

COLLECTIVE PHENOMENA IN INTERACTING PARTICLE SYSTEMS

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We consider the (kinetic) continuum limit for a class of stochastic interacting particle systems. We prove propagation of chaos and convergence to macroscopic equations of the "Reaction-Diffusion" type.

interacting particle systems * continuum limit * propagation of chaos * reaction-diffusion equations

Introduction

Collective phenomena, hydrodynamical behavior, self organization, local equilibrium and propagation of chaos are main features in the evolution of systems with many components. In this paper we consider a class of stochastic interacting particle systems where some of the above effects can be observed. In the "continuum limit" the macroscopic equations that we obtain are nonlinear PDE's of the "Reaction-Diffusion type".

The main feature of the models we consider is that in such continuum limit the generator splits into two parts, one "much larger" than the other. As a consequence we can distinguish two time scales; in the first the evolution seems ruled only by the main, larger, part of the generator; in the second, longer, time scale the effect of the "smaller" one enters into play. To make such a splitting evident it is convenient to describe the continuum limit in the way outlined below. Other equivalent procedures can and are widely used, we will come back to this later on.

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The microscopic models can be described as follows. Particles move in \mathbb{Z} (\mathbb{Z}^d , $d > 1$, can be considered as well. For technical reasons one sometimes considers bounded regions with periodic boundary conditions, but here we shall not need such an assumption). Particles move like independent symmetric random walks with nearest neighbor jumps and jump intensity equal to 1. We denote by L_0 the corresponding generator. Besides this, particles can also be created and/or die.

The birth intensity at any site x is $q_+(\eta(x))$, $\eta(x)$ being the occupation number at x and q_+ some increasing positive polynomial. Particles die with intensity $q_-(\eta(x))$, q_- being also some increasing positive polynomial. All the above events, i.e. births and deaths, are mutually independent, cf. Definition 1.1. To have a well defined process we also assume that the degree of the polynomial q_+ is smaller than that of q_- (it would be enough to assume that there is $c < \infty$ so that $q_+(n) - q_-(n) \leq c$ for any $n \geq 1$).

If births and deaths were absent the process would consist of independent symmetric random walks. The natural macroscopic scaling for such a process (the same for which a single random walk converges to a Brownian motion) is to scale down positions by ε and times by ε^2 . Namely one studies the averages $\langle \eta([\varepsilon^{-1}r], \varepsilon^{-2}t) \rangle$, i.e. the mean number of particles at time $\varepsilon^{-2}t$ and at site $[\varepsilon^{-1}r]$, ($[a]$ denotes the integer part of a). In the limit, when $\varepsilon \rightarrow 0$, $\langle \eta([\varepsilon^{-1}r], \varepsilon^{-2}t) \rangle$ goes to $p(r, t)$ which solves the equation

$$\partial_t p = \frac{1}{2} \partial_r^2 p, \quad p(r, 0) = p(r),$$

under the assumption that $\langle \eta([\varepsilon^{-1}r], 0) \rangle \rightarrow p(r)$ (and that $p(r)$ is smooth). Furthermore if at time $t=0$ the particle numbers at different sites are independent (or “weakly dependent”) variables, then, at any $t > 0$, the measure becomes close to a product (over all sites) of Poisson distributions.

The birth and death generator L_G , which will be defined exactly by (1.1b) below, is infinitesimally small, when $\varepsilon \rightarrow 0$, as compared to $\varepsilon^{-2}L_0$: in the time it takes for a particle to jump, the probability for a birth–death event at that site typically goes like ε^2 . In such a “short time scale” therefore the presence of L_G is negligible and the system behaves as if it were free, so that the particle distribution in the limit when $\varepsilon \rightarrow 0$ becomes again a direct product of Poisson laws. In a finite time scale (when particles have typically $\approx \varepsilon^{-2}$ jumps) L_G has some finite nonzero influence on the evolution. Such a picture is confirmed by our first result, which we give below after some definitions.

Definition 1.1. q_+ and q_- denote positive polynomials on the nonnegative integers N such that $q_{\pm}(0) = 0$ and such that degree of $q_+ <$ degree of q_- , actually it is enough to assume that (2.5b) below holds.¹

As pointed out by Metivier, the natural assumption would be that there exists $c > 0$ such that

$$q_+(n) - q_-(n) \leq cn \quad \forall n > 0.$$

Our analysis would work also in this case as well, modulo some changes in the proofs.

Let $L^\varepsilon \equiv \varepsilon^{-2}L_0 + L_G$, $\varepsilon > 0$, be the generator of the Markov process on $N^{\mathbb{Z}}$, which acts on the cylinder functions as follows: for any $\eta \in N^{\mathbb{Z}}$,

$$L_0 f(\eta) = \sum_{x \in \mathbb{Z}} \eta(x) \left\{ \frac{1}{2} f(\eta^{x,x+1}) + \frac{1}{2} f(\eta^{x,x-1}) - f(\eta) \right\}, \quad (1.1a)$$

$$L_G f(\eta) = \sum_{x \in \mathbb{Z}} \{ q_+(\eta(x)) [f(\eta^{x,+}) - f(\eta)] + q_-(\eta(x)) [f(\eta^{x,-}) - f(\eta)] \}, \quad (1.1b)$$

$$\eta^{x,x\pm 1}(y) = \eta(y) \quad \text{for } y \neq x, x \pm 1,$$

$$\eta^{x,x\pm 1}(x) = \eta(x) - 1,$$

$$\eta^{x,x\pm 1}(x \pm 1) = \eta(x \pm 1) + 1, \quad (1.2a)$$

$$\eta^{x,\pm}(y) = \eta(y) \quad \text{for } y \neq x, \quad \eta^{x,\pm}(x) = \eta(x) \pm 1. \quad (1.2b)$$

For what follows we need to define the polynomials

$$p(k, z) = \eta(z)(\eta(z) - 1) \cdots (\eta(z) - k + 1), \quad z \in \mathbb{Z}, k \in \mathbb{N}. \quad (1.3)$$

By $z = (z_1, \dots, z_k)$ we shall denote an element of \mathbb{Z}^k , $k \geq 1$. Furthermore we set

$$p(k, z) = \prod_{i=1, \dots, m} p(k_i, z_i) \quad (1.3a)$$

where m is the number of distinct elements of $z \in \mathbb{Z}^k$, and k_i is the multiplicity of each single element $z_i \in \mathbb{Z}$. Note that if μ_ρ is a product of Poisson distributions each having density ρ , then $\nu_\rho(p(k, x)) = \rho^k$.

μ^ε denotes a family of probability measures on $N^{\mathbb{Z}}$ such that for any $L > 0$, $k \geq 1$, $(x_1, \dots, x_k) \in \mathbb{Z}^k$ mutually distinct

$$\lim_{\varepsilon \rightarrow 0} \sup_{|x_i| \leq \varepsilon^{-1}L} \left| \mu^\varepsilon \left(\prod_{i=1, \dots, k} \eta(x_i) \right) - \prod_{i=1, \dots, k} \rho(\varepsilon x_i) \right| = 0 \quad (1.4)$$

where $\rho(r)$ is assumed² to be uniformly bounded and C^2 . Furthermore we assume that there exists c_0 such that for any $k \geq 1$ and all $(x_1, \dots, x_k) \in \mathbb{Z}^k$ (not necessarily distinct),

$$\mu^\varepsilon [p(k, x)] \leq c_0^k. \quad (1.5)$$

We are now ready to state the following.

Theorem 1.2. *For each $\varepsilon > 0$ consider the Markov process with generator L^ε and initial measure μ^ε , as in Definition 1.1. Then for all $r \in \mathbb{R}$ and $t \geq 0$,*

$$\lim_{\varepsilon \rightarrow 0} \mu^\varepsilon [\eta([\varepsilon^{-1}r], t)] = \rho(r, t) \quad (1.6)$$

² We do not need to assume convergence of μ^ε to a product of Poisson distributions, we only need convergence of the first moments in the sense of equation (1.4). In this way equations (1.4) [and (1.5)] can be satisfied by families μ^ε with support on configurations for which $\eta(x)$ is uniformly bounded. This remark might be useful for numerical simulation of such models. In fact our conditions in Definition 1.1 are not optimal, and can be weakened; we shall not discuss further this point.

where

$$\partial_t \rho = \frac{1}{2} \partial_r^2 \rho - V'(\rho), \quad \rho(r, 0) = \rho(r), \quad (1.7)$$

$$V'(\rho) = -\{v_+(\rho) - v_-(\rho)\}, \quad v_{\pm}[\rho] = v_{\rho}[q_{\pm}(\eta(0))], \quad (1.8)$$

v_{ρ} being the Poisson measure with parameter ρ .

Furthermore let μ_t^{ε} denote the law of the process at time t , then propagation of chaos holds at all times t , namely

$$\left\{ \mu_t^{\varepsilon} - \prod_{x \in \mathbb{Z}} \nu_{\rho(\varepsilon x, t)} \right\} \rightarrow 0 \quad (\text{weakly}).$$

In the proof of Theorem 1.2 we derive bounds on the moments of the occupation numbers which for any finite time interval are uniform in ε . From this and Theorem 1.2 we get the following

Corollary 1.3. *Let L^{ε} and μ^{ε} be as in Definition 1.1. Then for any $\varphi \in \mathcal{S}(\mathbb{R})$ (i.e. the Schwartz space of rapidly decreasing functions on \mathbb{R}) the “density field”*

$$X_t^{\varepsilon}(\varphi) = \varepsilon \sum \varphi(\varepsilon x) \eta(x, t) \quad (1.9)$$

converges in law to

$$\int dr \varphi(r) \rho(r, t) \quad (1.10)$$

where $\rho(r, t)$ solves (1.7).

Bibliographical notes

The above results, Theorem 1.2 and Corollary 1.3, were proven by Dittrich [7], for $q_{\pm} \equiv 0$. Microscopic models for the Reaction–Diffusion equations are discussed in [21] and [9] for instance.

A mathematically rigorous derivation of the Reaction–Diffusion equation, (1.7), and the analysis of the fluctuations of the density fields (1.9) around their averages are contained in [1], [2], [20] and [10] for some “mean field” versions of the model, cf. also [12]. Translated into our language these results correspond to replacing $q_{\pm}(\eta(x))$ by

$$v_{\pm} \left(\varepsilon^{\gamma} \sum_{|y-x| < \varepsilon^{-\gamma}/2} \eta(x) \right)$$

(cf. (1.8) for notation) where γ is some positive number less than one. That is one divides the lattice into intervals (cells) of length $\varepsilon^{-\gamma}$, each cell being then a point in a new lattice (which we will still denote by \mathbb{Z} , and the occupation numbers by $\eta(x)$). Typically therefore $\eta(x) \approx \varepsilon^{-\gamma}$. The new jump intensity is $\varepsilon^{-2(1-\gamma)}$, reflecting

the fact that the original lengths are now scaled differently. The new birth–death process has intensity $\varepsilon^{-\gamma} v_{\pm}(\varepsilon^{\gamma} \eta(x))$ and the density field becomes

$$X_t^{\varepsilon}(\varphi) = \varepsilon^{1-\gamma} \sum \varphi(\varepsilon^{1-\gamma} x) [\varepsilon^{\gamma} \eta(x, t)]$$

which, for a suitable choice of γ and of the initial conditions, is proven to converge (at least when the system is on a torus of length $\varepsilon^{-1}L$) to a deterministic field which solves (1.7) (as in our Corollary 1.3).

Another microscopic model for the Reaction–Diffusion equations has been introduced in [5]; cf. also [7] for a further analysis of such system. Our techniques are closer to those in [5], as noticed by Herbert Spohn who actually proposed to use them also in the present context.

In our proofs we use a perturbative approach relating the actual semigroup with generator L^{ε} to that with generator $\varepsilon^{-2}L_0$. We then obtain a hierarchy of equations as it typically occurs in the kinetic Boltzmann–Grad limit. In particular our strategy was inspired by the analysis in [16].

The analogy with the Boltzmann–Grad limit is in fact quite strict. The latter, for a gas of hard spheres, is a limit when the radius $R(\varepsilon)$ of each sphere vanishes when $\varepsilon \rightarrow 0$. Things are arranged so that, typically, each sphere has finitely many collisions per unit time (in the time-scale for which the Boltzmann equation holds). One can perform the Boltzmann–Grad limit keeping finite the initial interparticle distances, as we are doing here. In this case one has to increase velocities by a factor ε^{-1} (hence the radius $R(\varepsilon)$ is determined so that the typical number of collisions per unit time $R(\varepsilon)^{d-1} \varepsilon^{-1} \sim 1$, where d is the number of dimensions of the space where particles move). Therefore the free part of the Liouville generator is multiplied by a factor ε^{-1} (in our case by ε^{-2} because we consider diffusions without drift) and it is much larger, when $\dot{\varepsilon} \rightarrow 0$, than the collision generator.

To underline the analogy we shall call “kinetic” the continuum limit we consider here, to distinguish it from the “hydrodynamical limit” where only the initial distribution is scaled (as well as the time), while the generator is kept fixed.

In Section 2 and 3 we give the proof of Theorem 1.2. Section 4 is a “remarks section”, which sketches some possible future research.

Section 2

In this section we shall derive ε -uniform a priori bounds on the $t > 0$ averages of polynomials of the occupation numbers. In particular we shall prove that the function $(r, t) \rightarrow \langle \eta[\varepsilon^{-1}r] \rangle_t^{\varepsilon}$ (i.e. the average value at time t of the occupation number at site $[\varepsilon^{-1}r]$ in the process with generator L^{ε}) is equicontinuous and uniformly bounded [on the compact sets of $\mathbb{R} \times \mathbb{R}_+$], so that it converges by subsequences.

In the next section we shall identify its limits as the unique solution of (1.6). This will come together with the proof of the factorization property stated in Theorem 1.2, hence Theorem 1.2 will then be proved. For the polynomials $p(k, z)$ defined in

(1.3) the following “duality” formula holds³ (its proof is sketched below):

$$\langle p(k, \mathbf{x}) \rangle_t = \sum_z \pi_t(\mathbf{x} \rightarrow \mathbf{z}) \langle p(k, \mathbf{z}) \rangle_0 \quad (2.1)$$

where $\langle \cdot \rangle_0$ and $\langle \cdot \rangle_t$ denote averaging w.r.t. an initial measure μ_0 on N^Z and to the measure μ_0^t which gives the measure at time t when $\mu_0^0 = \mu_0$ for the evolution semigroup generated by L_0 , respectively. $\pi_t(\mathbf{x} \rightarrow \mathbf{z})$ are the transition probabilities of k independent random walks starting at \mathbf{x} . Equation (2.1) states that the “ k -body correlation functions $\langle p(k, \mathbf{x}) \rangle_t$ ” obey *closed equations* [the set of equations involving all the correlation functions is called the “BBGKY hierarchy”, which, in the present case, is decoupled].

Equation (2.1) can be proven by checking the following identity:

$$L_0 p(k, \mathbf{x}) = \frac{1}{2} \sum_i \Delta_i p(k, \mathbf{x})$$

where Δ_i is the discrete Laplacian acting on the variable x_i , $i = 1, \dots, k$. A similar formula was used in [11].

For the full evolution generated by L^ε the “BBGKY hierarchy” is no longer decoupled. We have in fact, by “the integration by parts formula” (see for instance the proof of Proposition VIII, 1.7 in [17]):

$$\langle p(k, \mathbf{x}) \rangle_t^\varepsilon = \sum \pi_t^\varepsilon(\mathbf{x} \rightarrow \mathbf{z}) \langle p(k, \mathbf{z}) \rangle_0^\varepsilon + \int_0^t ds \sum \pi_s^\varepsilon(\mathbf{x} \rightarrow \mathbf{z}) \langle L_G p(k, \mathbf{z}) \rangle_{t-s}^\varepsilon \quad (2.2)$$

where $\langle \cdot \rangle_t^\varepsilon$ denotes averaging w.r.t. the measure μ_t^ε , obtained from μ_0^ε by the evolution semigroup generated by L^ε , and $\pi_t^\varepsilon(\mathbf{x} \rightarrow \mathbf{z})$ are the transition rates of the speeded up random walk, i.e. with generator $\varepsilon^{-2} L_0$. For notational simplicity we assume that $q_\pm(\eta(z)) = p(k_\pm, z)$, $k_- > k_+$.

Equations (2.2) and (1.7) are very close to each other. Take (2.2) with $k = 1$ and consider the expression $\langle L_G p(1, z) \rangle_{t-s}^\varepsilon \equiv \langle q_+(\eta(z)) - q_-(\eta(z)) \rangle_{t-s}^\varepsilon$. Assume that when $\varepsilon \rightarrow 0$ such average becomes close to a Poisson average with some parameter $\rho_{t-s}(\varepsilon z)$ and that $\langle \eta(z) \rangle_{t-s}^\varepsilon - \rho_{t-s}(\varepsilon z)$ vanishes when $\varepsilon \rightarrow 0$. Then, formally, (2.2) with $k = 1$ converges to (1.7) in integral form.

Our strategy will be to prove that the functions $\langle p(k, \mathbf{x}) \rangle_t^\varepsilon$ are uniformly bounded (Proposition 2.1) and equicontinuous (Proposition 2.2), so that they converge by subsequences. In Section 3 we shall prove the factorization property (Proposition 3.1) and the above heuristic argument will be made rigorous.

Proposition 2.1. *Let μ^ε be as in Definition 1.1, and $T > 0$. Then for any $0 \leq t \leq T$ and $k \geq 1$ there is a function $f(\varepsilon, k, t)$ such that for any $k > 1$*

$$\lim_{\varepsilon \rightarrow 0} f(\varepsilon, k, T) = 0 \quad (2.3a)$$

³ An analogous formula holds for asymmetric independent random walks (in the dual process particles move with opposite drift). It was noticed by Claude Kipnis that in such case also another duality formula holds, corresponding to the existence of spatially nonhomogeneous invariant reversible measures.

and

$$\langle p(k, z) \rangle_i^\varepsilon \leq (c_0 e^{ct})^k + f(\varepsilon, k, t) \quad (2.3b)$$

where c_0 is the constant appearing in (1.5) and c is such that

$$q_+(n) - q_-(n) \leq c \quad \forall n \geq 0. \quad (2.4)$$

Proof. We have

$$\begin{aligned} L_G p(k, z) &= \sum_{i=1}^m k_i \{q_+(\eta(z_i)) - \hat{q}_-(\eta(z_i))[\eta(z_i) - k_i + 1]\} \\ &\quad \times p(k_i - 1, z_i) \left\{ \prod_{j \neq i} p(k_j, z_j) \right\} \end{aligned} \quad (2.5a)$$

where $\hat{q}_-(n) = (n-1)(n-2) \cdots (n-k_-+1)$. Clearly, for all $h \geq 1$,

$$\max_{n \in \mathbb{N}} (q_+(n) - \hat{q}_-(n)(n-h+1)) = c'_h < \infty. \quad (2.5b)$$

We set

$$\varphi_k(t) = \sup_{h \leq k} \sup_{x \in \mathbb{Z}^h, s \leq t, \varepsilon > 0} \langle p(k, x) \rangle_s^\varepsilon. \quad (2.6)$$

We shall first of all derive a rough estimate for $\langle p(k, z) \rangle_i^\varepsilon$ which will be afterwards improved to obtain (2.3b). By the hypotheses on the initial state and by (2.5) there are constants c_k so that

$$\varphi_k(t) \leq c_0^k + c_k \int_0^t ds \varphi_{k-1}(s) \quad (\varphi_0 = 1). \quad (2.7)$$

By (2.7) we get that for any $k \geq 1$ and $t \geq 0$ there is $c_k(t) < \infty$ (and nondecreasing with k and t) such that

$$\varphi_k(t) \leq c_k(t) < \infty, \quad t \in \mathbb{R}. \quad (2.8)$$

By the same relation (2.5), if $z \equiv (z_1, z_2, \dots, z_k) \in \mathbb{Z}^k$ and the z_i 's are all distinct, we have

$$\langle L_G p(k, z) \rangle_s^\varepsilon \leq ck \varphi_{k-1}(s) \quad (2.9)$$

where c is defined in (2.4).

On the other hand from (2.5a) using (2.5b), (2.6) and (2.8) we get that there exists $g^*(k, t)$ (nondecreasing in t) such that, for all $s \leq t$ and $z \in \mathbb{Z}^k$,

$$\langle L_G p(k, z) \rangle_s^\varepsilon \leq g^*(k, t). \quad (2.10)$$

We denote by Σ'' the sum over $\{z \equiv (z_1, \dots, z_k): z_i = z_j \text{ for some } i \neq j\}$. We then have that for any $k > 1$ there is c_k'' so that

$$\Sigma'' \pi_s^\varepsilon(x \rightarrow z) \leq c_k'' \varepsilon / \sqrt{s}$$

for any $s > 0$. We get

$$\begin{aligned} \left| \int_0^t ds \Sigma'' \pi_s^\varepsilon(x \rightarrow z) \langle L_G p(k, z) \rangle_{t-s}^\varepsilon \right| &\leq \varepsilon c_k'' \int_0^t ds s^{-1/2} g^*(k, t) \\ &\leq \varepsilon c_k'' 2\sqrt{t} g^*(k, t) \equiv \varepsilon g(k, t). \end{aligned} \quad (2.11)$$

Putting together (2.9) and (2.11) we get

$$\varphi_k(t) \leq (c_0)^k + ck \int_0^t ds \varphi_{k-1}(s) + \varepsilon g(k, T), \quad (2.12)$$

which gives (2.3b) with $f = \varepsilon g(k, T) e^{cT}$.

Proposition 2.2. *Let μ^ε be as in Definition 1.1. Then for any T and L positive and $k \geq 1$ the following relation holds*

$$\lim_{\delta \rightarrow 0} \limsup_{\varepsilon \rightarrow 0} \sup^{(L, T, \delta)} |\langle p(k, x) \rangle_{t'}^\varepsilon - \langle p(k, y) \rangle_t^\varepsilon| = 0, \quad (2.13)$$

where $\sup^{(L, T, \delta)}$ denotes the supremum over all $x, y \in \mathbb{Z}^k$, $t, t' \in [0, T]$, such that $|x| \leq \varepsilon^{-1}L$, $|y| \leq \varepsilon^{-1}L$, $|x - y| \leq \varepsilon^{-1}\delta$, $|t - t'| \leq \delta$.

Proof. For simplicity we give the proof only for $k = 1$. The extension to the case $k > 1$ can be done using similar arguments.

By assumption (1.4) it follows that we can find an $L_\varepsilon \rightarrow \infty$ as $\varepsilon \rightarrow 0$ such that

$$\lim_{\varepsilon \rightarrow 0} \sup_{|z| \leq \varepsilon^{-1}L_\varepsilon} |\langle \eta(z) \rangle_0^\varepsilon - \rho(\varepsilon z)| = 0.$$

Hence we get

$$\begin{aligned} &\sup^{(L, T)} \left| \sum_z \pi_t^\varepsilon(y \rightarrow z) (\langle \eta(z) \rangle_0^\varepsilon - \rho(\varepsilon z)) \right| \\ &\leq \sup^{(L, T)} \sum_{z: |z-y| \leq \varepsilon^{-1}L_\varepsilon} \pi_t^\varepsilon(y \rightarrow z) |\langle \eta(z) \rangle_0^\varepsilon - \rho(\varepsilon z)| \\ &\quad + 2c_0 \sum_{z: |z-y| > \varepsilon^{-1}L_\varepsilon} \pi_t^\varepsilon(y \rightarrow z) \rightarrow 0, \end{aligned} \quad (2.14)$$

where $\sup^{(L, T)}$ denotes the supremum over $|y| \leq \varepsilon^{-1}L$, $t \leq T$.

We first prove relation (2.13) for $t' = t$. We have

$$\sup_{|x-y| \leq \varepsilon^{-1}\delta} |\sum (\pi_s^\varepsilon(x \rightarrow z) - \pi_s^\varepsilon(y \rightarrow z))| \leq c^* \delta / \sqrt{s}$$

for some constant $c^* > 0$ and any $s > 0$. Hence

$$\left| \int_0^t ds \sum (\pi_s^\varepsilon(x \rightarrow z) - \pi_s^\varepsilon(y \rightarrow z)) \langle L_G p(1, z) \rangle_{t-s}^\varepsilon \right| \leq 2c^* \sqrt{T} \delta g^*(1, T).$$

The other terms can be written as

$$\sup^{(L, T)} \left| \sum_z \pi_t^\varepsilon(y \rightarrow z) (\rho(\varepsilon(z+w)) - \rho(\varepsilon z)) \right|,$$

where $w = x - y$. We can find $c_\delta \uparrow \infty$ as $\delta \rightarrow 0$ and correspondingly $c'_\delta = \sup_{|x| < c_\delta \sqrt{T}} |\rho'(x)|$ such that $\lim_{\delta \rightarrow 0} c'_\delta \delta = 0$.

If $|y - z| < (c_\delta/2)\varepsilon^{-1}\sqrt{T}$ we have

$$|\rho(\varepsilon(z + w)) - \rho(\varepsilon z)| \leq c'_\delta \delta \rightarrow 0 \quad \text{as } \delta \rightarrow 0. \tag{2.15}$$

Since

$$\lim_{\delta \rightarrow 0} \lim_{\varepsilon \rightarrow 0} \sum_{|y-z| > (C_\delta/2)\varepsilon^{-1}\sqrt{T}} \pi_t^\varepsilon(y \rightarrow z) = 0,$$

relation (2.13) is proved for $t = t'$.

Suppose now that $t' > t$, $t' - t < \delta$. Using (2.2) and taking t as initial time, we have

$$|\langle p(1, y) \rangle_{t'}^\varepsilon - \langle p(1, y) \rangle_t^\varepsilon - \sum \pi_{t'-t}^\varepsilon(y \rightarrow z) (\langle p(1, z) \rangle_{t'}^\varepsilon - \langle p(1, y) \rangle_t^\varepsilon)| \leq g^*(1, T) \delta$$

where $g^*(1, T)$ is defined in (2.10). Now, since $|\langle \eta(z) \rangle_t| \leq c_0 + g(1, T)T$, and

$$\lim_{\delta \rightarrow 0} \lim_{\varepsilon \rightarrow 0} \sum_{|y-z| > \varepsilon^{-1}\delta} \pi_{t'-t}^\varepsilon(y \rightarrow z) = 0,$$

the result follows from the relation

$$\lim_{\delta \rightarrow 0} \lim_{\varepsilon \rightarrow 0} \sup_{|y| \leq \varepsilon^{-1}L} \sum_{|y-z| < \varepsilon^{-1}\delta} \pi_{t'-t}^\varepsilon(y \rightarrow z) |\langle p(1, z) \rangle_{t'}^\varepsilon - \langle p(1, y) \rangle_t^\varepsilon| = 0,$$

which is a consequence of the previous result for equal times.

Remark 2.3. As a consequence of Propositions 2.1 and 2.2 one can find a continuous extension to R^k of $\langle p(k, x) \rangle_t^\varepsilon$, $p_k^\varepsilon(x, t)$ such that the family of functions $p_k^\varepsilon(\varepsilon x, t)$ is uniformly bounded and equicontinuous in any bounded set.

Section 3

If $\rho_t(r)$ denotes the solution of (1.7), then

$$\rho^* = \sup_{r,t} \rho_t(r) < \infty, \tag{3.1a}$$

as a consequence of the assumption $\sup \rho_0(r) < \infty$ (see [3]). From now on we assume that the constant c_0 of (1.5) is such that

$$c_0 > \rho^*. \tag{3.1b}$$

The proof of Theorem 1.2 is a corollary of Proposition 3.1 below.

Proposition 3.1. *Let $\rho(r)$ be as in Definition 1.1, and let μ^ε be any family of probabilities such that (i) and (ii) below hold:*

(i) *For any $L > 0$, $k \geq 1$,*

$$\lim_{\varepsilon \rightarrow 0} \sup^{(L)} \left| \mu^\varepsilon[p(k, x)] - \prod_{l=1}^k \rho(\varepsilon x_l) \right| = 0 \tag{3.2}$$

where $x = (x_1, \dots, x_k)$, $\sup^{(L)}$ is the sup over all $x \in \mathbb{Z}^k$ such that $|x_i| \leq \varepsilon^{-1}L$ and $x_i \neq x_j$ whenever $i \neq j$;

(ii) For any $k \geq 1$, $T > 0$, $0 \leq t \leq T$, $f(\varepsilon, k, t)$ exists such that

$$\lim_{\varepsilon \rightarrow 0} f(\varepsilon, k, T) = 0 \tag{3.3a}$$

and, for some $c_0 > 0$,

$$\sup \mu_i^\varepsilon[p(k, x)] \leq (c_0 e^{c t})^k + f(\varepsilon, k, T). \tag{3.3b}$$

Let $\tau > 0$ be such that

$$(1 - e^{-3\tau})3c_0 e^{c\tau} < 1 \tag{3.4}$$

where c is defined in (2.4). Then, for any $L > 0$ and $k \geq 1$,

$$\lim_{\varepsilon \rightarrow 0} \sup^{(L)} |\mu_\tau^\varepsilon[p(k, x)] - \prod_{i=1, \dots, k} \rho_\tau(\varepsilon x_i)| = 0 \tag{3.5}$$

where ρ_i solves (1.7) with initial value ρ .

Remark 3.2. Since the initial family μ^ε in Definition 1.1 satisfies condition (i) and (ii) Proposition 3.1 gives convergence to the Reaction-Diffusion equation in the first time interval $(0, \tau]$, where τ is a fixed number satisfying 3.4. We now want to iterate our procedure. Condition (i) of Proposition 3.1 holds for the initial measure μ_τ^ε as well, because of (3.5), but condition (3.3b) holds with c_0 changed into $c_0 e^{c\tau}$, which would give a smaller interval. In the next lemma we prove that, because of inequality (3.1), condition (3.3b) holds for μ_τ^ε with the same constant c_0 and perhaps a different function f .

Lemma 3.3. Let ν^ε be a family of probability measures satisfying (i) of Proposition 3.1 and the following condition. For any $k \geq 1$ and $T > 0$, two positive functions $d(t)$ and $g(\varepsilon, k, t)$ exist, nondecreasing in t and such that

$$\sup_x \nu_i^\varepsilon[p(k, x)] \leq (d(t))^k + g(\varepsilon, K, T), \quad t \leq T, \tag{3.6a}$$

$$\lim_{\varepsilon \rightarrow 0} g(\varepsilon, k, T) = 0. \tag{3.6b}$$

Then for ν^ε inequality (3.3b) holds for some f which satisfies relation (3.3a).

Proof. We proceed like in the proof of Proposition 2.1. We therefore get

$$\begin{aligned} \langle p(k, x) \rangle_i^\varepsilon &\leq \sum_{L \geq 0} \sum_{n=0, \dots, k} (t^n/n!) c^n k^n \pi^\varepsilon(\sup | \varepsilon x_i |(\varepsilon)[L, L+1]) \\ &\quad \times \min\{d(t)^{k-n}, [\rho^{*k-n} + h(\varepsilon, k, L)]\} + h^*(\varepsilon, k, t) \end{aligned} \tag{3.7}$$

for suitable h and h^* , as we are going to explain below.

The index n in (3.7) counts the number of iterations of the “integration by parts formula” (2.2). π^ε denotes the law of k independent random walks speeded up by

ε^{-2} . After n iterations we are left with a polynomial of degree $k - n$, cf. the proof of Proposition 2.1. We then use either (i) or (3.6a) according to which gives the better estimate and we get the term with the min in (3.7), for suitable $h(\varepsilon, k, L)$ (which is infinitesimal in ε). The contribution of the cases when more particles are at the same site is taken into account by h^* , which is also infinitesimal with ε , as in the proof of Proposition 2.1.

Since the sum of L is uniformly convergent in ε , by Lebesgue theorem the Lemma is proven.

Proof of Proposition 3.1. The proof of (3.5) goes as follows. By Proposition 2.2 and Remark 2.3 we can choose a subsequence ε_n such that for any $k, (r_1, \dots, r_k) \in \mathbb{R}^k, t \in [0, \tau]$, the limit of $\langle p(k; [\varepsilon^{-1}r_1], \dots, [\varepsilon^{-1}r_k]) \rangle_t^\varepsilon$ exists along the given subsequence and we call it $\vee(k, r_1, \dots, r_k, t)$. Now choose any $k \geq 1, (x_1, \dots, x_k) \in \mathbb{Z}^k$ and $t \leq \tau$. We use the integration by parts formula for the semigroup U_s^ε w.r.t. $\vee_s^\varepsilon e^{-3ks}$ where k is the same k as above and \vee_s^ε is the semigroup generated by $\varepsilon^{-2}L_0$ (see (1.1a)). The extra factor e^{-3ks} will be useful for controlling the combinatorics involved in the iteration of the formula. We have

$$\begin{aligned} \langle p(k, x) \rangle_t^\varepsilon &= e^{3kt} \sum_z \pi_i^\varepsilon(x \rightarrow z) \langle p(k, z) \rangle_0^\varepsilon + \int ds 3k e^{-3ks} \\ &\quad \times \left\{ \sum \pi_i^\varepsilon(x \rightarrow x) \mathbf{1}(z_i \neq z_j \forall i \neq j) k^{-1} \sum_{i=1, \dots, k} 3^{-1} \sum_{\beta \in \{-1, 0, 1\}} d(\beta) \right. \\ &\quad \left. \times \langle p(k + h(\beta)); z_1, \dots, z_k, z_i^{h(\beta)} \rangle_{t-s}^\varepsilon \right\} + R(\varepsilon; x; t) \end{aligned} \tag{3.8}$$

where $\pi_i^\varepsilon(x \rightarrow z)$ is the probability that k independent standard random walks starting from x are at z at time $\varepsilon^{-2}t$;

$$d(\beta) = \beta + 3 \mathbf{1}\{\beta = 0\}, \tag{3.9}$$

$$h(\pm 1) = \text{degree } q_\pm - 1, \tag{3.10a}$$

$$h(0) = 0, \tag{3.10b}$$

$z_i^{h(\beta)}$ is z_i repeated $h(\beta)$ times.

R is the remaining contribution, which, by (3.3), is such that

$$\limsup_{\varepsilon \rightarrow 0} \sup_x \sup_{t \leq \tau} R(\varepsilon; x; t) = 0.$$

(We have used that the probability that two random walks are at the same site after time $\varepsilon^{-2}s$ goes like $\varepsilon s^{-1/2}$.)

We shall now take the limit when $\varepsilon \rightarrow 0$ along the subsequence chosen at the beginning of the proof. So we get, by Lebesgue's dominated convergence (which

can be applied because of (3.3))

$$\begin{aligned} V(k, r_1, \dots, r_k; t) &= e^{-3kt} \int \pi_t(db_1 \cdots db_k) V(k, r_1, \dots, r_k; 0) \\ &+ \int ds 3k e^{-3ks} \int \pi_s(db_1 \cdots db_k) \frac{1}{k} \sum_i \frac{1}{3} \sum_{\beta} d(\beta) \\ &\times V(k+h(\beta); r_1, \dots, r_k, r_i^{h(\beta)}; s) \end{aligned} \quad (3.11)$$

where $b_1 \cdots b_k$ are independent standard Brownian motions starting respectively from r_1, \dots, r_k and π_t is their law at time t . (3.5) will be obtained by iteration of (3.11).

We notice that (3.11) has a nice probabilistic interpretation in terms of branching processes, as observed in [5]. Such interpretation is closely connected to the approach of McKean (cf. [18] and [4]), who in fact introduced branching processes to study the travelling wave solutions of some Reaction-Diffusion equations.

The r.h.s of (3.11) can be thought of as the expectation w.r.t. the following branching process: k independent Brownian motions start from r_1, \dots, r_k , and each one, after an exponential time of mean 1, branches. A value of $\beta \in \{-1, 0, 1\}$ is then chosen with probability $\frac{1}{3}$, and $h(\beta)$ indicates how many new particles are generated. Such new particles are created at the same place where the generating particle was.

Denote by $dP[\mathbf{b}(1) \cdots \mathbf{b}(k), \mathbf{t}(1) \cdots \mathbf{t}(k), \boldsymbol{\beta}(1) \cdots \boldsymbol{\beta}(k)]$ the law of such branching, where $\mathbf{t}(i)$ is the collection of branching times for the descendants of particle i , $\boldsymbol{\beta}(i)$ are the corresponding branching parameters and $\mathbf{b}(i, s)$ the positions of the particles of the i -th family at time s . Obviously the law of V factorizes w.r.t. the different families of branching.

By iterating (3.11) and letting N_t = the total number of branching times before t , we have, for any finite M ,

$$\begin{aligned} &V(k, r_1, \dots, r_k; t) \\ &= \sum \int_{n \leq M} dP[\mathbf{b}(1) \cdots \mathbf{b}(k), \mathbf{t}(1) \cdots \mathbf{t}(k), \boldsymbol{\beta}(k)] 1\{N_t = n\} \\ &\quad \times \prod_{i=1, \dots, k} [\Pi^{(i)} d(\boldsymbol{\beta}_j(i))] F(\mathbf{b}(1) \cdots \mathbf{b}(k), \mathbf{t}(1) \cdots \mathbf{t}(k), \boldsymbol{\beta}(1) \cdots \boldsymbol{\beta}(k)) \\ &\quad + R(M, k, r_1, \dots, r_k; t) \end{aligned} \quad (3.12)$$

where $\Pi^{(i)}$ is the product over all $\beta_j(i)$ for j such that $t_j(i) \leq t$.

$F(\mathbf{b}(1) \cdots \mathbf{b}(k), \mathbf{t}(1) \cdots \mathbf{t}(k), \boldsymbol{\beta}(1) \cdots \boldsymbol{\beta}(k))$ is a product of $\rho(\cdot)$ (remind that by (3.1), $V(k, r_1, \dots, r_k; 0) = \Pi \rho(r_i)$) which contains at most

$$k + [\text{degree } q_- - 1]M \quad (3.13)$$

factors. $R(M, k, r_1, \dots, r_k; t)$ takes into account the remainder. Such last term can be bounded as follows

$$R(M, k, r_1, \dots, r_k; t) < P[N_t \geq M] [c_0 e^{\alpha t}] \{k + [\text{degree } q_- - 1](M + 1)\}. \quad (3.14)$$

Since (cf. (A.21) of [5])

$$P[N_t \geq M] \leq d[1 - e^{-3t}]^M k M^{k/2-1} \quad (3.15)$$

where k is the initial number of particles and d is a suitable constant, the remainder term vanishes when $M \rightarrow \infty$ if $t \leq \tau$. Furthermore the corresponding series in (3.12) is absolutely convergent. As a consequence, since everything factorizes,

$$V(k; r_1, \dots, r_k; t) = \prod V(1; r_i; t),$$

hence (3.12) for $V(1; r; t)$ is the Reaction-Diffusion equation (1.7) in integral form. We have therefore proven (3.5).

Section 4

Convergence to macroscopic equations is just a first step. The long time behaviour is the next one, the question being how much about it can be inferred from the macroscopic equations. For instance are stability or instability of the microscopic orbits consequence of the corresponding properties of the macroscopic equations? A step in this direction, as proposed in [5], comes from the analysis of the covariance structure of the density fluctuation fields. The density fluctuation fields $Y_\tau^\varepsilon(\psi)$ are defined, as the “fluctuations” of the density fields $X_\tau^\varepsilon(\psi)$, cf. (1.9), namely

$$Y_\tau^\varepsilon(\psi) = \sqrt{\varepsilon} \sum \psi(\varepsilon x) (\eta(x, t) - \langle \eta(x, t) \rangle^\varepsilon) \quad (4.1)$$

where $\psi \in \mathcal{S}(\mathbb{R})$ and $\langle \cdot \rangle^\varepsilon$ is the average w.r.t. the process with generator L^ε .

The covariance of $Y_\tau^\varepsilon(\psi)$ is a natural estimate for the stability of the deterministic orbits. On the other hand, in the limit when $\varepsilon \rightarrow 0$ if the limiting law of the fluctuation fields converges to a generalized Ornstein-Uhlenbeck process, then it is believed in such case that it is possible to relate at least to some extent the parameters of the O.U. to those entering in the macroscopic equations, more precisely to its linearization, as predicted by the Fluctuations Dissipation theorem.

We believe that the techniques introduced in Sections 2 and 3 can be modified to deal with such problems as we hope to report in a future paper.

The analysis of the fluctuation fields is in a sense a linear theory, it studies small fluctuations around the deterministic equation which are, supposedly, governed by the linearized macroscopic equation.

In [7] a case was studied in which the macroscopic profile is stationary but not stable. It was then proved that after an initial time layer $T(\varepsilon)$ (which suitably diverges with ε) the state of the system becomes (close to) a nontrivial superposition of the extremal equilibrium states (for the free generator) and the law of the mixture is a statistical solution of the macroscopic equation. Several restrictions of technical origin had to be imposed in [7] among them the assumption that the system was in a macroscopically bounded region.

Presumably the models considered here are simpler to treat and for them it is conceivably possible to improve the results in [7], at least this has been one of the motivations for our analysis.

In Definition 1.1 we have considered models with only one species of particles. More naturally, in chemical reaction equations, one has several species and conservation laws, for instance when one particle of a species dies a particle of another is created. If different species have different mechanical properties the situation gets quite complicated.

The techniques we used so far are inadequate: the analysis of Section 3 goes through, what we miss are the a priori estimates of Section 2, which were based on bounding the birth with the death intensity.

We describe below two models whose kinetic continuum limit should yield the Carleman and the Broadwell equations respectively. These are Boltzmann equations with discrete velocities, hence, such result confirms that the continuum limit we are considering in this paper is in a sense a “kinetic continuum limit”.

Before introducing the models we briefly sketch their main features. We start with the one related to the Carleman equation, the other will be discussed only briefly. We consider two types of particles, distinguished by a spin which has values ± 1 . Particles move in \mathbb{Z} in a way which depends on their spins. Spin = +1 simulates particles with velocity +1, in fact particles with spin +1 after an exponential time of mean 1 jump to their right. Particles with spin -1 jump with the same intensity to their left (\approx negative velocity). Such process, whose generator is denoted by L_0 (warning: we are using the same symbols as before, but in the present context they have different meanings) is speeded up by a factor ε^{-1} (and not ε^{-2} because here we have a drift and not a diffusion). Furthermore the spin of a particle can change, the intensity for such event is proportional to the number of pairs of particles with the *same spin* sitting at the same site.

Let $L^\varepsilon = \varepsilon^{-1}L_0 + L_G$ be the corresponding generator. The initial measure is a family, μ^ε , $\varepsilon > 0$, of product measures on $N^{\mathbb{Z}} \times N^{\mathbb{Z}}$ such that, for all $r \in \mathbb{R}$,

$$\lim \mu^\varepsilon[\eta_\pm([\varepsilon^{-1}r])] = \rho_\pm(r) \quad (4.2)$$

where ρ_\pm are C^2 nonnegative uniformly bounded functions. As in Definition 1.1 we also assume that there exists $c_0 < \infty$ so that for all k and x_1, \dots, x_k mutually distinct

$$\mu^\varepsilon \left[\prod_{i=1, \dots, k} \eta(x_i) \right] \leq c_0^k. \quad (4.3)$$

We then have the following.

Conjecture 4.2. *Let L^ε and μ^ε be as above. Then for any $r \in \mathbb{R}$ and $t > 0$*

$$\lim \mu_t^\varepsilon[\eta_\pm([\varepsilon^{-1}r])] = \rho_\pm(r) \quad (4.4)$$

where

$$\partial_t \rho_\pm \pm \partial_r \rho_\pm = -(\rho_\pm^2 - \rho^2), \quad \rho_\pm(r, 0) = \rho_\pm(r). \quad (4.5)$$

The Carleman equation has been studied in the “hydrodynamical limit” by Kurtz [14], McKean [19], and Palczewski [22]. That is, one considers (4.7) with a parameter ε^{-1} which multiplies $\partial_r \rho_{\pm}$ and ε^{-2} in front of the collision term $-(\rho_{\pm}^2 - \rho^2)$. In the limit when $\varepsilon \rightarrow 0$ it is proven that $\rho_+ = \rho_- = \rho$ and that ρ solves the diffusion equation:

$$\partial_t \rho = 1/2 \partial_r (1/\rho \partial_r \rho). \quad (4.6)$$

We think it would be very interesting to obtain such limiting behaviour directly from the original microscopic system.

The particle system leading to the Broadwell equation is analogous to the previous one: we only give a brief description of it. We have four component spins corresponding to four velocities. Particles move in \mathbb{Z}^2 and they jump up or down, left or right according to their spin (hence hereafter called velocity) with exponential waiting times of mean 1. Such processes are speeded up by ε^{-1} as in the Carleman model.

Particles with horizontal velocities (say positive along the x -axis) and at a given site may change velocity which then becomes vertical (up or down with equal probability) with intensity proportional to the number of particles at that site which have negative horizontal velocity. Such process simulates elastic collisions between particles and leads in the macroscopic equation to that part of the collision kernel which contains the product of the local densities of particles with opposite horizontal velocity. Collisions among particles with opposite vertical velocities are defined analogously.

The interesting point in the Broadwell case is that the limiting hydrodynamical equation has still an Euler structure in contrast to what happens for the Carleman equation.

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