

Convergence of a Stochastic Particle Approximation for Measure Solutions of the 2D Keller-Segel System

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Abstract. The analysis of a stochastic interacting particle scheme for the approximation of measure solutions of the parabolic-elliptic Keller-Segel system in 2D is continued. In previous work it has been shown that solutions of a regularized scheme converge to solutions of the regularized Keller-Segel system, when the number of particles tends to infinity. In the present work, the regularization is eliminated in the particle model, which requires an application of the framework of time dependent measures with diagonal defects, developed by Poupaud. The subsequent many particle limit of the BBGKY hierarchy can be solved using measure solutions of the Keller-Segel system and the molecular chaos assumption. However, a uniqueness result for the limiting hierarchy and therefore a proof of propagation of chaos is missing. Finally, the dynamics of strong measure solutions, i.e. sums of smooth distributions and Delta measures, of the particle model is discussed formally for the cases of 2 and 3 particles. The blow-up behavior for more than 2 particles is not completely understood.

Key words: Keller-Segel model, Measure valued solutions, Stochastic interacting particle systems, BBGKY hierarchy, Defect measure.

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1 Introduction

This paper is concerned with the mathematical analysis of a stochastic interacting particle scheme [14] for the approximation of measure solutions of the 2D parabolic-elliptic Keller-Segel system for chemotaxis, a biological phenomenon in which living organisms direct their movements according to the distribution of certain chemicals in their environment. At the macroscopic level, the biological system is described by the number density of cells, $\varrho = \varrho(t, x)$, and the concentration of the chemoattractant, $S = S(t, x)$. The classical (Patlak-)Keller-Segel model [17], which we consider in its parabolic-elliptic nondimensional setting, reads

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \nabla S - \nabla \varrho) = 0, \quad (1)$$

$$-\Delta S = \varrho, \quad (2)$$

for $t > 0$ and $x \in \mathbb{R}^2$, subject to the initial condition

$$\varrho(t = 0, x) = \varrho_I(x) \quad \text{for all } x \in \mathbb{R}^2. \quad (3)$$

This system was extensively studied by many authors. The survey [21] gives a very good overview of the results and an extensive bibliography. In the spatially two-dimensional case, the Poisson equation (2) is usually replaced by the Newtonian potential solution

$$S[\varrho](x) = -\frac{1}{2\pi} \int_{\mathbb{R}^2} \log(|x - y|) \varrho(y) dy. \quad (4)$$

Substitution of (4) in (1) leads to a McKean-Vlasov equation with singular interaction potential. The classical result

$$\frac{d}{dt} \int |x|^2 \varrho(t, x) dx = \frac{M}{2\pi} (8\pi - M), \quad \text{with } M := \int_{\mathbb{R}^2} \varrho_I(x) dx, \quad (5)$$

indicates the well known dichotomy in the qualitative behavior of the system with the critical mass 8π , see [16, 10, 4, 3]. Biologically, the possible concentration of the cell density in the supercritical case $M > 8\pi$ represents aggregation of cells, and the description of the dynamics of these aggregates and of their interaction with the non-aggregated cells is of natural interest. This led to the study of various regularizations of (1), (4). The regularization

$$S_\varepsilon[\varrho](x) = -\frac{1}{2\pi} \int_{\mathbb{R}^2} \log(|x - y| + \varepsilon) \varrho(y) dy. \quad (6)$$

of the interaction potential has been studied in [11], the main result being convergence as $\varepsilon \rightarrow 0$ globally in time and for arbitrary initial mass to measure solutions. It is based on the framework developed by Poupaud in [22], which he applied to the two-dimensional incompressible Euler equations (extending earlier work by Schochet [25]) as well as to the Keller-Segel system without diffusion of the cells. Obviously, the main mathematical problem is an appropriate definition of the limiting convective flux $\varrho \nabla S[\varrho]$, when ϱ is only a signed bounded measure. The limit of the cell density is a distributional solution of the generalized Keller-Segel model

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (j[\varrho, \nu] - \nabla \varrho) = 0, \quad (7)$$

where $\nu \in \mathcal{M}_1((0, T) \times \mathbb{R}^2)^{2 \times 2}$ is a time dependent, symmetric and nonnegative matrix valued measure (the so-called *diagonal defect measure*), verifying the estimate

$$\text{tr}(\nu(t, x)) \leq \sum_{a \in S_{at}(\varrho(t))} \varrho(t)(\{a\})^2 \delta(x - a), \quad (8)$$

with $S_{at}(\varrho(t))$ denoting the atomic support of the bounded, nonnegative Radon measure $\varrho(t) \in \mathcal{M}_1^+(\mathbb{R}^2)$. The distributional definition of the convective flux $j[\varrho, \nu]$ with a test function $\varphi \in C_c^\infty((0, T) \times \mathbb{R}^2)$ is given by

$$\begin{aligned} & \int_0^T \int_{\mathbb{R}^2} j[\varrho, \nu](t, x) \varphi(t, x) \, dx \, dt = \\ & - \frac{1}{4\pi} \int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{K}(x - y) (\varphi(t, x) - \varphi(t, y)) \varrho(t, x) \varrho(t, y) \, dx \, dy \, dt \\ & - \frac{1}{4\pi} \int_0^T \int_{\mathbb{R}^2} \nu(t, x) \nabla \varphi(t, x) \, dx \, dt, \end{aligned}$$

with

$$\mathcal{K}(x) = \begin{cases} x/|x|^2 & \text{for } x \neq 0, \\ 0 & \text{for } x = 0. \end{cases}$$

An essential trick (already detected by Schochet [25]) is the symmetrization in the second line above, leading to the bounded factor $\mathcal{K}(x - y)(\varphi(t, x) - \varphi(t, y))$, whose discontinuity required the introduction of the defect measure.

In [11] a strong formulation of the limiting system has been given, based on the following ansatz for ϱ :

$$\varrho = \bar{\varrho} + \hat{\varrho}, \quad \text{with } \hat{\varrho}(t, x) = \sum_{n \in \mathcal{H}} M_n(t) \delta(x - x_n(t)),$$

for a finite set $\mathcal{H} \subset \mathbb{N}$, assuming that $\bar{\varrho}(t, x)$ is smooth and t varies in a time interval where the atomic support of ϱ consists of smooth paths $x_n(t)$ carrying smooth weights $M_n(t) \geq 8\pi$. The defect measure then takes the form

$$\nu(t, x) = \sum_{n \in \mathcal{H}} 4\pi M_n(t) \delta(x - x_n(t)) \text{Id},$$

where Id denotes the identity matrix in $\mathbb{R}^{2 \times 2}$, and the following system of equations is obtained:

$$\frac{\partial \bar{\varrho}}{\partial t} + \nabla \cdot (\bar{\varrho} \nabla S[\bar{\varrho}] - \nabla \bar{\varrho}) - \frac{1}{2\pi} \nabla \bar{\varrho} \cdot \sum_{n \in \mathcal{H}} M_n(t) \frac{x - x_n}{|x - x_n|^2} = 0, \quad (9)$$

$$\dot{M}_n = M_n \bar{\varrho}(x = x_n), \quad (10)$$

$$\dot{x}_n = \nabla S[\bar{\varrho}](x = x_n) - \frac{1}{2\pi} \sum_{n \neq m \in \mathcal{H}} M_m \frac{x_n - x_m}{|x_n - x_m|^2}. \quad (11)$$

A variant of this system has been derived by Velázquez [29, 30] and a local-in-time existence result for the initial value problem was given in [31]. In general, one has to expect blow-up events in the smooth part $\bar{\varrho}$ and/or collisions of point aggregates in finite time. At such instants, a restart would be required with either an additional point aggregate after a blow-up event or with a smaller number of point aggregates after a collision. A rigorous theory producing global solutions by such a procedure is missing, however.

Contrary to the large amount of literature dedicated to the analysis of the Keller-Segel system, only a few works are concerned with its numerical treatment, [26, 19, 8, 24, 12, 23, 2]. However, these are capable to produce an approximation of the solution in the smooth regime only. To fill this gap, we recently developed a method for approximation of the global in time solutions of the strong formulation of the Keller-Segel system after blow-up (9)–(11). Our method is based on the approximation of the smooth part of the cell density with a system of stochastic interacting particles,

$$\bar{\varrho}(t, x) \approx \sum_{n \in \mathcal{L}} M_n(t) \delta(x - x_n(t))$$

for some finite index set $\mathcal{L} \subset \mathbb{N}$, $\mathcal{L} \cap \mathcal{H} = \emptyset$, with point masses $0 < M_n(t) < 8\pi$ and particle paths $x_n(t)$. The point singularities of ϱ with $M_n(t) \geq 8\pi$ are, as before, collected in the finite set \mathcal{H} ,

$$\hat{\varrho}(t, x) = \sum_{n \in \mathcal{H}} M_n(t) \delta(x - x_n(t)).$$

The evolution of the particle paths is governed by the system of stochastic differential equations

$$dx_n = -\frac{1}{2\pi} \sum_{n \neq m \in \mathcal{L} \cup \mathcal{H}} M_m \frac{x_n - x_m}{|x_n - x_m|^2} dt + \sqrt{2} \beta_n dB_t^n, \quad (12)$$

for all $n \in \mathcal{L} \cup \mathcal{H}$, where B_t^n are mutually independent two-dimensional Brownian motions and the “switch” β_n is equal to 1 for $n \in \mathcal{L}$ and zero otherwise. Due to the singularity of the interaction kernel, a special treatment is necessary in the situation when two particles approach each other. In our scheme, such a situation is treated as an inelastic particle collision and the two particles are “glued” together, ensuring stability of the scheme. A blow-up instant in the cell density $\bar{\varrho}$ is detected as a collisional creation of a particle with mass larger or equal to 8π . This criterion is based upon the conjecture that a blow-up of the cell density is always manifested as a creation of the Dirac delta singularity with initial mass 8π . This conjecture is generally accepted to be valid, although a rigorous proof exists for the radially symmetric case only, see [15, 1, 20]. A detailed description of this method as well as numerical results are presented in [14]. There also the many particle limit of the regularized scheme has been studied, using the formally equivalent formulation of the stochastic system (12) in terms of the Kolmogorov forward equation and the corresponding *BBGKY hierarchy* for the marginals of the particle distribution function. We showed that the limiting *Boltzmann hierarchy* has a unique solution proving propagation of molecular chaos. This is an example of the approximation of a McKean-Vlasov equation with regular interaction potential by a stochastic particle system [27].

In this work we are concerned with the many particle limit after removing the regularization in the particle system, which is mathematically a much more demanding problem. We start with the Kolmogorov equation with the regularized interaction kernel

$$\mathcal{K}^\varepsilon(x) := \frac{x}{|x|(|x| + \varepsilon)} \quad \text{for } x \in \mathbb{R}^2. \quad (13)$$

For the corresponding BBGKY hierarchy (Section 2), only estimates in the sense of tight boundedness of measures are uniform with respect to ε (Section 3). The limit $\varepsilon \rightarrow 0$ is complicated by the fact that the limiting interaction terms contain products of discontinuous functions and (possibly) singular measures charging the set of discontinuities. However, if the discontinuity is of a particular type, one can apply the framework of time dependent measures with diagonal defects, developed by Poupaud in [22], to obtain a partial characterization of the limiting object. This is done in Section 4, as well as the subsequent passage $N \rightarrow \infty$, which yields the *Boltzmann hierarchy*. Then, in Section 5, we show that the Boltzmann hierarchy is compatible with the generalized Keller-Segel system, in the sense that measure solutions of the latter together with the molecular chaos assumption generate solutions of the former. However, there remains a gap in the theory, which is the lack of a uniqueness result for the Boltzmann hierarchy, meaning that propagation of chaos has not been proven. This difficulty does not come as a surprise since already for the one-particle problem (the generalized Keller-Segel system) a uniqueness result is not available. Finally, in Sections 6 and 7 we return to the stochastic particle system and study strong measure solutions for 2 and 3 particles, respectively. Whereas, on a formal level, we have a good understanding of the solution behaviour and of blow-up scenarios for 2 particles, the situation for 3 (or more) particles is less clear.

2 The BBGKY hierarchy

Our starting point is the regularized stochastic particle system

$$dx_n = -\frac{1}{2\pi} \frac{M}{N} \sum_{n \neq m=1}^N \mathcal{K}^\varepsilon(x_n - x_m) dt + \sqrt{2} dB_t^n, \quad n = 1, \dots, N, \quad (14)$$

with the parameter $\varepsilon > 0$ and the fixed set $\mathcal{L} = \{1, \dots, N\}$ of particles, approximating the smooth solution of the regularized Keller-Segel system (1), (6). For simplicity, we assume that each particle carries the same mass M/N , with $M > 0$ being the total mass of the system. B_t^n are mutually independent two-dimensional Brownian motions and \mathcal{K}^ε is given by (13). Our convergence proof is based on the (formally) equivalent formulation of (14) in terms of

the corresponding Kolmogorov forward equation,

$$\frac{\partial p^{N,\varepsilon}}{\partial t} + \sum_{n=1}^N \nabla_{x_n} \cdot \left[-\frac{1}{2\pi} \frac{M}{N} \sum_{m \neq n} \mathcal{K}^\varepsilon(x_n - x_m) p^{N,\varepsilon} - \nabla_{x_n} p^{N,\varepsilon} \right] = 0, \quad (15)$$

where $p^{N,\varepsilon} = p^{N,\varepsilon}(t, x_1, \dots, x_N)$ is the N -particle distribution function with $(x_1, \dots, x_N) \in \mathbb{R}^{2N}$ the vector of particle locations, subject to the initial condition

$$\begin{aligned} p^{N,\varepsilon}(t=0, x_1, \dots, x_N) &= p_I^N(x_1, \dots, x_N), \\ p_I^N &\geq 0 \text{ a.e. and } \int_{\mathbb{R}^{2N}} p_I^N dx_1 \dots dx_N = 1, \end{aligned} \quad (16)$$

Existence of unique, nonnegative smooth solutions to (15), (16) is obtained by standard arguments (observe that $\mathcal{K}^\varepsilon \in L^\infty$ for $\varepsilon > 0$). Moreover, we postulate the *indistinguishability of particles*: The initial condition p_I^N is indifferent to permutations of its arguments (x_1, \dots, x_N) , i.e., for any permutation π of the N arguments, we have

$$p_I^N(x_1, \dots, x_N) = p_I^N(\pi(x_1, \dots, x_N)) \quad \text{for all } (x_1, \dots, x_N) \in \mathbb{R}^{2N}. \quad (17)$$

Then, as a consequence of the symmetry of the Kolmogorov equation (15) with respect to interchange of the x -arguments and the uniqueness of its solutions, the indistinguishability is propagated in time, i.e., $p^{N,\varepsilon}(t, \cdot)$ satisfies (17) as well, for all $t \geq 0$.

In the following section, the limit $\varepsilon \rightarrow 0$ will be carried out. Assuming a regular limit $p^N = \lim_{\varepsilon \rightarrow 0} p^{N,\varepsilon}$, a counterpart of the classical virial calculation (5) carried out for solutions of (15) followed by the limit $\varepsilon \rightarrow 0$ gives

$$\frac{d}{dt} \int_{\mathbb{R}^{2N}} \sum_{n=1}^N |x_n|^2 p^N dx_1 \dots dx_N = \frac{N-1}{2\pi} \left(\frac{N}{N-1} 8\pi - M \right). \quad (18)$$

Consequently, for $M > \frac{N}{N-1} 8\pi$ we expect formation of singularities in the particle distribution function p^N in finite time. In the limit $N \rightarrow \infty$ the classical 8π -criterion for the Keller-Segel system is recovered. However, the analysis of Section 6 will show that for finite N the above criterion cannot be expected to be sharp.

For $k = 1, \dots, N$ we define the k -particle marginals

$$P_k^{N,\varepsilon}(t, x_1, \dots, x_k) := \int_{\mathbb{R}^{2(N-k)}} p^{N,\varepsilon}(t, x_1, \dots, x_N) dx_{k+1} \dots dx_N, \quad (19)$$

with $P_N^{N,\varepsilon} \equiv p^{N,\varepsilon}$. An integration of (15) with respect to x_{k+1}, \dots, x_N yields

$$\begin{aligned} \frac{\partial P_k^{N,\varepsilon}}{\partial t} + \sum_{n=1}^k \nabla_{x_n} \cdot \left[-\frac{M}{2\pi N} \sum_{n \neq m=1}^N \int_{\mathbb{R}^{2(N-k)}} \mathcal{K}^\varepsilon(x_n - x_m) p^{N,\varepsilon} dx_{k+1} \dots dx_N \right. \\ \left. - \nabla_{x_n} P_k^{N,\varepsilon} \right] = 0. \end{aligned} \quad (20)$$

Obviously, $P_k^{N,\varepsilon}$ also satisfies the indistinguishability property. We split the inner sum in (20) into the part with $m > k$ (interaction of the first k particles with the other $N - k$) and $m \leq k$ (interaction among the first k particles) to obtain

$$\begin{aligned} & \frac{M}{2\pi N} \sum_{m \neq n} \int_{\mathbb{R}^{2(N-k)}} \mathcal{K}^\varepsilon(x_n - x_m) p^{N,\varepsilon} dx_{k+1} \dots dx_N \\ &= \frac{M(N-k)}{2\pi N} \int_{\mathbb{R}^2} \mathcal{K}^\varepsilon(x_n - y) P_{k+1}^{N,\varepsilon}(t, x_1, \dots, x_k, y) dy \\ &+ \frac{M}{2\pi N} \sum_{m \leq k, m \neq n} \mathcal{K}^\varepsilon(x_n - x_m) P_k^{N,\varepsilon}(t, x_1, \dots, x_k). \end{aligned} \quad (21)$$

This, inserted into (20), constitutes the *BBGKY hierarchy* for our system of interacting particles (see, for instance, [9]). A simple consideration reveals that in its weak formulation it is sufficient to work with symmetric test functions $\varphi = \varphi(x_1, \dots, x_k) \in C_c^\infty(\mathbb{R}^{2k})$ only (with respect to interchange of their x -arguments), since the antisymmetric part of φ does not contribute to the value of the integrals. Consequently, using the classical Schochet trick [25], the weak formulation of the BBGKY hierarchy may be written in a symmetrized form, which in fact is crucial for the forthcoming analysis. It is based on the antisymmetry of the kernel \mathcal{K}^ε and on the following observation: Let us consider a symmetric test function φ of k two-dimensional arguments, collected in the vector $x = (x_1, \dots, x_k)$. Then, for any n, m with $n \neq m$, one has the relation $\nabla_n \varphi(x) = \nabla_m \varphi([x_m, x_n; \tilde{x}_{n,m}])$, where $\nabla_n \varphi(x)$ denotes the gradient of φ with respect to its n -th argument, evaluated at

x , and $\nabla_m \varphi([z, y; \tilde{x}_{n,m}])$ denotes the gradient of φ with respect to its m -th argument, evaluated at x with (z, y) replacing (x_n, x_m) . Analogously, the notation $\nabla_n \varphi([y; \tilde{x}_m])$ denotes the gradient of φ with respect to its n -th argument, evaluated at x with $y \in \mathbb{R}^2$ replacing x_m . With this notation, the symmetrized weak formulation of the BBGKY hierarchy reads

$$\begin{aligned}
& \frac{d}{dt} \int_{\mathbb{R}^{2k}} P_k^{N,\varepsilon}(t, x) \varphi(x) dx \\
& + \frac{M(N-k)}{4\pi N} \sum_{n=1}^k \int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^2} \mathcal{K}^\varepsilon(x_n - y) P_{k+1}^{N,\varepsilon}(t, x, y) \cdot (\nabla_n \varphi(x) - \nabla_n \varphi([y; \tilde{x}_n])) dy dx \\
& + \frac{M}{2\pi N} \sum_{n=1}^k \sum_{m>n} \int_{\mathbb{R}^{2k}} \mathcal{K}^\varepsilon(x_n - x_m) P_k^{N,\varepsilon}(t, x) \cdot (\nabla_n \varphi(x) - \nabla_n \varphi([x_m, x_n; \tilde{x}_{n,m}])) dx \\
& - \sum_{n=1}^k \int_{\mathbb{R}^{2k}} P_k^{N,\varepsilon}(t, x) \Delta_{x_n} \varphi(x) dx = 0. \tag{22}
\end{aligned}$$

In our previous work [14] we studied the limit of (22) when $N \rightarrow \infty$ with fixed $\varepsilon > 0$ and recovered the solution of the regularized Keller-Segel system, which in fact is an instance of a McKean-Vlasov equation with a regular interaction kernel. Approximation of its solutions by large systems of interacting particles, evolving according to systems of coupled stochastic differential equations, was studied in [18, 5, 6, 27, 28] using the tools of stochastic analysis. In contrast, our approach is PDE-based and deals with the corresponding Kolmogorov forward equation.

Theorem 1 ([14]) *For each $\varepsilon > 0$ and $N \geq 2$, the regularized Kolmogorov forward equation (15)–(16) with the initial condition $p_1^N \in L^2(\mathbb{R}^{2N})$ satisfying the molecular chaos property has a unique global weak solution $p^N \in L^2_{loc}([0, \infty); W^{1,2}(\mathbb{R}^{2N})) \cap C([0, \infty); L^2(\mathbb{R}^{2N}))$. This solution verifies the indistinguishability property and conserves the total mass. The k -particle marginals $P_k^{N,\varepsilon}$ given by (19) have weakly converging subsequences in $L^2_{loc}([0, \infty); W^{1,2}(\mathbb{R}^{2k}))$ as $N \rightarrow \infty$ for each $k \geq 1$ and the respective limits P_k^ε satisfy the molecular chaos property*

$$P_k^\varepsilon(t, x_1, \dots, x_k) = \prod_{n=1}^k P_1^\varepsilon(t, x_n) \quad \text{for a.e. } x \in \mathbb{R}^{2k}, \quad t \geq 0, \tag{23}$$

with $\varrho^\varepsilon(t, x) := MP_1^\varepsilon(t, x)$ being the weak solution of the regularized Keller-Segel model (1), (6) with the initial condition $\varrho^\varepsilon(t=0) = MP_1^\varepsilon(t=0)$.

The proof is based on uniform (with respect to N but not with respect to ε) a priori estimates in the space $L^2_{loc}([0, \infty); W^{1,2}(\mathbb{R}^{2k}))$ for the sequence $\{P_k^{N,\varepsilon}\}_{N=k}^\infty$ for each fixed $k \in \mathbb{N}$, and profits essentially from the chain property of the marginals,

$$\int_{\mathbb{R}^2} P_{k+1}^{N,\varepsilon}(t, x_1, \dots, x_k, y) dy = P_k^{N,\varepsilon}(t, x_1, \dots, x_k). \quad (24)$$

Then, it is simple to pass to the limit $N \rightarrow \infty$ to obtain the so-called Boltzmann hierarchy for $P_k = \lim_{N \rightarrow \infty} P_k^N$. We showed that the Boltzmann hierarchy admits solutions given by the molecular chaos formula (23), and since, by regularity, the solutions are unique, they necessarily factorize.

3 Uniform a priori estimates in ε and N

In the limit $\varepsilon \rightarrow 0$ of the BBGKY hierarchy one cannot expect any better convergence than in the sense of measures and, as for the Keller-Segel system, the main difficulty lies in the characterization of the product of the discontinuous limiting interaction kernel and the (possibly) singular limiting measure, charging the set of discontinuities. Similarly to [11] we apply the framework of time dependent measures with diagonal defects, developed by Poupaud [22].

Let us recall that a sequence of bounded, nonnegative Radon measures $\mu^n \in \mathcal{M}_1^+(\mathbb{R}^d)$ converges tightly to $\mu \in \mathcal{M}_1^+(\mathbb{R}^d)$ if it converges vaguely (this is, $\mathcal{M}_1(\mathbb{R}^d)$ -weak*) and, moreover, $\mu^n(\mathbb{R}^d) \rightarrow \mu(\mathbb{R}^d)$. In this case one has

$$\int_{\mathbb{R}^d} \varphi(x) \mu^n(x) dx \rightarrow \int_{\mathbb{R}^d} \varphi(x) \mu(x) dx, \quad \text{as } n \rightarrow \infty,$$

for every bounded continuous test function φ (in contrast to vague convergence, where the test function has to be compactly supported). We say that a sequence $\mu^n \in \mathcal{M}_1^+(\mathbb{R}^d)$ is tightly bounded if for some $M > 0$

$$\begin{aligned} \mu^n(\mathbb{R}^d) &< M \quad \forall n \geq 1, \\ \sup_{n \geq 1} \mu^n(\mathbb{R}^d \setminus B_R) &\rightarrow 0 \quad \text{as } R \rightarrow \infty, \end{aligned}$$

where B_R denotes the ball with center in the origin and with diameter R in \mathbb{R}^d . By the Prokhorov criterion, tight boundedness is equivalent to compactness in the tight topology of measures, see for instance [7].

For the forthcoming analysis, we introduce the family of 2×2 -matrix valued functions

$$\mathbf{m}_k^{N,\varepsilon}(t, z, x) := \int_{\mathbb{R}^2} \mathcal{N}^\varepsilon(z - y) P_{k+1}^{N,\varepsilon}(t, y, z, x) dy \quad \text{for } 1 \leq k \leq N - 1, \quad (25)$$

with $z \in \mathbb{R}^2$ and $x \in \mathbb{R}^{2(k-1)}$, where

$$\mathcal{N}^\varepsilon(z) := \frac{z \otimes z}{|z|(|z| + \varepsilon)} \quad \text{for } z \in \mathbb{R}^2.$$

Following [22], we consider $P_k^{N,\varepsilon}(t, \cdot)$ and $\mathbf{m}_k^{N,\varepsilon}(t, \cdot)$ as time dependent measures $P_k^{N,\varepsilon}(t) \in \mathcal{M}_1^+(\mathbb{R}^{2k})$ and $\mathbf{m}_k^{N,\varepsilon}(t) \in (\mathcal{M}_1^+(\mathbb{R}^{2k}))^{2 \times 2}$. Moreover, we introduce a shorthand notation for the interaction terms of (22):

$$\mathbf{A}_{k+1}^{N,\varepsilon}(n; \varphi)(t) := \int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^2} \mathcal{K}^\varepsilon(x_n - y) P_{k+1}^{N,\varepsilon}(t, x, y) \cdot (\nabla_n \varphi(x) - \nabla_n \varphi([y; \tilde{x}_n])) dy dx$$

and

$$\mathbf{B}_k^{N,\varepsilon}(n, m; \varphi)(t) := \int_{\mathbb{R}^{2k}} \mathcal{K}^\varepsilon(x_n - x_m) P_k^{N,\varepsilon}(t, x) \cdot (\nabla_n \varphi(x) - \nabla_m \varphi([x_m, x_n; \tilde{x}_{n,m}])) dx.$$

Lemma 1 *For each fixed k , the two-parameter family $\{P_k^{N,\varepsilon}(t)\}_{N,\varepsilon}$ of weak solutions to the BBGKY hierarchy (22) is tightly bounded locally uniformly in t and tightly equicontinuous in t , uniformly with respect to $N < \infty$ and $\varepsilon > 0$. The family $\{\mathbf{m}_k^{N,\varepsilon}(t)\}_{N,\varepsilon}$ given by (25) is tightly bounded locally uniformly in t , uniformly with respect to $N < \infty$ and $\varepsilon > 0$.*

Proof: The existence of weak solutions $P_k^{N,\varepsilon}$ to (22) in $L_{loc}^2([0, \infty); W^{1,2}(\mathbb{R}^{2k})) \cap C([0, \infty); L^2(\mathbb{R}^{2k}))$ is established by Theorem 1. The forthcoming estimates are based on the total mass conservation

$$\int_{\mathbb{R}^{2k}} P_k^{N,\varepsilon}(t, x) dx = 1 \quad \text{for all } t > 0, \varepsilon > 0, N < \infty, k \leq N. \quad (26)$$

Let $\varphi \in C_c^\infty(\mathbb{R}^{2k})$. From the mean value theorem

$$|\nabla_n \varphi(x) - \nabla_n \varphi([y; \tilde{x}_n])| \leq \|\nabla_{n,n}^2 \varphi\|_{L^\infty} |x_n - y|$$

and the uniform boundedness $|\mathcal{N}_{i,j}^\varepsilon| \leq 1$ we immediately obtain

$$\sum_{n=1}^k \left| \mathbf{A}_{k+1}^{N,\varepsilon}(n; \varphi) \right| \leq \sum_{n=1}^k \|\nabla_{n,n}^2 \varphi\|_{L^\infty} \leq |\varphi|_{2,\infty},$$

and, similarly,

$$\sum_{n=1}^k \sum_{m>n} \left| \mathbf{B}_k^{N,\varepsilon}(n, m; \varphi) \right| \leq \sum_{n=1}^k \sum_{m>n} \left(\|\nabla_{n,n}^2 \varphi\|_{L^\infty} + \|\nabla_{n,m}^2 \varphi\|_{L^\infty} \right) \leq k|\varphi|_{2,\infty}, \quad (27)$$

where $|\varphi|_{2,\infty}$ is the $W^{2,\infty}(\mathbb{R}^{2k})$ -seminorm of φ (i.e., L^∞ -norm of the second order partial derivatives). Consequently, we have

$$\left| \frac{d}{dt} \int_{\mathbb{R}^{2k}} P_k^{N,\varepsilon}(t, x) \varphi(x) dx \right| \leq \left(\frac{M}{2\pi} + 1 \right) |\varphi|_{2,\infty}.$$

This implies equicontinuity in $W^{2,\infty}(\mathbb{R}^{2N})'$:

$$\left| \int_{\mathbb{R}^{2k}} P_k^{N,\varepsilon}(t, x) \varphi(x) dx - \int_{\mathbb{R}^{2k}} P_k^{N,\varepsilon}(s, x) \varphi(x) dx \right| \leq C|\varphi|_{2,\infty}|t - s|.$$

Now let $\varphi \in C_b(\mathbb{R}^{2k})$. For every $\delta > 0$ there exists $\varphi_\delta \in W^{2,\infty}(\mathbb{R}^{2k})$ such that $\|\varphi - \varphi_\delta\|_{L^\infty(\mathbb{R}^{2k})} \leq \delta$. By the above inequality and the conservation of mass (26), we have

$$\left| \int_{\mathbb{R}^{2k}} P_k^{N,\varepsilon}(t, x) \varphi(x) dx - \int_{\mathbb{R}^{2k}} P_k^{N,\varepsilon}(s, x) \varphi(x) dx \right| \leq 2\delta + C|\varphi_\delta|_{2,\infty}|t - s|,$$

implying the tight equicontinuity of $P_k^{N,\varepsilon}$, uniformly with respect to N and ε .

With a test function $\varphi_R(x) = 1 - \beta(|x|^2/R^2)$ with β nonincreasing, $\beta(r) = 1$ for $0 \leq r \leq 1/2$ and $\beta(r) = 0$ for $r \geq 1$, the above inequality gives

$$P_k^{N,\varepsilon}(t)(\mathbb{R}^{2k} \setminus B_R) \leq P_I^{N,k}(\mathbb{R}^{2k} \setminus B_{R/2}) + \frac{ct}{R^2},$$

where B_R is a ball in \mathbb{R}^{2k} with radius R . This immediately implies the locally uniform tight boundedness.

The result for \mathbf{m}^ε is a simple consequence of the tight boundedness of $P_k^{N,\varepsilon}$ and the uniform bound $|\mathcal{N}_{i,j}^\varepsilon| \leq 1$. ■

4 The limit $\varepsilon \rightarrow 0$, followed by $N \rightarrow \infty$

By the Prokhorov criterion [7], for every $k \leq N$ there exist nonnegative bounded time dependent measures $P^{N,k}(t)$ and $\mathbf{m}^{N,k}(t)$ such that, restricting

to subsequences, as $\varepsilon \rightarrow 0$, $P_k^{N,\varepsilon}(t)$ converges to $P_k^N(t)$ tightly and locally uniformly in t and

$$\int_0^T \int_{\mathbb{R}^{2k}} \mathbf{m}_k^{N,\varepsilon}(t,x) \varphi(t,x) dx dt \rightarrow \int_0^T \int_{\mathbb{R}^{2k}} \mathbf{m}_k^N(t,x) \varphi(t,x) dx dt$$

for all $T > 0$ and $\varphi \in C_b([0, T] \times \mathbb{R}^{2k})$. We can easily pass to the limit in the time derivative and diffusive terms of the distributional formulation of (22), but due to the discontinuity of the limiting interaction kernels,

$$\mathcal{K}(x_n - y) \cdot (\nabla_n \varphi(x) - \nabla_n \varphi([y; \tilde{x}_n]))$$

and

$$\mathcal{K}(x_n - x_m) \cdot (\nabla_n \varphi(x) - \nabla_n \varphi([x_m, x_n; \tilde{x}_{n,m}]))$$

where \mathcal{K} is the pointwise limit of \mathcal{K}^ε as $\varepsilon \rightarrow 0$, we cannot directly pass to the limit here. Instead, we characterize the discontinuities in the $\mathbf{A}_{k+1}^{N,\varepsilon}$ -terms by performing the Taylor expansion

$$\varphi_{n,i}(x) - \varphi_{n,i}([y; \tilde{x}_n]) = \sum_{j=1}^2 \frac{\partial \varphi_{n,i}}{\partial x_{n,j}}(x) (x_n - y) + \mathcal{O}(|x_n - y|^2),$$

where $\varphi_{n,i} := \frac{\partial \varphi}{\partial x_{n,i}}$, $i = 1, 2$, with $x_{n,i}$ being the i -th coordinate of x_n . Therefore, the integrand of the interaction term $\mathbf{A}_{k+1}^{N,\varepsilon}(n; \varphi)(t)$ in the neighbourhood of the diagonal $x_n = y$ is equivalent to

$$\sum_{i,j=1}^2 \mathcal{N}_{i,j}^\varepsilon(x_n - y) \frac{\partial \varphi_{n,i}}{\partial x_{n,j}}(x) P_{k+1}^{N,\varepsilon}(t, x) + \mathcal{O}(|x_n - y|).$$

This suggests to define, for $i = 1, 2$ and $n \leq k$, the operators

$$\mathcal{A}_{k+1,i}^\varepsilon(n; \eta)(y, x) := \mathcal{K}_i^\varepsilon(x_n - y) (\eta(x) - \eta([y; \tilde{x}_n])) - \sum_{j=1}^2 \mathcal{N}_{i,j}^\varepsilon(x_n - y) \frac{\partial \eta}{\partial x_{n,j}}(x),$$

with $y \in \mathbb{R}^2$ and $x \in \mathbb{R}^{2k}$, such that the $\mathbf{A}_{k+1}^{N,\varepsilon}$ -interaction terms can be written as

$$\begin{aligned} \mathbf{A}_{k+1}^{N,\varepsilon}(n; \varphi)(t) &= \int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^2} \sum_{i=1}^2 \mathcal{A}_{k+1,i}^\varepsilon(n; \varphi_{n,i})(y, x) P_{k+1}^{N,\varepsilon}(t, y, x) dy dx \\ &+ \int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^2} \sum_{i,j=1}^2 \mathcal{N}_{i,j}^\varepsilon(x_n - y) \frac{\partial \varphi_{n,i}}{\partial x_{n,j}}(x) P_{k+1}^{N,\varepsilon}(t, y, x) dy dx. \end{aligned}$$

The functions $\mathcal{A}_{k+1;i}^\varepsilon(n; \varphi_{n,i})$ are continuous and bounded, and converge uniformly to $\mathcal{A}_{k+1;i}(n; \varphi_{n,i})$; consequently, we can pass to the limit directly in the integrals involving them. Next, we realize that

$$\int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^2} \mathcal{N}_{i,j}^\varepsilon(x_n - y) \frac{\partial \varphi_{n,i}}{\partial x_{n,j}}(x) P_{k+1}^{N,\varepsilon}(t, y, x) dy dx = \int_{\mathbb{R}^{2k}} \mathbf{m}_k^{N,\varepsilon}(t, x_n, \tilde{x}_n) \frac{\partial \varphi_{n,i}}{\partial x_{n,j}}(x) dx,$$

and the limit passage is facilitated by the uniform tight boundedness of $\mathbf{m}_k^{N,\varepsilon}(t)$. Let us note that the somehow weird notation $\mathbf{m}_k^{N,\varepsilon}(x_n, \tilde{x}_n)$ is enforced by the fact that the functions $\mathbf{m}_k^{N,\varepsilon}$ (as functions of k 2D-arguments) are indifferent with respect to interchange of their $k - 1$ last arguments, the first one being solicited, as explained by the definition (25).

Consequently, in the limit $\varepsilon \rightarrow 0$, with $\varphi \in C_c^\infty(\mathbb{R}^{2k})$, we obtain the distributional formulation

$$\begin{aligned} & \int_{\mathbb{R}^{2k}} P_k^N(T, x) \varphi(x) dx - \int_{\mathbb{R}^{2k}} P_k^N(0, x) \varphi(x) dx \\ & + \frac{M(N-k)}{4\pi N} \sum_{n=1}^k \int_0^T \int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^2} \sum_{i=1}^2 \mathcal{A}_{k+1;i}(n; \varphi_{n,i})(y, x) P_{k+1}^N(t, y, x) dy dx dt \\ & + \int_0^T \int_{\mathbb{R}^{2k}} \sum_{i,j=1}^2 \mathbf{m}_{k;i,j}^N(t, x_n, \tilde{x}_n) \frac{\partial \varphi_{n,i}}{\partial x_{n,j}}(x) dx dt \\ & + \frac{M}{2\pi N} \sum_{n=1}^k \sum_{m>n} \int_0^T \mathbf{B}_k^N(n, m; \varphi)(t) dt \\ & + \sum_{n=1}^k \int_0^T \int_{\mathbb{R}^{2k}} P_k^N(t, x) \Delta_{x_n} \varphi(x) dx dt = 0. \end{aligned} \tag{28}$$

Here, \mathbf{B}_k^N denotes the pointwise limit of $\mathbf{B}_k^{N,\varepsilon}$, which exists in $L^1(0, T)$ due to the estimate (27). We could have characterized the limit of the \mathbf{B} -terms in the same way as we did for the \mathbf{A} -terms, however, since our next step is to pass to $N \rightarrow \infty$, the double sum of the \mathbf{B} -terms, multiplied by the factor $1/N$, will vanish.

The limit passage $N \rightarrow \infty$ is facilitated by the fact that the tight boundedness estimates for $P_k^{N,\varepsilon}$ and $\mathbf{m}_k^{N,\varepsilon}$ of Lemma 1 are uniform with respect to N . Due to the locally uniform (with respect to t) tight boundedness of \mathbf{m}_k^N , there exist time dependent, matrix valued measures $\mathbf{m}_k(t) \in (\mathcal{M}_1^+(\mathbb{R}^{2k}))^{2 \times 2}$,

such that in the limit $N \rightarrow \infty$, (a subsequence of) the **A**-type interaction terms tends to

$$\begin{aligned} & \int_0^T \int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^2} \sum_{i=1}^2 \mathcal{A}_{k+1;i}(n; \varphi_{n,i})(y, x) P_{k+1}(t, y, x) dy dx dt \\ & + \int_0^T \int_{\mathbb{R}^{2k}} \sum_{i,j=1}^2 \mathbf{m}_{k+1;i,j}(t, x_n, \tilde{x}_n) \frac{\partial \varphi_{n,i}}{\partial x_{n,j}}(x) dx dt, \end{aligned}$$

where P_k is the limit of (a subsequence of) P_k^N . Inspired by [22], we introduce the defect measure

$$\nu_k(t, z, \tilde{x}) := \mathbf{m}_k(t, z, \tilde{x}) - \int_{\mathbb{R}^2} \mathcal{N}(z - y) P_{k+1}(t, z, y, \tilde{x}) dy,$$

for $z \in \mathbb{R}^2$ and $\tilde{x} \in \mathbb{R}^{2(k-1)}$, where \mathcal{N} is the pointwise limit of \mathcal{N}^ε as $\varepsilon \rightarrow 0$. Then, the distributional formulation of the *Boltzmann hierarchy* for P_k with a test function $\varphi \in C_c^\infty(\mathbb{R}^{2k})$ reads

$$\begin{aligned} & \int_{\mathbb{R}^{2k}} P_k(T, x) \varphi(x) dx - \int_{\mathbb{R}^{2k}} P_k(0, x) \varphi(x) dx \\ & + \frac{M}{4\pi} \sum_{n=1}^k \int_0^T \int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^2} \mathcal{K}(x_n - y) P_{k+1}(t, x, y) \cdot (\nabla_n \varphi(x) - \nabla_n \varphi([y; \tilde{x}_n])) dy dx dt \\ & + \frac{M}{4\pi} \sum_{n=1}^k \int_0^T \int_{\mathbb{R}^{2k}} \nu_k(t, x_n, \tilde{x}_n) : \nabla_{n,n}^2 \varphi(x) dx dt \\ & + \sum_{n=1}^k \int_0^T \int_{\mathbb{R}^{2k}} P_k(t, x) \Delta_{x_n} \varphi(x) dx dt = 0, \end{aligned} \tag{29}$$

where \mathcal{K} is the pointwise limit of \mathcal{K}^ε and $A : B$ denotes the scalar product of the 2×2 -matrices A and B . Let us note that the interaction integrals are well defined, since $\mathcal{K}(x_n - y)(\nabla_n \varphi(x) - \nabla_n \varphi([y; \tilde{x}_n]))$ are bounded functions.

Lemma 2 *For every $k \geq 1$, the defect measure ν_k is symmetric, nonnegative and satisfies, in the sense of distributions, the estimate*

$$\text{tr}(\nu_k(t, z, \tilde{x})) \leq P_{k+1}(t, z, \{z\}, \tilde{x}) := \int_{\mathbb{R}^2} \chi(z - y) P_{k+1}(t, z, y, \tilde{x}) dy, \tag{30}$$

for $z \in \mathbb{R}^2$, $\tilde{x} \in \mathbb{R}^{2(k-1)}$, where $\chi(0) = 1$ and $\chi(z) = 0$ for $z \neq 0$.

Proof: The proof follows along the lines of [22] and we present its outline only. Symmetry is obvious. For a test function $\varphi \in C_c^\infty(\mathbb{R}^{2k})$, $z, y \in \mathbb{R}^2$, $\tilde{x} \in \mathbb{R}^{2(k-1)}$, $(\varphi(z, y, \tilde{x}) - \varphi(z, z, \tilde{x}))\mathcal{N}^\varepsilon(z - y)$ converges uniformly to the continuous function $(\varphi(z, y, \tilde{x}) - \varphi(z, z, \tilde{x}))\mathcal{N}(z - y)$. Therefore,

$$\begin{aligned} & \int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{N}^\varepsilon(z - y) P_{k+1}^{N,\varepsilon}(t, z, y, \tilde{x}) (\varphi(z, y, \tilde{x}) - \varphi(z, z, \tilde{x})) dz dy d\tilde{x} \\ & \xrightarrow{\varepsilon \rightarrow 0} \int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{N}(z - y) P_{k+1}^N(t, z, y, \tilde{x}) (\varphi(z, y, \tilde{x}) - \varphi(z, z, \tilde{x})) dz dy d\tilde{x} \\ & \xrightarrow{N \rightarrow \infty} \int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{N}(z - y) P_{k+1}(t, z, y, \tilde{x}) (\varphi(z, y, \tilde{x}) - \varphi(z, z, \tilde{x})) dz dy d\tilde{x}. \end{aligned}$$

By the definitions of $\mathbf{m}_k^{N,\varepsilon}$ and ν_k , this implies

$$\begin{aligned} & \int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{N}^\varepsilon(z - y) P_{k+1}^{N,\varepsilon}(t, z, y, \tilde{x}) \varphi(z, y, \tilde{x}) dz dy d\tilde{x} \\ & \xrightarrow{\varepsilon \rightarrow 0, N \rightarrow \infty} \int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{N}(z - y) P_k(t, z, y, \tilde{x}) \varphi(z, y, \tilde{x}) dz dy d\tilde{x} \\ & + \int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \nu_k(t, z, \tilde{x}) \varphi(z, z, \tilde{x}) dz d\tilde{x}. \end{aligned}$$

Since \mathcal{N}^ε is nonnegative, so is the right hand side for a nonnegative test function. Choosing $\varphi(z, [y; \tilde{x}]) = \eta(R(z - y))\psi(z, \tilde{x})$ with an arbitrary nonnegative $\psi \in C_c^\infty(\mathbb{R}^{2(k-1)})$ and a nonnegative $\eta \in C_c^\infty(\mathbb{R}^2)$ with $\eta(0) = 1$, the first term on the right hand side vanishes for $R \rightarrow \infty$, proving nonnegativity of ν_k . The convergence is due to the Lebesgue theorem of dominated convergence, using the fact that $\mathcal{N}(z - y)\eta(R(z - y))$ is bounded and converges to 0 pointwise.

For the second statement, note that $\text{tr}(\mathcal{N}^\varepsilon) \leq 1$, and, consequently

$$\begin{aligned} & \text{tr} \left(\int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{N}^\varepsilon(z - y) P_{k+1}^{N,\varepsilon}(t, z, y, \tilde{x}) \varphi(z, y, \tilde{x}) dz dy d\tilde{x} \right) \\ & \leq \int_{\mathbb{R}^{2(k+1)}} P_{k+1}^{N,\varepsilon}(t, x) \varphi(x) dx. \end{aligned}$$

Passing to the limit, this gives

$$\int_{\mathbb{R}^{2(k+1)}} P_{k+1}(t, x) \varphi(x) dx$$

$$\begin{aligned}
&\geq \operatorname{tr} \left(\int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{N}(z-y) P_{k+1}(t, z, y, \tilde{x}) \varphi(z, y, \tilde{x}) \, dz \, dy \, d\tilde{x} \right) \\
&\quad + \operatorname{tr} \left(\int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \nu_k(t, z, \tilde{x}) \varphi(z, z, \tilde{x}) \, dz \, d\tilde{x} \right) \\
&= \int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} (1 - \chi(z-y)) P_{k+1}(t, z, y, \tilde{x}) \varphi(z, y, \tilde{x}) \, dz \, dy \, d\tilde{x} \\
&\quad + \operatorname{tr} \left(\int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \nu_k(t, z, \tilde{x}) \varphi(z, z, \tilde{x}) \, dz \, d\tilde{x} \right),
\end{aligned}$$

where we have used the identity $\operatorname{tr}(\mathcal{N}(z)) = 1 - \chi(z)$ with the above definition of χ . Finally, we arrive at

$$\begin{aligned}
&\operatorname{tr} \left(\int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \nu_k(t, z, \tilde{x}) \varphi(z, z, \tilde{x}) \, dz \, d\tilde{x} \right) \\
&\leq \int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \chi(z-y) P_{k+1}(t, z, y, \tilde{x}) \varphi(z, y, \tilde{x}) \, dz \, dy \, d\tilde{x} \\
&= \int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} P_{k+1}(t, z, \{z\}, \tilde{x}) \varphi(z, z, \tilde{x}) \, dz \, d\tilde{x},
\end{aligned}$$

which completes the proof. \blacksquare

5 Compatibility with the Keller-Segel system

We show that the Boltzmann hierarchy (29) has solutions that are generated by scaled measure solutions ϱ of the Keller-Segel system (7) and by the molecular chaos assumption:

$$P_k(t, x_1, \dots, x_k) = \prod_{i=1}^k P_1(t, x_i) \quad \text{for all } k \geq 1, \quad (31)$$

where $P_1 := \varrho/M$. Then, the usual procedure would be to prove uniqueness of the solutions to the Boltzmann hierarchy and conclude that they always factorize. However, not surprisingly we did not succeed in proving such a uniqueness result. In fact, even for the single particle model (7), (8) uniqueness is an open problem. Therefore, we are merely able to show the *compatibility* of the Boltzmann hierarchy with the Keller-Segel system:

Theorem 2 *Let (ϱ, ν) be a solution of the Keller-Segel system (7) in the sense of [11], with ϱ a time dependent, bounded, nonnegative Radon measure $\varrho(t) \in \mathcal{M}_1^+(\mathbb{R}^2)$ and $\nu \in \mathcal{M}_1((0, T) \times \mathbb{R}^2)^{2 \times 2}$ a time dependent, symmetric and nonnegative matrix valued measure. Then the measures*

$$P_k(t, x_1, \dots, x_k) := \prod_{i=1}^k P_1(t, x_i) \quad \text{and} \quad (32)$$

$$\nu_k(t, z, x_1, \dots, x_{k-1}) := \nu_1(t, z) \prod_{i=1}^{k-1} P_1(t, x_i) \quad (33)$$

with $P_1 := \varrho/M$ and $\nu_1 := \nu/M^2$, are a distributional solution to the Boltzmann hierarchy (29) subject to the initial condition $P_k(t=0, x_1, \dots, x_k) = \prod_{i=1}^k P_1(t=0, x_i)$. Moreover, the defect measures ν_k are symmetric and nonnegative, and satisfy the estimate (30).

Proof: We will show that the pairs (P_k, ν_k) defined by (32) verify the distributional formulation (29). Let us fix $k \in \mathbb{N}$ and the test function $\varphi = \varphi(x_1, \dots, x_k) \in C_c^\infty(\mathbb{R}^{2k})$, symmetric with respect to the interchange of its x_i -arguments. Moreover, we define

$$\psi(t, z) := \int_{\mathbb{R}^{2(k-1)}} \left(\prod_{i=1}^{k-1} P_1(t, x_i) \right) \varphi(z, x) dx, \quad \text{for all } z \in \mathbb{R}^2, t > 0.$$

Let us note that we have the regularity $P_1 \in W^{1,\infty}(0, T; W^{-2,\infty}(\mathbb{R}^2))$ (see the proof of Lemma 1 in [11]), which implies $\psi \in C_b(0, T; C_c^\infty(\mathbb{R}^2))$. Consequently, the time derivative term (first line) of (29) can be written with (32) as follows:

$$\begin{aligned} & \int_{\mathbb{R}^{2k}} P_k(T, x) \varphi(x) dx - \int_{\mathbb{R}^{2k}} P_k(0, x) \varphi(x) dx \\ &= \int_0^T \frac{d}{dt} \left[\int_{\mathbb{R}^{2k}} \left(\prod_{i=1}^k P_1(t, x_i) \right) \varphi(x) dx \right] dt \\ &= k \int_0^T \int_{\mathbb{R}^2} \frac{\partial P_1}{\partial t}(t, z) \psi(t, z) dz. \end{aligned}$$

The convective term (second line) of (29) yields

$$\frac{M}{4\pi} \sum_{n=1}^k \int_0^T \int_{\mathbb{R}^{2k}} \int_{\mathbb{R}^2} \mathcal{K}(x_n - y) P_{k+1}(t, x, y) \cdot (\nabla_n \varphi(x) - \nabla_n \varphi([y; \tilde{x}_n])) dy dx dt$$

$$\begin{aligned}
&= \frac{M}{4\pi} \sum_{n=1}^k \int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{K}(x_n - y) P_1(t, x_n) P_1(t, y) \\
&\quad \times \left(\int_{\mathbb{R}^{2(k-1)}} \prod_{i=1}^{k-1} P_1(t, x_i) (\nabla_n \varphi(x) - \nabla_n \varphi([y; \tilde{x}_n])) dx \right) dy \\
&= \frac{kM}{4\pi} \int_0^T \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \mathcal{K}(z - y) P_1(t, z) P_1(t, y) \cdot (\nabla \psi(t, z) - \nabla \psi(t, y)) dz dy.
\end{aligned}$$

The defect measure term (third line) and diffusive term (fourth line) of (29) are treated similarly,

$$\frac{M}{4\pi} \sum_{n=1}^k \int_0^T \int_{\mathbb{R}^{2k}} \nu_k(t, x_n, \tilde{x}_n) : \nabla_{n,n}^2 \varphi(x) dx dt = \frac{kM}{4\pi} \int_0^T \int_{\mathbb{R}^2} \nu_1(t, z) : \nabla^2 \psi(t, z) dz dt$$

and, respectively,

$$\sum_{n=1}^k \int_0^T \int_{\mathbb{R}^{2k}} P_k(t, x) \Delta_{x_n} \varphi(x) dx dt = k \int_0^T \int_{\mathbb{R}^2} P_1(t, z) \Delta \psi(t, z) dt dz.$$

We conclude that, since $(\varrho, \nu) = (MP_1, M^2\nu_1)$ satisfy the weak formulation of the limiting Keller-Segel system (7), the sequence (P_k, ν_k) given by (32) is a distributional solution of the Boltzmann hierarchy (29).

Finally, symmetry and nonnegativity of ν_k follow trivially from the corresponding properties of ν , so we only need to verify the validity of the estimate (30) on $\text{tr}(\nu_k)$. With the same test functions φ and ψ as above, the distributional formulation of the left hand side of (30) reads

$$\begin{aligned}
\int_{\mathbb{R}^2} \int_{\mathbb{R}^{2(k-1)}} \text{tr}(\nu_k(t, z, x)) \varphi(z, x) dx dz &= \int_{\mathbb{R}^2} \text{tr}(\nu_1(t, z)) \psi(t, z) dz \\
&\leq \sum_{a \in S_{at}(P_1(t))} P_1(t) (\{a\})^2 \psi(t, a),
\end{aligned}$$

where the last estimate follows from (8). This is indeed equal to the distributional formulation of the right hand side of (30), since

$$\begin{aligned}
&\int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \chi(z - y) P_{k+1}(t, z, y, x) \varphi(z, x) dy dz dx \\
&= \int_{\mathbb{R}^{2(k-1)}} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \chi(z - y) P_1(t, y) P_1(t, z) \prod_{i=1}^{k-1} P_1(t, x_i) \varphi(z, x) dy dz dx
\end{aligned}$$

$$\begin{aligned}
&= \sum_{a \in S_{at}(P_1(t))} \sum_{b \in S_{at}(P_1(t))} P_1(t)(\{a\})P_1(t)(\{b\})\chi(a=b)\psi(t,a) \\
&= \sum_{a \in S_{at}(P_1(t))} P_1(t)(\{a\})^2\psi(t,a).
\end{aligned}$$

■

6 A detailed study of the system with two particles

In the introduction, the strong formulation (9)–(11) of the Keller-Segel system for measure solutions has been given. This and the following section deal with the corresponding question for the stochastic particle formulation. We restrict the discussion to the cases of two (this section) and three (following section) particles, since already in the case of three particles our results are incomplete.

The Kolmogorov equation (15) in the case $N = 2$ takes the form

$$\frac{\partial p^\varepsilon}{\partial t} + (\nabla_x - \nabla_y) \cdot j^\varepsilon - (\Delta_x + \Delta_y)p^\varepsilon = 0, \quad (34)$$

for the particle distribution function $p^\varepsilon = p^\varepsilon(t, x, y)$, $t \geq 0$, $x, y \in \mathbb{R}^2$, with $j^\varepsilon(t, x, y) = -\frac{M}{4\pi}\mathcal{K}^\varepsilon(x-y)p^\varepsilon(t, x, y)$.

With the coordinate transformation

$$u = \frac{x+y}{2}, \quad v = \frac{x-y}{2},$$

this equation becomes

$$\frac{\partial p^\varepsilon}{\partial t} + \nabla_v \cdot j^\varepsilon - \frac{1}{2}(\Delta_u + \Delta_v)p^\varepsilon = 0, \quad j^\varepsilon = -\frac{M}{4\pi}\mathcal{K}^\varepsilon(2v)p^\varepsilon. \quad (35)$$

It is inspiring to study the evolution of the marginals $g^\varepsilon(t, v) := \int_{\mathbb{R}^2} p^\varepsilon(t, u, v) du$ and $h^\varepsilon(t, u) := \int_{\mathbb{R}^2} p^\varepsilon(t, u, v) dv$, which turns out to be decoupled:

$$\begin{aligned}
\frac{\partial g^\varepsilon}{\partial t} - \frac{M}{4\pi}\nabla_v \cdot (\mathcal{K}^\varepsilon(2v)g^\varepsilon) - \frac{1}{2}\Delta_v g^\varepsilon &= 0, \\
\frac{\partial h^\varepsilon}{\partial t} - \frac{1}{2}\Delta_u h^\varepsilon &= 0.
\end{aligned} \quad (36)$$

The first equation describes the distribution of the distance of the particles, while the second one stands for the distribution of the center of mass of the system. Comparing the virial calculation for the formal limits $g = \lim_{\varepsilon \rightarrow 0} g^\varepsilon$ and $p = \lim_{\varepsilon \rightarrow 0} p^\varepsilon$ (see (18)),

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^2} g |v|^2 dv &= \frac{1}{8\pi} (8\pi - M), \\ \frac{d}{dt} \int_{\mathbb{R}^4} p (|x|^2 + |y|^2) dx dy &= \frac{1}{2\pi} (16\pi - M), \end{aligned}$$

we observe that the latter does not provide a sharp criterion for concentration. We conjecture that, even for a finite number of particles, the criterion $M > 8\pi$ is sharp.

For the Keller-Segel system concentration goes hand in hand with L^∞ -blow-up. In the following, formal arguments will be given for the claim that the probability density of the stochastic particle system is always unbounded, and this fact is not necessarily connected to concentration of mass. To this end, we examine local approximations of the distribution of the particle distance by introducing the coordinate transformation $\vartheta = \frac{2v}{\varepsilon}$, $\tilde{g}(\vartheta) = \varepsilon^2 g^\varepsilon(v)$, and performing the formal limit $\varepsilon \rightarrow 0$ in (36):

$$\frac{M}{4\pi} \nabla_{\vartheta} \cdot \frac{\vartheta \tilde{g}}{|\vartheta|(|\vartheta| + 1)} + \Delta_{\vartheta} \tilde{g} = 0.$$

The rotationally symmetric solutions, decaying as $\vartheta \rightarrow \infty$, have the form

$$\tilde{g}(\vartheta) = c(|\vartheta| + 1)^{-M/4\pi},$$

where c is a constant. This expression has finite mass if and only if $M > 8\pi$. Consequently, in this case g^ε contains an approximation of a Dirac delta at $v = 0$. On the other hand, if $M < 8\pi$, g does not concentrate. To obtain the profile of g in the neighbourhood of $v = 0$, we integrate (36) with $\varepsilon = 0$ over $\mathbb{R}^2 \setminus B_r(0)$:

$$\frac{d}{dt} \int_{|v|>r} g dv = \int_{|v|=r} \left(\frac{M}{4\pi} \frac{g}{r} + \frac{\partial g}{\partial n} \right) dS(v),$$

where dS is the surface measure and $\frac{\partial g}{\partial n}$ denotes the derivative of g with respect to the outer normal. Since the total mass of g is conserved, for small r we approximately have

$$\frac{M}{4\pi} \frac{g(r)}{r} + \frac{\partial g}{\partial r}(r) = 0,$$

with $g(v) = g(|v|)$. Therefore, in the subcritical case g behaves asymptotically like $r^{-M/4\pi}$ close to the origin, i.e., it is unbounded with an integrable singularity. In this situation we expect 'diffusion to win', i.e. a long time behavior governed by dispersion. This can be examined by an intermediate asymptotics showing self similar decay: With the standard diffusive rescaling $\tau = \log t$, $\xi = x/\sqrt{t}$, $\eta = y/\sqrt{t}$, and $\lim_{\varepsilon \rightarrow 0} p^\varepsilon(t, x, y) = p(t, x, y) = q(\log t, x/\sqrt{t}, y/\sqrt{t})/t^2$, the function q satisfies

$$\begin{aligned} \partial_\tau q + \nabla_\xi \cdot J_\xi + \nabla_\eta \cdot J_\eta &= 0, \\ J_\xi &= -\frac{\xi}{2}q - \frac{M}{4\pi} \frac{\xi - \eta}{|\xi - \eta|^2}q - \nabla_\xi q, \quad J_\eta = -\frac{\eta}{2}q - \frac{M}{4\pi} \frac{\xi - \eta}{|\xi - \eta|^2}q - \nabla_\eta q. \end{aligned}$$

The steady state making these fluxes vanish, is given by

$$q_\infty(\xi, \eta) = c|\xi - \eta|^{-M/(4\pi)} \exp\left(-\frac{|\xi|^2 + |\eta|^2}{4}\right)$$

The value of c can be determined from initial conditions by mass conservation. The standard computation leads to entropy decay:

$$\frac{d}{d\tau} \int_{\mathbb{R}^4} q \log \frac{q}{q_\infty} d\xi d\eta = - \int_{\mathbb{R}^4} \frac{|J_\xi|^2 + |J_\eta|^2}{q} d\xi d\eta.$$

This computation is only formal and has to be taken with care because of the singularities in the integrands. However, we still conjecture, for $M < 8\pi$:

$$p(t, x, y) \approx ct^{\frac{M}{8\pi}-2} |x - y|^{-\frac{M}{4\pi}} \exp\left(-\frac{|x|^2 + |y|^2}{4t}\right), \quad \text{as } t \rightarrow \infty.$$

After these observations, let us come back to (35), now for arbitrary M . The same steps as in Sections 3 and 4 for the BBGKY hierarchy lead to the limit $\varepsilon \rightarrow 0$ in the interaction term:

$$\frac{M}{8\pi} \int_{\mathbb{R}^4} \mathcal{K}(2v) \cdot (\nabla_v \varphi(u, v) - \nabla_v \varphi(u, -v)) p \, du \, dv + \frac{M}{8\pi} \int_{\mathbb{R}^2} \nu : \nabla_v^2 \varphi(u, 0) \, du.$$

The defect measure ν is symmetric, nonnegative, and satisfies

$$\text{tr}(\nu(t, u)) \leq p(t, u, \{0\}) := \int_{\mathbb{R}^2} p(t, u, v) \chi(v) \, dv.$$

Therefore, in the subcritical case $M < 8\pi$, when p does not concentrate, the defect measure vanishes and the corresponding strong formulation of the limiting system is obtained by choosing $\varepsilon = 0$ in (35).

To derive the strong formulation in the supercritical case $M > 8\pi$, we make an ansatz for p of the form

$$p(t, u, v) = p_0(t, u, v) + \delta(v)p_1(t, u), \quad (37)$$

where p_0 (the distribution function of free particles) and p_1 (the distribution function of the particle aggregate) are smooth functions of u and v . Inserting this ansatz into the weak formulation, we obtain

$$\begin{aligned} & \frac{d}{dt} \int_{\mathbb{R}^4} p_0 \varphi(u, v) \, du \, dv + \frac{d}{dt} \int_{\mathbb{R}^2} p_1 \varphi(u, 0) \, du \\ & + \frac{M}{8\pi} \int_{\mathbb{R}^4} \mathcal{K}(2v) p_0 \cdot (\nabla_v \varphi(u, v) - \nabla_v \varphi(u, -v)) \, du \, dv \\ & + \frac{M}{8\pi} \int_{\mathbb{R}^2} \nu : \nabla_v^2 \varphi(u, 0) \, du \\ & - \frac{1}{2} \int_{\mathbb{R}^4} p_0 (\Delta_u + \Delta_v) \varphi(u, v) \, du \, dv - \frac{1}{2} \int_{\mathbb{R}^2} p_1 (\Delta_u + \Delta_v) \varphi(u, 0) \, du = 0. \end{aligned}$$

We require that the defect measure term balances the term $\frac{1}{2} \int_{\mathbb{R}^2} p_1 \Delta_v \varphi(u, 0) \, du$, which leads to $\nu(t, u) = \frac{4\pi}{M} p_1(t, u) \text{Id}_{2 \times 2}$.

The estimate $\text{tr}(\nu(t, u)) \leq p(t, u, \{0\}) = p_1(t, u)$ implies that the ansatz (37) is only valid if $M \geq 8\pi$. The strong formulation is obtained by integration by parts and taking into account the calculation $\nabla_v \cdot \frac{v}{2|v|^2} = \pi \delta(v)$:

$$\begin{aligned} \frac{\partial p_0}{\partial t} - \frac{M}{4\pi} \mathcal{K}(2v) \cdot \nabla_v p_0 - \frac{1}{2} (\Delta_u + \Delta_v) p_0 &= 0, \\ \frac{\partial p_1}{\partial t} - \frac{1}{2} \Delta_u p_1 &= \frac{M}{4} p_0(v=0). \end{aligned}$$

With this system, we can make several interesting observations. First of all, note that the equation for p_0 is not in divergence form. Indeed, the “mass” of p_0 is not conserved, since it is being transported to p_1 via the source term on the right hand side of the second equation. Therefore, the mass of the aggregate increases with time which, being in the supercritical case $M > 8\pi$, is indeed to be expected. Moreover, defining the mass $m_0(t) = \int_{\mathbb{R}^4} p_0(t, u, v) \, du \, dv$

and the v -second-order moment $u_0(t) = \int_{\mathbb{R}^4} p_0(t, u, v) |v|^2 du dv$ of p_0 , we easily compute

$$\dot{u}_0(t) + \left(\frac{M}{4\pi} - 2 \right) m_0(t) = 0.$$

Thus, $u_0(t)$ is a nonincreasing quantity, and, if $u_0(t = 0)$ is finite, $m_0 \in L^1(0, \infty)$. We see that the flow of mass from p_0 to p_1 must be fast enough, so that the total mass of p_0 is integrable on the time interval $(0, \infty)$.

Finally, let us give the limiting strong formulation in the original variables x and y . For $M < 8\pi$, it is (34) with $\varepsilon = 0$. For $M > 8\pi$, we have $p(t, x, y) = p_0(t, x, y) + p_1(t, x)\delta(x - y)$ with

$$\begin{aligned} \frac{\partial p_0}{\partial t} - \frac{M}{4\pi} \mathcal{K}(x - y) \cdot (\nabla_x - \nabla_y) p_0 - (\Delta_x + \Delta_y) p_0 &= 0, \\ \frac{\partial p_1}{\partial t} - \frac{1}{2} \Delta_x p_1 &= \frac{M}{4} p_0(x, x). \end{aligned}$$

7 Systems with three or more particles

We give an overview of some observations concerning the three particle problem (see [13] for details). The ansatz corresponding to (37) for the case of three particles reads

$$\begin{aligned} p(t, x, y, z) &= p_0(t, x, y, z) + \delta(x - y) p_1(t, x, z) + \delta(y - z) p_1(t, y, x) \\ &\quad + \delta(z - x) p_1(t, z, y) + \delta(x - y) \delta(y - z) p_2(t, x), \end{aligned}$$

where p_0 describes three free particles, $p_1(t, x, z)$ one two-particle aggregate at position x and one free particle at position z , and p_2 a three-particle aggregate. The three terms containing p_1 have to occur due to particle indistinguishability. Note that p_1 is in general not symmetric in its two position arguments. If for the diagonal defect measures corresponding to this ansatz, the inequalities (30) are checked, it turns out that, for p_2 not to vanish, $M > 8\pi$ is required, whereas the corresponding condition for p_1 is $M > 12\pi$. Thus, for $M < 8\pi$ no concentration happens and $p_1 = p_2 = 0$. For $M > 12\pi$, a system of PDEs for p_0, p_1, p_2 can be derived from the distributional formulation (28), where mass is transferred from p_0 to p_1 (by collisions of 2 particles) and from p_1 to p_2 (by collisions of a two-particle aggregate with the third particle). The condition $M > 12\pi$ (curiously agreeing with the

concentration condition obtained from (18)) again can be seen as a version of the 8π -criterion since it is needed for the collision of 2 particles, whose total mass $2\frac{M}{3}$ has to be bigger than 8π .

The strong formulation of the dynamics in the case $8\pi < M < 12\pi$ is an open problem. The difficulty lies in the fact that in this case only an aggregate of three (but not of two) particles can be stable, which therefore has to be created by a three-particle collision intuitively expected to be an event with zero probability. This question as well as the strong formulation of the dynamics of more than three particles remain the subject of further investigations.

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