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Chemotaxis: from kinetic equations to aggregate dynamics

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Abstract

The hydrodynamic limit for a kinetic model of chemotaxis is investigated. The limit equation is a non local conservation law, for which finite time blow-up occurs, giving rise to measure-valued solutions and discontinuous velocities. An adaptation of the notion of duality solutions, introduced for linear equations with discontinuous coefficients, leads to an existence result. Uniqueness is obtained through a precise definition of the nonlinear flux as well as the complete dynamics of aggregates, i.e. combinations of Dirac masses. Finally a particle method is used to build an adapted numerical scheme.

Keywords: duality solutions, non local conservation equations, hydrodynamic limit, measure-valued solutions, chemotaxis.

2010 AMS subject classifications: 35B40, 35D30, 35L60, 35Q92.

1 Introduction

Kinetic frameworks have been investigated to describe the chemotactic movement of cells in the presence of a chemical substance since in the 80’s experimental observations showed that the motion of bacteria (e.g. *Escherichia Coli*) is due to the alternation of ‘runs and tumbles’. The so-called Othmer-Dunbar-Alt model [1, 12, 19, 21] describes the evolution of the distribution function of cells at time t , position x and velocity v , assumed to have a constant modulus $c > 0$, as well as the concentration $S(t, x)$ of the involved chemical. A general formulation for this model can be written as

$$\begin{cases} \partial_t f_\varepsilon + v \cdot \nabla_x f_\varepsilon &= \frac{1}{\varepsilon} \int_{|v'|=c} (T[S_\varepsilon](v' \rightarrow v) f_\varepsilon(v') - T[S_\varepsilon](v \rightarrow v') f_\varepsilon(v)) dv', \\ -\Delta S_\varepsilon + S_\varepsilon &= \rho_\varepsilon(t, x) := \int_{|v|=c} f_\varepsilon(t, x, v) dv. \end{cases} \quad (1.1)$$

The transport operator on the left-hand side of the first equation stands for the unbiased movement of cells, while the right-hand side governs the chemotactic orientation, or taxis, through the turning kernel $T[S](v' \rightarrow v)$, that is the rate of cells changing their velocity from v' to v .

The parameter ε corresponds to the time interval of information sampling for the bacteria, usually $\varepsilon \ll 1$, and when it goes to zero, one expects to recover the collective behaviour of the population, that is a macroscopic equation for the density $\rho(t, x)$ of cells. Such derivations have been proposed by several authors. When the taxis is small compared to the unbiased movement of cells, the scaling must be of diffusive type, so that the limit equations are of diffusion or drift-diffusion type, see for instance [9] for a rigorous proof. In [14, 20], the authors show that the classical Patlak-Keller-Segel model can be obtained in a diffusive limit for a given smooth chemoattractant concentration.

We focus here on the opposite case, that is when taxis dominates the unbiased movements. This is accounted for in the model by the choice of the scaling in equation (1.1). Moreover, we consider positive chemotaxis, which means that the involved chemical is attracting cells, and therefore is called chemoattractant. The model has been proposed in [10], several works have been devoted to the mathematical study of this kinetic system. Existence of solutions have been obtained for various assumptions on the turning kernel in [9, 7, 11, 15]. Numerical simulations of this system are proposed in [26]. The limit problem is usually of hyperbolic type, see for instance [13, 22, 23] for a hyperbolic limit model which consists in a conservation equation for the cell density and a momentum balance equation.

It is not difficult to obtain the following formal hydrodynamic limit to equation (1.1), more precisely on the total density of particles $\rho = \lim_{\varepsilon} \rho_{\varepsilon}$:

$$\partial_t \rho + \operatorname{div}_x (a[S] \rho) = 0, \quad -\Delta_{xx} S + S = \rho. \quad (1.2)$$

Here the macroscopic velocity $a[S]$ depends on the chemoattractant concentration S through the turning kernel. This system of equations has been obtained in [10], with a rigorous proof in the two-dimensional setting for a fixed smooth S , and therefore a bounded density ρ . The aim of this paper is to obtain rigorously this limit for the whole coupled system. Severe difficulties arise then mainly due to the lack of estimates for the solutions to the kinetic model when ε goes to zero and consequently to the very weak regularity of the solutions to the limit problem.

It turns out that the limit equation is in some sense a weakly nonlinear conservation equation on the density ρ . Indeed the expected velocity field depends on ρ , but through S , and therefore in a non local way. Actually it can be written as a variant of the so-called aggregation equation, for which blow-up in finite time is evidenced (see e.g. [3]), leading to measure-valued solutions. In this respect, this equation behaves also like linear equations with discontinuous coefficients. In particular Dirac masses can arise, this is the mathematical formulation of the aggregation of bacteria. Therefore S is no longer smooth, and a major difficulty in this study will be to define properly the velocity field $a = a[S]$ and the product $a\rho$.

The viewpoint of the aggregation equation has been extensively studied by Carrillo *et al.* [8] through optimal transport techniques. Existence and uniqueness are obtained in a very weak sense, and the dynamics of aggregates is also given. We propose here another approach, based on the notion of duality solutions, as introduced in the linear case by Bouchut and James [4]. The main drawback is that presently we have to restrict ourselves to the one-dimensional case, since the theory in higher dimensions is not complete yet (see [6]). The approach proposed by Poupaud and Rasle [25], which coincides with duality in the 1-d case, could also be explored.

Notice however, that the properties of the expected velocity field a in the two-dimensional case are not obvious either.

More precisely, we propose to proceed in a similar way as in [5], where the nonlinear system of zero pressure gas dynamics is interpreted as a system of two linear conservation equations coupled through the definition of the product. This last point turns out to be crucial in order to obtain a proper uniqueness result for the system (1.2). In this work, the product $a\rho$ will be defined thanks to the limiting flux of the kinetic system (1.1) (see also [16] for another application of the same idea). As we shall see, this is closely related to the dynamics of aggregates, that is combinations of Dirac masses, which reflect some kind of collective behaviour of the population. Finally, an important application of this aggregate dynamics is the development of a numerical scheme, based on a particle method. The motion and collapsing of Dirac masses is clearly evidenced.

The paper is organized as follows. In Section 2 we precisely state the model. Section 3 is devoted to the notion of duality solutions, and contains the main results of this article. Some technical properties which will be useful for the rest of the paper are given in Section 4. Then we investigate in Section 5 the proof of the existence and uniqueness result of duality solution for system (2.8)–(2.10) stated in Theorem 3.9. In Section 6 we prove the rigorous derivation of the hydrodynamical system from the kinetic system. Finally, the dynamics of aggregates and the numerical scheme for the limit equation are described in the last section, where numerical illustrations are also provided.

2 Modelling

From now on we focus on the one dimensional version of the problem, so that $x \in \mathbb{R}$. We first recall the main assumptions leading to the kinetic equation, next we proceed to the formal limit.

2.1 Kinetic model

In this work, cells are supposed to be large enough to sense the gradient of the chemoattractant instantly. Therefore the turning kernel takes the form (independent on v)

$$T[S](v' \rightarrow v) = \Phi(v' \partial_x S). \quad (2.1)$$

The function Φ is the turning rate, obviously it has to be positive. More precisely, for attractive chemotaxis, the turning rate is smaller if cells swim in a favourable direction, that is $v \cdot \nabla_x S \geq 0$. Thus Φ should be a non increasing function. A simplified model for this phenomenon is the following choice for Φ : we fix a positive parameter α , a mean turning rate $\phi_0 > 0$ and take

$$\Phi(x) = \phi_0(1 + \phi(x)), \quad (2.2)$$

where ϕ is an odd function such that

$$\phi \in C^\infty(\mathbb{R}), \quad \phi' \leq 0, \quad \phi(x) = \begin{cases} +\lambda & \text{if } x < -\alpha, \\ -\lambda & \text{if } x > \alpha, \end{cases} \quad (2.3)$$

where $0 < \lambda < 1$ is a given constant.

Now since the transport occurs in \mathbb{R} the set of velocities is $V = \{-c, c\}$, and the expression of the turning kernel simplifies in such a way that (1.1) rewrites

$$\partial_t f_\varepsilon + v \partial_x f_\varepsilon = \frac{1}{\varepsilon} (\Phi(-v \partial_x S) f_\varepsilon(-v) - \Phi(v \partial_x S) f_\varepsilon(v)), \quad v \in V. \quad (2.4)$$

$$- \partial_{xx} S_\varepsilon + S_\varepsilon = \rho_\varepsilon = f_\varepsilon(v) + f_\varepsilon(-v). \quad (2.5)$$

The existence of weak solutions in a L^p setting for a slightly different system in a more general framework has been obtained for instance in [7, 15]. Concerning precisely this model, we refer to [26] for the existence theory in any space dimension. Notice that no uniform L^∞ bounds can be expected. The reader is referred to [26] for some numerical evidences of this phenomenon, which is the mathematical translation of the concentration of bacteria. This is some kind of “blow-up in infinite time”, which for $\varepsilon = 0$ leads to actual blow-up in finite time, and creation of Dirac masses. Moreover the balanced distribution vanishing the right hand side of (2.4) depends on S_ε ; thus the techniques developed e.g. in [9] cannot be applied.

2.2 Formal hydrodynamic limit

We formally let ε go to 0 assuming that S_ε and f_ε admit a Hilbert expansion

$$f_\varepsilon = f_0 + \varepsilon f_1 + \dots, \quad S_\varepsilon = S_0 + \varepsilon S_1 + \dots$$

Multiplying (2.4) by ε and taking $\varepsilon = 0$, we find

$$\Phi(-c \partial_x S_0) f_0(-c) = \Phi(c \partial_x S_0) f_0(c). \quad (2.6)$$

Summing equations (2.4) for c and $-c$, we obtain

$$\partial_t (f_\varepsilon(c) + f_\varepsilon(-c)) + c \partial_x (f_\varepsilon(c) - f_\varepsilon(-c)) = 0. \quad (2.7)$$

Moreover, from equation (2.6) we deduce that

$$f_0(c) - f_0(-c) = \frac{\Phi(-c \partial_x S_0) - \Phi(c \partial_x S_0)}{\Phi(-c \partial_x S_0) + \Phi(c \partial_x S_0)} (f_0(c) + f_0(-c)).$$

The density at equilibrium is defined by $\rho := f_0(c) + f_0(-c)$. Taking $\varepsilon = 0$ in (2.7) we finally obtain

$$\partial_t \rho + \partial_x (a(\partial_x S_0) \rho) = 0,$$

where a is defined by

$$a(\partial_x S_0) = c \frac{\Phi(-c \partial_x S_0) - \Phi(c \partial_x S_0)}{\Phi(-c \partial_x S_0) + \Phi(c \partial_x S_0)} = -c \phi(c \partial_x S_0),$$

and we have used (2.2) for the last identity. Notice that a is actually a macroscopic quantity, since we can rewrite

$$a(\partial_x S_0) = - \frac{\int_V v \Phi(v \partial_x S_0) dv}{\int_V \Phi(v \partial_x S_0) dv},$$

so that this expression is independent the sign of c .

We couple this equation with the limit of the elliptic problem (2.5) for the chemoattractant concentration, so that, in summary, and dropping the index 0, the formal hydrodynamic limit is the following system

$$\partial_t \rho + \partial_x(a(\partial_x S)\rho) = 0, \quad (2.8)$$

$$a(\partial_x S) = -c\phi(c\partial_x S), \quad (2.9)$$

$$-\partial_{xx}S + S = \rho, \quad (2.10)$$

complemented with the boundary conditions

$$\rho(t=0, x) = \rho^{ini}(x), \quad \lim_{x \rightarrow \pm\infty} \rho(t, x) = 0, \quad \lim_{x \rightarrow \pm\infty} S(t, x) = 0. \quad (2.11)$$

We now give the precise formulation of the limit system in terms of aggregate equation. Noticing that a solution to (2.10) has the explicit expression

$$S(t, x) = K * \rho(t, \cdot)(x), \quad \text{where } K(x) = \frac{1}{2}e^{-|x|}, \quad (2.12)$$

the macroscopic conservation equation for ρ (2.8) can be rewritten

$$\partial_t \rho + \partial_x(a(\partial_x K * \rho)\rho) = 0.$$

When a is the identity function, this is exactly the so-called aggregation equation, and since the potential is non-smooth, blow-up in finite time is expected. We refer the reader to e.g. [3, 8], and [17] in the context of chemotaxis.

Similar problems were encountered for instance in [18], where the authors investigate the high field limit of the Vlasov-Poisson-Fokker-Planck model in one space dimension. The limit system is a scalar conservation law coupled to the Poisson equation, and a proper definition of the product is needed to pass to the limit. This definition has been extended in two dimensions by Poupaud [24] using defect measures but losing uniqueness.

3 Duality solutions

3.1 Notations

Let $C_0(Y, Z)$ be the set of continuous functions from Y to Z whose limit vanishes at infinity and $C_c(Y, Z)$ the set of continuous functions with compact support from Y to Z . All along the paper, we denote $\mathcal{M}_{loc}(\mathbb{R})$ the space of local Borel measures on \mathbb{R} . For $\rho \in \mathcal{M}_{loc}$ we denote by $|\rho|(\mathbb{R})$ its total variation. We will denote $\mathcal{M}_b(\mathbb{R})$ the space of measures in $\mathcal{M}_{loc}(\mathbb{R})$ whose total variation is finite. From now on, the space of measure-valued function $\mathcal{M}_b(\mathbb{R})$ is always endowed with the weak topology $\sigma(\mathcal{M}_b, C_0)$. We denote $\mathcal{S}_{\mathcal{M}} := C([0, T]; \mathcal{M}_b(\mathbb{R}) - \sigma(\mathcal{M}_b, C_0))$.

We recall that if a sequence of measure $(\mu_n)_{n \in \mathbb{N}}$ in $\mathcal{M}_b(\mathbb{R})$ satisfies $\sup_{n \in \mathbb{N}} |\mu_n|(\mathbb{R}) < +\infty$, then we can extract a subsequence that converges for the weak topology $\sigma(\mathcal{M}_b, C_0)$.

The coupled system (2.8)–(2.9)–(2.10) is interpreted in this context as a linear conservation equation (2.8), the velocity a of which depends on the solution S to the elliptic equation (2.10).

This actually means that equation (2.8) is somehow nonlinear. One convenient tool to handle such conservation equations

$$\partial_t \rho + \partial_x(a\rho) = 0, \quad a \text{ being a given function,} \quad (3.1)$$

whose solutions eventually are measures in space, is the notion of duality solutions, introduced in [4].

3.2 Linear conservation equations

Duality solutions are defined as weak solutions, the test functions being Lipschitz solutions to the backward linear transport equation

$$\partial_t p + a(t, x)\partial_x p = 0, \quad p(T, \cdot) = p^T \in \text{Lip}(\mathbb{R}). \quad (3.2)$$

A key point to ensure existence of smooth solutions to (3.2) is that the velocity field has to be compressive, in the following sense.

Definition 3.1 *We say that the function a satisfies the so-called one-sided Lipschitz condition (OSL condition) if*

$$\partial_x a(t, \cdot) \leq \beta(t) \quad \text{for } \beta \in L^1(0, T) \text{ in the distributional sense.} \quad (3.3)$$

A formal computation shows that $\partial_t(p\rho) + \partial_x[a(t, x)p\rho] = 0$, and thus

$$\frac{d}{dt} \left(\int_{\mathbb{R}} p(t, x)\rho(t, dx) \right) = 0, \quad (3.4)$$

which defines the duality solutions for suitable p 's. It is now quite classical that (3.3) ensures existence for (3.2), but not uniqueness, which is of great importance here to obtain stability results and make a convenient use of (3.4).

Therefore, the corner stone in the construction of duality solutions is the introduction of the notion of *reversible* solutions to (3.2). A complete statement of the definitions and properties of reversible solutions would be too long in the present context, so that merely a few hints are given. Let \mathcal{L} denote the set of Lipschitz continuous solutions to (3.2), and define the set of *exceptional solutions*:

$$\mathcal{E} = \left\{ p \in \mathcal{L} \text{ such that } p^T \equiv 0 \right\}.$$

The possible loss of uniqueness corresponds to the case where \mathcal{E} is not reduced to zero.

Definition 3.2 *We say that $p \in \mathcal{L}$ is a **reversible solution** to (3.2) if p is locally constant on the set*

$$\mathcal{V}_e = \left\{ (t, x) \in [0, T] \times \mathbb{R}; \exists p_e \in \mathcal{E}, p_e(t, x) \neq 0 \right\}.$$

This definition leads quite directly to the uniqueness results of [4]. It turns out that the class of reversible solutions is also stable by perturbations of the coefficient a .

We now restrict ourselves to those p 's in (3.4). More precisely, we state the following definition.

Definition 3.3 We say that $\rho \in \mathcal{S}_{\mathcal{M}} := C([0, T]; \mathcal{M}_b(\mathbb{R}) - \sigma(\mathcal{M}_b, C_0))$ is a **duality solution** to (3.1) if for any $0 < \tau \leq T$, and any **reversible** solution p to (3.2) with compact support in x , the function $t \mapsto \int_{\mathbb{R}} p(t, x) \rho(t, dx)$ is constant on $[0, \tau]$.

Remark 3.4 A similar notion of duality solution for the transport equation is available $\partial_t u + a \partial_x u = 0$, and ρ is a duality solution of (3.1) iff $u = \int^x \rho$ is a duality solution to transport equation (see [4]).

We shall need the following facts concerning duality solutions.

Theorem 3.5 (Bouchut, James [4])

1. Given $\rho^\circ \in \mathcal{M}_b(\mathbb{R})$, under the assumptions (3.3), there exists a unique $\rho \in \mathcal{S}_{\mathcal{M}}$, duality solution to (3.1), such that $\rho(0, \cdot) = \rho^\circ$.
Moreover, if ρ° is nonnegative, then $\rho(t, \cdot)$ is nonnegative for a.e. $t \geq 0$. And we have the mass conservation

$$|\rho(t, \cdot)|(\mathbb{R}) = |\rho^\circ|(\mathbb{R}), \quad \text{for a.e. } t \in]0, T[.$$

2. Backward flow and push-forward: the duality solution satisfies

$$\forall t \in [0, T], \forall \phi \in C_0(\mathbb{R}), \quad \int_{\mathbb{R}} \phi(x) \rho(t, dx) = \int_{\mathbb{R}} \phi(X(t, 0, x)) \rho^0(dx), \quad (3.5)$$

where the **backward flow** X is defined as the unique reversible solution to

$$\partial_t X + b(t, x) \partial_x X = 0 \quad \text{in }]0, s[\times \mathbb{R}, \quad X(s, s, x) = x.$$

3. For any duality solution ρ , we define the **generalized flux** corresponding to ρ by $a_\Delta \rho = -\partial_t u$, where $u = \int^x \rho dx$.

There exists a bounded Borel function \widehat{a} , called **universal representative** of a , such that $\widehat{a} = a$ almost everywhere, and for any duality solution ρ ,

$$\partial_t \rho + \partial_x(\widehat{a} \rho) = 0 \quad \text{in the distributional sense.}$$

4. Let (a_n) be a bounded sequence in $L^\infty(]0, T[\times \mathbb{R})$, such that $a_n \rightharpoonup a$ in $L^\infty(]0, T[\times \mathbb{R}) - w^*$. Assume $\partial_x a_n \leq \alpha_n(t)$, where (α_n) is bounded in $L^1(]0, T[)$, $\partial_x a \leq \alpha \in L^1(]0, T[)$. Consider a sequence $(\rho_n) \in \mathcal{S}_{\mathcal{M}}$ of duality solutions to

$$\partial_t \rho_n + \partial_x(a_n \rho_n) = 0 \quad \text{in }]0, T[\times \mathbb{R},$$

such that $\rho_n(0, \cdot)$ is bounded in $\mathcal{M}_b(\mathbb{R})$, and $\rho_n(0, \cdot) \rightharpoonup \rho^\circ \in \mathcal{M}_b(\mathbb{R})$.

Then $\rho_n \rightharpoonup \rho$ in $\mathcal{S}_{\mathcal{M}}$, where $\rho \in \mathcal{S}_{\mathcal{M}}$ is the duality solution to

$$\partial_t \rho + \partial_x(a \rho) = 0 \quad \text{in }]0, T[\times \mathbb{R}, \quad \rho(0, \cdot) = \rho^\circ.$$

Moreover, $\widehat{a}_n \rho_n \rightharpoonup \widehat{a} \rho$ weakly in $\mathcal{M}_b(]0, T[\times \mathbb{R})$.

The set of duality solutions is clearly a vector space, but it has to be noted that a duality solution is not *a priori* defined as a solution in the sense of distributions. However, assuming that the coefficient a is piecewise continuous, we have the following equivalence result :

Theorem 3.6 *Let us assume that in addition to the OSL condition (3.3), a is piecewise continuous on $]0, T[\times \mathbb{R}$ where the set of discontinuity is locally finite. Then there exists a function \widehat{a} which coincides with a on the set of continuity of a .*

With this \widehat{a} , $\rho \in \mathcal{S}_{\mathcal{M}}$ is a duality solution to (3.1) if and only if $\partial_t \rho + \partial_x(\widehat{a}\rho) = 0$ in $\mathcal{D}'(\mathbb{R})$. Then the generalized flux $a_{\Delta}\rho = \widehat{a}\rho$. In particular, \widehat{a} is a universal representative of a .

This result comes from the uniqueness of solutions to the Cauchy problem for both kinds of solutions (see Theorem 4.3.7 of [4]).

3.3 Main results

We are now in position to give the definition of duality solutions for the limit system (2.8)–(2.10).

Definition 3.7 *We say that $(\rho, S) \in C([0, T]; \mathcal{M}_b(\mathbb{R})) \times C([0, T]; W^{1,\infty})$ is a duality solution to (2.8)–(2.10) if there exists $a \in L^\infty((0, T) \times \mathbb{R})$ and $\alpha \in L^1_{loc}(0, T)$ satisfying $\partial_x a \leq \alpha$ in \mathcal{D}' , such that*

1. for all $0 < t_1 < t_2 < T$

$$\partial_t \rho + \partial_x(a\rho) = 0 \quad \text{in the sense of duality on }]t_1, t_2[,$$

2. (2.9) is satisfied in the weak sense :

$$\forall \psi \in C^1(\mathbb{R}), \forall t \in [0, T], \quad \int_{\mathbb{R}} (\partial_x S \partial_x \psi + S\psi)(t, x) dx = \int \psi(x) \rho(t, dx),$$

3. $a = a(\partial_x S) \quad \text{a.e.}$

Remark 3.8 *For S in $C([0, T]; W^{1,\infty})$ and ϕ as in (2.3), we have $a(\partial_x S) \in C([0, T]; L^\infty(\mathbb{R}))$. Therefore equation (2.8) is meaningful in the duality sense. The key property is then the one-sided Lipschitz condition.*

Unfortunately, Definition 3.7 does not ensure uniqueness, as we shall evidence in Section 5. This is due to the fact that the product $a(\partial_x S)\rho$ is not properly defined. Indeed the definition of this product relies on the definition of the flux of the system, and we introduce now a flux J , which is defined in a more physical way, and will turn out to be of great importance in the following. Let A be an antiderivative of a such that $A(0) = 0$, we set

$$J = -\partial_x(A(\partial_x S)) + a(\partial_x S)S. \tag{3.6}$$

We can now establish the following uniqueness Theorem:

Theorem 3.9 *Let us assume that ρ^{ini} is given in $\mathcal{M}_b(\mathbb{R})$. Then, for all $T > 0$ there exists a unique duality solution (ρ, S) of (2.8)–(2.10) which satisfies in the distributional sense :*

$$\partial_t \rho + \partial_x J = 0, \quad (3.7)$$

where J is defined in (3.6). It means that the universal representative in Theorem 3.5 satisfies

$$\widehat{a}\rho = J, \quad \text{in the sense of measures.}$$

Moreover, we have $\rho = X_{\#}\rho^{ini}$ where X is the backward flow corresponding to $a(\partial_x S)$.

The second result concerns the rigorous proof of hydrodynamical limit for the kinetic model. Let $(f_\varepsilon, S_\varepsilon)$ be a solution of the system (2.4)–(2.5), complemented with boundary condition null at infinity and with the following initial data:

$$f_\varepsilon(0, \cdot, \cdot) = f_\varepsilon^{ini}, \quad (3.8)$$

such that $\rho_\varepsilon^{ini} = \eta_\varepsilon * \rho^{ini}$ where η_ε is a mollifier and ρ^{ini} is given in $\mathcal{M}_b(\mathbb{R})$. We recall that for fixed $\varepsilon > 0$, there exists $(f_\varepsilon, S_\varepsilon)$ such that f_ε belongs to $C([0, T] \times \mathbb{R} \times V)$ and therefore $S_\varepsilon \in C([0, T]; C^2(\mathbb{R}))$, see [7], or [26] in the present context.

Theorem 3.10 *Let us assume that ρ^{ini} is given in $\mathcal{M}_b(\mathbb{R})$. Let $(f_\varepsilon, S_\varepsilon)$ be a solution to the kinetic–elliptic equation (2.4)–(2.5) with initial data (3.8). Then, as $\varepsilon \rightarrow 0$, $(f_\varepsilon, S_\varepsilon)$ converges in the following sense:*

$$\begin{aligned} \rho_\varepsilon := f_\varepsilon(v) + f_\varepsilon(-v) &\rightharpoonup \rho && \text{in } \mathcal{S}_{\mathcal{M}} := C([0, T]; \mathcal{M}_b(\mathbb{R}) - \sigma(\mathcal{M}_b, C_0)), \\ S_\varepsilon &\rightharpoonup S && \text{in } C([0, T]; W^{1, \infty}(\mathbb{R})) - \text{weak}, \end{aligned}$$

where (ρ, S) is the unique duality solution of the system (2.8)–(2.10) satisfying

$$\widehat{a}\rho = J, \quad \text{in the sense of measures.}$$

4 Properties of S

We gather in this section a set of properties for the solution S to (2.10) that will be used throughout the paper.

Lemma 4.1 *Let $\rho \in C([0, T], \mathcal{M}_b(\mathbb{R}))$. Then the solution S of equation (2.10) satisfies*

1. $\rho \geq 0 \implies S \geq 0$
2. one sided estimate: $-\partial_{xx} S \leq S$ if and only if $\rho \geq 0$
3. for all $p \in [1, +\infty]$, $S \in C([0, T], L^p(\mathbb{R}))$ and $\partial_x S \in C([0, T], L^p(\mathbb{R}))$

Proof. The first two items are easy consequences of the expression (2.12) for the first one, of the equation (2.10) for the second. For the third item, from convolution properties, we have for any $p \in [1, +\infty]$

$$\|S(t, \cdot)\|_{L^p(\mathbb{R})} = \frac{1}{2} \|e^{-|\cdot|} * \rho(t, \cdot)\|_{L^p(\mathbb{R})} \leq |\rho(t, \cdot)|(\mathbb{R}) \frac{1}{2} \|e^{-|\cdot|}\|_{L^p(\mathbb{R})} = \frac{1}{2} \sup_{t \in [0, T]} |\rho(t, \cdot)|(\mathbb{R}),$$

where $|\rho|(\mathbb{R})$ stands for the total mass of the nonnegative measure ρ . We proceed in the same way for $\partial_x S$. \square

As precised above, the key point to use the duality solutions is that the velocity field satisfies the OSL condition (3.3).

Lemma 4.2 *Let $\rho \in \mathcal{S}_{\mathcal{M}}$. Then the coefficient $a(\partial_x S)$ defined by (2.9)-(2.10) satisfies the OSL condition (3.3) if and only if $\rho \geq 0$*

Proof. Straightforward computations lead to

$$\partial_x(a(\partial_x S)) = -c^2 \phi'(c \partial_x S) \partial_{xx} S.$$

With (2.10) and since ϕ is a nonincreasing function, we deduce from the one sided estimate of Lemma 4.1

$$\partial_x(a(\partial_x S)) \leq \max\{c^2 \|\phi'\|_{L^\infty} S, 0\}.$$

We conclude thanks to the bound on S in L^∞ . \square

Finally, we turn to a convergence result for a sequence of such functions S .

Lemma 4.3 *Let $(\rho_n)_{n \in \mathbb{N}}$ be a sequence of measures that converges weakly towards ρ in $\mathcal{S}_{\mathcal{M}}$ as n goes to $+\infty$. Let $S_n(t, x) = (K * \rho_n(t, \cdot))(x)$ and $S(t, x) = (K * \rho(t, \cdot))(x)$, where K is defined in (2.12). Then when $n \rightarrow +\infty$ we have*

$$\begin{aligned} \partial_x S_n(t, x) &\longrightarrow \partial_x S(t, x) && \text{for a.e. } t \in [0, T], x \in \mathbb{R}, \\ \partial_x S_n(t, x) &\rightharpoonup \partial_x S(t, x) && \text{in } L_{t,x}^\infty \text{ weak} - *. \end{aligned}$$

Proof. The proof of this result is obtained by regularization of the convolution kernel (see Lemma 3.1 of [17]). \square

5 Existence and uniqueness for the hydrodynamical problem

In this Section, we focus on the proof of Theorem 3.9, which can be split in 3 steps. The first one consists in obtaining the dynamics of aggregates, or in other words of combinations of Dirac masses. Next we obtain the existence of duality solutions in the sense of Definition 3.7 by approximation. Finally, uniqueness follows from a careful definition of the flux of the equation.

In this respect, we first underline the fact Definition 3.7 as it stands does not give uniqueness of solutions.

Indeed, let us consider (2.8)–(2.10) with boundary condition (2.11) where the initial datum is assumed to be a Dirac mass in 0 : $\rho^{ini} = \delta_0$. We have that $(\delta_0, K * \delta_0)$ is a solution to (2.8)–(2.10) with initial data δ_0 . More generally, the pair

$$\rho_1(t, x) = \delta_{x_1(t)}(x); \quad S_1(t, x) = K * \rho_1(t, x) = \frac{1}{2}e^{-|x-x_1(t)|}. \quad (5.1)$$

turn out to define a solution in the sense of duality in Definition 3.7 for several choices of curves x_1 with $x_1(0) = 0$. Indeed set $b(t, x) = a(\partial_x S_1)(t, x)$, according to Remark 3.4, ρ_1 is a duality solution if $u_1 := \int^x \rho_1 dx = H(x - x_1(t))$ is a duality solution of the transport equation. From Lemma 4.2, b satisfies the OSL condition, therefore u_1 is a duality solution of the transport equation if $a(1/2) > x_1'(t) > a(-1/2)$, which furnishes an infinity of solution.

However, we have on the one hand that the generalized flux (Theorem 3.5 3) is $b_{\Delta} \rho_1 = -\partial_t u_1 = -x_1'(t) \delta_{x_1(t)}$. On the other hand, we compute the flux J given by (3.6). For the clarity of computations, we set here $\alpha = 0$ in the definition (2.3) of Φ . With this convention, we get

$$a(\partial_x S_1)(t, x) = \begin{cases} -\lambda c, & x < x_1(t), \\ \lambda c, & x > x_1(t), \end{cases} \quad A(\partial_x S_1)(t, x) = \frac{1}{2} \begin{cases} -\lambda c e^{x-x_1(t)}, & x < x_1(t), \\ -\lambda c e^{-x+x_1(t)}, & x > x_1(t). \end{cases}$$

Obviously we have $J = 0$, so that the condition $\hat{a}\rho = J$ selects $x_1'(t) = 0$, so that finally $x_1 \equiv 0$ since $x_1(0) = 0$.

5.1 Dynamics of aggregates

Let us first consider the motion of aggregates. We assume then that ρ_n^{ini} is given by a finite sum of Dirac masses : $\rho_n^{ini} = \sum_{i=1}^n m_i \delta_{x_i^0}$ where $x_1^0 < x_2^0 < \dots < x_n^0$. We look for a couple (ρ_n, S_n) solving in the distributional sense $\partial_t \rho_n + \partial_x J_n = 0$ where the flux J_n is given by (3.6) and S_n solves (2.10). We recall that it means that $S_n = K * \rho_n$ where K is defined in (2.12). Let us set $\rho_n(t, x) = \sum_{i=1}^n m_i \delta_{x_i(t)}$. Such a function is a solution in the sense of distributions of (3.7) if u_n is a solution in the sense of distributions of

$$\partial_t u_n - \partial_x A(\partial_x S_n) + a(\partial_x S_n) S_n = 0, \quad (5.2)$$

where u_n is defined by

$$u_n(t, x) := \int^x \rho_n dx = \sum_{i=1}^n m_i H(x - x_i(t)), \quad (5.3)$$

where H denotes the Heaviside function. We have

$$S_n(t, x) = \sum_{i=1}^n \frac{m_i}{2} e^{-|x-x_i(t)|},$$

$$\partial_x S_n(t, x) = - \sum_{i=1}^n \frac{m_i}{2} \text{sign}(x - x_i(t)) e^{-|x-x_i(t)|}. \quad (5.4)$$

Then after calculations, we have in the distributional sense

$$\partial_x A(\partial_x S_n) = a(\partial_x S_n)S_n + \sum_{i=1}^n [A(\partial_x S_n)]_{x_i} \delta_{x_i}, \quad (5.5)$$

where $[f]_{x_i} = f(x_i^+) - f(x_i^-)$ is the jump of the function f in x_i . Injecting (5.3) and (5.5) in (5.2), we find

$$-\sum_{i=1}^n m_i x'_i(t) \delta_{x_i(t)} = \sum_{i=1}^n [A(\partial_x S_n)]_{x_i} \delta_{x_i}.$$

Thus the dynamics of aggregates is finally given by

$$m_i x'_i(t) = -[A(\partial_x S_n)]_{x_i(t)}, \quad \text{for } i = 1, \dots, n.$$

We complement this system of ODE by the initial data $x_i(0) = x_i^0$. More precisely, recalling that $K(x) = \frac{1}{2}e^{-|x|}$, using (5.4) this latter system can be rewritten :

$$m_i x'_i(t) = A\left(\frac{m_i}{2} + \sum_{j \neq i} m_j \partial_x K(x_j - x_i)\right) - A\left(-\frac{m_i}{2} + \sum_{j \neq i} m_j \partial_x K(x_j - x_i)\right). \quad (5.6)$$

From the definition of the coefficient a in (2.9) with (2.3), we deduce that a is nondecreasing and odd. Therefore A is a convex function and we deduce that for $i = 1, \dots, n-1$, $x'_i \geq x'_{i+1}$. Therefore, aggregates can collapse in finite time and an aggregate can not split. This is a direct consequence of the fact that we are considering positive chemotaxis, i.e. a is nondecreasing. If there exists a time t_1 for which we have for instance $x_i(t_1) = x_{i+1}(t_1)$, then the dynamics for $t > t_1$ is defined as above except that we replace m_i by $m_i + m_{i+1}$ and $x_i(t) = x_{i+1}(t)$ for $t > t_1$. Moreover A is even, then when $n = 1$, we have $x'_1 = 0$ and $x_1(t) = x_1^0$. Thus if aggregates collapse such that they form a single aggregate of mass $\sum_i m_i$, then this aggregate does not move for larger times.

5.2 Existence of duality solutions

We have constructed (ρ_n, S_n) which is a solution of (3.7)-(3.6)-(2.10) in the distributional sense for the given initial data ρ_n^{ini} . We recall the following result due to Vol'pert [27] (see also [2]) : if u belongs to $BV(\mathbb{R})$ and $f \in C^1(\mathbb{R})$ with $f(0) = 0$, then $v = f \circ u$ belongs to $BV(\mathbb{R})$ and

$$\exists \bar{f}_u \quad \text{with } \bar{f}_u = f'(u) \text{ a.e.} \quad \text{such that } (f \circ u)' = \bar{f}_u u'.$$

We recall that A is an antiderivative of a such that $A(0) = 0$. Then, using this result, there exists a function \widehat{a}_n such that

$$J_n := -\partial_x(A(\partial_x S_n)) + a(\partial_x S_n)S_n = \widehat{a}_n \rho_n, \quad \text{and} \quad \widehat{a}_n = a(\partial_x S_n) \text{ a.e.}$$

Thus ρ_n is a solution in the distributional sense of

$$\partial_t \rho_n + \partial_x(\widehat{a}_n \rho_n) = 0.$$

Moreover, we deduce from (5.4) that $a(\partial_x S_n)$ is piecewise continuous with the discontinuity lines defined by $x = x_i$, $i = 1, \dots, n$. We can apply Theorem 3.6 which gives that ρ_n is a duality solution and that \widehat{a}_n is a universal representative of $a(\partial_x S_n)$. Then the flux is given by $a(\partial_x S_n) \Delta \rho_n = J_n$.

Let us yet consider the case of any initial data $\rho^{ini} \in \mathcal{M}_b(\mathbb{R})$. We approximate ρ^{ini} by $\rho_n^{ini} = \sum_{i=1}^n m_i \delta_{x_i^0}$ with $\rho_n^{ini} \rightharpoonup \rho^{ini}$ in $\mathcal{M}_b(\mathbb{R})$. By the same token as above, we can construct a solution $(\rho_n, S_n = K * \rho_n)$ which solves

$$\partial_t \rho_n + \partial_x (a(\partial_x S_n) \rho_n) = 0$$

in the sense of duality,

$$\partial_t \rho_n + \partial_x J_n = 0, \quad J_n = -\partial_x A(\partial_x S_n) + a(\partial_x S_n) S_n$$

in the sense of distributions and

$$\widehat{a}_n \rho_n = J_n, \quad \widehat{a}_n = a(\partial_x S_n) \text{ a.e.}$$

and which is such that $\rho_n(t=0) = \rho_n^{ini} = \sum_{i=1}^n m_i \delta_{x_i^0}$. Moreover, since $\partial_x S_n$ is bounded in L^∞ uniformly with respect to n by construction, we can extract a subsequence of $(a(\partial_x S_n))_n$ that converges in $L^\infty - weak^*$ towards b . Since from Lemma 4.2, $a(\partial_x S_n)$ satisfies the OSL condition, we deduce from Theorem 3.5 4) that, up to an extraction, $\rho_n \rightharpoonup \rho$ in \mathcal{S}_M and $\widehat{a}_n \rho_n \rightharpoonup \widehat{a} \rho$ weakly in $\mathcal{M}_b([0, T] \times \mathbb{R})$, ρ being a duality solution of the scalar conservation law with coefficient b . With Lemma 4.3, we deduce that $\partial_x S_n \rightarrow \partial_x S$ a.e., it implies in particular that $J_n \rightarrow J := -\partial_x A(\partial_x S) + a(\partial_x S) S$ in $\mathcal{D}'(\mathbb{R})$ and that $a(\partial_x S_n) \rightarrow a(\partial_x S)$ a.e. By uniqueness of the weak limit, we have $b = a(\partial_x S)$. Moreover $J = \widehat{a} \rho$ a.e. and ρ satisfies then (3.7). Then (ρ, S) is a solution as in Theorem 3.9, this concludes the proof of the existence.

5.3 Uniqueness of solutions

Let us consider yet the study of the uniqueness. As shown above, Definition 3.7 is not enough to get the uniqueness. Therefore, we will use the fact that we have a duality solution ρ that satisfies (3.7) in $\mathcal{D}'([0, T] \times \mathbb{R})$ with the initial data ρ^{ini} and with the flux J given by (3.6). This equation will lead to a non-local evolution equation on S as stated in the following Lemma :

Lemma 5.1 *Let (ρ, S) be a duality solution of (2.8)–(2.10) such as in Theorem 3.9 then $\partial_x S \in C([0, T], BV(\mathbb{R}))$ and S is a weak solution of*

$$\partial_t S - \partial_x K * \partial_x (A(\partial_x S)) + \partial_x K * (a(\partial_x S) S) = 0. \quad (5.7)$$

Proof. We have $\rho \in \mathcal{S}_M$ and $\partial_{xx} S = S - \rho$. Then $\partial_x S \in C([0, T], BV(\mathbb{R}))$. We recall that we have $S = K * \rho$ where $K(x) = \frac{1}{2} e^{-|x|}$. Thus taking the convolution by K of (3.7)–(3.6), we get that S is weak solutions of (5.7). Differentiating (5.7), we get moreover

$$\partial_t \partial_x S + \partial_x (A(\partial_x S)) - \partial_x K * A(\partial_x S) + K * (a(\partial_x S) S) - a(\partial_x S) S = 0. \quad (5.8)$$

□

Proposition 5.2 *Let S_1 and S_2 be two weak solutions in $C([0, T]; W^{1,1}(\mathbb{R}))$ of (5.7) with initial data S_1^{ini} and S_2^{ini} respectively and such that $\partial_x S_1$ and $\partial_x S_2$ belongs to $L^\infty([0, T]; BV(\mathbb{R}))$. Then there exists a nonnegative constant C such that*

$$\|S_1 - S_2\|_{L^\infty([0, T]; W^{1,1}(\mathbb{R}))} \leq C \|S_1^{ini} - S_2^{ini}\|_{W^{1,1}(\mathbb{R})}.$$

Proof. Let us denote $a_1 = a(\partial_x S_1)$ and $a_2 = a(\partial_x S_2)$. We deduce from (5.8) that

$$\partial_t \partial_x (S_1 - S_2) + \partial_x (A(\partial_x S_1) - A(\partial_x S_2)) = \partial_x K * (A(\partial_x S_1) - A(\partial_x S_2)) + a_1 S_1 - a_2 S_2 - K * (a_1 S_1 - a_2 S_2).$$

Multiplying this equation by $\text{sign}(\partial_x (S_1 - S_2))$, integrating with respect to x and using the properties of the convolution product, we deduce

$$\frac{d}{dt} \int_{\mathbb{R}} |\partial_x (S_1 - S_2)| dx \leq \|\partial_x K\|_\infty \int_{\mathbb{R}} |A(\partial_x S_1) - A(\partial_x S_2)| dx + (1 + \|K\|_\infty) \int_{\mathbb{R}} |a_1 S_1 - a_2 S_2| dx.$$

The function a being regular, we have

$$\frac{d}{dt} \int_{\mathbb{R}} |\partial_x (S_1 - S_2)| dx \leq C_0 \int_{\mathbb{R}} |\partial_x (S_1 - S_2)| dx + C_1 \int_{\mathbb{R}} |S_1 - S_2| dx. \quad (5.9)$$

By the same token with equation (5.7), it leads to

$$\frac{d}{dt} \int_{\mathbb{R}} |S_1 - S_2| dx \leq C_2 \int_{\mathbb{R}} |\partial_x (S_1 - S_2)| dx + C_3 \int_{\mathbb{R}} |S_1 - S_2| dx. \quad (5.10)$$

Summing (5.10) and (5.9), we deduce that there exists a nonnegative constant C such that

$$\frac{d}{dt} \|S_1 - S_2\|_{W^{1,1}(\mathbb{R})} \leq C \|S_1 - S_2\|_{W^{1,1}(\mathbb{R})}.$$

Applying the Gronwall Lemma allows to conclude the proof. \square

Proof of the uniqueness of Theorem 3.9. Let us assume that we have two dual-ity solutions (ρ_1, S_1) and (ρ_2, S_2) such as in Theorem 3.9. Therefore, from Lemma 5.1, S_1 and S_2 are weak solutions of (5.7). Using Proposition 5.2, we conclude that $S_1 = S_2$. Thus $\rho_1 = K * S_1 = K * S_2 = \rho_2$. \square

Remark 5.3 *We deduce from the proof above that equations (5.7) and (5.8) are a key point for the uniqueness of solutions. These equations relies strongly on the definition of the flux J in (3.6). This fact has already been noticed by the authors in [16], which can be viewed as a particular case of the one studied in this paper by replacing the elliptic equation for S (2.10) by the Poisson equation $-\partial_{xx} S = \rho$. In this case, the product of $a(\partial_x S)$ by ρ is naturally defined by $a(\partial_x S)\rho = -\partial_x A(\partial_x S)$ and the equation on S corresponding to (5.8) is given by*

$$\partial_t \partial_x S + \partial_x A(\partial_x S) = 0.$$

Contrary to (5.8), this equation is local and since $\partial_x S$ is monotonous ($-\partial_{xx} S = \rho \geq 0$), we are looking for an entropy solutions of this equation and for A convex or concave (i.e. for a non-decreasing or non-increasing), there exists a unique entropy solution. Uniqueness in [16] is obtained in this way.

6 Convergence for the kinetic model

In this section we investigate the rigorous derivation of (2.8)–(2.10) from the microscopic model (2.4). We first state some estimates on the moments of the solution of the kinetic problem.

Lemma 6.1 *Let $(f_\varepsilon, S_\varepsilon)$ be a solution of the kinetic problem (2.4)–(2.5). Then for all $t \in [0, T]$ and all $\varepsilon > 0$ we have*

$$\int_{\mathbb{R}} \int_V |v|^k f_\varepsilon dx dv = |v|^k |\rho^{ini}|(\mathbb{R}), \quad k \in \mathbb{N}.$$

Proof. Since $v \in V = \{-c, c\}$, $|v|$ is constant therefore

$$\int_{\mathbb{R}} \int_V |v|^k f_\varepsilon dx dv = |v|^k \int_{\mathbb{R}} \rho_\varepsilon dx.$$

The result follows then directly from the mass conservation in (2.4). \square

Proof of Theorem 3.10. Let $(f_\varepsilon, S_\varepsilon)$ be a solution of (2.4)–(2.5). For fixed $\varepsilon > 0$, we have $f_\varepsilon \in C([0, T] \times \mathbb{R} \times V)$. Define $\rho_\varepsilon := \int_V f_\varepsilon dv$, $J_\varepsilon := \int_V v f_\varepsilon dv$ and $a(\partial_x S_\varepsilon) = -c\phi(c\partial_x S_\varepsilon)$. We can rewrite the kinetic equation (2.4) as

$$\partial_t f_\varepsilon + v \partial_x f_\varepsilon = \frac{1}{\varepsilon} (\Phi(-v \partial_x S_\varepsilon) \rho_\varepsilon - 2f_\varepsilon).$$

Taking the zeroth and first order moments, we get

$$\partial_t \rho_\varepsilon + \partial_x J_\varepsilon = 0, \tag{6.1}$$

$$\partial_t J_\varepsilon + v^2 \partial_x \rho_\varepsilon = \frac{2}{\varepsilon} (a(\partial_x S_\varepsilon) \rho_\varepsilon - J_\varepsilon). \tag{6.2}$$

From (6.1), we deduce that

$$\forall t \in [0, T], \quad |\rho_\varepsilon(t, \cdot)|(\mathbb{R}) = |\rho^{ini}|(\mathbb{R}).$$

Therefore, for all $t \in [0, T]$ the sequence $(\rho_\varepsilon(t, \cdot))_\varepsilon$ is relatively compact in $\mathcal{M}_b(\mathbb{R}) - \sigma(\mathcal{M}_b(\mathbb{R}), C_0(\mathbb{R}))$. Moreover, there exists $u_\varepsilon \in L^\infty([0, T], BV(\mathbb{R}))$ such that $\rho_\varepsilon = \partial_x u_\varepsilon$. From (6.1), we get that $\partial_t u_\varepsilon = -J_\varepsilon$ and with Lemma 6.1 we deduce that u_ε is bounded in $\text{Lip}([0, T], L^1(\mathbb{R}))$. It implies the equicontinuity in t of $(\rho_\varepsilon)_\varepsilon$. Thus the sequence $(\rho_\varepsilon)_\varepsilon$ is relatively compact in $\mathcal{S}_\mathcal{M}$ and we can extract a subsequence still denoted $(\rho_\varepsilon)_\varepsilon$ that converges towards ρ in $\mathcal{S}_\mathcal{M}$.

We recall that $S_\varepsilon(t, x) = (K * \rho_\varepsilon(t, \cdot))(x)$ where $K(x) = \frac{1}{2}e^{-|x|}$. Denoting $S(t, x) := (K * \rho(t, \cdot))(x)$, since $\rho \in \mathcal{S}_\mathcal{M}$, we have $\partial_x S \in L^\infty([0, T]; BV(\mathbb{R}))$. From Lemma 4.3, the sequence $(\partial_x S_\varepsilon)_\varepsilon$ converges in $L^\infty w - *$ and a.e. to $\partial_x S$ as ε goes to 0. Lemma 4.2 ensures that both $a(\partial_x S_\varepsilon)$ and $a(\partial_x S)$ satisfy the OSL condition.

From (6.1)–(6.2), we have in the distributional sense

$$\partial_t \rho_\varepsilon + \partial_x (a(\partial_x S_\varepsilon) \rho_\varepsilon) = \partial_x (a(\partial_x S_\varepsilon) \rho_\varepsilon - J_\varepsilon) = \frac{\varepsilon}{2} \partial_x (\partial_t J_\varepsilon + v^2 \partial_x \rho_\varepsilon) = R_\varepsilon. \tag{6.3}$$

Now, for all $\psi \in C_c^2((0, T) \times \mathbb{R})$, we deduce from Lemma 6.1

$$\left| \int (\partial_t J_\varepsilon + v^2 \partial_x \rho_\varepsilon) \partial_x \psi \, dx dt \right| \leq |v| |\rho^{ini}|(\mathbb{R}) \|\partial_t \partial_x \psi\|_{L^\infty} + |v|^2 |\rho^{ini}|(\mathbb{R}) \|\partial_{xx} \psi\|_{L^\infty}.$$

This implies that the limit in the distributional sense of the right-hand side R_ε of (6.3) vanishes.

On the one hand, multiplying equation (2.5) by $a(\partial_x S_\varepsilon)$ and introducing the real-valued function A such that $A' = a$, we get

$$a(\partial_x S_\varepsilon) \rho_\varepsilon = -\partial_x (A(\partial_x S_\varepsilon)) + a(\partial_x S_\varepsilon) S_\varepsilon, \quad (6.4)$$

so that we can rewrite the conservation equation (6.3) as follows, in $\mathcal{D}'(\mathbb{R})$:

$$\partial_t \rho_\varepsilon + \partial_x (-\partial_x A(\partial_x S_\varepsilon) + a(\partial_x S_\varepsilon) S_\varepsilon) = \frac{\varepsilon}{2} \partial_x (\partial_t J_\varepsilon + v^2 \partial_x \rho_\varepsilon). \quad (6.5)$$

Taking the limit $\varepsilon \rightarrow 0$ at the distributional sense of equation (6.5), we get that in $\mathcal{D}'(\mathbb{R})$

$$\partial_t \rho + \partial_x (-\partial_x A(\partial_x S) + a(\partial_x S) S) = 0, \quad (6.6)$$

where $S(t, x) = (K * \rho(t, \cdot))(x)$. We recall that we have chosen the initial data such that $\rho_\varepsilon^{ini} = \eta_\varepsilon * \rho^{ini}$ where η_ε is a mollifier. Therefore $\rho_\varepsilon^{ini} \rightharpoonup \rho^{ini}$ in $\mathcal{M}_b(\mathbb{R}) - \sigma(\mathcal{M}_b(\mathbb{R}), C_0(\mathbb{R}))$.

On the other hand, first taking the convolution with K of (6.6) we find that S and $\partial_x S$ satisfy in the distributional sense

$$\partial_t S - \partial_x K * \partial_x (A(\partial_x S)) + \partial_x K * (a(\partial_x S) S) = 0. \quad (6.7)$$

Next, differentiating this (or taking the convolution of (6.6) with $\partial_x K$), and noticing that K satisfies $-\partial_{xx} K + K = \delta_0$, we get

$$\partial_t \partial_x S + \partial_x (A(\partial_x S)) - \partial_x K * A(\partial_x S) + K * (a(\partial_x S) S) - a(\partial_x S) S = 0. \quad (6.8)$$

The definition of S , $S(t, x) = (K * \rho(t, \cdot))(x)$, implies that $\partial_x S$ belongs to $L^\infty(0, T; BV(\mathbb{R}))$. Therefore equations (6.7)–(6.8) have a sense in their weak formulation. It is proved in Section 5.3 that we have a bound on S in $C([0, T]; W^{1,1}(\mathbb{R}))$ and that such a S satisfying (6.7)–(6.8) is unique. Thus ρ is unique. In fact, if we assume that there exist ρ_1 and ρ_2 satisfying (6.6) in the distributional sense, then by the uniqueness of the solution of (6.7)–(6.8), we have that $K * \rho_1 = K * \rho_2$ which implies that $\rho_1 = \rho_2$. Finally, thanks to the uniqueness, all the sequence ρ_ε converges to ρ in \mathcal{S}_M .

Thus we have constructed a solution that satisfies (6.6) in the distributional sense, in other words, we have defined a solution of the problem (2.8)–(2.10) thanks to its flux. A natural question is to know whether we can define a velocity corresponding to this flux. From the theory of duality solutions (see Theorem 3.5), it boils down to show that the above constructed solution is a duality solution. From the Vol'pert calculus [27] there exists a_S such that $a_S = a(\partial_x S)$ a.e. and

$$\partial_x (A(\partial_x S)) = a_S \partial_{xx} S.$$

Therefore

$$-\partial_x (A(\partial_x S)) + a(\partial_x S) S = a_S \rho \text{ a.e.}, \quad \text{with } a_S = a(\partial_x S) \text{ a.e.} \quad (6.9)$$

Using equation (6.6) we have in the distributional sense

$$\partial_t \rho + \partial_x(a_S \rho) = 0. \quad (6.10)$$

However, we have proved in Section 5.3 that such a solution is unique. We deduce that the solution (ρ, S) obtained by the hydrodynamical limit above is the duality solution of Theorem 3.9. It concludes the proof of Theorem 3.10. \square

Remark 6.2 *In the proof above, the macroscopic flux J defined in (3.6) appears to be the limit of the microscopic flux J_ϵ . Indeed from (6.2) and (6.4) we deduce that, in the distributional sense,*

$$J_\epsilon \longrightarrow J := -\partial_x A(\partial_x S) + a(\partial_x S)S.$$

This natural definition of the flux allows to get the uniqueness of the solutions of the coupled system (2.8)–(2.10) thanks to equations (6.7)–(6.8). Such a technique to establish the hydrodynamic limit has been proposed in [18]. But the authors do not state that their limit is a duality solution and do not define a velocity and therefore a flow corresponding to their flux. In the limit of the Vlasov-Poisson-Fokker-Planck system, this result has been investigated in [16].

7 Numerical issue

7.1 Finite time of collapse

Before focusing on the numerical simulations, let us clarify the dynamics of the model. In the case of n Dirac masses located at positions $x_1 < \dots < x_n$, we recall that the time evolution is governed by system (5.6):

$$m_i x'_i(t) = A \left(\frac{m_i}{2} + \sum_{j \neq i} m_j \partial_x K(x_j - x_i) \right) - A \left(-\frac{m_i}{2} + \sum_{j \neq i} m_j \partial_x K(x_j - x_i) \right), \quad (7.1)$$

for $i = 1, \dots, n$, where we recall that A is an antiderivative of a such that $A(0) = 0$. We deduce that for all $t > 0$, and for $i = 1, \dots, n$,

$$\begin{aligned} \exists \gamma_i \in \left(-\frac{m_i}{2} + \sum_{j \neq i} m_j \partial_x K(x_j - x_i), \frac{m_i}{2} + \sum_{j \neq i} m_j \partial_x K(x_j - x_i) \right) \\ \text{such that } x'_i(t) = a(\gamma_i(t)). \end{aligned} \quad (7.2)$$

Proposition 7.1 *Let us assume that there exists $n \in \mathbb{N}^*$ such that*

$$\rho^{ini}(x) = \sum_{i=1}^n m_i^0 \delta_{x_i^0}(x).$$

We assume moreover that a is a nondecreasing and odd real function and A its antiderivative such that $A(0) = 0$. Then the duality solution ρ of Theorem 3.9 has the following properties :

1. *If $n = 1$, $x_1(t) = x_1^0$ for all $t > 0$. Then $\rho(t) = \rho^{ini}$ for all $t > 0$.*

2. For $i = 1, \dots, n-1$, $x'_i(t) \geq x'_{i+1}(t)$ therefore $x_{i+1} - x_i \leq x_{i+1}^0 - x_i^0$.

3. There exists $c^* \in [x_1^0, x_n^0]$ and $T^* > 0$ such that $\rho(t, x) = \delta_{c^*}(x)$ for all $t > T^*$.

Proof. The first point is a direct consequence of the even character of A whereas the second point comes from the convexity of A . Let us then prove the third point. By convexity of the function A and with (7.1), we have

$$m_1 x'_1 \geq A \left(\frac{m_1}{2} + \sum_{j=2}^n \frac{m_j}{2} e^{x_1^0 - x_j^0} \right) - A \left(-\frac{m_1}{2} + \sum_{j=2}^n \frac{m_j}{2} e^{x_1^0 - x_j^0} \right) > 0,$$

and

$$m_n x'_n \leq A \left(-\sum_{j=1}^{n-1} \frac{m_j}{2} e^{x_j^0 - x_n^0} + \frac{m_n}{2} \right) - A \left(-\sum_{j=1}^{n-1} \frac{m_j}{2} e^{x_j^0 - x_n^0} - \frac{m_n}{2} \right) < 0.$$

As for (7.2), we can rewrite these last inequalities as :

$$x'_1(t) \leq a(\gamma_1(0)), \quad x'_n \geq a(\gamma_n(0)).$$

We deduce that there exists a time $T^* > 0$ such that all masses collapse for $t = T^*$ in a single Dirac mass. Moreover, we have

$$T^* < (x_n^0 - x_1^0) / (a(\gamma_1(0)) - a(\gamma_n(0))).$$

□

Corollary 7.2 *Let us assume that $\rho^{ini} \in C_c(\mathbb{R})$ with compact support $[0, L]$. Let us denote ρ the duality solution of Theorem 3.9 with initial data ρ^{ini} . Then there exists $c^* \in [0, L]$ and $T^* > 0$ such that $\rho(t, x) = \delta_{c^*}(x)$ for all $t > T^*$.*

Proof. Let us approximate ρ^{ini} by

$$\rho_n^{ini}(x) = \sum_{i=1}^n m_i^0 \delta_{x_i^0}(x),$$

with $x_i^0 = (i-1)L/n$, for $i = 1, \dots, n$ and $m_i^0 = \int_{x_i^0}^{x_{i+1}^0} \rho^{ini}(dx)$. From Proposition 7.1, we deduce that there exists $c_n^* \in [0, L]$ and $T_n^* > 0$ such that the duality solution of Theorem 3.9 with initial data ρ_n^{ini} is such that $\rho_n(t, x) = \delta_{c_n^*}$ for all $t > T_n^*$. Moreover, we have $T_n^* < L / (a(\gamma_1^n(0)) - a(\gamma_n^n(0)))$ where we recall that

$$-m_1^0 + \sum_{j=1}^n \frac{m_j^0}{2} e^{-(j-1)L/n} < \gamma_1^n(0) < \sum_{j=1}^n \frac{m_j^0}{2} e^{-(j-1)L/n}, \quad (7.3)$$

and

$$-\sum_{j=1}^n \frac{m_j^0}{2} e^{(j-n)L/n} < \gamma_n^n(0) < m_n^0 - \sum_{j=1}^n \frac{m_j^0}{2} e^{(j-n)L/n}. \quad (7.4)$$

By stability results on duality solutions in Theorem 3.5 (see also subsection 5.1), we deduce that $\rho_n \rightharpoonup \rho$ in \mathcal{S}_M as $n \rightarrow +\infty$. Taking the limit in (7.3) and (7.4), we deduce by continuity of ρ^{ini} that

$$\lim_{n \rightarrow +\infty} \gamma_1^n(0) = \int_0^L \rho^{ini}(x) e^{-x} dx$$

and

$$\lim_{n \rightarrow +\infty} \gamma_n^n(0) = - \int_0^L \rho^{ini}(x) e^{-L+x} dx.$$

Moreover, since ρ^{ini} is continuous with compact support in $[0, L]$ we have $\rho^{ini}(0) = \rho^{ini}(L) = 0$. We deduce that the sequence $(T_n^*)_{n \in \mathbb{N}^*}$ is bounded. Thus there exists a time T^* independent of n such that $\rho_n(t) = \delta_{c_n^*}$ for all $t > T^*$. Taking the limit when $n \rightarrow +\infty$, we conclude that there exists $c \in [0, L]$ such that $\rho(t) = \delta_c$ for all $t > T^*$. \square

Remark 7.3 Taking $a = Id$, therefore $A(x) = x^2/2$, we deduce from (7.1) that

$$x'_i = \sum_{j \neq i} m_j \partial_x K(x_j - x_i).$$

We recover the dynamics of the aggregation equation as noticed by Carrillo et al. in [8]. They prove in particular the concentration in finite time of the total mass in the center of mass. In the framework of this work, focusing on applications in chemotaxis, a is not assumed to be the identity function, so that the center of mass is not conserved. A numerical evidence of this phenomenon will be proposed in the last subsection of this paper.

7.2 Discretization

The numerical resolution of system (2.8)–(2.10) is far from obvious. A first naive idea consists in applying a standard splitting method where we treat separately the scalar conservation law (2.8) and the elliptic equation (2.10). It turns out that such a scheme is unable to recover the correct definition of the flux and therefore of the product $a(\partial_x S)$ by ρ . In particular, it leads to stationary Dirac masses.

A second idea consists in solving the distributional conservation law (3.7) by a finite volume method. It involves a discretization of the flux J on the interface of each cell of the mesh, and thus one could expect a correct computation of the flux, and therefore a convenient interpretation of the product. However, this definition of the flux involves the calculation of two derivatives of S . Using a centered scheme to discretize this quantity induces spurious oscillations as it is usually noticed for centered scheme on scalar conservation laws. We can then unwind the scheme depending on the sign of $a(\partial_x S)$ computed at previous iteration. But in doing so, we actually specify a value for $a(\partial_x S)$ in the definition of the product $a(\partial_x S)$ with ρ , and this can lead to capture wrong solutions.

Next, one can think of solving the equation (6.7) on S , motivated by the fact that it plays a key part in the uniqueness, and that ρ can be recovered readily from S . However the equation is non local and its numerical resolution appears to be quite complicated and with a high computational cost (even in the one dimensional setting).

Thus we prefer to use a method based on the dynamics of aggregates, detailed in Section 5.1. We use the principle of a particle method in which we approximate the density by a sum of Dirac masses. Then the motion of these pseudo-particles is approximated by discretizing system (5.6) with an explicit Euler scheme. More precisely, let us assume that we have an approximation of ρ at time $t_n = n\Delta t$, given by

$$\rho^n(x) = \sum_{i=1}^{I^n} m_i^n \delta_{y_i^n}(x), \quad (7.5)$$

where $m_i^n > 0$ is the mass allocated to the pseudo-particle at the position y_i^n with $y_1^n < y_2^n < \dots < y_{I^n}^n$ for $I^n \in \mathbb{N}^*$. Then an approximation of the potential at time t^n is given by

$$S^n(x) = \sum_{i=1}^{I^n} m_i^n e^{-|x-y_i^n|}.$$

Using an explicit Euler scheme, we compute the new position

$$\begin{aligned} y_i^{n+1} = & y_i^n + \frac{\Delta t}{m_i^n} A \left(- \sum_{j=1}^{i-1} \frac{m_j^n}{2} e^{y_j^n - y_i^n} + \frac{m_i^n}{2} + \sum_{j=i+1}^{I^n} \frac{m_j^n}{2} e^{y_i^n - y_j^n} \right) \\ & - \frac{\Delta t}{m_i^n} A \left(- \sum_{j=1}^{i-1} \frac{m_j^n}{2} e^{y_j^n - y_i^n} - \frac{m_i^n}{2} + \sum_{j=i+1}^{I^n} \frac{m_j^n}{2} e^{y_i^n - y_j^n} \right). \end{aligned}$$

Next, we test if some pseudo-particles have collided during the time step Δt . If $y_{j+1}^{n+1} \leq y_j^{n+1}$ for $j \geq 1$, then the pseudo-particles j and $j+1$ have collapsed and form a unique pseudo-particle which has the mass $m_j^n + m_{j+1}^n$. In this case, we decide to set this pseudo-particle at the position $\frac{1}{2}(y_{j+1}^{n+1} + y_j^{n+1})$ and set $m_j^{n+1} = m_j^n + m_{j+1}^n$, moreover we have therefore $I^{n+1} = I^n - 1$. Finally, for given initial sequences $(y_i^0)_{i=1, \dots, I^0}$ and $(m_i^0)_{i=1, \dots, I^0}$ of size I^0 , we can construct (y_i^n) and (m_i^n) of size I^n as above.

Using well-known result on the convergence of Euler scheme, we deduce that, for given initial data $(y_i^0)_{i=1, \dots, I^0}$, $(m_i^0)_{i=1, \dots, I^0}$ and I^0 , y_i^n defined above converges to the solution $x_i(t)$ of (5.6) when Δt tends to 0 such that $t_n \rightarrow t$. Using the result of Section 5.1, we deduce that the function ρ^n in (7.5) converges in \mathcal{S}_M to the unique duality solution of Theorem 3.9. Then the method introduced above is convergent provided we discretize the initial data ρ^{ini} in such a way that $\rho^0(x) := \sum_{i=1}^{I^0} m_i^0 \delta_{y_i^0}(x)$ converges in \mathcal{M}_b to ρ^{ini} . Moreover, we verify easily that we have

$$\sum_{i=1}^{I^0} m_i^0 = \sum_{i=1}^{I^n} m_i^n, \quad \text{and } I^n \leq I^0, \quad \text{for all } n \in \mathbb{N},$$

and that the approximation ρ^n of $\rho(t_n)$ is nonnegative.

7.3 Numerical results

In this Section, we present numerical simulations of model (2.8)–(2.10) using the algorithm described above. We first approximate the initial data $\rho^{ini} \geq 0$, which is assumed to be compactly supported for numerical purpose, in the following way: we introduce a discretization

$x_j = x_0 + j\Delta x$ of the bounded domain which includes the compact support of ρ^{ini} and we define

$$m_i^0 = \int_{x_i - \frac{\Delta x}{2}}^{x_i + \frac{\Delta x}{2}} \rho^{ini}(x) dx.$$

Then the sequence $(y_j^0)_j$ is defined by the nodes (x_i) for which m_i^0 is not zero, and I^0 correspond to the number of $i \in \mathbb{N}$ such that m_i^0 is not zero. We construct then the approximation of ρ^{ini} by

$$\rho^0(x) := \sum_{i=1}^{I^0} m_i^0 \delta_{y_i^0}(x).$$

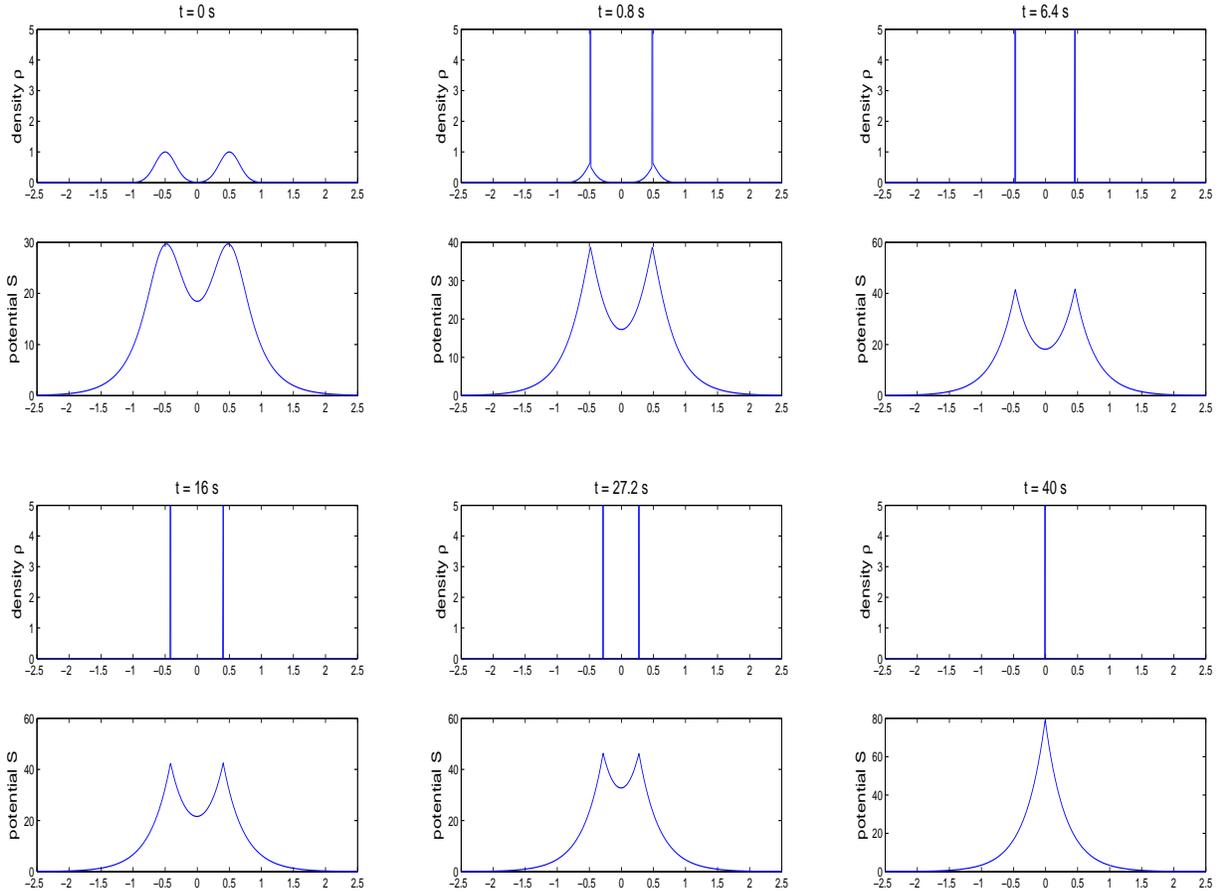


Figure 1: Dynamics of the density ρ and of the potential S for an initial density given by the sum of two Gaussian.

We present in Figure 1 the dynamics of the density ρ and of the chemoattractant concentration S for an initial data ρ^{ini} given by the sum of two Gaussian functions, more precisely

$$\rho^{ini}(x) = e^{-20(x-0.5)^2} + e^{-20(x+0.5)^2}.$$

As expected, we first observe the formation of two Dirac masses at the position where $\partial_x S$ initially vanishes. Then, the two aggregates collapse in the center. Looking at the time evolution, we notice that the first step of formation of aggregates is fast compared to the time of collapse.

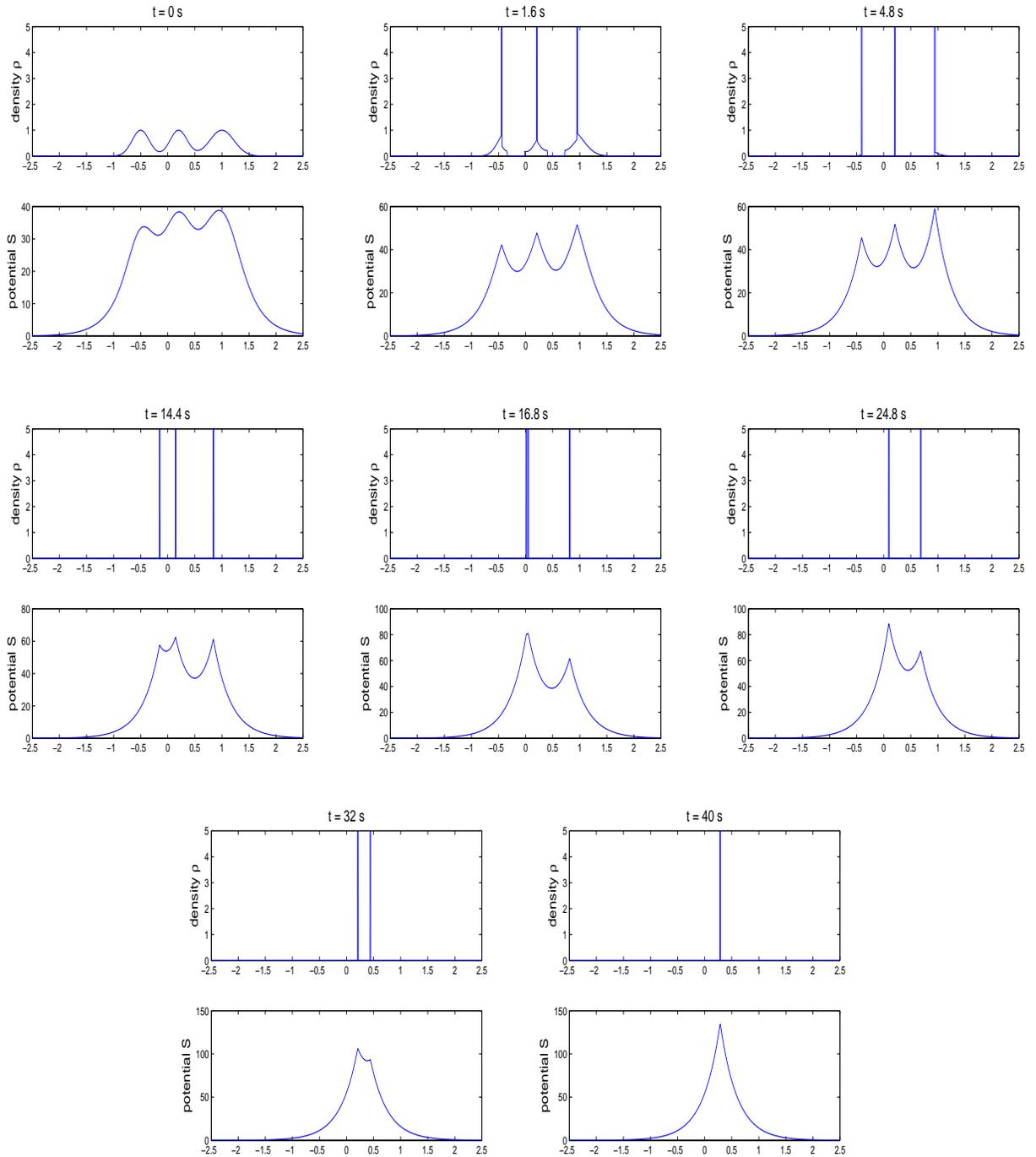


Figure 2: Dynamics of the density ρ and of the potential S for an initial density given by the sum of three Gaussian.

In Figure 2 we display the dynamics for an initial data given by the sum of three Gaussian functions:

$$\rho^{ini}(x) = e^{-10(x-1)^2} + e^{-20(x-0.2)^2} + e^{-20(x+0.5)^2}.$$

We observe the formation of three Dirac masses that moves according to the dynamical system (7.1). They collapse then in finite time.

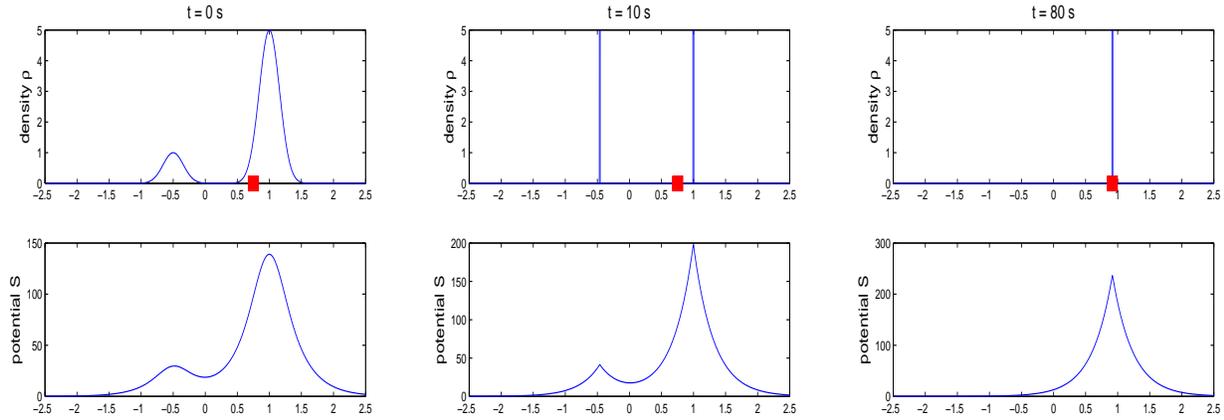


Figure 3: Dynamics of the density ρ and of the potential S with the dynamics of the center of mass represented by a red square. The center of mass moves.

Finally, as we have already noticed, we evidence that the center of mass is not fixed. For instance, Figure 3 represents the dynamics of the density and of the potential for an initial data made of one big bump with one small bump:

$$\rho^{ini}(x) = 5e^{-20(x-1)^2} + 0.5e^{-20(x+0.5)^2}.$$

The square shows the time dynamics of the center of mass. We observe that the center of mass at the final time is not located at the same position as at the initial time.

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