SENSITIVITY FOR SMOLUCHOWSKI EQUATION

I.F. BAILLEUL

Abstract. This article investigates the question of sensitivity of the solutions μ_t^λ of the Smoluchowski equation on $\mathbb{R}_+^*$ with respect to parameters λ in the interaction kernel K^λ. It is proved that μ_t^λ is a $\mathcal{C}^1$ function of (t,λ) with values in a good space of measures under the hypotheses $K^\lambda(x,y) \leqslant \varphi(x)\,\varphi(y)$, for some sub-linear function φ, and $\displaystyle\int \varphi^{4+\varepsilon}(x)\,\mu_0(dx) < \infty$, and that the derivative is the unique solution of a related equation.

1. Introduction

a) Smoluchowski equation. Many chemical reactions, such as soot formation [1] or flame synthesis of organic or inorganic nanoparticles [2], have in common a microscopic mechanism where particles of different masses evolve in a homogeneous medium. Each of them performs a free thermal motion, with diffusivity depending on its mass, until it approaches enough any other particle. These two particles will then coagulate to create a new one, whose stucture will be a combination of the strucutres of each of its ancestors [3], [4].

The experimentor has only access to macroscopic quantities such as the concentration of the different masses along time. How can he describe the evolution of these quantities from this microscopic description of the dynamics? Mathematically, we can describe these concentrations as measures μ_t on the space $\mathbb{R}_+^* := (0,+\infty)$ of masses of species. What comes out from experimental measurements are quantities such like the concentration of particles with a mass between such and such number, or, more generally, quantities of the form $(f,\mu_t) \equiv \int f(x)\mu_t(dx)$, for some functions f. Smoluchowski has proposed in [5] to describe the evolution of the observations (f,μ_t) in a well mixed system using some symmetric kernel $K(x,y)$ describing the rates at which coagulations occur:

$$\frac{d}{ds}\big(f,\mu_s\big) = \frac{1}{2}\int \big\{f(x+y) - f(x) - f(y)\big\}K(x,y)\,\mu_s(dx)\,\mu_s(dy). \tag{1.1}$$

Roughly speaking, a particle of mass x coagulates with a particle of mass y at rate $K(x,y)$ to create a particle of mass $x+y$. Numerous works have been devoted to this equation, both in the physics/engeneering and mathematics litteratures, motivated by different questions. The reviews by Aldous [6] and Leyvraz [7] give a good overview of the state of the art a few years ago. The main trends of mathematical research are concerned with the well-posedness problem [8], [9] of Smoluchowski equation (1.1), the gelation problem [10], [11], [12], [13], [14], [15], [16], the structure of self-similar or asymptotically self-similar solutions [7], [17], [18], [19], [20], and the mean-field approximation of Smoluchowski equation by random microscopic dynamics [21], [22]; simulation and numerical issues are also of great importance [23], [24], [25], for practical purposes.

b) Sensitivity. The parameters of an experiment are incorporated into the model dynamics (1.1) as parameters $\lambda \in \mathbb{R}^d$ in the interaction kernel $K = K^\lambda$. Binder granulation a priori requires for instance around 10 parameters to describe it, [26]. Finding the relevant parameters, given the experimental data (the so-called "inverse problem") is the fundamental step which will allow future simulations to provide law cost predictions – see e.g. [27] for some theoretical background on that

---

Date: April 7, 2011.
2000 *Mathematics Subject Classification.* Primary: 34A34, Secondary 34A12.
Key words and phrases. Smoluchowski's coagulation equation, sensitivity.

problem, and [28] for a global approach of the inverse problem for general population balances. From a different and as important point of view, the fact that all experimental measurements are approximate emphasizes the crucial need for a study of the dependence on parameters in practical applications.

Let denote by λ a generic multi-dimensional parameter, K^λ the corresponding coagulation kernel and μ_t^λ the solution to Smoluchowksi equation associated with K^λ. A simple and largely used method for tuning the parameter to data consists in formally applying a method of steepest descent so as to minimize some distance between μ_T^λ and μ_T^{obs}, in the typical case where we are interested in the value at time T of the system, [29]. The measure μ_T^{obs} is given by experiments. To be effective, the algorithm requires the knowledge of the differential σ_λ^t of μ_t^λ with respect to λ so as to choose the steepest descent direction at each step. Note that σ_t^λ is a priori a signed measure. Engineers usually estimate it by a finite difference corresponding to two close values of λ. The main approach to do that consists in approximating the differences $\frac{\mu_t^{\lambda+\epsilon e_i}-\mu_t^\lambda}{\epsilon}$ (for a basis vector e_i of $\mathbb{R}^d$) by the corresponding difference for the approximating particle systems – see [30] for a non-trivial and efficient way of doing that, and refer to the bibliographies of the works [29], [30] or [31] for more references on the computational analysis of dependence of μ_t^λ on λ. However, no justification that $\partial_\lambda\mu_t^\lambda$ is well-defined (in the mathematical sense) and well-behaved has ever been given up to now, which puts the previous investigations on a somewhat hazy mathematical framework.

The aim of this article is to prove that μ_t^λ is a $\mathcal{C}^1$ function of (t,λ) (under proper conditions and in a suitable sense) and that it is the unique solution to some equation ("sensitivity equation"). Not only does this fact put the existing approaches on a firm ground, but it also leads to a new particle approximation [31] for sensitivity which happens to be more accurate than any other method. In the same way as one can associate some finite interacting particle systems to Smoluchowski equation, the so-called Marcus-Lushnikov processes [32], one can associate a pair of coupled interacting particle systems to the equation associated with the sensitivity (§2.2.2), such that their difference converges weakly to a solution of the sensitivity equation, as a consequence of a kind of law of large numbers – a fact proved in [31]. The well-posedness of the sensitivity equation obtained in the present work justifies theoretically the use of that particle system for simulating the sensitivity.

Notation. Given a locally bounded non-negative kernel $F(x,y)$ on $\mathbb{R}_+^*\times\mathbb{R}_+^*$ and Radon measures μ,ν on $\mathbb{R}_+^*$, one defines a signed Radon measure $F(\mu,\nu)$ setting

$$F(\mu,\nu)=\int\left\{\delta_{x+y}-\delta_x-\delta_y\right\}F(x,y)\,\mu(dx)\,\nu(dy). \tag{1.2}$$

c) Strategy for studying the sensitivity of Smoluchowski equation. We describe in the remainder of this section the approach we use to prove the above mentionned differentiability result. From a mathematical point of view, the main difficulty in solving Smoluchowski equation comes from the fact that whilst the weak formulation (1.1) is always a well-defined problem (although it may have no solution), it is not easy to find a Banach or a Fréchet space of (signed) measures where the differential equation

$$\dot{\mu}_s=\frac{1}{2}K(\mu_s,\mu_s) \tag{1.3}$$

itself is meaningful. This difficulty disappears for bounded kernels, where Smoluchowski equation can be solved in the Banach framework of Radon signed measures equipped with total variation norm. The computation of $\partial_\lambda\mu_t^\lambda$ is formally straightforward and leads to a representation formula involving essentially only $\{\mu_s^\lambda\}_{s\leqslant t}$. The map $t\to\mu_t^\lambda$ solving equation (1.3), its derivative with respect to λ solves formally the equation

$$\dot{\sigma}_t^\lambda=K^\lambda\left(\mu_t^\lambda,\sigma_t^\lambda\right)+\frac{1}{2}\partial_\lambda K^\lambda\left(\mu_t^\lambda,\mu_t^\lambda\right) \tag{1.4}$$

obtained by differentiating equation (1.3) with respect to λ; we have written $\partial_\lambda K^\lambda(x,y)$ for the partial derivative of $K^\lambda(x,y)$ with respect to λ. This equation can be solved, considering first the linearized problem

$$\dot\rho_s^\lambda = K^\lambda(\mu_s^\lambda, \rho_s^\lambda) \tag{1.5}$$

before using the variation of constants method.

(i) We introduce a dual evolution equation on functions to study the linear equation (1.5). To that end, define some time dependent operators Λ_s^λ on functions setting

$$\Lambda_s^\lambda f(x) = \int \{f(x+y) - f(x) - f(y)\} K^\lambda(x,y)\mu_s^\lambda(dy). \tag{1.6}$$

These operators satisfy the identity

$$\big(\Lambda_s^\lambda f, \rho\big) = \big(f, K(\mu_s^\lambda, \rho)\big).$$

Now, if one considers the backward linear equation

$$\dot f_s = -\Lambda_s^\lambda f_s, \quad s \in [0,t] \text{ and } f_t = f,$$

its solution $\{f_s\}_{0\leqslant s\leqslant t}$ depends linearly on f, so we can write it in the form $U_{s,t}^\lambda f$, for a linear operator $U_{s,t}^\lambda$. This function $U_{s,t}^\lambda f$ has two important properties. As a function of t it satisfies the identity $\frac{d}{dt}U_{s,t}^\lambda f = U_{s,t}^\lambda \Lambda_t^\lambda f$, and if $\{\rho_s^\lambda\}_{s\geqslant 0}$ denotes a solution of equation (1.5), then

$$\begin{aligned}
\frac{d}{ds}\big(U_{s,t}^\lambda f, \rho_s^\lambda\big) &= \big(-\Lambda_s^\lambda U_{s,t}^\lambda f, \rho_s^\lambda\big) + \big(U_{s,t}^\lambda f, \dot\rho_s^\lambda\big) \\
&= -\big(U_{s,t}^\lambda f, K(\mu_s^\lambda, \rho_s^\lambda)\big) + \big(U_{s,t}^\lambda f, K(\mu_s^\lambda, \rho_s^\lambda)\big) \\
&= 0.
\end{aligned}$$

So we see that the solution to the linear equation (1.5) needs to be given by the formula

$$\big(f, \rho_t^\lambda\big) = \big(U_{0,t}^\lambda f, \rho_0\big). \tag{1.7}$$

(ii) To implement the variation of constants method and solve the affine equation (1.4), introduce as in equation (1.6) the operator

$$\Lambda_s^{\partial\lambda} f(x) = \int \{f(x+y) - f(x) - f(y)\} \partial_\lambda K^\lambda(x,y)\mu_s^\lambda(dy).$$

Note the relations

$$\big(\Lambda_s^\lambda f, \mu_s^\lambda\big) = \Big(f, K^\lambda\big(\mu_s^\lambda, \mu_s^\lambda\big)\Big) \quad \text{and} \quad \big(\Lambda_s^{\partial\lambda} f, \mu_s^\lambda\big) = \Big(f, \partial_\lambda K^\lambda\big(\mu_s^\lambda, \mu_s^\lambda\big)\Big).$$

Defining the measures σ_t^λ by the formula

$$\big(f, \sigma_t^\lambda\big) = \frac{1}{2}\int_0^t \Big(\Lambda_s^{\partial\lambda} U_{s,t}^\lambda f, \mu_s^\lambda\Big)\, ds \tag{1.8}$$

one can easily check that it satisfies a weak form of equation (1.4):

$$\begin{aligned}
\frac{d}{dt}\big(f, \sigma_t^\lambda\big) &= \frac{d}{dt}\left(\frac{1}{2}\int_0^t U_{0,s}^\lambda \Lambda_s^{\partial\lambda} U_{s,t}^\lambda f\, ds\,,\, \mu_0\right) \\
&= \left(\frac{1}{2}\int_0^t U_\lambda^{0,s} \Lambda_s^{\partial\lambda} U_{s,t}^\lambda \Lambda_t^\lambda f\, ds, \mu_0\right) + \frac{1}{2}\Big(U_{0,t}^\lambda \Lambda_t^{\partial\lambda} f, \mu_0\Big) \\
&= \Big(\Lambda_t^\lambda f, \sigma_t^\lambda\Big) + \frac{1}{2}\Big(\Lambda_t^{\partial\lambda} f, \mu_t^\lambda\Big) \\
&= \Big(f, K^\lambda\Big(\mu_t^\lambda, \sigma_t^\lambda\Big)\Big) + \Big(f, \frac{1}{2}K^{\partial\lambda}\Big(\mu_t^\lambda, \mu_t^\lambda\Big)\Big).
\end{aligned}$$

d) Organisation of the article. How far from full justification is this argument? In the case of uniformly bounded kernels K^λ, we shall see in section 2 that everything is meaningful in the Banach framework of signed measures equipped with the total variation distance. Yet, no such satisfactory framework is available for unbounded kernels; we shall thus use an approximation procedure in section 3 to extend the result; it relies crucially on the representation formula (1.8) for the sensitivity which comes from equation (1.4). We explain in §2.2.2 how this equation can be used in a practical way to simulate the sensitivity. The main result (theorem 6) states that the function $(t,\lambda) \mapsto \mu_t^\lambda$ is a $\mathcal{C}^1$ function with values in a good space of measures and that it is the only solution of a weak version of equation (1.4) under some proper conditions.

The idea to investigate the linearized Smoluchowski equation was first used in Kolokoltsov's paper [33] to see how μ_t depends on its initial value – see also [34] where similar ideas are used in a different context. We use here the same tools (theorems 13, 15, 16) as in Kolokoltsov's paper. We compare in section 4, **a)** the present work with the work [33]. Note that the simplified proof of a useful lemma of Kolokoltsov (theorem 13), given in section 4, **b)** and used in section 3.1, might be of some interest for itself.

Notations. All functions and measures are defined on $\mathbb{R}_+^*$ throughout the text.

- We shall use the notation $\mu^{\otimes 2}(dxdy)$ for the product measure $\mu(dx)\mu(dy)$.
- As the expression $f(x+y)-f(x)-f(y)$ will appear numerous times in the text, it will be useful to abbreviate it into $\{f\}(x,y)$. In these terms, the weak version (1.1) of Smoluchowski equation may be written

$$\frac{d}{dt}(f,\mu_t) = \frac{1}{2}\int \{f\}(x,y)\, K(x,y)\, \mu_t(dx)\, \mu_t(dy).$$

2. Sensitivity for bounded kernels

We consider in this section Smoluchowski equation (1.1) for a family $\{K^\lambda\}_\lambda$ of interaction kernels, bounded some constant M. We recall in section 2.1 why the strong version (1.3) of Smoluchowski equation is well defined in a good Banach framework. The classical tools of differential equations will then give us for free existence, uniqueness and regularity results of the solutions $\{\mu_t^\lambda\}_{t\geqslant 0}$ to equation (1.3). We shall then take profit in section 2.2 of the fact that the derivative $\sigma_t^\lambda = \partial_\lambda \mu_t^\lambda$ solves a time-non-homogeneous *affine* equation to get an explicit formula for it which will be useful in the sequel.

2.1. Existence and uniqueness in the bounded case: a quick overview.

Denote by B_0 the Banach space of bounded measurable functions, equipped with the supremum norm $\|.\|_0$. Denote also by $\|\rho\|_0$ the total variation of a signed Radon measure ρ, and by

$$\mathcal{M}_0 = \{\mu \text{ Radon measure };\, \|\rho\|_0 < \infty\}.$$

Note that $\|\rho\|_0 = \sup\big\{(f,\rho)\,;\, f \in B_0, \|f\|_0 \leqslant 1\big\}$, and that the space $(\mathcal{M}_0, \|.\|_0)$ is complete since it is the dual space of the complete space $\big(\mathcal{C}_b(\mathbb{R}_+,\mathbb{R}), \|.\|_\infty\big)$. We shall denote by $\mathcal{M}_0^+$ the cone of non-negative elements of $\mathcal{M}_0$.

The main reason why everything works well in the bounded case is that since we have

$$\big|\big(f, K(\mu,\mu)\big)\big| \leqslant 3\|f\|_0 M \|\mu\|_0^2$$

for any $f \in B_0$, the Radon measure $K(\mu,\mu)$ belongs to $\mathcal{M}_0$ if μ does; so Smoluchowski equation (1.3): $\dot\mu_s = \frac{1}{2}K(\mu_s,\mu_s)$, is a well-defined ordinary differential equation in the Banach space $\mathcal{M}_0$.

Proposition **1.** *Equation* (1.3) *has a well defined flow of solutions in* $\big(\mathcal{M}_0, \|.\|_0\big)$*, which preserves the cone* $\mathcal{M}_0^+$*. The solution* μ_t *is defined for all times if* $\mu \in \mathcal{M}_0^+$*.*

PROOF – It suffices to see that the vector field K is locally Lipschitz. But given μ and ν in $\mathcal{M}_0$, one can write

$$\big(\mu^{\otimes 2}-\nu^{\otimes 2}\big)(dxdy)=\mu(dx)(\mu-\nu)(dy)+\nu(dy)(\mu-\nu)(dx).$$

Nothing more is needed to get, for any $f\in B_0$, the inequality

$$\begin{aligned}\big|\big(f,K(\mu,\mu)\big)-\big(f,K(\nu,\nu)\big)\big| &= \Big|\int\{f\}(x,y)K(x,y)\big(\mu^{\otimes 2}-\nu^{\otimes 2}\big)(dxdy)\Big|\\ &\leqslant 3\|f\|_0 M\big(\|\mu\|_0+\|\nu\|_0\big)\|\mu-\nu\|_0,\end{aligned}$$

which implies

$$\big\|K(\mu,\mu)-K(\nu,\nu)\big\|_0\leqslant 3M\big(\|\mu\|_0+\|\nu\|_0\big)\|\mu-\nu\|_0. \tag{2.1}$$

To see that μ_t is non-negative if μ_0 is non-negative we find a non-negative function θ_t on $\mathbb{R}_+^*$ such that the transformed measure $\rho_t:=\theta_t\mu_t$ solves a differential equation which preserves $\mathcal{M}_0^+$ in a obvious way[1]. See [8], proposition 2.2, for instance.

Given an initial condition μ_0, denote by $\big[0,T(\mu_0)\big)$ the maximal interval on which the solution started from μ_0 is defined. If μ_0 is non-negative, one has

$$\frac{d}{dt}\|\mu_t\|_0=\frac{d}{dt}(1,\mu_t)=-\frac{1}{2}\int K(x,y)\mu_t(dx)\mu_t(dy)\leqslant 0$$

and the path $\{\mu_t\}_{0\leqslant t<T(\mu_0)}$ stays in a ball where the vector field K is (globally) Lipschitz. This explains why the solution is actually defined on $[0,\infty)$. ▷

2.2. **Sensitivity.** We prove in this section that if the coagulation kernel depends nicely on a parameter λ then the solution to Smoluchowski equation is a $\mathcal{C}^1$ function of (t,λ). Its derivative with respect to λ has a representation involving only $(\mu_s)_{s\geqslant 0}$.

2.2.1. *Dependence on a parameter.* Let now $\{K^\lambda(.,.)\}_{\lambda\in\mathcal{U}}$ be a family of symmetric non-negative kernels on $\mathbb{R}_*^+$ depending in a $\mathcal{C}^2$ way in a parameter λ belonging to some open set $\mathcal{U}$ of some $\mathbb{R}^p$. Denote by $K^{\partial\lambda}(x,y)$ the derivative of $K^\lambda(x,y)$ with respect to λ and define the Radon signed measure $K^{\partial\lambda}(\mu,\mu)$ setting

$$\big(f,K^{\partial\lambda}(\mu,\mu)\big)=\int\{f(x+y)-f(x)-f(y)\}K^{\partial\lambda}(x,y)\,\mu(dx)\mu(dy).$$

Denote by $\big[0,T^\lambda(\mu_0)\big)$ the maximal interval on which the solution to Smoluchowski equation (1.3) with interaction kernel $K^\lambda(\cdot,\cdot)$ started from μ_0 is defined

THEOREM **2** (Sensitivity for bounded kernels)**.** *Suppose $K^\lambda(\cdot,\cdot)$ and its first two derviatives are bounded by a constant M, uniformly in $\lambda\in\mathcal{U}$. Then the map $(t,\lambda)\in\big[0,T^\lambda(\mu_0)\big)\times\mathcal{U}\mapsto\mu_t^\lambda\in(\mathcal{M}_0,\|.\|_0)$ is differentiable with respect to λ and its derivatives σ_t^λ (called "sensitivity") is the unique solution of the equation*

$$\dot\sigma_t^\lambda=K^\lambda\left(\mu_t^\lambda,\sigma_t^\lambda\right)+\frac{1}{2}K^{\partial\lambda}\left(\mu_t^\lambda,\mu_t^\lambda\right). \tag{2.2}$$

PROOF – As is classically done in the study of ordinary differential equations in Banach spaces (e.g. consult [35]), the result is a consequence the following four properties.

(1) For each $\mu\in\mathcal{M}_0$, the map $\lambda\in\mathcal{U}\mapsto K^\lambda(\mu,\mu)\in(\mathcal{M}_0,\|.\|_0)$ is differentiable, with a derivative $K^{\partial\lambda}(\mu,\mu)\in(\mathcal{M}_0,\|.\|_0)$ depending continuously on $\mu\in(\mathcal{M}_0,\|.\|_0)$.
(2) The map $(s,\lambda)\mapsto\mu_s^\lambda\in(\mathcal{M}_0,\|.\|_0)$ is continuous on $[0,T]\times\mathcal{U}$.
(3) The linear map $\nu\mapsto K(\mu_s,\nu)$ takes $(\mathcal{M}_0,\|.\|_0)$ into itself and has a uniformly bounded norm for $s\in[0,T]$. The same result holds for the map $\nu\mapsto K^{\partial\lambda}(\mu_s,\nu)$.

[1]Which is not the case of Smoluchowski equation. One uses the same method in the study of Boltzmann equation.

(4) Let C be a compact set of $(\mathcal{M}_0, \|.\|_0)$. There exists an $(\mathcal{M}_0, \|.\|_0)$-valued function $O_2(\mu,\mu')$ such that $\|O_2(\mu,\mu')\|_0 \leqslant m\|\mu-\mu'\|_0^2$ for some constant m, and

$$\forall\, \mu,\, \mu' \in C, \quad K^{\lambda_0}(\mu',\mu') - K^{\lambda_0}(\mu,\mu) = 2K^{\lambda_0}(\mu,\mu'-\mu) + O_2(\mu,\mu'). \tag{2.3}$$

$K^{\partial\lambda_0}$ has the same property.

We prove points 1 and 2 and leave the elementary proofs of points 3 and 4 to the reader.

1. Given $f \in B_0$, apply Taylor formula in a small neighbourhood $\mathcal{V}$ of λ_0 to get

$$\begin{aligned}&\Big|\big(f, K^{\lambda}(\mu,\mu) - K^{\lambda_0}(\mu,\mu) - (\lambda-\lambda_0)K^{\partial\lambda}(\mu,\mu)\big)\Big| = \\ &\Big|\int \{f\}(x,y)\big(K^{\lambda}(x,y) - K^{\lambda_0}(x,y) - (\lambda-\lambda_0)K^{\partial\lambda}(x,y)\big)\mu(dx)\mu(dy)\Big| \\ &\leqslant 3\|f\|_0 \frac{|\lambda-\lambda_0|^2}{2} \max_{\widetilde{\lambda}\in\mathcal{V}} \big|\partial^2_{\widetilde{\lambda}} K^{\widetilde{\lambda}}(x,y)\big| \|\mu\|_0^2.\end{aligned}$$

This proves the differentiability assertion. The map $\mu \in \mathcal{M}_0 \to K^{\partial\lambda}(\mu,\mu)$ can be seen to be locally Lipschitz using the same reasonning as was used in the proof of proposition 1 to prove that the vector field K is locally Lipschitz.

2. It is a classical fact in dynamics[2] that it is sufficient to check that the map $(\lambda,\mu) \in \mathcal{U}\times\mathcal{M}_0 \to K^{\lambda}(\mu,\mu)$ is locally Lipschitz to get the continuity of $(s,\lambda) \mapsto \mu_s^{\lambda} \in (\mathcal{M}_0, \|.\|_0)$. Writing

$$K^{\lambda}(\mu,\mu) - K^{\lambda'}(\nu,\nu) = K^{\lambda}(\mu,\mu) - K^{\lambda}(\nu,\nu) + \left(K^{\lambda} - K^{\lambda'}\right)(\nu,\nu),$$

and using inequality (2.1), Taylor formula, and the fact that $\sup_{x,y\,;\,\ell}\big|K^{\partial\ell}(x,y)\big| \leqslant M$, one obtains

$$\|K^{\lambda}(\mu,\mu) - K^{\lambda'}(\nu,\nu)\|_0 \leqslant 3M\big(\|\mu\|_0 + \|\nu\|_0\big)\|\mu-\nu\|_0 + 3M\|\nu\|_0^2|\lambda-\lambda'|.$$

▷

2.2.2. *A representation formula for the sensitivity.* We fix μ_0 throughout this section and work on a fixed time interval $[0,T] \subset \big[0, T^{\lambda}(\mu_0)\big)$, for all $\lambda \in \mathcal{U}$. As explained in the introduction, one can solve explicitly the sensitivity equation (2.2) by solving first its linearized version before using the variation of constant method. The first step is made solving a dual problem to the homogeneous equation, on the space B_0.

a) Dual linearized Smoluchowski equation. Define for each $\lambda \in \mathcal{U}$, a time-dependent linear vector field Λ_s^{λ} on B_0, setting for any $f \in B_0$

$$\Lambda_s^{\lambda} f(x) = \int \big\{f(x+y) - f(x) - f(y)\big\} K^{\lambda}(x,y)\mu_s^{\lambda}(dy). \tag{2.4}$$

As $\|\Lambda_s^{\lambda}\|_0 \leqslant 3M(1,\mu_s^{\lambda}) \leqslant 3M\|\mu_0\|_0$, and μ_s^{λ} depends continuously on s, the vector field Λ_s^{λ} on B_0 is continuous with respect to $f \in B_0$ and s. So, given some time $t > 0$, the backward and forward differential equations

$$\dot{f}_s(x) = -\Lambda_s^{\lambda} f_s(x), \quad f_t \text{ given}, \tag{2.5}$$

are meaningful in B_0, and elementary results on linear differential equations on Banach spaces give the following proposition[3].

---

[2] Consult Martin's book [35] for instance.

[3] Consult Martin's book [35].

PROPOSITION **3.** *The differential backwards and forwards equations* (2.5) *in* $(B_0, \|.\|_0)$ *have a unique solution, defined for all time. It is of the form* $f_s = U^\lambda_{s,t} f_t$*, for a continuous linear operator* $U^\lambda_{s,t}$ *on* B_0*, with norm* $\leqslant e^{3M\|\mu_0\|_0|t-s|}$*. We also have for any* $f \in B_0$

$$\frac{d}{dt} U^\lambda_{s,t} f = U^\lambda_{s,t} \Lambda^\lambda_t f. \tag{2.6}$$

This operator $U^\lambda_{s,t}$ can be used to solve explicitly the linear equation on $\mathcal{M}_0$

$$\dot{\rho}^\lambda_s = K^\lambda(\mu^\lambda_s, \rho^\lambda_s);$$

this equation has a unique solution on the time interval $[0,T]$ as the time non-homogeneous vector field $K^\lambda(\mu^\lambda_s, \cdot)$ is continuous and bounded. Indeed, one gets from Smoluchowski equation (1.3) and equation (2.5)

$$\begin{aligned}
&\frac{d}{ds}\big(U^\lambda_{s,t} f, \rho_s\big) = -\big(\Lambda^\lambda_s U^\lambda_{s,t} f, \rho_s\big) + \big(U^\lambda_{s,t} f, \dot{\rho}_s\big) \\
&= -\big(U^\lambda_{s,t} f, K(\mu_s, \rho_s)\big) + \big(U^\lambda_{s,t} f, K(\mu_s, \rho_s)\big) \\
&= 0;
\end{aligned}$$

so the identity $\big(U^\lambda_{0,t} f, \rho_0\big) = (f, \rho^\lambda_t)$ holds for any $f \in B_0$; thus

$$\rho^\lambda_t = \big(U^\lambda_{0,t}\big)^* \rho_0.$$

b) A representation formula for σ^λ_t. The second step to solve the affine equation (2.2) is to use the variation of constant method as explained in the introduction. The following lemma will be used on the way.

LEMMA **4.** *The function* $t \in [0,T] \mapsto \sigma^\lambda_t \in \mathcal{M}_0$ *is the only solution in* $\big(\mathcal{M}_0, \|.\|_0\big)$ *of the weak differential equation*

$$\forall\, f \in B_0, \quad \frac{d}{dt}(f, \sigma_t) = \Big(f, K^\lambda\big(\mu^\lambda_t, \sigma_t\big)\Big) + \frac{1}{2}\Big(f, K^\lambda\big(\mu^\lambda_t, \mu^\lambda_t\big)\Big), \quad \sigma_0 \text{ given.}$$

PROOF – Note first that since the function $t \in [0,T] \mapsto \sigma^\lambda_t \in \mathcal{M}_0$ satisfies the strong equation (2.2) it also satisfies the above weak equation. Given two solutions σ_t and $\overline{\sigma}_t$ of the latter, one has for any $f \in B_0$

$$\big(f, \sigma_t - \overline{\sigma}_t\big) = \int_0^t \Big(f, K^\lambda\big(\mu^\lambda_s, \overline{\sigma}_s - \sigma_s\big)\Big) ds = \int_0^t \big(\Lambda^\lambda_s f, \overline{\sigma}_s - \sigma_s\big) ds.$$

But as the operator Λ^λ_s on $\big(B_0, \|.\|_0\big)$ has norm $\leqslant 3M\|\mu_0\|_0$, we must have

$$\big(f, \sigma_t - \overline{\sigma}_t\big) \leqslant 3M\|\mu_0\|_0 \|f\|_0 \int_0^t \|\sigma_t - \overline{\sigma}_t\|_0 ds,$$

and so

$$\|\sigma_t - \overline{\sigma}_t\|_0 \leqslant 3M\|\mu_0\|_0 \int_0^t \|\sigma_s - \overline{\sigma}_s\|_0 \, ds.$$

One deduces from Gronwall's formula that $\overline{\sigma}_t = \sigma_t$. ▷

Define the map $\Lambda^{\partial\lambda}_s$ on B_0 by the formula

$$\Lambda^{\partial\lambda}_s f(x) = \int \big\{f(x+y) - f(x) - f(y)\big\} K^{\partial\lambda}(x,y) \mu^\lambda_s(dy);$$

notice the identities

$$\big(\Lambda^{\partial\lambda}_s f, \mu^\lambda_s\big) = \big(f, K^{\partial\lambda}_s(\mu^\lambda_s, \mu^\lambda_s)\big), \quad \text{and} \quad \big(\Lambda^\lambda_s f, \mu^\lambda_s\big) = \big(f, K^\lambda_s(\mu^\lambda_s, \mu^\lambda_s)\big), \quad f \in B_0.$$

Proposition **5** (Representation formula for the sensitivity). *One has*

$$(f,\sigma_t^\lambda) = \frac{1}{2}\int_0^t \left(\Lambda_s^{\partial\lambda} U_{s,t}^\lambda f, \mu_s^\lambda\right) ds \tag{2.7}$$

for any $f \in B_0$.

Proof – Denote temporarily by $\widehat{\sigma}_t^\lambda$ the measure $f \in B_0 \mapsto \frac{1}{2}\int_0^t \left(\Lambda_s^{\partial\lambda} U_{s,t}^\lambda f, \mu_s^\lambda\right) ds$; it belongs to $\mathcal{M}_0$. The following calculus is fully justified in the Banach framework of $(B_0, \|.\|_0)$. For any $f \in B_0$, one has

$$\begin{aligned}
\frac{d}{dt}(f,\widehat{\sigma}_t^\lambda) = \frac{d}{dt}\left(\frac{1}{2}\int_0^t \Lambda_s^{\partial\lambda} U_{s,t}^\lambda f \, ds \,,\, \mu_s^\lambda\right) &= \left(\frac{1}{2}\int_0^t \Lambda_s^{\partial\lambda} U_{s,t}^\lambda \Lambda_t^\lambda f \, ds, \mu_s^\lambda\right) + \frac{1}{2}\left(\Lambda_t^{\partial\lambda} f, \mu_t^\lambda\right) \\
&= \left(\Lambda_t^\lambda f, \widehat{\sigma}_t^\lambda\right) + \frac{1}{2}\left(\Lambda_t^{\partial\lambda} f, \mu_t^\lambda\right) \\
&= \left(f, K^\lambda\left(\mu_t^\lambda, \widehat{\sigma}_t^\lambda\right)\right) + \left(f, \frac{1}{2}K^{\partial\lambda}\left(\mu_t^\lambda, \mu_t^\lambda\right)\right).
\end{aligned}$$

Since $\widehat{\sigma}_t^\lambda$ satisfies a weak version of equation (2.2) it coincides with σ_t^λ according to lemma 4. $\triangleright$

Remark on the sensitivity equation (2.2). Since solving explicitly equation (2.2) requires the explicit knowledge of $(\mu_t^\lambda)_{t\geqslant 0}$, from which an explicit formula for the sensitivity follows by differentiation, the above representation formula is useful not in providing some explicit formula for the sensitivity, but in so far as it enables to get some a priori information on σ_t^λ from some quantitative informations on $(\mu_t^\lambda)_{t\geqslant 0}$. As Smoluchowski equation is solvable in only a few cases, this is the best kind of information one can hope to get in a general framework. We shall use it crucially in the next section where we extend the regularity result stated in theorem 2 to a class of unbounded coagulation kernels by showing that the representation formula for the sensitivity still makes sense and provides indeed the derivative of the solution to Smoluchowski equation with respect to λ.

Note, however, that equation (2.2) can be usefully used for simulation purposes. One can indeed associate to it some Marcus-Lushnikov-like [32] interacting particle system converging to its unique solution as the number of particles increases indefinitely; we briefly describe it here and refer the reader to the article [31] for the mathematical details and a numerical study of the associated algorithm. We write for simplicity σ_t for σ_t^λ as λ is fixed here.

The measure σ_t is a non-positive; denote by $\sigma_t^{+/-}$ its positive and negative parts. Set also $K'_+ = \max\{K', 0\}$ and $K'_- = \max\{-K', 0\}$. The particle system we introduce is motivated by the following formal re-writting of equation (2.2)

$$\dot{\sigma}_t = \dot{\sigma}_t^+ - \dot{\sigma}_t^- = \left(K(\mu_t, \sigma_t^+) + \frac{1}{2}K'_+(\mu_t,\mu_t)\right) - \left(K(\mu_t, \sigma_t^-) + \frac{1}{2}K'_-(\mu_t,\mu_t)\right).$$

Three coupled systems of particles $\Theta_t^N = \left(\mu_t^N, \sigma_t^{+,N}, \sigma_t^{-,N}\right)$ simulate μ_t, σ_t^+ and σ_t^- respectively, the first being the usual Marcus-Lushnikov particle system. Set

$$\Theta_0 = \frac{1}{N}\left(\sum_{i=1..m} \delta_{y_i}, \sum_{k=1..p} \delta_{z_k}, \sum_{\ell=1..q} \delta_{z'_\ell}\right),$$

and associate to each pair

- $1 \leqslant i < j \leqslant m$, some exponential random variables R_{ij}, S_{ij} et T_{ij}, with parameters $K(y_i, y_j)$, $K'_+(y_i, y_j)$ and $K'_-(y_i, y_j)$, respectively,
- $(i,k) \in [\![1,m]\!] \times [\![1,p]\!]$, some exponential random variables U_{ik} with parameters $K(y_i, z_k)$,
- $(i,\ell) \in [\![1,m]\!] \times [\![1,q]\!]$, some exponential random variables $V_{i\ell}$ with parameters $K(y_i, z'_\ell)$.

All these exponential times are independent. Let W be the first time where one of these clocks ring. If

$$\begin{array}{lll} W = R_{ij}, & \text{then} & \Delta\Theta = \big(\delta_{x_i+x_j} - \delta_{x_i} - \delta_{x_j}\big) \oplus 0 \oplus 0, \\ W = S_{ij}, & \text{then} & \Delta\Theta = 0 \oplus \delta_{x_i+x_j} \oplus \big(\delta_{x_i} + \delta_{x_j}\big), \\ W = T_{ij}, & \text{then} & \Delta\Theta = 0 \oplus \big(\delta_{x_i} + \delta_{x_j}\big) \oplus \delta_{x_i+x_j}, \\ W = U_{ik}, & \text{then} & \Delta\Theta = 0 \oplus \big(\delta_{x_i+y_k} - \delta_{y_k}\big) \oplus \delta_{x_i}, \\ W = V_{i\ell}, & \text{then} & \Delta\Theta = 0 \oplus \delta_{x_i} \oplus \big(\delta_{x_i+z_\ell} - \delta_{z_\ell}\big). \end{array}$$

The process Θ_t is constant over the time interval $[0, W)$ and has a jump $\frac{1}{N}\Delta\Theta$ at time W; the dynamics is Markovian. Some classical methods of weak convergence of measure-valued processes can be used to prove that this interacting particle system converges in some sense to the unique solution of the sensitivity equation (2.2) provided by theorem 2 and theorem 6 below – see [31].

3. From bounded to unbounded kernels

We show in this section that one can extend the regularity result theorem 2 to some unbounded coagulation kernels under some conditions. Suppose for that purpose that one has

$$\forall \lambda \in \mathcal{U}, \forall x, y \in \mathbb{R}_+^*, \quad K^\lambda(x,y) \leqslant \varphi(x)\,\varphi(y) \quad \text{and} \quad \big|K^{\partial\lambda}(x,y)\big| \leqslant \varphi(x)\,\varphi(y), \tag{3.1}$$

for some sub-additive function φ([4]), greater than 1. Suppose also that there exists a (small) $\varepsilon > 0$ such that

$$(\varphi^{4+\varepsilon}, \mu_0) < \infty. \tag{3.2}$$

In his paper [8], J. Norris proved that $(\varphi^2, \mu_t^\lambda)$ remains finite on some time interval $\big[0, T(\mu_0)\big)$ if (φ^2, μ_0) is finite. The same argument shows that $(\varphi^{4+\varepsilon}, \mu_t^\lambda)$ also remains finite (on a possibly different time interval, still denoted $\big[0, T(\mu_0)\big)$) if $(\varphi^{4+\varepsilon}, \mu_0)$ is finite. Given some $T < T(\mu_0)$ denote by $C(T)$ a positive constant such that

$$\forall t \leqslant T, \quad (\varphi^{4+\varepsilon}, \mu_t) \leqslant C(T). \tag{3.3}$$

The function φ being greater than 1, the other moments $(\varphi^p, \mu_t^\lambda)$, with $1 \leqslant p \leqslant 4 + \varepsilon$, are also bounded above by $C(T)$ on $[0, T]$.

In order to estimate the tail behaviour of measures, we introduce the following spaces of measures, indexed by non-negative reals p:

$$\mathcal{M}_p = \big\{\mu\,;\, \|\mu\|_p := \big(\varphi^p, |\mu|\big) < \infty\big\}.$$

Using this notation condition (3.3) reads: $\mu_t \in \mathcal{M}_{4+\varepsilon} \subset \mathcal{M}_1$, for all $0 \leqslant t \leqslant T$. To compare the behaviour of non-bounded functions with the behaviour of φ, one defines the increasing family of function spaces, indexed by non-negative reals p:

$$B_p = \Big\{f\,;\, \sup \frac{|f|}{\varphi^p} < \infty\Big\};$$

we shall write $\|f\|_p$ for this supremum. Note that $\|\mu\|_p = \sup\{(f,\mu)\,;\, f \in B_p,\, \|f\|_p \leqslant 1\}$. The purpose of this section is to prove our main result.

Theorem **6** (Sensitivity for unbounded kernels)**.** *Assume condition* (3.1) *and the moment condition* (3.2)*. Then the map* $(t,\lambda) \in [0,T] \times \mathcal{U} \mapsto \mu_t^\lambda \in \big(\mathcal{M}_1, \|.\|_1\big)$*, is a* $\mathcal{C}^1$ *function and its derivative* σ_t^λ *satisfies the following equation for any* $f \in B_0$*.*

$$(f, \sigma_t^\lambda) = (f, \sigma_0^\lambda) + \int_0^t \int \{f\}(x,y) K^\lambda(x,y) \mu_s^\lambda(dx) \sigma_s^\lambda(dy) ds + \frac{1}{2}\int_0^t \int \{f\}(x,y) K^{\partial\lambda}(x,y) \mu_s^\lambda(dx) \mu_s^\lambda(dy) ds$$

The function $\sigma_\cdot^\lambda$ *is the only* $\big(\mathcal{M}_1, \|.\|_1\big)$*-valued solution of this equation.*

---

[4] We have $\varphi(x+y) \leqslant \varphi(x) + \varphi(y)$, for all $x, y \in \mathbb{R}_+^*$.

We prove this statement by an approximation procedure. Let $\{K^{\lambda\,;\,N}\}_{N\geqslant 0}$ be a sequence of bounded symmetric kernels converging towards K, and such that $\partial_\lambda K^{\lambda\,;\,N}$ and $\partial_\lambda^2 K^{\lambda\,;\,N}$ are also bounded, with $\big|K^{\lambda\,;\,N}(x,y)\big|$ and $\big|\partial_\lambda K^{\lambda\,;\,N}(x,y)\big|$ bounded above by $\varphi(x)\,\varphi(y)$. Let $\mu_t^{\lambda\,;\,N}$ and $\sigma_t^{\lambda\,;\,N}$ be the measures associated with $K^{\lambda\,;\,N}$ and $\partial_\lambda K^{\lambda\,;\,N}$, constructed in section 2. Theorem 6 is proved by showing that

(1) the map $(t,\lambda)\in[0,T]\times\mathcal{U}\mapsto\mu_t^{\lambda\,;\,N}\in\big(\mathcal{M}_1,\|.\|_1\big)$ is, for each N, a $\mathcal{C}^1$ function, and $\partial_\lambda\,\mu_t^{\lambda\,;\,N}=\sigma_t^{\lambda\,;\,N}$ in $\big(\mathcal{M}_1,\|.\|_1\big)$.
(2) the sequence $\{\mu_t^{\lambda\,;\,N}\}_{N\geqslant 0}$ converges towards μ_t^λ in $\big(\mathcal{M}_1,\|.\|_1\big)$, uniformly with respect to $(t,\lambda)\in[0,T]\times\mathcal{U}$;
(3) the sequence $\{\sigma_t^{\lambda\,;\,N}\}_{N\geqslant 0}$ of its derivatives converges in $\big(\mathcal{M}_1,\|.\|_1\big)$ towards some σ_t^λ, uniformly with respect to $(t,\lambda)\in[0,T]\times\mathcal{U}$.

Points 2 and 3 will be proved sections 3.1 and 3.2 respectively. We prove the first point here. Denote by M an upper bound of $K^{\lambda\,;\,N}$. Notice first that the inequality $\big|\{f\}(x,y)\big|\leqslant 2\|f\|_1\big(\varphi(x)+\varphi(y)\big)$, gives for any $\mu\in\mathcal{M}_1$

$$
\begin{aligned}
\big|\big(f,K^{\lambda\,;\,N}(\mu,\mu)\big)\big| &\leqslant 2M\|f\|_1\int\big(\varphi(x)+\varphi(y)\big)\mu(dx)\mu(dy)\\
&\leqslant 4M\|f\|_1\|\mu\|_1^2;
\end{aligned}
\tag{3.4}
$$

so the Radon measure $K^{\lambda\,;\,N}(\mu,\mu)$ belongs to $\mathcal{M}_1$ if μ does. Now, the following inequalities enable us to see that the vector field $\mu\mapsto K^{\lambda\,;\,N}(\mu,\mu)$ on $\big(\mathcal{M}_1,\|.\|_1\big)$ is Lipschitz. The function $f\in B_1$ has norm no greater than 1 and $\mu,\nu\in\mathcal{M}_1$.

$$
\begin{aligned}
\Big|\Big(f,K^{\lambda\,;\,N}(\mu,\mu)-K^{\lambda\,;\,N}(\nu,\nu)\Big)\Big| &= 2M\int\big(\varphi(x)+\varphi(y)\big)\big(|\mu|(dx)|\mu-\nu|(dy)+|\nu|(dy)|\mu-\nu|(dx)\big)\\
&\leqslant 2M\big(\|\mu\|_1\|\mu-\nu\|_0+\|\mu\|_0\|\mu-\nu\|_1+\|\nu\|_0\|\mu-\nu\|_1+\|\nu\|_1\|\mu-\nu\|_0\big)\\
&\leqslant 4M\big(\|\mu\|_1+\|\nu\|_1\big)\|\mu-\nu\|_1.
\end{aligned}
$$

The differentiability of the map $\lambda\in\mathcal{U}\mapsto\mu_t^{\lambda\,;\,N}\in\big(\mathcal{M}_1,\|.\|_1\big)$ can be proved in the same way as was done in section 2.2 in the framework of $\big(\mathcal{M}_0,\|.\|_0\big)$. To prove the continuity of $\mu_t^{\lambda\,;\,N}$ and $\sigma_t^{\lambda\,;\,N}$ with respect to $(t,\lambda)\in[0,T]\times\mathcal{U}$, one checks that the vector fields appearing in equations (1.3) and (2.2) are Lipschitz in $(\lambda,\mu)\in\mathcal{U}\times\mathcal{M}_1$, mimicking what was done in the proof of theorm 2 in the framework of $\mathcal{U}\times\mathcal{M}_0$. This completes the proof of the first point.

Note that the operators $\Lambda_s^{\lambda\,;\,N}$ and $\Lambda_s^{\partial\lambda\,;\,N}$ are bounded in $\big(\mathcal{M}_1,\|.\|_1\big)$, with norm no greater than $4M\|\mu_s^\lambda\|_1$, so that the representation formula for $\sigma_t^{\lambda\,;\,N}$ given in (2.7) also holds in $\big(\mathcal{M}_1,\|.\|_1\big)$. The remainder of this section is dedicated to the proofs of points 2 and 3. After a preliminary result in section 3.1, we prove a stronger version of point 2, useful in the sequel. The proof of point 3 is made in section 3.2.

As we shall prove these results for a fixed λ, we shall drop the λ in μ_t^λ and σ_t^λ in the sequel. The following elementary result will be used repeatedly; its proof is left to the reader.

Lemma 7. *For any $p\geqslant 1$ and any $f\in B_p$, $\big|\{f\}(x,y)\big|\leqslant 2^p\|f\|_p\big(\varphi^p(x)+\varphi^p(y)\big)$.*

As a last remark, note that the measures μ_t^N satisfy for any $0\leqslant t\leqslant T$ and $N\geqslant 0$ the same moment inequality (3.3) as μ_t.

3.1. Convergence of μ_t^N to μ_t in $(\mathcal{M}_{2+\varepsilon},\|.\|_{2+\varepsilon})$.

Let $\{\mu_t\}_{0\leqslant t<T(\mu_0)}$ be the solution given by Norris' theorem; choose $T<T(\mu_0)$. It is worth noting that using dominated convergence and the moment estimate (3.3), the measures $\{\mu_t\}_{0\leqslant t\leqslant T}$ satisfy the weak version (1.1) of Smoluchowski equation for any $f\in B_{3+\varepsilon}$. We start this section showing that they depend regularly on t.

PROPOSITION **8.** *The path $\{\mu_t\}_{0\leqslant t\leqslant T}$ is a $\mathcal{C}^1$ path in $\big(\mathcal{M}_{2+\varepsilon}, \|.\|_{2+\varepsilon}\big)$.*

PROOF – One proves that the path $\{\mu_t\}_{0\leqslant t\leqslant T}$ is ***1)*** Lipschitz in $\big(\mathcal{M}_{3+\varepsilon}, \|.\|_{3+\varepsilon}\big)$, ***2)*** $\mathcal{C}^1$ in $\big(\mathcal{M}_{2+\varepsilon}, \|.\|_{2+\varepsilon}\big)$.

1) Take a function $f \in B_{3+\varepsilon}$. One establishes the following inequalities using the inequality $K(x,y) \leqslant \varphi(x)\varphi(y)$ and the sub-additivity of φ.

$$\begin{aligned}
\big|(f, \mu_t - \mu_s)\big| &\leqslant \frac{1}{2}\int_s^t \int \big|\{f\}(x,y)\big| K(x,y)\mu_r(dx)\mu_r(dy)\,dr \\
&\leqslant \frac{c_\varepsilon \|f\|_{3+\varepsilon}}{2}\int_s^t \int \big\{\varphi^{3+\varepsilon}(x) + \varphi^{3+\varepsilon}(y)\big\}\varphi(x)\varphi(y)\mu_r(dx)\mu_r(dy)\,dr \\
&\leqslant 2c_\varepsilon\|f\|_{3+\varepsilon}\int_s^t \int \varphi^{4+\varepsilon}(x)\varphi(y)\mu_r(dx)\mu_r(dy)\,dr \\
&\leqslant 2c_\varepsilon\|f\|_{3+\varepsilon}(\varphi, \mu_0)\sup_{s\leqslant r\leqslant t}\|\mu_r\|_{4+\varepsilon}\,|t-s|.
\end{aligned}$$

Taking the supremum of the left hand side, with $\|f\|_{3+\varepsilon} \leqslant 1$, this shows that the path $\{\mu_t\}_{0\leqslant t\leqslant T}$ is Lipschitz in $\big(\mathcal{M}_{3+\varepsilon}, \|.\|_{3+\varepsilon}\big)$, with Lipschitz constant $\leqslant 2c_\varepsilon C(T)^2$.

It follows from this fact that the formula

$$(f, \nu_t) := \frac{1}{2}\int \{f\}(x,y)K(x,y)\mu_t(dx)\mu_t(dy)$$

defines an element ν_t of $\big(\mathcal{M}_{2+\varepsilon}, \|.\|_{2+\varepsilon}\big)$ which is continuous with respect to t. Indeed, since one has for any $f \in B_{2+\varepsilon}$,

$$\begin{aligned}
\big|(f, \nu_t - \nu_s)\big| &= \frac{1}{2}\left|\int \{f\}(x,y)K(x,y)\big\{\mu_t(dx)(\mu_t-\mu_s)(dy) + \mu_s(dy)(\mu_t-\mu_s)(dx)\big\}\right| \\
&\leqslant \frac{c'_\varepsilon\|f\|_{2+\varepsilon}}{2}\int \big(\varphi^{2+\varepsilon}(x) + \varphi^{2+\varepsilon}(y)\big)\varphi(x)\varphi(y)\big(\mu_t(dx)|\mu_t-\mu_s|(dy) + \mu_s(dy)|\mu_t-\mu_s|(dx)\big) \\
&\leqslant 2c'_\varepsilon\|f\|_{2+\varepsilon}C(T)\|\mu_t-\mu_s\|_{3+\varepsilon},
\end{aligned}$$

we have $\|\nu_t - \nu_s\|_{2+\varepsilon} \leqslant 8c_\varepsilon c'_\varepsilon C(T)^3\,|t-s|$.

2) Finally, write for any $f \in B_{2+\varepsilon}$

$$\big(f, \mu_t - \mu_s - (t-s)\nu_s\big) = \int_s^t (f, \nu_r - \nu_s)dr,$$

and note that the integral is uniformly $o(t-s)$, for $\|f\|_{2+\varepsilon} \leqslant 1$; this proves that the path $\{\mu_t\}_{0\leqslant t\leqslant T}$ is differentiable, as a path in $\big(\mathcal{M}_{2+\varepsilon}, \|.\|_{2+\varepsilon}\big)$, with continuous derivative ν_t. ▷

We shall use this result in the form: *The path $\{\varphi^{2+\varepsilon}\mu_t\}_{0\leqslant t\leqslant T}$ is a $\mathcal{C}^1$ path in $\big(\mathcal{M}_0, \|.\|_0\big)$.* This enables us to apply a useful lemma of Kolokoltsov (see the appendix of [36]) of which we give a clear and short proof in section 4.

LEMMA **9** (Kolokoltsov [36])**.** *Let $\{\rho_s\}_{0\leqslant s\leqslant T}$ be a $\mathcal{C}^1$ path in $(\mathcal{M}_0, \|.\|_0)$, with derivative $\{\dot\rho_s\}_{0\leqslant s\leqslant T}$. There exists a $\{\pm1, 0\}$-valued measurable function $(s,x) \in \mathbb{R}_+ \times \mathbb{R}_+^* \mapsto \varepsilon_s(x)$ such that we have*

- $\|\rho_t\|_0 = \|\rho_0\|_0 + \int_0^t (\varepsilon_s, \dot\rho_s)\,ds,$ *for any $t \in [0,T]$,*
- $\big(f, |\rho_t|\big) = (f\varepsilon_t, \rho_t)$*, for all $f \in \mathcal{B}, t \in [0,T]$.*

PROPOSITION **10.** *The sequence of measures $\{\mu_t^N\}_{N\geqslant 0}$ converges to μ_t in $\big(\mathcal{M}_{2+\varepsilon}, \|.\|_{2+\varepsilon}\big)$, uniformly with respect to $t \in [0,T]$.*

PROOF – Applying Kolokoltsov's lemma to the $\mathcal{C}^1$ path $\{\varphi^{2+\varepsilon}(\mu_t^N-\mu_t)\}_{0\leqslant t\leqslant T}$ in $(\mathcal{M}_0,\|.\|_0)$, and denoting by ε_s^N the function given by theorem 13, we can write

$$\begin{aligned}
\|\mu_t^N-\mu_t\|_{2+\varepsilon} = \int \varphi^{2+\varepsilon}(x)|\mu_t^N-\mu_t|(dx) &= \int_0^t \big(\varepsilon_s^N\varphi^{2+\varepsilon},\dot\mu_s^N-\dot\mu_s\big)ds \\
&= \int_0^t \{\varepsilon_s^N\varphi^{2+\varepsilon}\}(x,y)\left(K^N(x,y)\mu_s^{N\otimes 2}-K(x,y)\mu_s^{\otimes 2}\right)(dx\otimes dy) \\
&= \int_0^t\int \{\varepsilon_s^N\varphi^{2+\varepsilon}\}(x,y)K^N(x,y)\big(\mu_s^{N\otimes 2}-\mu_s^{\otimes 2}\big)(dx\otimes dy)\,ds \\
&+ \int_0^t\int \{\varepsilon_s^N\varphi^{2+\varepsilon}\}(x,y)\big(K^N-K\big)(x,y)\mu_s^{\otimes 2}(dx\otimes dy)\,ds.
\end{aligned}$$

The second term converges to 0 by dominated convergence and the fact that $\|\mu_s\|_{3+\varepsilon}$ is bounded; call it $o_N(1)$. To handle the first term, write it as

$$\begin{aligned}
&\int_0^t\int \{\varepsilon_s^N\varphi^{2+\varepsilon}\}(x,y)K^N(x,y)\Big((\mu_s^N-\mu_s)(dx)\mu_s^N(dy)+\mu_s(dx)(\mu_s^N-\mu_s)(dy)\Big) \\
&= \int_0^t\int \{\varepsilon_s^N\varphi^{2+\varepsilon}\}(x,y)K^N(x,y)\varepsilon_s^N(x)|\mu_s^N-\mu_s|(dx)\big(\mu_s+\mu_s^N\big)(dy) =: (*);
\end{aligned}$$

we have used the symmetry of the expressions with respect to x and y. Now, using the fact that $|\varepsilon_s^N|\leqslant 1$, one can find some constant C_ε such that

$$\begin{aligned}
\{\varepsilon_s^N\varphi^{2+\varepsilon}\}(x,y)\varepsilon_s^N(x) &\leqslant \varepsilon_s^N(x)\varphi^{2+\varepsilon}(x+y)-\varphi^{2+\varepsilon}(x)-\varepsilon_s^N(y)\varepsilon_s^N(x)\varphi^{2+\varepsilon}(y) \\
&\leqslant \varphi^{2+\varepsilon}(x+y)-\varphi^{2+\varepsilon}(x)-\varepsilon_s^N(y)\varepsilon_s^N(x)\varphi^{2+\varepsilon}(y).
\end{aligned}$$

To deal with the upper bound, note that there exists a constant C_ε such that the inequality

$$(a+b)^\alpha-a^\alpha\leqslant C_\alpha\left(a^{\alpha-1}b+b^\alpha\right).$$

holds for any $a,b\geqslant 0$. It follows that

$$\{\varepsilon_s^N\varphi^{2+\varepsilon}\}(x,y)\varepsilon_s^N(x)\leqslant C_\varepsilon\big(\varphi^{2+\varepsilon}(y)+\varphi^{1+\varepsilon}(x)\varphi(y)\big),$$

so

$$\begin{aligned}
(*) &\leqslant c_\varepsilon\int_0^t\int \big(\varphi^{2+\varepsilon}(y)+\varphi^{1+\varepsilon}(x)\varphi(y)\big)K^N(x,y)\big(\mu_s+\mu_s^N\big)(dy)|\mu_s^N-\mu_s|(dx)\,ds \\
&\leqslant c_\varepsilon\int_0^t\Big(2\big(\|\mu_s\|_{3+\varepsilon}\vee\|\mu_s^N\|_{3+\varepsilon}\big)\|\mu_s^N-\mu_s\|_1+2\big(\|\mu_s\|_2\vee\|\mu_s^N\|_2\big)\|\mu_s^N-\mu_s\|_{2+\varepsilon}\Big)\,ds \\
&\leqslant 4C_\varepsilon C(T)\int_0^t\|\mu_s^N-\mu_s\|_{2+\varepsilon}\,ds.
\end{aligned}$$

Putting the pieces together, we have obtained

$$\|\mu_t^N-\mu_t\|_{2+\varepsilon}\leqslant o_N(1)+4C_\varepsilon C(T)\int_0^t\|\mu_s^N-\mu_s\|_{2+\varepsilon}\,ds,$$

where $o_N(1)$ is uniform in $t\in[0,T]$; Gronwall's lemma enables to conclude. ▷

All the estimates above do not depend on the implicit parameter λ; this proposition proves (a stronger version of) point 2 in our strategy of proof.

3.2. **Convergence of σ_t^N to σ_t in $\big(\mathcal{M}_1, \|.\|_1\big)$.** We prove the third point of our strategy in this section. For that purpose, we rely crucially on the representation formula (2.7) for σ_t for bounded kernels, as it brings back the problem of proving the convergence of σ_t^N to a convergence problem for $(\mu_s^N)_{0\leqslant s\leqslant t}$ and its functionals $U_{s,t}^N$. Given $\ell \geqslant 0$, denote by B_ℓ^0 the set of real-valued functions f on $\mathbb{R}_+$ such that $\frac{|f|}{\varphi^\ell}$ is bounded and converges to 0 at infinity.

PROPOSITION **11.** (1) *There exists a uniformly bounded family of operators $\{U_{s,t}\}_{0\leqslant s\leqslant t\leqslant T}$ on $\big(B_3^0, \|.\|_3\big)$ such that the functions $s,t \mapsto U_{s,t}f$ are differentiable in $\big(B_3^0, \|.\|_0\big)$, when $f \in B_{1+\varepsilon}$, with derivatives $-\Lambda_s U_{s,t} f$ and $U_{s,t}\Lambda_t f$, respectively.*

(2) *These operators $U_{s,t}$ preserve $B_{1+\varepsilon}^0$, and are bounded in $\big(B_{1+\varepsilon}^0, \|.\|_{1+\varepsilon}\big)$.*

PROOF – This proposition is a direct application of theorems 15 and 16 on propagators, in section 5; we apply them to the two pairs $\big(\varphi^{1+\varepsilon}, \varphi^3\big)$ and $\big(\varphi^{\frac12}, \varphi^{1+\varepsilon}\big)$. We adopt the notations

$$\mathbf{J}_s f(x) \equiv \int \big\{f(x+y) - f(x)\big\} K(x,y)\mu_s(dy), \quad \mathbf{M}_s f(x) \equiv \int f(y) K(x,y)\mu_s(dy)$$

used in section 5.

1. Applying theorems 15 and 16, we only need to check that the inequalities
- $\mathbf{J}_s\varphi^\alpha \leqslant C(\alpha)\|\mu_s\|_{\alpha+1}\varphi^\alpha$,
- $\big|\mathbf{M}_s\big(\varphi^\alpha\big)\big| \leqslant \|\mu_s\|_{\alpha+1}\varphi$,
- for any $f \in B_\beta$, $\qquad \mathbf{J}_s f \leqslant 2^{\beta+1}\big(\varphi^{\beta+1}(x)\|\mu_s\|_1 + \varphi(x)\|\mu_s\|_{\beta+1}\big)$.

hold for any α and $\beta \geqslant 1$, which is done by elementary algebra.

2. To apply theorems 15 and 16 to the pair $\big(\varphi^{\frac12}, \varphi^{1+\varepsilon}\big)$, one needs to verify that $\mathbf{J}_s\varphi^{\frac12} \leqslant \dfrac{C(T)}{2}\varphi^{\frac12}$. This can be done by writing

$$\begin{aligned}\int \big\{\varphi^{\frac12}(x+y) - \varphi^{\frac12}(x)\big\} K(x,y)\mu_s(dy) &\leqslant \int \Big\{\big(\varphi(x)+\varphi(y)\big)^{\frac12} - \varphi^{\frac12}(x)\Big\} K(x,y)\mu_s(dy) \\ &\leqslant \int \frac{\varphi(y)}{2\varphi^{\frac12}(x)}\varphi(x)\varphi(y)\mu_s(dy) = \frac{\|\mu_s\|_2}{2}\varphi^{\frac12}(x) \\ &\leqslant \frac{C(T)}{2}\varphi^{\frac12}(x).\end{aligned}$$

▷

Theorem 16 provides us with an additional information: $U_{s,t}$ and all its approximations $U_{s,t}^N$ have a norm on $B_{1+\varepsilon}^0$ controlled by the right hand side of equation (5.7), which is independent of N.

Since $U_{s,t}$ sends $B_{1+\varepsilon}^0$ in itself, and $\Lambda_s^{\partial\lambda}$ is easily verified to be a bounded operator from $B_{1+\varepsilon}$ into $B_{2+\varepsilon}$, with a uniformly bounded norm for $0 \leqslant s \leqslant t \leqslant T$, the formula

$$(f, \sigma_t) = \frac12 \int_0^t \Big(\Lambda_s^{\partial\lambda} U_{s,t} f, \mu_s\Big)\, ds \tag{3.5}$$

defines a measure σ_t belonging to $\mathcal{M}_1$. By proposition 11, the quantities $\big(f, \sigma_t^N\big)$ and $\big(f, \sigma_t\big)$ are bounded uniformly in $t \in [0,T]$, $N \geqslant 0$ and $\lambda \in \mathcal{U}$, given any $f \in B_1$.

THEOREM **12.** *The sequence $\big\{\sigma_t^N\big\}_{N\geqslant 0}$ converges to σ_t in $(\mathcal{M}_1, \|.\|_1)$, uniformly for $t \in [0,T]$.*

PROOF – We need to prove that the limit

$$\big(f, \sigma_t^N\big) = \frac12 \int_0^t \int \big\{U_{s,t}^N f\big\} K^{\partial\lambda\,;\,N}\big(\mu_s^N, \mu_s^N\big)\, ds \underset{N,+\infty}{\longrightarrow} \frac12 \int_0^t \int \big\{U_{s,t} f\big\} K^{\partial\lambda}\big(\mu_s, \mu_s\big)\, ds = (f, \sigma_t)$$

holds uniformly for $\|f\|_1 \leqslant 1$ and $0 \leqslant t \leqslant T$. If one can prove that $U_{s,t}^N f$ converges to $U_{s,t}f$ in $B_{1+\varepsilon}$, uniformly in $0 \leqslant s \leqslant t \leqslant T$, then
- the inequality $\big|K^{\partial\lambda\,;\,N}\big|(x,y) \leqslant \varphi(x)\varphi(y)$,

- and the fact that μ_s^N converges to μ_s in $\big(\mathcal{M}_{2+\varepsilon}, \|.\|_{2+\varepsilon}\big)$, uniformly in $s \in [0,T]$,

will enable us to apply dominated convergence to get the result. We are thus led to prove that there exists a decreasing sequence $\{a_N\}_{N\geqslant 0}$, converging to 0, such that one has

$$\big\|U_{s,t}f - U_{s,t}^N f\|_{1+\varepsilon} \leqslant a_N \big\|f\|_1,$$

for any $0 \leqslant s \leqslant t \leqslant T$ and any $f \in B_1$.
Since $f \in B_1 \subset B_{1+\varepsilon}$ one can use the differentiability property of $U_{s,t}$ as a function of s and t to write

$$U_{s,t}f - U_{s,t}^N f = \int_s^t \frac{d}{du}\big(U_{s,u}U_{u,t}^N\big)\, f\, du = \int_s^t \big(U_{s,u}\big(\Lambda_u - \Lambda_u^N\big)U_{u,t}^N\big)\, f\, du.$$

As $U_{u,t}^N f$ belongs to $B_{1+\varepsilon}^0$, with a norm uniformly controlled for $\|f\|_1 \leqslant 1$, and as $U_{s,u}$ is a uniformly bounded operator on $B_{2+\varepsilon}$, it suffices to prove that *there exists a decreasing sequence* $\{a_N\}_{N\geqslant 0}$ *converging to* 0 *such that one has*

$$\big\|\big(\Lambda_u - \Lambda_u^N\big)g\big\|_{2+\varepsilon} \leqslant a_N,$$

for any $g \in B_{1+\varepsilon}$, *with* $\|g\|_{1+\varepsilon} \leqslant 1$. To prove this fact, write

$$\begin{aligned}
\Big|\big(\Lambda_u^\lambda - \Lambda_u^{\lambda\,;\,N}\big)g(x)\Big| &= \Big|\int \{g\}(x,y)\Big(K(x,y)\mu_s(dy) - K^N(x,y)\mu_s^N(dy)\Big)\Big| \\
&\leqslant c_\varepsilon \int \big(\varphi^{1+\varepsilon}(x)+\varphi(y)\big)\Big(K(x,y)|\mu_s - \mu_s^N|(dy) + |K-K^N|(x,y)\mu_s(dy) + 2\varphi(x)\varphi(y)|\mu_s^N - \mu_s|(dy)\Big) \\
&\leqslant c_\varepsilon\varphi^{2+\varepsilon}(x)\,\|\mu_s^N - \mu_s\|_1 + c_\varepsilon\varphi(x)\,\|\mu_s - \mu_s^N\|_{2+\varepsilon} + c_\varepsilon\varphi^{1+\varepsilon}(x)\,\big(|K-K^N|(x,.),\mu_s\big) \\
&\qquad + c_\varepsilon\Big(\varphi^{1+\varepsilon}(\cdot)\,\big|K-K^N\big|(x,\cdot),\mu_s\Big) + c_\varepsilon\varphi^{2+\varepsilon}(x)\,\|\mu_s^N - \mu_s\|_1 + c_\varepsilon\varphi(x)\,\|\mu_s^N - \mu_s\|_{2+\varepsilon}.
\end{aligned}$$

This formula makes it clear that we shall get the existence of these a_N's if we can prove that the sequence of functions $x \mapsto \big(\varphi^{1+\varepsilon}(\cdot)\,\big|K-K^N\big|(x,\cdot),\mu_s\big)$ converges to 0 in $B_{2+\varepsilon}$ as $N \to +\infty$. This fact is clearly seen on the following inequality where M is an arbitrary positive constant.

$$\begin{aligned}
\frac{1}{\varphi^{2+\varepsilon}(x)}\int \varphi^{1+\varepsilon}(y)|K-K^N|(x,y)\mu_s(dy) &\leqslant \frac{1}{\varphi^{2+\varepsilon}(x)}\int \varphi^{2+\varepsilon}(y)\varphi(x)\mathbf{1}_{\varphi(x)\varphi(y)\geqslant N}\,\mu_s(dy) \\
&\leqslant \frac{1}{\varphi^{1+\varepsilon}(x)}\int \varphi^{2+\varepsilon}(y)\mathbf{1}_{\varphi(x)\varphi(y)\geqslant N}\,\mu_s(dy) \\
&\overset{\varphi\geqslant 1}{\leqslant} \frac{\|\mu_s\|_{2+\varepsilon}}{M^{1+\varepsilon}}\mathbf{1}_{\varphi(x)\geqslant M} + \left(\int \varphi^{2+\varepsilon}(y)\mathbf{1}_{\varphi(y)\geqslant\frac{N}{M}}\mu_s(dy)\right)\mathbf{1}_{\varphi(x)\leqslant M}
\end{aligned}$$

$\triangleright$

Proposition 10 and theorem 12 together prove point (2) and (3) of our strategy of proof for theorem 6, showing that μ_t^λ is a $\mathcal{C}^1$ function of its arguments. To complete the proof of theorem 6, it remains to prove that σ_t^λ is the unique solution in $\mathcal{M}_1$ of the equation

(3.6)
$$\big(f,\sigma_t^\lambda\big) = \big(f,\sigma_0^\lambda\big) + \int_0^t\int \{f\}(x,y)K^\lambda(x,y)\,\mu_s^\lambda(dx)\sigma_s^\lambda(dy)ds + \frac{1}{2}\int_0^t\int \{f\}(x,y)K^{\partial\lambda}(x,y)\,\mu_s^\lambda(dx)\mu_s^\lambda(dy)ds$$

where f is any *bounded* function.

We have seen in section 2.2 that this identity holds if one replaces σ_t^λ and μ_t^λ by $\sigma_t^{\lambda\,;\,N}$ and $\mu_t^{\lambda\,;\,N}$ resspectively. Use then the above convergence results $\sigma_t^{\lambda\,;\,N} \to \sigma_t^\lambda$, in $\mathcal{M}_1$, and $\mu_t^{\lambda\,;\,N} \to \mu_t^\lambda$, in $\mathcal{M}_{2+\varepsilon}$, together with the inequalities

$$\Big|\big(f,K^\lambda(\mu_t^\lambda,\sigma_t^\lambda)\big) - \big(f,K^\lambda(\mu_t^{\lambda\,;\,N},\sigma_t^{\lambda\,;\,N})\big)\Big| \leqslant 3\|f\|_\infty\Big(\|\mu_t^\lambda - \mu_t^{\lambda\,;\,N}\|_1\,\|\sigma_t^\lambda\|_1 + \|\mu_t^{\lambda\,;\,N}\|_1\,\|\sigma_t^\lambda - \sigma_t^{\lambda\,;\,N}\|_1\Big),$$
$$\Big|\big(f,K^{\partial\lambda}(\mu_t^\lambda,\mu_t^\lambda)\big) - \big(f,K^{\partial\lambda}(\mu_t^{\lambda\,;\,N},\mu_t^{\lambda\,;\,N})\big)\Big| \leqslant 3C(T)\,\|f\|_\infty\Big(\|\mu_t^\lambda - \mu_t^{\lambda\,;\,N}\|_1 + \|\sigma_t^\lambda - \sigma_t^{\lambda\,;\,N}\|_1\Big),$$

to pass to the limit properly.

To prove uniqueness of the solution to equation (3.6) in $\big(\mathcal{M}_1, \|\cdot\|_1\big)$ it suffices to show that the equation

$$\forall\, f \in B_c, \quad (f, \gamma_t) = \int_0^t \int \big\{ f(x+y) - f(x) - f(y) \big\} K(x,y) \mu_s(dx) \gamma_s(dy) ds$$

has at most one solution in $\big(\mathcal{M}_1, \|\cdot\|_1\big)$. We have written here B_c for the set of bounded Borel functions with compact support. Rewrite this equation under the form

$$(f, \gamma_t) = \int_0^t \big(\Lambda_s f, \gamma_s\big) ds.$$

Repeating the proof of corollary 11, it is seen that there exists bounded propagators $U_{s,t}$ on $\big(B_1^0, \|\cdot\|_1\big)$ such that the function $s \in [0,t] \mapsto U_{s,t} f$ solves the equation $\frac{d}{ds} U_{s,t} f = -\Lambda_s U_{s,t} f$ for any $f \in B_c (\subset B_1^0)$ and $t \in [0,T]$. It follows that the expression $(U_{s,t} f, \gamma_s)$ is well defined and that

$$\frac{d}{ds} (U_{s,t} f, \gamma_s) = \big(-\Lambda_s U_{s,t} f, \gamma_s\big) + \big(\Lambda_s U_{s,t} f, \gamma_s\big) = 0;$$

so $(f, \gamma_t) = (U_{0,t} f, \gamma_0)$, implying the uniqueness of γ_t. This ends the proof of theorem 6.

4. Comments

4.1. **Related works.** One can see the main roots of theorem 6 in section 4 of Kolokoltsov's pioneering article [33] on the central limit theorem for the Marcus-Lushnikov dynamics. He develops in this section tools for the analysis of the rate of convergence of the semi-group of Marcus-Lushnikov process to the semi-group of solutions of Smoluchowski equation. Recall the Marcus-Lushnikov process $\big\{X_t^n\big\}_{t \geqslant 0}$ is a strong Markov jump process on the space of discrete measures whose jumps are as follows. If its state at time t is $\frac{1}{n} \sum \delta_{x_i(t)}$, for i in a finite set I_t depending on t, define, for $i < j$ in I_t, independent exponential random times T_{ij} with parameter $\frac{K\big(x_i(t), x_j(t)\big)}{n}$ and set

$$T = \min\{T_{ij}\,;\, i < j\}.$$

The process remains constant on the time interval $[t, t+T[$ and has a jump $\frac{1}{n}\big(\delta_{x_p(t)+x_q(t)} - \delta_{x_p(t)} - \delta_{x_q(t)}\big)$ at time $t+T$, if $T = T_{pq}$. The dynamics then starts afresh. The convergence of this sequence $\{X^n\}_{n \geqslant 0}$ of processes to the deterministic solution of Smoluchowski equation was first proved under general conditions in [8]. Yet, no fine analysis of the convergence of the corresponding semi-group was done before [33]. We explain roughly his idea to see how similar equations to the 'variation' equations (1.3), (1.4) appear in his context.

Suppose we are in a situation where existence and uniqueness of solutions to Smoluchowski equation hold into a proper sense, and denote by $\{T_t\}$ and $\{T_t^n\}$ the semi-groups of Smoluchowski and Marcus-Lushnikov dynamics. Also, denote by L and L^n their generators. Then, given any (good) function F and a measure μ

$$\big(T_t - T_t^n\big) F(\mu) = \int_0^t \Big(T_{t-s}^n \big(L^n - L\big) T_s F\Big)(\mu)\, ds.$$

The choice of a function F of the form $F(\mu) = \int g(\mathbf{x}) \mu^{\otimes k}(d\mathbf{x})$, for some symmetric function g of k variables, provides a 'measure' of the moments of μ. One has $T_s F\,(\mu) = F(\mu_s)$, where $\mu_0 = \mu$.

Introducing some derivation operation δ on functions on measures:

$$\delta F(\mu\,;\, x) = \lim_{\varepsilon \to 0} \frac{F(\mu + \varepsilon \delta_x) - F(\mu)}{\varepsilon},$$

one can write for any function G

$$(L^n - L)G(\mu) = -\frac{1}{2n}\int \big(\delta G(\mu\,;\,2x) - 2\delta G(\mu\,;\,x)\big)K(x,x)\mu(dx) + O\big(n^{-3/2}\big). \tag{4.1}$$

One thus sees that taking $G = T_sF$, with the above F, leads to consider the quantity

$$\delta\big((g,\mu_t^{\otimes k})\big) = k\,\big((g,\mu_t^{\otimes k-1}\otimes\delta\mu_t)\big),$$

where

$$\delta\mu_t = \lim_{\varepsilon\to 0}\frac{\mu_t(\mu+\varepsilon\delta_x)-\mu_t(\mu)}{\varepsilon}$$

is 'the' derivative of μ_t with respect to its initial condition. Terms of the form $\delta(\delta\mu_t)$ arise in the $O\big(n^{-3/2}\big)$ term of equation (4.1). This analysis brings back the estimate of $\big(T_t - T_t^n\big)F(\mu)$ to estimates on $\mu_s, \delta\mu_s$ and $\delta^2\mu_s$. To do so, Kolokoltsov shows that $\delta\mu_s$ is a solution of the linear equation

$$\frac{d}{ds}\delta\mu_s = K\big(\mu_s,\delta\mu_s\big)$$

in some sense, and that $\delta^2\mu_s$ is a solution of the affine equation

$$\frac{d}{ds}\delta^2\mu_s = K\big(\mu_s,\delta^2\mu_s\big) + K\big(\delta\mu_s,\delta\mu_s\big)$$

in some sense. The tools used to solve these equations are essentially the same as those used above; the reader may will find the details given here helpful to unzip the section 4 of [33]. We have used yet a slightly different approach in the implementation of the variation of constant method. Note also that we have been able to go from the framework of 'sub-linear' kernels of [33]: $K(x,y)\leqslant C(1+x+y)$, to the framework of an essentially 'sub-multiplicative' kernel: $K(x,y)\leqslant\varphi(x)\,\varphi(y)$, an improvement which is of some practical interest.

4.2. **Kolokoltsov's lemma.** This paragraph contains a simple proof of Kolokoltsov's lemma, which was used in a crucial way to prove a uniqueness result in the original article [36] where it was first introduced. We prove it here in a slightly less general framework than in [36], sufficient for our purposes as well as for its use in [36]; the gain in clarity and volume of the proof is substantial.

Let $(\Omega,\mathcal{F})$ be a measurable space with a σ-algebra $\mathcal{F}$ generated by a filtration $\{\mathcal{F}_n\}_{n\geqslant 0}$ made up of finite σ-algebras. We shall denote by $\{A_n^p\}_p$ the atoms of $\mathcal{F}_n$. We shall write $(\mathcal{M},\|.\|)$ for the space of finite signed-measures on $(\Omega,\mathcal{F})$, equipped with the total variation distance. We shall define, for each $n\geqslant 1$, the total variation of a measure with respect to $\mathcal{F}_n$:

$$\forall\,\mu\in\mathcal{M},\quad \|\mu\|_{(n)} = \sup\big\{(f,\mu)\,;\, f\in\mathcal{F}_n,\,|f|\leqslant 1\big\}.$$

These quantities have the property

$$\forall\,\mu\in\mathcal{M},\quad \|\mu\|_{(n)} \underset{n+\infty}{\longrightarrow} \|\mu\|. \tag{4.2}$$

Recall that the topological dual space of $(\mathcal{M},\|.\|)$ is the space $(\mathcal{B},|.|)$ of bounded measurable functions on $(\Omega,\mathcal{F})$, equipped with the supremum norm. We shall write $\widehat{\mathcal{B}}$ for the set of bounded functions g on $[0,T]\times\Omega$, with norm $\widehat{\|g\|} = \sup\big\{g_s(x)\,;\,s\in[0,T],\,x\in\Omega\big\}$, and shall define $\Big(\widehat{\mathcal{M}},\|.\|_{TV}\Big)$ as the space of finite signed measures on $[0,T]\times\Omega$, equipped with the total variation norm.

Theorem **13** (Kolokoltsov's lemma [36], Appendix)**.** *Let $\{\rho_s\}_{0\leqslant s\leqslant T}$ be a $\mathcal{C}^1$ path in $(\mathcal{M},\|.\|)$, with derivative $\{\dot\rho_s\}_{0\leqslant s\leqslant T}$. There exists a $\{\pm 1,0\}$-valued measurable function $\varepsilon_s(x)$ such that we have*

- $\|\rho_t\| = \|\rho_0\| + \int_0^t(\varepsilon_s,\dot\rho_s)\,ds$, *for any* $t\in[0,T]$,
- $\forall\,f\in\mathcal{B},\forall\,t\in[0,T],\quad \big(f,|\rho_t|\big) = (f\varepsilon_t,\rho_t)$.

We shall make use of the following elementary lemma in the course of the proof of theorem 13.

LEMMA **14.** *By convention,* $\mathrm{sgn}(0) = 0$. *We have for any* $\mathcal{C}^1$ *function* $g : \mathbb{R}_+ \to \mathbb{R}$

$$\big|g(t)\big| = \big|g(0)\big| + \int_0^t \mathrm{sgn}\big(g(s)\big)\, g'(s)ds.$$

PROOF – Using lemma 14 in each set A_n^p, we can define a $\{\pm 1, 0\}$-valued function $s \mapsto \varepsilon_s^{n;p}$ such that

$$\big|\rho_t(A_n^p)\big| = \big|\rho_0(A_n^p)\big| + \int_0^t \varepsilon_s^{n;p} \dot\rho_s(A_n^p)\, ds.$$

Define then the function $\varepsilon_s^n(x)$ as being equal to $\varepsilon_s^{n;p}$ on A_n^p; the preceding identity yields

$$\|\rho_t\|_{(n)} = \|\rho_0\|_{(n)} + \int_0^t (\varepsilon_s^n, \dot\rho_s)\, ds. \tag{4.3}$$

The functions ε^n belong to the set $\widehat{\mathcal{B}}$ of bounded functions on $[0,T] \times \Omega$, and have supremum norm no greater than 1. Using the duality between $\widehat{\mathcal{M}}$ and $\widehat{\mathcal{B}}$ provided by integration, equation (4.3) can be written

$$\|\rho_t\|_{(n)} = \|\rho_0\|_{(n)} + \big(\varepsilon^n, \dot\rho_s \otimes ds\big). \tag{4.4}$$

Now, since $\Big(\widehat{\mathcal{B}}, \widehat{\|.\|}\Big)$ is the topological dual space of $\Big(\widehat{\mathcal{M}}, \|.\|_{TV}\Big)$, its unit sphere is weakly-* compact. We can thus find a sub-sequence $\{\varepsilon^{n_k}\}_{k \geqslant 1}$ and an element ε of $\widehat{\mathcal{B}}$, with norm less than 1, such that

$$\forall\, \mu \in \widehat{\mathcal{M}}, \quad (\varepsilon^{n_k}, \mu) \underset{k+\infty}{\longrightarrow} (\varepsilon, \mu).$$

Together with formulas (4.2) and (4.4), this convergence result, applied to the measures $\dot\rho_s(dx) \otimes \mathbf{1}_{[0,t]}(s)ds$, gives

$$\forall\, t \in [0,T], \quad \|\rho_t\| = \|\rho_0\| + \int_0^t (\varepsilon_s, \dot\rho_s)\, ds. \tag{4.5}$$

To prove the second point of theorem 13, remark that since

$$\int_0^T \|\rho_s\|_{(n)} ds = \int_0^T (\varepsilon_s^n, \rho_s) ds = (\varepsilon^n, \rho_s \otimes \mathbf{1}_{[0,T]} ds),$$

we have

$$\||\rho_s| \otimes ds\|_{TV} = (\varepsilon, \rho_s \otimes \mathbf{1}_{[0,T]} ds).$$

It follows that

$$\varepsilon_s \rho_s = |\rho_s|$$

for almost all s. Define ε_s to be equal to $\frac{d\rho_s}{d|\rho_s|}$ on the exceptional set. This modification of ε_s preserves identity (4.5) and proves the second point of theorem 13. ▷

5. APPENDIX ON PROPAGATORS

We collect in this appendix the material on propagators needed in section 3.2 to prove the convergence of σ_t^N to σ_t in $\big(\mathcal{M}_1, \|\cdot\|_1\big)$. Recall that a ***propagator*** is a family $\{U_{s,t}\}_{s \leqslant t}$ of operators such that $U_{tt} = \mathrm{Id}$ and one has $U_{st}U_{tr} = U_{sr}$ for all $s \leqslant t \leqslant r$. Define an (a priori) unbounded operator on functions setting

$$\Lambda_s f(x) = \int \{f\}(x,y) K(x,y) \mu_s(dy).$$

Theorem 16 below states conditions under which the backward/forward differential equation

$$\dot u_s = -\Lambda_s u_s,\ 0 \leqslant s \leqslant t \leqslant T, \quad u_t \text{ given}, \tag{5.1}$$

can be solved in some Banach space of functions. Some notations are needed. Set

$$\mathbf{J}_s f(x) \equiv \int \big\{f(x+y) - f(x)\big\} K(x,y)\mu_s(dy) = \int f(x+y)K(x,y)\mu_s(dy) - \left(\int K(x,y)\mu_s(dy)\right) f(x) \equiv \mathbf{L}_s f(x) - \tau_s(x) f(x), \tag{5.2}$$

and

$$\mathbf{M}_s f(x) \equiv \int f(y)K(x,y)\mu_s(dy), \quad T_s(x) \equiv \int_0^s \tau_r(x)dr. \tag{5.3}$$

Considering the backward/forward differential equation

$$\dot{f}_s = -\mathbf{J}_s f_s,\ 0 \leqslant s \leqslant t \leqslant T, \quad f_t \text{ given}, \tag{5.4}$$

as a perturbation of the integrable equation $\dot{f}_s = \tau_s f_s$, one sees that equation (5.4) is formally equivalent to the integral equation

$$f_s = e^{T_s - T_t} f_t + \int_s^t e^{T_s - T_r} \mathbf{L}_r f_r\, dr. \tag{5.5}$$

Given some positive function h, set $B_h = \big\{f\,;\, \sup \frac{|f|}{h} < \infty\big\}$, and define $\|f\|_h = \sup \frac{|f|}{h}$, for $f \in B_h$. The space $\big(B_h, \|.\|_h\big)$ is a Banach space. Define also B_h^0 as the set of functions $f \in B_h$ such that $\frac{f}{h}$ goes to 0 as h goes to infinity. The following two theorems are part of the folkore; they are stated under this form in the appendix of Kolokoltsov's article [33].

Theorem **15** (Existence of propagators, first part)**.** *1) Suppose that there exists two continuous positive functions h and h', and positive constants c and c' such that*

a. $0 < h' \leqslant h,\ h' \in B_h,$
$\forall\, s \in [0,T], \quad \mathbf{J}_s h' \leqslant c' h',\ \mathbf{J}_s h \leqslant ch.$

Then, given $t \in [0,T]$ and some function $u_t \in B_h$, the minimal solution of the backwards/forwards integral problem (5.5) with final/initial condition u_t is of the form $\{S_{s,t}u_t\}_s$ for some bounded operators $S_{s,t}$ on $(B_h^0, \|.\|_h)$ depending continuously on s and t, with norm no greater than $e^{c|t-s|}$.

If now one considers the backward/forward differential equation

$$\dot{f}_s = -\Lambda_s f_s = -\big(\mathbf{J}_s - \mathbf{M}_s\big) f_s,\ 0 \leqslant s \leqslant t \leqslant T, \quad f_t = f \ \text{ given},$$

as a perturbation of equation (5.4), the preceding differential equation is formally equivalent to the integral equation

$$f_s = S_{s,t} f - \int_s^t S_{s,r}\mathbf{M}_r f_r\, dr. \tag{5.6}$$

Theorem **16** (Existence of propagators, second part)**.** *2) Suppose, in addition to the hypothesis of theorem 15, that the following hypothesis on the perturbations $\mathbf{M}_s$ hold.*

b. *The family $\{\mathbf{M}_s\}_{0 \leqslant s \leqslant T}$ is a bounded family of linear transforms of $(B_h, \|.\|_h)$.*

Denote by $\|\mathbf{M}_s\|_h$ the norm operator of $\mathbf{M}_s$. Then the series

$$U_{s,t} f = S_{s,t} f - \int_s^t S_{s,r}\mathbf{M}_r S_{r,t} f\, dr + \int_{s \leqslant r_1 \leqslant r_2 \leqslant t} S_{s,r_1}\mathbf{M}_{r_1} S_{r_1,r_2}\mathbf{M}_{r_2} S_{r_2,t} f\, dr_1 dr_2 + \cdots,$$

converges in $(B_h, \|.\|_h)$ for any $f \in B_h$. It defines a propagator on $\big(B_h^0, \|.\|_h\big)$ depending continuously on s and t, and with norm

$$\leqslant e^{\left(c + \sup_{s \leqslant r \leqslant t} \|\mathbf{M}_r\|_h\right)|t-s|} \tag{5.7}$$

The map $s \mapsto U_{s,t}f$ is the minimal solution of the backwards/forwards integral problem (5.6) *with final/initial condition f.*

3) If finally

c. • *for any $f \in B_{h'}$, the function $s \mapsto \mathbf{J}_s f \in (B_h^0, \|.\|_h)$ is well defined and continuous,*
• *each $\mathbf{M}_s$ sends continuously $(B_h, \|.\|_h)$ in $(B_{h'}, \|.\|_{h'})$,*

then for any $f \in B_{h'}$, the function $s \mapsto U_{s,t}f \in \left(B_h^0, \|.\|_h\right)$ is differentiable, with derivative $-\Lambda_s U^{s,t} f$. It is also differentiable as a function of t, with derivative $U_{s,t}\Lambda_t f$.

Acknoledgements. The author would like to thank James Norris for his interest about this work.

References

[1] M. Kraft and R.I. Patterson. Weighted particle methods for the Smoluchowski coagulation equation. *Technical Report 47, c4e-Preprint Series,Cambridge*, 2007.

[2] M. Kraft. Modelling of particulate processes. *American Chemical Society: Preprint Papers, Division of Fuel Chemistry, 51 (1)*, pages 172–173, 2006.

[3] J. R. Norris. Cluster coagulation. *Comm. Math. Phys.*, 209(2):407–435, 2000.

[4] M. Mobilia, P.L. Krapivsky, and S. Redner. Kinetic anomalies in addition-aggregation processes. *J. Phys. A: Math. Gen*, 36:4533–4542, 2003.

[5] M. van Smoluchowski. Drei vortrage uber diffusion. *Brownsche Bewegung und Koagulation von Kolloidteilchen. Physik. Z.*, pages 557–585, 1916.

[6] D. Aldous. Deterministic and stochastic models for coalescence (aggregation and coagulation): a review of the mean-field theory for probabilists. *Bernoulli*, 5(1):3–48, 1999.

[7] F. Leyvraz. Scaling theory and exactly solved models in the kinetics of irreversible aggregation. *Physics Reports*, 383:95–212, 2003.

[8] J. R. Norris. Smoluchowski's coagulation equation: uniqueness, nonuniqueness and a hydrodynamic limit for the stochastic coalescent. *Ann. Appl. Probab.*, 9(1):78–109, 1999.

[9] N. Fournier and Ph. Laurençot. Well-posedness of Smoluchowski's coagulation equation for a class of homogeneous kernels. *J. Funct. Anal.*, 233(2):351–379, 2006.

[10] M.H. Ernst, R.M. Ziff, and E.M. Hendricks. Coagulation processes with a phase transition. *Journal of Colloid and Interface Science*, 97:266–277, 1984.

[11] P. B. Dubovskiĭ and I. W. Stewart. Existence, uniqueness and mass conservation for the coagulation-fragmentation equation. *Math. Methods Appl. Sci.*, 19(7):571–591, 1996.

[12] Yu Jiang. Instantaneous gelation in the generalized smoluchovski coagulation equation. *J. Phys. A: Math. Gen.*, 29:7893, 1996.

[13] I. Jeon. Existence of gelling solutions for coagulation-fragmentation equations. *Comm. Math. Phys.*, 194(3):541–567, 1998.

[14] M. Escobedo, Ph. Laurençot, S. Mischler, and B. Perthame. Gelation and mass conservation in coagulation-fragmentation models. *J. Differential Equations*, 195(1):143–174, 2003.

[15] E. Brunel, R. G. Owens, and H. van Roessel. Gelation time in the discrete coagulation-fragmentation equations with a bilinear coagulation kernel. *J. Phys. A: Math. Theor.*, 40:11749, 2007.

[16] A. A. Lushnikov. Exact post-critical behavior of a source-enhanced gelling system. *J. Phys. A: Math. Theor.*, 41:072001, 2008.

[17] M. Escobedo. Stationary and self-similar solutions for coagulation and fragmentation equations. In *Elliptic and parabolic problems*, volume 63 of *Progr. Nonlinear Differential Equations Appl.*, pages 243–258. Birkhäuser, Basel, 2005.

[18] Ph. Laurençot. Self-similar solutions to a coagulation equation with multiplicative kernel. *Phys. D*, 222(1-2):80–87, 2006.

[19] M. Escobedo and S. Mischler. Dust and self-similarity for the Smoluchowski coagulation equation. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 23(3):331–362, 2006.

[20] Ph. Laurencot and H. van Roessel. Nonuniversal self-similarity in a coagulation-annihilation model with constant kernels. *J. Phys. A: Math. Theor.*, 43:455210, 2010.

[21] J. R. Norris. Notes on Brownian coagulation. *Markov Process. Related Fields*, 12(2):407–412, 2006.

[22] M. R. Yaghouti, F. Rezakhanlou, and A. Hammond. Coagulation, diffusion and the continuous Smoluchowski equation. *Stochastic Process. Appl.*, 119(9):3042–3080, 2009.

[23] A. Eibeck and W. Wagner. Stochastic particle approximations for Smoluchoski's coagulation equation. *Ann. Appl. Probab.*, 11(4):1137–1165, 2001.

[24] S. Rjasanow and W. Wagner. Stochastic weighted particle method, theory and numerical examples. *Bull. Inst. Math. Acad. Sin. (N.S.)*, 2(2):461–493, 2007.
[25] H. L. Man. A survey of numerical solutions to the coagulation equation. *J. Phys. A: Math. Gen.*, 34:10219, 2001.
[26] A. Braumann, M. Goodson, M. Kraft, and P. Mort. Modelling and validation of granulation with heterogeneous binder dispersion and chemical reaction. *Chemical Engeneering Science*, 62:4717–4728, 2007.
[27] H. Wright, R. Muralidhar, T. Tobin, and D. Ramkrishna. Inverse problems of aggregation processes. *Journal of Statistical Physics*, 61(3-4):843–863, 1990.
[28] D. Ramkrishna. *Population balances*. Academic Press, 2000.
[29] M. Kraft and A. Vikhansky. Single-particle method for stochastic simulation of coagulation processes. *Chemical Engineering Science*, 60:963–967, 2005.
[30] I. Bailleul, M. Kraft, P. Man, and J. Norris. Coupling algorithm for calculating sensitivities in smoluchowski equation. *SIAM J. on Scientific Computing*, 32 (2):635–655, 2010.
[31] I. Bailleul, P. Man, and M. Kraft. A stochastic algorithm for sensitivity in Smoluchowski equation. *SIAM J. on Numerical Analysis*, 48 (3):1064–1086, 2010.
[32] Allan H. Marcus. Stochastic coalescence. *Technometrics*, 10:133–143, 1968.
[33] V.N. Kolokoltsov. The central limit theorem for the Smolukovski coagulation model. *Prob. Th. and Rel. Fields*, 146(2), 2010.
[34] V. Kolokoltsov. On the regularity of solutions to the spatially homogeneous Boltzmann equation with polynomially growing collision kernel. *Adv. Stud. Contemp. Math. (Kyungshang)*, 12(1):9–38, 2006.
[35] R. H. Martin, Jr. *Nonlinear operators and differential equations in Banach spaces*. Robert E. Krieger Publishing Co. Inc., Melbourne, FL, 1987.
[36] V. N. Kolokoltsov. Kinetic equations for the pure jump models of k-nary interacting particle systems. *Markov Process. Related Fields*, 12(1):95–138, 2006.

Statistical Laboratory, Cambridge, Email: i.bailleul@statslab.cam.ac.uk, This research was supported by the EPSRC grant EP/E01772X/1.

E-mail address: i.bailleul@statslab.cam.ac.uk
URL: http://www.statslab.cam.ac.uk/~ismael/