = \langle f^0, \phi \rangle + \int_0^t \langle F(s), \phi \rangle ds \quad \text{for almost all } t \in (0, T). \quad (10.12)$$

**Definition 10.1.14.** Let  $D \subseteq X'$  be dense in the weak-\* topology. We say that  $f : (0, T) \rightarrow X$  is a solution to the initial value problem (10.2) if the conditions in definition 10.1.13 hold for for all  $\phi \in D$  (instead of all  $\phi \in X'$ ).

**Definition 10.1.15 (Weak solution).** We say that  $f : (0, T) \rightarrow X$  is a *weak solution* to the initial value problem (10.1) if for all  $\phi \in X'$  we have that  $t \mapsto \langle f(s), \phi \rangle$  is locally integrable in  $(0, T)$  and

$$\int_0^T \langle f(s), \phi \rangle \frac{d}{ds} \psi(s) ds = - \langle f^0, \phi \rangle \psi(0) - \int_0^T \langle F(s), \phi \rangle \psi(s) ds$$

for all  $\phi \in X' \quad \psi \in \mathcal{C}_c^1([0, T])$ . (10.13)

**Definition 10.1.16.** Let  $D \subseteq X'$  be dense in the weak-\* topology. We say that  $f : (0, T) \rightarrow X$  is a solution to the initial value problem (10.2) if the conditions in definition 10.1.15 hold for for all  $\phi \in D$  (instead of all  $\phi \in X'$ ).

The following definitions are easily seen to be equivalent to definitions 10.1.10 and 10.1.12, respectively:

**Definition 10.1.17.** We say that  $f : (0, T) \rightarrow X$  is a *mild solution* (or *solution in the sense of semigroups*) to the initial value problem (10.2) if it is a mild solution to equation (10.1) and  $\|f(t) - f^0\| \rightarrow 0$  when  $t \rightarrow 0^+$ .

**Definition 10.1.18.** We say that  $f : (0, T) \rightarrow X$  is a *solution in the sense of moments* to the initial value problem (10.2) if it is a solution in the sense of moments to equation (10.1) and  $f(t) \rightharpoonup f^0$  in the weak topology when  $t \rightarrow 0^+$ .

### 10.1.3. Equivalence of the definitions

Under the previous assumptions, these definitions are equivalent: a solution in the sense of any of them is also a solution in the sense of all the others, possibly after being changed in a set of measure zero. The key assumption is the regularity of the function  $F$  in equation (10.1); some of these solutions make sense when  $F$  is less regular and then it may happen that not all of these concepts are equivalent; however, they are when  $F$  is integrable.

**Theorem 10.1.19 (Equivalence of the concepts of solution to the equation).** *If a function  $f : (0, T) \rightarrow X$  is a solution to equation (10.1) in the sense of any of the previous definitions, then it can be modified in a set of measure zero so that it becomes a solution to equation (10.1) in the sense of all of the previous definitions.*

**Theorem 10.1.20.** *If a function  $f : (0, T) \rightarrow X$  is a solution to the initial value problem (10.2) in the sense of any of the definitions in section 10.1.2, then it can be modified in a set of measure zero so that it becomes a solution to the initial value problem in the sense of all of the definitions in section 10.1.2.*

## 10.2. Solutions in $L^1$

Let  $\Omega$  be an open subset of  $\mathbb{R}^N$  and  $\mu$  a positive Borel measure on  $\Omega$ . We can put  $X = L^1(\Omega, \mu)$  (which we denote as  $L^1(\Omega)$ , understanding the measure  $\mu$ ) in the previous section and obtain several definitions of solution of an evolution equation in  $L^1(\Omega)$ , which have been proved to be equivalent when the  $F$  in equation (10.1) is regular enough. Here we want to particularize the definitions in this case and add another one when  $\mu$  is finite on compact sets, that of *renormalized solution*, which does not have a direct analogy in an abstract Banach space.

Of course, definitions in the previous section *do* directly apply to the case  $X = L^1(\Omega)$ , but it is sometimes more convenient to phrase them in slightly different terms: equality between functions in  $L^1$  is usually expressed as equality a.e., and an integrable function  $F : (0, T) \rightarrow L^1(\Omega)$  is more commonly regarded as a real integrable function on  $(0, T) \times \Omega$ . We start by stating this latter relationship precisely, after [32, theorem III.11.16]:

**Theorem 10.2.1.** *Let  $0 < T \leq +\infty$  and  $(S, \mathcal{A}, \mu)$  be a positive measure space. We consider the Lebesgue measure  $dt$  on  $(0, T)$  and the product measure  $dt \otimes \mu$  on  $(0, T) \times S$ .*

1. *If  $\tilde{f} : (0, T) \rightarrow L^1(S)$  is integrable, then there exists an integrable function  $f : (0, T) \times S \rightarrow \mathbb{R}$  such that  $f(t, \cdot) = \tilde{f}(t)$  for almost all  $t \in (0, T)$ .*
2. *Let  $f : (0, T) \times S \rightarrow \mathbb{R}$  be an integrable function. Then the function  $\tilde{f} : (0, T) \rightarrow L^1(S)$  defined for almost all  $t \in (0, T)$  by  $\tilde{f}(t) := f(t, \cdot)$  is integrable.*

*In any of these cases  $\int_0^T f(t, x) dt$  (which exists for almost all  $x \in S$ ) is a.e. equal to  $\int_0^T \tilde{f}(t) dt$ .*

This enables us to speak interchangeably of integrable functions from  $(0, T)$  to  $L^1(\Omega)$  and integrable functions on  $(0, T) \times \Omega$ . Definitions 10.1.1–10.1.9 and the corresponding definitions of solution to the initial value problem can easily be rewritten in this case.

### 10.2.1. Renormalized solutions

The following definition is different from the above ones:



**Definition 10.2.2 (Renormalized solution).** We say that a measurable function  $f : (0, T) \times \Omega \rightarrow \mathbb{R}$  is a *renormalized solution* of equation (10.1) if, in the sense of distributions in  $(0, T) \times \Omega$ ,

$$\frac{d}{dt}\beta(f) = \beta'(f)F \quad \text{for all } \beta \in \mathcal{C}^{1,b}(\mathbb{R}). \quad (10.14)$$

*Remark 10.2.3.* The notation  $\mathcal{C}^{1,b}(A)$  represents the set of all bounded functions with continuous and bounded first-order derivatives in a set  $A \subseteq \mathbb{R}^N$ .

*Remark 10.2.4.* Note that the expressions in the definition make sense:  $\beta$  being continuous and bounded,  $\beta(f)$  is measurable and bounded, so it is a distribution; for similar reasons  $\beta'(f)$  is in  $L^\infty((0, T) \times \Omega)$ , so  $\beta'(f)F$  is integrable on  $(0, T) \times \Omega$  and in particular is a distribution.

The following results are well-known:

**Theorem 10.2.5.** *Let  $f$  be a renormalized solution to equation (10.1). If  $f$  is in  $L^1((0, T) \times \Omega)$ , then  $f$  is almost everywhere equal to a solution to (10.1) in the sense of all of our previous definitions.*

**Theorem 10.2.6.** *Let  $f$  be a solution in  $L^1$  to equation (10.1) in the sense of any of the definitions 10.1.1–10.1.8. Then,  $f$  is also a renormalized solution to equation (10.1).*

**Theorem 10.2.7.** *Let  $f$  be a mild solution to the initial value problem (10.2) in the space  $X = L^1(\Omega)$ . Then for all piecewise differentiable  $\beta : \mathbb{R} \rightarrow \mathbb{R}$  such that  $\beta'(f)F \in L^1((0, T) \times \Omega)$  and  $\beta(f^0) \in L^1(\Omega)$  it happens that  $\beta(f) : (0, T) \rightarrow L^1(\Omega)$  is continuous in the norm topology and*

$$\beta(f(t)) = \beta(f^0) + \int_0^t \beta'(f(s))F(s) ds \quad \text{for all } t \in (0, T). \quad (10.15)$$

(This is,  $\beta(f)$  is a mild solution of the initial value problem  $\frac{d}{dt}g = \beta'(f)F$ ,  $g(0) = \beta(f^0)$ ; note that this is stronger than (10.14)). As a consequence, for all  $\psi \in L^\infty(\Omega)$ , we have that  $\int_\Omega \beta(f)\psi d\mu(x)$  is absolutely continuous on  $[0, T)$  and

$$\frac{d}{dt} \int_\Omega \beta(f)\psi d\mu(x) = \int_\Omega \beta'(f)F\psi d\mu(x).$$

# Chapter 11

## Appendix D: Some useful inequalities

When estimating the size of the coagulation and fragmentation terms in the continuous coagulation-fragmentation equation, one often needs to find inequalities of the kind

$$(x^\alpha y^\beta + y^\alpha x^\beta)((x+y)^k - x^k - y^k) \leq \pm C (x^\mu y^\nu + y^\mu x^\nu) \quad \text{for } x, y > 0, \quad (11.1)$$

$$(x^\alpha y^\beta + y^\alpha x^\beta)((x+y)^k - x^k - y^k) \geq \pm C (x^\mu y^\nu + y^\mu x^\nu) \quad \text{for } x, y > 0, \quad (11.2)$$

where  $\alpha, \beta, k, \mu, \nu$  are real numbers and  $C > 0$  is a positive constant. Sometimes the inequality is needed only for small or large values of  $x, y$ . Here we deduce the optimal exponents  $\mu, \nu$  for this kind of bound. Inequalities of this kind have been proved in various works on the coagulation-fragmentation equations (e.g. [33, 20, 16, 34]), but to our knowledge a complete study of the possible cases, though not difficult, is new.

First of all, observe that for any  $x, y > 0$ ,

$$\begin{aligned} (x+y)^k - x^k - y^k &\leq 0 & \text{if } k \leq 1 \\ (x+y)^k - x^k - y^k &\geq 0 & \text{if } k \geq 1. \end{aligned}$$

Hence, some inequalities of the kind 11.1, 11.2 are trivial; namely, the following hold for any  $\alpha, \beta, \mu, \nu \in \mathbb{R}$  and any  $C, x, y > 0$ :

$$\begin{aligned} (x^\alpha y^\beta + y^\alpha x^\beta)((x+y)^k - x^k - y^k) &\leq C (x^\mu y^\nu + y^\mu x^\nu) & \text{when } k \leq 1, \\ (x^\alpha y^\beta + y^\alpha x^\beta)((x+y)^k - x^k - y^k) &\geq -C (x^\mu y^\nu + y^\mu x^\nu) & \text{when } k \geq 1. \end{aligned}$$

We say that an inequality of the kind (11.1) or (11.2) is *nontrivial* when it is not one of the above (this is, when both terms are of the same sign). Note that for  $k = 1$  the inequality is always trivial: the left hand side is zero and the inequality has no interest.

As the functions involved are all homogeneous, it is useful to write them in a different form with a polar change of variables:

$$\begin{aligned}x &:= r\cos\theta \equiv rc \\ y &:= r\sin\theta \equiv rs.\end{aligned}$$

(We write  $c$  for  $\cos\theta$  and  $s$  for  $\sin\theta$  for convenience in the calculations below.) Then, one has

$$\begin{aligned}(x^\alpha y^\beta + y^\alpha x^\beta)((x+y)^k - x^k - y^k) &= r^{\alpha+\beta+k} ((c^\alpha s^\beta + s^\alpha c^\beta)((c+s)^k - c^k - s^k)) \\ x^\mu y^\nu + y^\mu x^\nu &= r^{\mu+\nu} (c^\mu s^\nu + s^\mu c^\nu).\end{aligned}$$

and the inequalities (11.1), (11.2) are translated into

$$r^{\alpha+\beta+k} ((c^\alpha s^\beta + s^\alpha c^\beta)((c+s)^k - c^k - s^k)) \leq \pm C r^{\mu+\nu} (c^\mu s^\nu + s^\mu c^\nu) \quad (11.3)$$

$$r^{\alpha+\beta+k} ((c^\alpha s^\beta + s^\alpha c^\beta)((c+s)^k - c^k - s^k)) \geq \pm C' r^{\mu+\nu} (c^\mu s^\nu + s^\mu c^\nu). \quad (11.4)$$

Any of the inequalities (11.1), (11.2) holds for all  $x, y > 0$  if and only if (11.3), (11.4), respectively, holds for all  $r > 0$  and all  $0 < \theta < \pi/2$ . Then it is clear that the following are true:

**Lemma 11.0.8.** *Suppose that any nontrivial inequality of the kind (11.1) or (11.2) holds for all  $x, y > 0$ . Then,*

$$\alpha + \beta + k = \mu + \nu.$$

To make notation easier, let us call

$$\begin{aligned}f(\theta) &:= (c^\alpha s^\beta + s^\alpha c^\beta)((c+s)^k - c^k - s^k) \\ g(\theta) &:= r^{\mu+\nu} (c^\mu s^\nu + s^\mu c^\nu).\end{aligned}$$

By fixing  $r$  or  $\theta$ , it is also clear that a nontrivial inequality of the kind (11.1) or (11.2) holds if and only if the inequalities

$$\begin{aligned}r^{\alpha+\beta+k} &\leq [\geq] C' r^{\mu+\nu} \\ f(\theta) &\leq [\geq] \pm C' g(\theta)\end{aligned}$$

hold for some other constant  $C'$ , in the right direction (which can be easily deduced, and which we do not explicitly list to avoid a cumbersome statement), and for the same range of values of  $r, \theta$ . As it is easy to compare  $r^{\alpha+\beta+k}$  and  $r^{\mu+\nu}$ , all we need is to be able to compare  $f(\theta)$  and  $g(\theta)$ . Additionally, to compare these two functions we only need to study their order near  $\theta = 0$ , as they are positive for  $\theta \in (0, \pi/2)$  and symmetric about  $\theta = \pi/4$ . We will do this next.

In the following we repeatedly use that for  $\theta < 0$  sufficiently small (i.e.  $\theta < \pi/8$ ), there is some constant  $0 < C < 1$  such that

$$C\theta \leq s = \sin\theta < \theta$$

$$C \leq c = \cos\theta < 1.$$

We also assume that

$$\alpha \leq \beta$$

$$\mu \leq \nu.$$

### **Bounds for $g(\theta)$**

For all  $\theta$  sufficiently small, we have that

$$g(\theta) \leq \theta^\mu + \theta^\nu \leq 2\theta^\mu \tag{11.5}$$

$$g(\theta) \geq C^{\mu+\nu}\theta^\mu. \tag{11.6}$$

### **Bounds for $f(\theta)$**

First of all, observe that thanks to the mean value theorem we can find positive constants  $C_1, C_2$  which depend on  $k \in \mathbb{R} \setminus \{0\}$  such that, for all  $\theta$  sufficiently small (depending on  $k$ ),

$$C_1\theta \leq (s+c)^k - c^k \leq C_2\theta \quad \text{for } k > 0$$

$$-C_2\theta \leq (s+c)^k - c^k \leq -C_1\theta \quad \text{for } k < 0.$$

(one can take  $C_1 = |k| \min\{C^{k-1}, 2^{k-1}\}$ ,  $C_2 = |k| \max\{C^{k-1}, 2^{k-1}\}$ ). Also, for all  $k \in \mathbb{R} \setminus \{0\}$  we can find constants  $C_3, C_4$  (which depend on  $k$ ) such that, for all  $\theta$  sufficiently small,

$$C_3\theta^k \leq s^k \leq C_4\theta^k.$$

With these two bounds, by comparing the two powers  $\theta$  and  $\theta^k$ , it is easy to prove the following:

- For  $k > 1$ , there are constants  $C_1, C_2 > 0$  and  $\epsilon > 0$  such that

$$C_1\theta < (s+c)^k - c^k - s^k < C_2\theta \quad \text{for } 0 < \theta < \epsilon.$$

- For  $k < 1$ , there are constants  $C_1, C_2 > 0$  and  $\epsilon > 0$  such that

$$-C_1\theta^k < (s+c)^k - c^k - s^k < -C_2\theta^k \quad \text{for } 0 < \theta < \epsilon.$$

This gives bounds for one of the factors in  $f(\theta)$ ; observe that the other factor is of the same form as  $g(\theta)$  with different exponents, so (11.5) and (11.6) give bounds for it (with  $\alpha$  instead of  $\mu$ ). We deduce that

- For  $k > 1$ , there are constants  $C_1, C_2 > 0$  and  $\epsilon > 0$  such that

$$C_1\theta^{\alpha+1} < f(\theta) < C_2\theta^{\alpha+1} \quad \text{for } 0 < \theta < \epsilon.$$

- For  $k < 1$ , there are constants  $C_1, C_2 > 0$  and  $\epsilon > 0$  such that

$$-C_1\theta^{\alpha+k} < f(\theta) < -C_2\theta^{\alpha+k} \quad \text{for } 0 < \theta < \epsilon.$$

## 11.1. Inequalities

With the bounds of the previous sections we can find which inequalities of the kind (11.1), (11.2) hold for any range of values of  $y, y'$ ; we will study them in two different cases: for small  $y, y'$  and for large  $y, y'$  (in particular we obtain the inequalities that hold for all  $y, y' > 0$ ).

First of all, observe that some expressions of the form  $x^\mu y^\nu + y^\mu x^\nu$  are comparable. The bounds for  $g(\theta)$  obtained before give the following:

**Lemma 11.1.1.** *Take  $\mu \leq \nu \in \mathbb{R}$ ,  $\mu' \leq \nu' \in \mathbb{R}$ , and any  $R > 0$ . We consider whether the following inequality holds for some  $C > 0$  and  $y, y'$  in some set:*

$$x^\mu y^\nu + y^\mu x^\nu \leq C x^{\mu'} y^{\nu'} + y^{\mu'} x^{\nu'} \quad (11.7)$$

*It happens that:*

- *Inequality (11.7) holds for all  $y, y' > 0$  with  $y + y' \leq R$  and some constant  $C > 0$  if and only if*

$$\begin{aligned} \mu + \nu &\geq \mu' + \nu' \\ \mu &\geq \mu'. \end{aligned}$$

- *Inequality (11.7) holds for all  $y, y' > 0$  with  $y + y' \geq R$  and some constant  $C > 0$  if and only if*

$$\begin{aligned} \mu + \nu &\leq \mu' + \nu' \\ \mu &\geq \mu'. \end{aligned}$$

It is clear then that, for a given range of values of  $y, y'$ , some inequalities of the kind (11.1), (11.2) are consequences of others by using the above inequalities. We will say that a nontrivial inequality  $A$  of the form (11.1) or (11.2) is *better* than another inequality  $B$  of the same form if  $B$  is directly deduced from  $A$  by one of the inequalities in the previous lemma (this is, if their right hand sides are comparable for the range of values of  $y, y'$  in question).

**Proposition 11.1.2 (Inequalities with  $\leq$ ).** *Take  $\alpha < \beta \in \mathbb{R}$ ,  $\mu < \nu \in \mathbb{R}$ ,  $k \in \mathbb{R}$ ,  $R > 0$ .*

- *If  $k > 1$ , we consider the inequality*

$$(x^\alpha y^\beta + y^\alpha x^\beta)((x + y)^k - x^k - y^k) \leq C(x^\mu y^\nu + y^\mu x^\nu). \quad (11.8)$$

- *Inequality (11.8) holds for all  $y, y' < R$  and some  $C > 0$  if and only if*

$$\begin{aligned} \alpha + \beta + k &\geq \mu + \nu \\ \alpha + 1 &\geq \mu. \end{aligned}$$

- Inequality (11.8) holds for all  $y, y' \geq R$  and some  $C > 0$  if and only if

$$\begin{aligned}\alpha + \beta + k &\leq \mu + \nu \\ \alpha + 1 &\geq \mu.\end{aligned}$$

- If  $k < 1$ , we consider the inequality

$$(x^\alpha y^\beta + y^\alpha x^\beta)((x + y)^k - x^k - y^k) \leq -C(x^\mu y^\nu + y^\mu x^\nu). \quad (11.9)$$

- Inequality (11.9) holds for all  $y, y' < R$  and some  $C > 0$  if and only if

$$\begin{aligned}\alpha + \beta + k &\leq \mu + \nu \\ \alpha + k &\leq \mu.\end{aligned}$$

- Inequality (11.9) holds for all  $y, y' \geq R$  and some  $C > 0$  if and only if

$$\begin{aligned}\alpha + \beta + k &\geq \mu + \nu \\ \alpha + k &\leq \mu.\end{aligned}$$

**Proposition 11.1.3 (Inequalities with  $\geq$ ).** Take  $\alpha < \beta \in \mathbb{R}$ ,  $\mu < \nu \in \mathbb{R}$ ,  $k \in \mathbb{R}$ ,  $R > 0$ .

- If  $k > 1$ , we consider the inequality

$$(x^\alpha y^\beta + y^\alpha x^\beta)((x + y)^k - x^k - y^k) \geq C(x^\mu y^\nu + y^\mu x^\nu). \quad (11.10)$$

- Inequality (11.10) holds for all  $y, y' < R$  and some  $C > 0$  if and only if

$$\begin{aligned}\alpha + \beta + k &\leq \mu + \nu \\ \alpha + 1 &\leq \mu.\end{aligned}$$

- Inequality (11.10) holds for all  $y, y' \geq R$  and some  $C > 0$  if and only if

$$\begin{aligned}\alpha + \beta + k &\geq \mu + \nu \\ \alpha + 1 &\leq \mu.\end{aligned}$$

- If  $k < 1$ , we consider the inequality

$$(x^\alpha y^\beta + y^\alpha x^\beta)((x + y)^k - x^k - y^k) \geq -C(x^\mu y^\nu + y^\mu x^\nu). \quad (11.11)$$

- Inequality (11.11) holds for all  $y, y' < R$  and some  $C > 0$  if and only if

$$\begin{aligned}\alpha + \beta + k &\geq \mu + \nu \\ \alpha + k &\geq \mu.\end{aligned}$$

- Inequality (11.11) holds for all  $y, y' \geq R$  and some  $C > 0$  if and only if

$$\begin{aligned}\alpha + \beta + k &\leq \mu + \nu \\ \alpha + k &\geq \mu.\end{aligned}$$



# Bibliography

- [1] D. J. Aldous. Deterministic and stochastic models for coalescence (aggregation, coagulation): a review of the mean-field theory for probabilists. *Bernoulli*, 5:3–48, 1999.
- [2] A. Arnold, J. L. López, P. A. Markowich, and J. Soler. An analysis of quantum Fokker-Planck models: a Wigner function approach. *Rev. Mat. Iberoamericana*, 20(3):771–814, 2004.
- [3] J. M. Ball and J. Carr. Asymptotic behaviour of solutions to the Becker-Döring equations for arbitrary initial data. *Proc. Roy. Soc. Edinburgh Sect. A*, 108:109–116, 1988.
- [4] J. M. Ball and J. Carr. The discrete coagulation-fragmentation equations: existence, uniqueness and density conservation. *J. Stat. Phys.*, 61:203–234, 1990.
- [5] J. M. Ball, J. Carr, and O. Penrose. The Becker-Döring cluster equations: basic properties and asymptotic behaviour of solutions. *Comm. Math. Phys.*, 104:657–692, 1986.
- [6] R. Becker and W. Döring. Kinetische Behandlung der Keimbildung in übersättigten Dämpfen. *Ann. Phys. (Leipzig)*, 24:719–752, 1935.
- [7] N. Bellomo, A. Bellouquid, and M. Delitala. Mathematical topics on the modelling complex multicellular systems and tumor immune cells competition. *Math. Models Methods Appl. Sci.*, 14(11):1683–1733, 2004.
- [8] L. L. Bonilla, A. Carpio, and J. C. Neu. Igniting homogeneous nucleation. In F. J. Higuera, J. Jiménez, and J. M. Vega, editors, *Simplicity, Rigor and Relevance in Fluid Mechanics*. CIMNE, Barcelona, 2004.
- [9] F. Bouchut. Smoothing effect for the non-linear Vlasov-Poisson-Fokker-Planck equation. *J. Diff. Eqs.*, 122:225–238, 1995.
- [10] H. Brézis. *Analyse Fonctionnelle*. Masson, Paris, 1983.



- [11] R. Caffisch and G. C. Papanicolaou. Dynamic theory of suspensions with Brownian effects. *SIAM J. Appl. Math.*, 43(4):885–906, 1983.
- [12] A. O. Caldeira and A. J. Leggett. Path integral approach to quantum Brownian motion. *Physica A*, 121:587–616, 1983.
- [13] J. A. Cañizo, J. L. López, and J. J. Nieto. Global  $L^1$  theory and regularity for the 3D nonlinear Wigner-Poisson-Fokker-Planck system. *J. Differential Equations*, 198(2):356–373, 2004.
- [14] J. A. Cañizo Rincón. Asymptotic behaviour of solutions to the generalized Becker-Döring equations for general initial data. *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.*, 461(2064):3731–3745, 2005.
- [15] J. Carr. Asymptotic behaviour of solutions to the coagulation-fragmentation equations. I. The strong fragmentation case. *Proc. Roy. Soc. Edinburgh Sect. A*, 121:231–244, 1992.
- [16] J. Carr and F. P. da Costa. Asymptotic behavior of solutions to the coagulation-fragmentation equations. II. Weak fragmentation. *J. Stat. Phys.*, 77:98–123, 1994.
- [17] J. A. Carrillo, J. Soler, and J. L. Vázquez. Asymptotic behaviour and self-similarity for the three dimensional Vlasov-Poisson-Fokker-Planck system. *J. Funct. Anal.*, 141:99–132, 1996.
- [18] F. Castella, L. Erdős, F. Frommlet, and P. A. Markowich. Fokker-Planck equations as scaling limits of reversible quantum systems. *J. Stat. Phys.*, 100:543–601, 2000.
- [19] J. F. Collet, T. Goudon, F. Poupaud, and A. Vasseur. The Becker-Döring system and its Lifshitz-Slyozov limit. *SIAM J. Appl. Math.*, 62:1488–1500, 2002.
- [20] F. P. da Costa. Asymptotic behaviour of low density solutions to the generalized Becker-Döring equations. *NoDEA Nonlinear Differential Equations Appl.*, 5:23–37, 1998.
- [21] E. B. Davies. *Quantum Theory of Open Systems*. Academic Press, New York, 1976.
- [22] C. Dellacherie and P. A. Meyer. *Probabilités et potentiel*, chapter I-IV, pages 85–115. Hermann, Paris, 1975.
- [23] J. Dieudonné. Sur les espaces de Köthe. *J. Analyse Math.*, 1:85–115, 1951.
- [24] L. Diósi. Caldeira-Leggett master equation and medium temperatures. *Physica A*, 199:517–526, 1993.

- [25] L. Diósi. On high-temperature Markovian equation for quantum Brownian motion. *Europhys. Lett.*, 22:1–3, 1993.
- [26] L. Diósi, N. Gisin, J. Halliwell, and I. C. Percival. Decoherent histories and quantum state diffusion. *Phys. Rev. Lett.*, 74 (2):203–207, 1995.
- [27] R. L. Drake. A general mathematical survey of the coagulation equation. In G. M. Hidy and J. R. Brock, editors, *Topics in Current Aerosol Research (Part 2)*, volume 3 of *International Reviews in Aerosol Physics and Chemistry*, pages 201–376. Pergamon, 1972.
- [28] P. B. Dubovskii. *Mathematical Theory of Coagulation*, volume 23 of *Lecture Notes*. Global Analysis Research Center, Seoul National University, 1994.
- [29] P. B. Dubovskii and I. W. Stewart. Existence, uniqueness and mass conservation for the coagulation-fragmentation equation. *Math. Methods Appl. Sci.*, 19:571–591, 1996.
- [30] N. Dunford. A mean ergodic theorem. *Duke Math. J.*, 5:635–646, 1939.
- [31] N. Dunford and B. J. Pettis. Linear operators on summable functions. *Trans. Amer. Math. Soc.*, 47:323–392, 1940.
- [32] N. Dunford and J. T. Schwartz. *Linear Operators (Part I)*. John Wiley & Sons Inc., New York, 1963.
- [33] M. Escobedo, P. Laurençot, S. Mischler, and B. Perthame. Gelation and mass conservation in coagulation-fragmentation models. *J. Differential Equations*, 195(1):143–174, 2003.
- [34] M. Escobedo and S. Mischler. Dust and self-similarity for the Smoluchowski coagulation equation. To appear.
- [35] M. Escobedo, S. Mischler, and B. Perthame. Gelation in coagulation and fragmentation models. *Comm. Math. Phys.*, 231:157–188, 2002.
- [36] M. Escobedo, S. Mischler, and M. R. Ricard. On self-similarity and stationary problem for fragmentation and coagulation models. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 22(1):99–125, 2005.
- [37] W. R. Frensley. Boundary conditions for open quantum systems driven far from equilibrium. *Rev. Mod. Phys.*, 62(3):745–791, 1990.
- [38] V. A. Galkin and P. B. Dubovskii. Solution of the coagulation equations with unbounded kernels. *Differential Equations*, 2:373–378, 1986.
- [39] U. Gasser, E. Weeks, A. Schofield, P. N. Pursey, and D. A. Weitz. *Science*, 292(258), 2001.

- [40] T. Goudon, P.-E. Jabin, and A. Vasseur. Hydrodynamic limit for the Vlasov-Navier-Stokes equations. I. Light particles regime. *Indiana Univ. Math. J.*, 53(6):1495–1515, 2004.
- [41] T. Goudon, P.-E. Jabin, and A. Vasseur. Hydrodynamic limit for the Vlasov-Navier-Stokes equations. II. Fine particles regime. *Indiana Univ. Math. J.*, 53(6):1517–1536, 2004.
- [42] M. Grabe, J. Neu, G. Oster, and P. Nollert. Protein interactions and membrane geometry. *Biophysical Journal*, 84:654–868, 2003.
- [43] M. P. Gualdani, A. Jüngel, and G. Toscani. Exponential decay in time of solutions of the viscous quantum hydrodynamic equations. To appear in *Appl. Math. Lett.*
- [44] M. A. Herrero and M. Rodrigo. A note on Smoluchowski’s equations with diffusion. *Appl. Math. Lett.*, 18(9):969–975, 2005.
- [45] M. A. Herrero, J. J. L. Velázquez, and D. Wrzosek. Sol-gel transition in a coagulation-diffusion model. *Phys. D*, 141(3-4):221–247, 2000.
- [46] J. N. Israelachvili. *Intermolecular and surface forces*. Academic Press, New York, second edition, 1991.
- [47] P.-E. Jabin and B. Niethammer. On the rate of convergence to equilibrium in the Becker-Döring equations. *J. Differential Equations*, 191:518–543, 2003.
- [48] P.-E. Jabin and F. Otto. Identification of the dilute regime in particle sedimentation. *Comm. Math. Phys.*, 250(2):415–432, 2004.
- [49] P.-E. Jabin and J. Soler. A kinetic description of particle fragmentation. To appear in *Math. Mod. Meth. Appl. Sci.*
- [50] A. Kufner, O. John, and S. Fučík. *Function Spaces*. Noordhoff International Publishing, Leyden, 1977.
- [51] J. C. Lasheras, C. Eastwood, C. Martínez-Bazán, and J. L. Montañés. A review of statistical models for the break-up of an immiscible fluid immersed into a fully developed turbulent flow. *Int. J. Multiphase Flow*, 28:247–278, 2002.
- [52] P. Laurençot. On a class of continuous coagulation-fragmentation equations. *J. Differential Equations*, 167:145–174, 2000.
- [53] P. Laurençot. The discrete coagulation equation with multiple fragmentation. *Proc. Edinburgh Math. Soc.*, 45:67–82, 2002.
- [54] P. Laurençot and S. Mischler. The continuous coagulation-fragmentation equations with diffusion. *Arch. Rational Mech. Anal.*, 162:45–99, 2002.

- [55] P. Laurençot and S. Mischler. From the Becker-Döring to the Lifshitz-Slyozov-Wagner equations. *J. Statist. Phys.*, 106(5–6):957–991, 2002.
- [56] P. Laurençot and S. Mischler. From the discrete to the continuous coagulation-fragmentation equations. *Proc. Roy. Soc. Edinburgh Sect. A*, 132:1219–1248, 2002.
- [57] P. Laurençot and S. Mischler. Global existence for the discrete diffusive coagulation-fragmentation equation in  $L^1$ . *Rev. Mat. Iberoamericana*, 18:731–745, 2002.
- [58] P. Laurençot and S. Mischler. On coalescence equations and related models. In P. Degond, L. Pareschi, and G. Russo, editors, *Topics in Current Aerosol Research (Part 2)*, Modelling and Simulation in Science, Engineering and Technology. Birkhauser, 2004.
- [59] E. M. Lifshitz and L. P. Pitaevskii. *Physical Kinetics*. Pergamon Press, New York, 1981.
- [60] I. M. Lifshitz and V. V. Slyozov. The kinetics of precipitation from supersaturated solid solutions. *J. Phys. Chem. Solids*, 19:35–50, 1961.
- [61] G. Lindblad. On the generators of quantum dynamical semigroups. *Comm. Math. Phys.*, 48:119–130, 1976.
- [62] P. L. Lions and T. Paul. Sur les mesures de Wigner. *Revista Matemática Iberoamericana*, 48(3):553–618, 1993.
- [63] A. A. Lushnikov. Coagulation in finite systems. *J. Colloid Interface Sci.*, 65:276–285, 1978.
- [64] A. H. Marcus. Stochastic coalescence. *Technometrics*, 10:133–143, 1968.
- [65] S. P. Marsh and M. E. Glicksman. *Acta Mater.*, 44:3761, 1996.
- [66] J. B. McLeod. On an infinite set of non-linear differential equations. *Quart. J. Math. Oxford Ser. (2)*, 13:119–128, 1962.
- [67] J. B. McLeod. On an infinite set of non-linear differential equations (II). *Quart. J. Math. Oxford Ser. (2)*, 13:193–205, 1962.
- [68] J. B. McLeod. On the scalar transport equation. *Proc. London Math. Soc. (3)*, 14:445–458, 1964.
- [69] Z. A. Melzak. A scalar transport equation. *Trans. Amer. Math. Soc.*, 85:445–458, 1964.
- [70] S. Mischler. Quelques outils d’analyse fonctionnelle. Unpublished notes, 2004.

- [71] S. Mischler and M. R. Ricard. Existence globale pour l'équation de Smoluchowski continue non homogène et comportement asymptotique des solutions. *C. R. Acad. Sci. Paris Sér. I Math*, 336:407–412, 2003.
- [72] H. Müller. Zur allgemeinen Theorie der raschen Koagulation. *Kolloidchemische Beihefte*, 27:223–250, 1928.
- [73] J. Neu, J. A. Cañizo, and L. L. Bonilla. Three eras of micellization. *Physical Review E*, 66:061406, 2002.
- [74] B. Niethammer. On the evolution of large clusters in the Becker-Döring model. *J. Nonlinear Science*, 13(1):115–155, 2003.
- [75] J. J. M. Nieto and J. L. López. Global solutions of the mean-field, very-high temperature Caldeira-Leggett master equation. *Quart. Appl. Math.*, (64):189–199, 2006.
- [76] K. Ono and W. Strauss. Regular solutions of the Vlasov-Poisson-Fokker-Planck system. *Discrete Contin. Dynam. Systems*, 6(4):751–772, 2000.
- [77] A. Pazy. *Semigroups of Linear Operators and Applications to Partial Differential Equations*. Springer-Verlag, New York, 1983.
- [78] O. Penrose. The Becker-Döring equations at large times and their connection with the LSW theory of coarsening. *J. Stat. Phys.*, 19:243–267, 1997.
- [79] O. Penrose and J. L. Lebowitz. Towards a rigorous theory of metastability. volume VII of *Studies in Statistical Mechanics*. North-Holland, 1979.
- [80] S. M. Ph. Laurençot. Notes on the Becker-Döring equation. Personal notes.
- [81] Y. B. Rumer. *Thermodynamics, Statistical Physics and Kinetics*. MIR publishers, Moscow, Russia, 1980. ISBN 5-88417-021-1.
- [82] M. Slemrod. *The Becker-Döring equations*, pages 149–171. Modelling and Simulation in Science, Engineering and Technology. Birkhäuser, Boston, 2000.
- [83] M. Smoluchowski. Drei Vorträge über Diffusion, Brownsche Molekularbewegung und Koagulation von Kolloidteilchen. *Physik. Zeitschr.*, 17:557–599, 1916.
- [84] M. Smoluchowski. Versuch einer mathematischen Theorie der Koagulationskinetik kolloider Lösungen. *Zeitschrift für physik. Chemie*, 92:129–168, 1917.
- [85] J. L. Spouge. An existence theorem for the discrete coagulation-fragmentation equations. *Math. Proc. Cambridge Philos. Soc.*, 96:351–357, 1984.
- [86] I. W. Stewart. A global existence theorem for the general coagulation-fragmentation equation with unbounded kernels. *Math. Methods Appl. Sci.*, 11:627–648, 1989.

- [87] I. W. Stewart. On the coagulation-fragmentation equation. *Z. Angew. Math. Phys.*, 41:917–924, 1990.
- [88] I. I. Vrabie. *Compactness methods for nonlinear evolutions*, volume 75 of *Pitman Monogr. Surveys Pure Appl. Math.* Longman, Harlow, second edition, 1995.
- [89] S. Q. Xiao and P. Haasen. On the coagulation-fragmentation equation. *Acta Metall. Mater.*, 39:651, 1991.