

Microscopic Models of Hydrodynamic Behavior

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We review recent developments in the rigorous derivation of hydrodynamic-type macroscopic equations from simple microscopic models: continuous time stochastic cellular automata. The deterministic evolution of hydrodynamic variables emerges as the "law of large numbers," which holds with probability one in the limit in which the ratio of the microscopic to the macroscopic spatial and temporal scales go to zero. We also study fluctuations in the microscopic system about the solution of the macroscopic equations. These can lead, in cases where the latter exhibit instabilities, to complete divergence in behavior between the two at long macroscopic times. Examples include Burgers' equation with shocks and diffusion-reaction equations with traveling fronts.

KEY WORDS: Stochastic particle systems; hydrodynamic limit; fluctuation theory.

1. INTRODUCTION

Nature has a hierarchical structure and to a great extent it is possible, even necessary, to study different levels independently. For the world of atoms and molecules, the nuclei are point charges despite the complicated dynamics of the hadrons, and the hydrodynamic equations for fluids, the elucidation of which is the subject of this article, were established long before the atomistic structure of matter was fully accepted. Indeed, hydrodynamicists can be (and sometimes are) quite ignorant of atomic theory and of statistical mechanics.

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The different levels are of course not completely isolated—there is no sharp demarcation line between an atomic beam and the jet stream. In fact, one of the basic dogmas of science is that the behavior at any level can be deduced, at least in principle, entirely from the dynamics of the level below it, i.e., there are no new physical laws, only new phenomena, as one goes from atoms to fluids. The apparent independence is due to the really remarkable fact that the microscopic dynamics give rise to approximate, but in most cases extremely accurate, autonomous macroscopic laws. The main physical motivation for elucidating the micro–macro connection comes therefore from situations where the hydrodynamic laws fail, partially or entirely, to describe all the phenomena of interest.

These laws generally take the form of nonlinear partial differential equations,

$$\frac{\partial}{\partial t} \mathbf{M}(\mathbf{r}, t) = \mathbf{F}(\mathbf{M}(\mathbf{r}, t), \text{grad } \mathbf{M}(\mathbf{r}, t), \dots) \quad (1.1)$$

where $\mathbf{M}(\mathbf{r}, t)$ denotes a “full” set of macroscopic variables depending on space and time. Examples include the heat equation and the Euler and Navier–Stokes equations. While \mathbf{M} and \mathbf{F} are specific to the phenomena considered, their dependence on the nature of the microscopic constituents of the macroscopic objects studied is in general small. Thus, Fourier’s law of heat conduction has the same form for solid gold and liquid water and the same Navier–Stokes equations describe the flow of air and the flow of milk. Even more remarkable, diffusion–reaction equations of similar form can describe both chemically reacting molecular mixtures and the propagation of genetic traits.⁽¹⁾ The details of microscopic structure generally enter in \mathbf{F} only through the numerical value of some parameters, e.g., heat conductivity, viscosity.

The origin of the hydrodynamic laws is a consequence of the existence of very different spatial and temporal scales for microscopic and macroscopic phenomena and some very general features of the microscopic dynamics. Chief among these are the approximate locality and additivity of the interactions and the resulting local conservation laws. Consequently, our microscopic models can be rather crude, even blatantly wrong, and still give rise to correct macroscopic behavior. All that is necessary is that the models contain the essential features responsible for the phenomena of interest.

The utility of simple models is well established for equilibrium behavior. The Ising spin system is used successfully to model such diverse phenomena as liquid–vapor transitions, phase segregation (or ordering) in alloys, or spontaneous magnetization in anisotropic magnets.

There are at present no such universal Ising models for hydrodynamic laws. This is due in part to the fact that the phenomena are more complicated, so that even the solutions of the macroscopic equations are far from being clearly understood in interesting cases. This makes the analysis of models to give laws of type (1.1) much more difficult mathematically. Nevertheless the recent advances in the ability of computers to implement microscopic dynamics for “large” numbers of particles has shown dramatically how similar indeed are self-organized macroscopic evolutions resulting from very different microscopic models—including Ising-like cellular automata.⁴

While there is no rigorous derivation of fluid dynamical equations even for the simple lattice gas automaton of Frisch *et al.*⁽³⁾ there has been much recent progress in the derivation of hydrodynamic-type laws of form (1.1) for models with stochastic dynamics. We believe that these models capture the essential features of the transition from microscopic to macroscopic evolutions in real physical systems. It is our purpose here to describe some of these results, particularly those that shed light on behavior beyond that contained in the macroscopic equations, in a non-technical way. (It is also possible to make these models entirely deterministic, albeit in a rather artificial way. We shall not discuss this here.)

Before discussing specific models, we describe some of the general ideas and methods used in obtaining the macroscopic equations and going beyond them. We focus attention on the fact that deterministic equations like (1.1) correspond to the “law of large numbers” in the theory of probability—they are obeyed with probability approaching one (with respect to a given dynamics and initial ensemble) as the ratio of microscopic to macroscopic spatial and temporal scales goes to zero. When the ratio is finite there will be deviations. These will usually be small, but may become large in interesting cases.

1.1. The Formulation of Macroscopic Laws

The essential element in the transition from microscopic to macroscopic evolution is best formulated mathematically in terms of suitable rescalings of space and time.^(4,5) By such rescalings one can take account in a precise way of the central fact that there are a very large number of atoms in a macroscopic drop of fluid, each undergoing a very large number of “changes” (e.g., collisions) in a macroscopic instant “*dt*.” The macroscopic view is therefore a “blurred” one: summing over a large

⁴ Access to the rapidly growing literature can be had via the August 1987 issue of *Complex Systems*.⁽²⁾

number of elementary events. This brings in the "law of large numbers," which is crucial for obtaining deterministic autonomous macroscopic equations like (1.1), *not just for ensemble averages*, but for the *almost sure value* of quantities that fluctuate on the microscopic scale, i.e., the macroscopic equations describe the actual evolution of single configurations of the physical system.

This is not just a mathematical nicety; it goes to the heart of what the hydrodynamic equations are all about. In particular, the phenomena of bifurcations and the presence of multiple stationary states might be missed entirely if one only looks at ensemble averages. We have here a close correspondence to the situation at phase transitions in equilibrium systems,⁽⁶⁻⁸⁾ where it is well established that ensemble averages may not represent any actual realization of the system. For example, the state of zero magnetization of an Ising system below the critical temperature, obtained with periodic boundary conditions, is really a superposition of the pure phases with magnetizations $\pm m^*$, $m^* \neq 0$, e.g., the magnetization/volume has a double-humped distribution sharply peaked at $\pm m^*$. In a similar way an ensemble average in the Rayleigh-Benard problem may yield a zero velocity field that really corresponds to a superposition of different states with rolls. Also, in Burgers' equation, which we shall discuss later, an ensemble average may superimpose shocks with different locations giving an apparent broadening not present in actual configurations of the system.

Even aside from phase transitions, it is clearly important to have convergence on a configuration basis if the deterministic equations are to describe what is actually observed in an experiment. If the difference between actual and average behavior is overlooked, one might also come to the erroneous conclusion that the origin of macroscopic phenomena, such as diffusion, is directly attributable to the highly irregular behavior of trajectories of nonlinear dynamical systems. This behavior, which occurs already in systems with a *few* degrees of freedom, may in fact be important for the validity of the hydrodynamic laws; it does not, however, by itself have any intrinsic mechanism for suppression of fluctuations. Thus, the ensemble average of the spatial density of three hard spheres in a cube will approach a uniform value, but the actual behavior of any initial configuration will not be described by the kind of deterministic equation associated with macroscopic variables discussed here.

We can illustrate some aspects of the micro-macro relation by considering the simplest example of independent, identically distributed random variables x_1, x_2, \dots . Let $\varphi(x_i)$ be the distribution of x_i , with $m = \langle x_i \rangle$ its mean and $\sigma^2 = \langle (x_i - m)^2 \rangle$ its variance. Suppose now that we can only

see or are only interested in the effect produced by a sum of many such variables. The law of large numbers then asserts that the random variable

$$X_N = \frac{1}{N} \sum_{i=1}^N x_i \tag{1.2}$$

takes the value m , with probability approaching one, as $N \rightarrow \infty$, i.e., in the macroscopic limit we have deterministic behavior. To see the deviation in the value of X_N from m for N very large, we have to magnify the scale on which we are looking. This can be done by considering the fluctuation variable

$$\xi_N = N^{1/2} [X_N - m] = N^{-1/2} \sum_{i=1}^N (x_i - m) \tag{1.3}$$

Then, as $N \rightarrow \infty$, ξ_N tends to a Gaussian *random variable* ξ with mean zero and variance σ^2 . We thus have here both a deterministic behavior and fluctuations about it which depend very little on the details of the microscopic distribution $\varphi(x)$. We did not even have to say whether x is continuous or discrete.

A crucial step in going from this zero-dimensional example to equations determining the space-time evolutions of macroscopic variables is that the microscopic dynamics produces “local equilibrium” states parametrized by the instantaneous values of the slowly varying fields $\mathbf{M}(\mathbf{r}, t)$. These local distributions will naturally also produce fluctuations about the $\mathbf{M}(\mathbf{r}, t)$. As long as these fluctuations remain small, they can be “added to \mathbf{M} ” and will evolve according to the linearization of (1.1) about a given solution $\mathbf{M}(\mathbf{r}, t)$ with a “random source term” (Section 6). In fact, such fluctuations are often added in a purely heuristic way to the macroscopic equations⁽⁹⁾—we justify them in some cases. In particular, when the solutions of (1.1) are smooth and stable the fluctuations are Gaussian fields whose covariance does not grow with time. In those cases, however, where the hydrodynamic equations produce shock waves or have other instabilities these fluctuations get amplified. This leads, then, to significant deviations between the actual behavior of the system and that predicted by (1.1) over “long” times. These are the physically interesting situations on which we focus in this very selective review.

The outline of the rest of this article is as follows: In Section 2 we give the simplest example of a microscopic dynamics, independent asymmetric jumps on a lattice, which leads to a (linear) equation of type (1.1) for the density. Interactions are introduced in Section 3 by imposing a hard core exclusion. This leads to Burgers’ equation, which can give rise to the

formation of shocks. The stability of these shocks is analyzed from the microscopic model. We present arguments that show that the shock remains sharp on the microscopic scale, with the exact location of the interface, however, undergoing a random walk. This is in contrast to the independent case, where an initially sharp interface is smeared out in the course of time.

In Section 4 we discuss the case of jumps with a small bias. We then obtain Burgers' equation with viscosity—in the proper scaling. Section 5 describes microscopic models in which the particle number is not strictly conserved, but can vary “slowly.” These models lead to diffusion–reaction-type equations. For certain initial conditions these evolve to configurations having traveling fronts with speeds $c \geq c^* > 0$: the microscopic significance of the minimal speed c^* is given. The general theory of fluctuations in these microscopic model systems is discussed in Section 6 and applied to the long-time dynamics of shocks and traveling fronts. Finally, some concluding remarks are made in Section 7.

2. LATTICE GASES WITH STOCHASTIC DYNAMICS

As mentioned in the introduction, there has been much progress in recent years in deriving hydrodynamic equations for systems whose microscopic dynamics involves some stochastic elements, e.g., particles on a lattice with stochastic dynamics. These systems have a single locally conserved field—the (mass) density. The stochastic dynamics maintains locally an equilibrium distribution characterized by a density $\rho(\mathbf{r}, t)$. This density varies on a macroscopic scale and its time evolution is governed by a partial differential equation of the form (1.1) with conservation,

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) + \text{div } \mathbf{j}(\rho(\mathbf{r}, t), \text{grad } \rho(\mathbf{r}, t)) = 0 \quad (2.1)$$

To understand how such a deterministic macroscopic equation arises from the dynamics of many particles, we discuss first a simple example. We consider a system of particles on a one-dimensional lattice with lattice spacing a , a being a microscopic length, say a few angstroms. The particles jump independently with rate p/τ to the right and $(1-p)/\tau$ to the left, $0 \leq p \leq 1$, τ a typical microscopic time. The system has a continuum of stationary states “labeled” by the average number of particles per site, $\rho \geq 0$. In each steady state the number of particles n at a given site has the Poisson distribution $(1/n!) \rho^n e^{-\rho}$ and the numbers of particles at different lattice sites are independent of each other. The average current across any bond in the steady state is $j(\rho) = (a/\tau)(2p - 1) \rho$.

Now let us assume that at some initial time $t=0$ our system has a nonuniform density, which, however, varies slowly on the microscopic scale, i.e., over many lattice spacings the density is essentially constant. We make this notion of slow variation precise by choosing some smooth function $\rho_0(q)$, $\rho_0(q) \geq 0$, and assuming that, as in the stationary state, each site has at time $t=0$ an independent Poisson distribution, with the average number of particles on the j th lattice site given by

$$\rho_0^\varepsilon(j) = \rho_0(\varepsilon j) \tag{2.2}$$

$j \in aZ$, the lattice with spacing a . Clearly the density gradient, measured on the microscopic scale (units of a), is of order ε and vanishes as $\varepsilon \rightarrow 0$. The macroscopic density profile $\rho_0(q)$, on the other hand, has some finite slope in general.

Because locally the density of particles is almost stationary in time, many jumps are needed to produce appreciable changes. In fact, for the asymmetric case $p \neq 1/2$ the time needed is of order $\varepsilon^{-1}\tau$. The scale appropriate for the phenomenon is then the *macroscopic* scale: space and time units in which the lattice spacing is εa and the mean jump time $\varepsilon\tau$. Since particles move independently, the *average* density is clearly governed by the *linear* equation

$$\begin{aligned} \frac{\partial}{\partial t} \rho^\varepsilon(q, t) = & \frac{1}{\varepsilon\tau} \{ p[\rho^\varepsilon(q - \varepsilon a, t) - \rho^\varepsilon(q, t)] \\ & + (1 - p)[\rho^\varepsilon(q + \varepsilon a, t) - \rho^\varepsilon(q, t)] \} \end{aligned} \tag{2.3}$$

where $q \in (\varepsilon a)Z$. In the limit $\varepsilon \rightarrow 0$ any smooth interpolation of $\rho^\varepsilon(q, t)$ converges to the solution of the macroscopic continuum equation

$$\frac{\partial}{\partial t} \rho(q, t) + \frac{a}{\tau} (2p - 1) \frac{\partial}{\partial q} \rho(q, t) = 0 \tag{2.4}$$

which is to be solved with the initial condition $\rho(q, 0) = \rho_0(q)$.

This is not the whole story. Let $n^\varepsilon([q, q + \delta], t)$ be the actual number of particles at time t in the (macroscopic) interval $[q, q + \delta]$ containing $\delta/\varepsilon a$ lattice sites. The actual density is therefore $n^\varepsilon([q, q + \delta], t)/(\delta/\varepsilon a)$, which is of course a random variable. What happens now as $\varepsilon \rightarrow 0$ is that this random variable converges with probability one to the number

$$\frac{1}{\delta} \int_q^{q+\delta} dq' \rho(q', t) \tag{2.5}$$

where $\rho(q, t)$ is the solution of (2.4). This is the famous law of large numbers already alluded to in the Introduction. If it did not hold, the

macroscopic equation would in fact be quite useless. After all, in a hydrodynamic experiment we follow just one particular fluid flow. To put it somewhat differently: Suppose that we produce a Monte Carlo simulation of the lattice gas dynamics by means of a computer. Then a *single* run follows the macroscopic equation, with probability approaching one, as we make the lattice finer and finer.⁽⁵⁾

We may even go one step further and sample the distribution of particles at the (macroscopic) time t at a set of lattice sites next to some point q . We find that for all ε the distributions at different sites are independent Poisson with densities that, in the limit $\varepsilon \rightarrow 0$, become equal to the density $\rho(q, t)$, characteristic of this local equilibrium. To be more precise, the joint distribution of particles at any fixed set of lattice sites $\{\varepsilon^{-1}q + j_1, \dots, \varepsilon^{-1}q + j_m\}$ is, in the limit $\varepsilon \rightarrow 0$, the same as in a uniform equilibrium system with average density $\rho = \rho(q, t)$.

The reader might find the introduction of the parameter ε fairly artificial. It should be regarded just as a mathematically convenient device to separate the microscopic and macroscopic scales. In the limit $\varepsilon \rightarrow 0$ the separation is perfect. For a real fluid we should think of ε as the magnitude of typical fractional changes of the density or velocity on the scale of intermolecular distances. So ε is small, but not strictly zero. By how much the limit $\varepsilon \rightarrow 0$ is an overidealization depends on the particular situation and we will discuss later possibly large corrections to the deterministic hydrodynamic equations that arise when $\varepsilon \neq 0$, i.e., due to the graininess of matter.

3. THE BURGERS EQUATION AND THE PROPAGATION OF SHOCKS

The linearity of Eq. (2.4) comes from the absence of any interaction between the particles in our model. Let us now introduce a very simple interaction: we require that there can be at most one particle per lattice site. The dynamics is as before, except that when a particle tries to jump to a site that is already occupied, it just does not. The analysis of the model is difficult, because the hard core exclusion produces dynamic correlations. Fortunately, the steady states are still simple: At each site, independently of the others, there is a particle with probability ρ and no particle with probability $1 - \rho$, ρ the same at all sites. As in the case of independent particles, there is a one-parameter family of steady states, one for each ρ , $0 \leq \rho \leq 1$, $\rho = 1$ being the maximal number of particles per site. The steady-state particle current is now

$$j(\rho) = (a/\tau) p\rho(1 - \rho) - (a/\tau)(1 - p)\rho(1 - \rho) = (a/\tau)(2p - 1)\rho(1 - \rho) \quad (3.1)$$

This suggests that the appropriate macroscopic equation is

$$\frac{\partial}{\partial t} \rho(q, t) + \frac{a}{\tau} (2p - 1) \frac{\partial}{\partial q} \{ \rho(q, t) [1 - \rho(q, t)] \} = 0 \quad (3.2)$$

which is the well-known Burgers equation with zero viscosity.⁽¹⁰⁾ Indeed, it has been proven that, under the same scaling as before (lattice spacing ϵa , average jump time $\epsilon \tau$), the actual density of particles converges to the solution of Burgers' equation.⁽¹¹⁻¹³⁾

Burgers' equation is a textbook example for shock formation. Even with smooth initial data, the solution may develop discontinuities in the course of time due to the fact that the "velocity" of a fluid element, $j(\rho)/\rho = (a/\tau)(2p - 1)(1 - \rho)$, decreases with density. Solving the equation, one finds that the motion of the shock is determined only if the Burgers equation is supplemented with the condition that the entropy has to increase. This agrees with the solution obtained by first adding a viscosity term $v \partial^2 \rho(q, t) / \partial q^2$ on the right side of (3.2) and then considering the solution when $v \rightarrow 0$. There is of course no room for such extra conditions in our microscopic model—the dynamics of particles is sufficient now to produce a unique evolution. In fact, the theorem mentioned asserts that as $\epsilon \rightarrow 0$, the convergence of the actual particle density is to the "right" solution, namely the one satisfying the entropy condition.

The shock formation has a disturbing aspect: the Burgers equation itself tells us that our basic assumption of slow variation breaks down completely along the exceptional space-time curves where there is a discontinuity in the density. For sure, the density at the shock does not vary slowly. To understand what happens *at the shock* we have to study finer, more microscopic structural details of the lattice gas; Burgers' equation itself is too crude a description of the phenomenon.

We might as well then impose a "pure" shock initially by setting

$$\rho_0(q) = \begin{cases} \rho_- & \text{for } q < 0 \\ \rho_+ & \text{for } q > 0 \end{cases} \quad (3.3)$$

with $0 \leq \rho_- < \rho_+ \leq 1$. If $p < 1/2$, then the shock spreads out linearly in a rarefaction fan. On the other hand, if $p > 1/2$, i.e., drift to the right, the sharp shock is maintained and travels with velocity

$$v_s = \frac{a}{\tau} (2p - 1)(1 - \rho_- - \rho_+) \quad (3.4)$$

as required by mass conservation. To the left of $v_s t$ the density is ρ_- and to the right of $v_s t$ it is ρ_+ . In the limit $\epsilon \rightarrow 0$, this is also the evolution of the

particle model on the *macroscopic* scale of length and time. Note that, because of piling up, v_s may be negative, although particles are pushed to the right.

In order to understand the shock dynamics on a *microscopic* scale when $\varepsilon \neq 0$ it is useful to first have a look at the independent particle model with the same step initial condition (3.3). Solving Eq. (2.3), we obtain approximately an error function which interpolates between ρ_- and ρ_+ , has center at $(a/\tau)(2p-1)$, and has a typical width $a(et/\tau)^{1/2}$. Therefore, on the time scale $\varepsilon^{-1}\tau$ the shock is sharp, i.e., of the order of the lattice spacing, and travels with velocity $(a/\tau)(2p-1)$. For longer times the shock gets washed out. Near the symmetry point the statistics of particles is local equilibrium, corresponding to independent Poisson distributions, with density $(\rho_+ + \rho_-)/2$.

One may be tempted to conjecture that due to viscosity there should be a similar behavior for the model with hard core exclusion. We note, however, that in contrast to the linear case, the solution to the Burgers equation with an added viscosity term $v \partial^2 \rho(q, t) / \partial q^2$ has a shape that remains fixed for all times and travels with velocity v_s . In addition, for the lattice gas with $1 - \rho_+ - \rho_- = 0$, i.e., $v_s = 0$, one can prove^(14,15) that if one samples the statistics of particles on lattice sites around the origin, then in the long run one will find half of the time the density ρ_+ and half of the time the density ρ_- . This is completely different from the behavior of independent particles. Apparently the discontinuity remains "sharp" even on a microscopic scale, but fluctuates back and forth in a random fashion. Numerical simulations of the lattice gas indicate a shock width of about ten lattice sites.⁽¹⁶⁾

Clearly, the issue here is to understand how the microscopic density fluctuations manifest themselves on a macroscopic scale. In a phenomenological approach, one would add *ad hoc* fluctuations to Burgers' equation. A better founded approach is the use of hydrodynamic fluctuation theory, of interest in its own right. In our case the fluctuations are dictated by the lattice gas model. Let us here just describe what fluctuating hydrodynamics predicts about the shock dynamics, postponing a more detailed analysis of fluctuations to Section 6.

The central point is that, on the time scale considered, the completely uncorrelated equilibrium fluctuations present initially just propagate deterministically according to the linearized equation. To the left of the shock these fluctuations propagate with velocity $(a/\tau)(2p-1)(1-2\rho_-)$ and to the right with velocity $(a/\tau)(2p-1)(1-2\rho_+)$. When they meet they have to satisfy mass balance. This results in an instantaneous shock velocity $v(t) = v_s + \sqrt{\varepsilon} \xi(t)$, where $\xi(t)$ is white noise with a strength depending on ρ_+ and ρ_- . Thus, the shock makes a random walk with mean square dis-

placement of order εt . To have an amplification to the macroscopic scale we have to follow the shock over a much longer time scale than considered before. Only after ε^{-2} jumps per particle is there a displacement macroscopic size. Such long times go beyond the domain of validity of the hydrodynamic fluctuation theory. *A priori*, it is not clear whether the dynamical behavior hinted at actually persists on the macroscopic scale. Nevertheless, as already mentioned, a detailed dynamical analysis proves the picture set forth to be correct, at least for particular cases. The analysis is more complete and gives the same results for a closely related model in which the macroscopic equation is Burgers' equation with viscosity. This is described in the next section.

4. WEAKLY ASYMMETRIC LATTICE GAS

We have deliberately saved the symmetric case $p = 1/2$. Equations (2.4) and (3.2) then degenerate to

$$\frac{\partial}{\partial t} \rho(q, t) = 0 \quad (4.1)$$

which tells us that after ε^{-1} jumps per particle the macroscopic density profile has not yet changed. For $p = 1/2$ the average steady-state current vanishes by symmetry, so to lowest order the current should be proportional to the density gradient (Fick's law of diffusion), i.e., of order ε . Therefore we expect to see appreciable changes in the density only after ε^{-2} jumps per particle. The macroscopic equation on the new time scale is the (generally nonlinear) diffusion equation,

$$\begin{aligned} \frac{\partial}{\partial t} \rho(q, t) + \frac{\partial}{\partial q} j(q, t) &= 0 \\ j(q, t) &= -D(\rho(q, t)) \frac{\partial}{\partial q} \rho(q, t) \end{aligned} \quad (4.2)$$

with $D(\rho)$ the bulk diffusion coefficient.

For independent particles, going back to Eq. (2.3), it is easy to verify that our reasoning is correct. On the time scale $\varepsilon^{-2}\tau$ the density is governed by the diffusion equation

$$\frac{\partial}{\partial t} \rho(q, t) = \frac{a^2}{\tau} \frac{\partial^2}{\partial q^2} \rho(q, t) \quad (4.3)$$

Because there is no interaction, D is independent of ρ . The hard core lattice gas requires a little more analysis. The net result is that the macroscopic

equation, on the time scale $\varepsilon^{-2}\tau$, is again (4.3). That D turns out to be independent of ρ for this case is due to particular cancellations. In fact, recently the *nonlinear* diffusion equation was derived for a large class of interacting stochastic particle systems,^(17,18) one of the most beautiful results in the field.

We want now to bias the lattice gas in such a way that the macroscopic equation is the Burgers equation with a viscosity term. This is very analogous to going from the Euler to the Navier–Stokes equations. Since the effect of dissipation manifests itself only on the diffusive time scale $\varepsilon^{-2}\tau$, the proper choice of microscopic dynamics is: particles jump with rate $(1 + \varepsilon\alpha)/2\tau$ to the right and with rate $(1 - \varepsilon\alpha)/2\tau$ to the left, subject to the hard core exclusion. This is called, for obvious reasons, the weakly asymmetric jump process with exclusion. It has been proven that on the macroscopic scale the density is governed by the viscous Burgers equation

$$\frac{\partial}{\partial t} \rho(q, t) + \alpha \frac{\partial}{\partial q} [\rho(q, t)(1 - \rho(q, t))] = v \frac{\partial^2}{\partial q^2} \rho(q, t) \quad (4.4)$$

with $v = a^2/\tau$. Together with the validity of (4.4), one also proves for this model the law of large numbers and the local equilibrium structure in the form already explained in Section 3.⁽¹⁹⁾

We note here that Eqs. (2.4) and (3.2) are invariant under the transformation $q \rightarrow \lambda q, t \rightarrow \lambda t$, while (4.2) and (4.3) have as their invariance group $q \rightarrow \lambda q, t \rightarrow \lambda^2 t$. This permitted the construction of particle models from which the above equations were obtained *solely* by going from the microscopic to the macroscopic scale (the appropriate scalings dictated by the invariance groups of the macroscopic equation) without any modification of the dynamics. Equation (4.4), on the other hand, does not have any such scale invariance. Consequently, its derivation from a microscopic model involved the modification of the dynamics with ε . We sometimes refer to models of this type as *kinetic-like* in contrast to *pure hydrodynamic* models in which the dynamics is independent of ε . While kinetic-like models are in some ways less satisfactory from the mathematical point of view, this is not so important physically, where ε is fixed anyway. It does indicate, however, that while one may hope to derive the Euler equations, which have the $q \rightarrow \lambda q, t \rightarrow \lambda t$ invariance, as a scaling limit, the Navier–Stokes equations, which are analogous to (4.4), must be considered as the first term in some kind of asymptotic series.

5. REACTION–DIFFUSION EQUATIONS

Propagating fronts or traveling waves are common structures, which appear also in equations not of conservation type. Some of these exhibit

interesting “velocity selection” mechanisms and various kinds of instabilities. The long-time dynamics in these systems can be expected to exhibit correspondingly varying phenomena on the microscopic level. These may be quite different from that found for the shock dynamics described by the Burgers equation. To illustrate this, we now discuss equations of the reaction–diffusion type exhibiting such structures.

One of the (many) physical examples that can be modeled by such an equation is a system in which various chemicals diffuse in an aqueous solution and react with each other. If we restrict our attention to one species, then its mass is no longer conserved. We model the diffusing particles again as a lattice gas with the constraint of single-site occupancy. No external force is driving the system. Therefore we set $p = 1/2$. In addition to particles jumping to neighboring empty sites, it is now also possible to create new particles at empty sites and annihilate particles at occupied sites. Let $c_j^+(\eta)$ be the rate for creating a particle at site j when the configuration is η . Correspondingly, let $c_j^-(\eta)$ be the rate for annihilating a particle at site j . Typically $c_j^\pm(\eta)$ will depend only on the occupancy of lattice sites in the neighborhood of j and it does so in a translation–invariant manner.

To have a meaningful scaling limit, in which there is a finite creation and destruction rate per unit volume, these rates have to be taken proportional to ε^2 on the microscopic scale, i.e., during times of the order of an average jump time the creation/annihilation per lattice site is only of the order ε^2 . This is to be compared with the weakly asymmetric lattice gas, where the corresponding coefficient was ε , since the whole process is conservative. Thus, between any two creation/annihilation events the diffusion has plenty of time to equilibrate the system *locally*. Therefore, in the macroscopic equation the (local) equilibrium production rate will appear. Indeed, it can be shown,^(20–22) for very general rates $\varepsilon^2 c_j^\pm(\eta)$, that in the scaling limit $\varepsilon \rightarrow 0$ the density is governed by the reaction–diffusion equation

$$\frac{\partial}{\partial t} \rho(q, t) = v \frac{\partial^2}{\partial q^2} \rho(q, t) + F(\rho(q, t)) \tag{5.1}$$

$F(\rho)$ is obtained by averaging the rates c^+ , c^- over a local equilibrium distribution in which the sites are occupied with probability ρ and empty with probability $1 - \rho$, independent of each other. If we denote this equilibrium average by $\langle \cdot \rangle_\rho$, then

$$F(\rho) = \langle c_j^+(\eta) \rangle_\rho - \langle c_j^-(\eta) \rangle_\rho \tag{5.2}$$

which, by translation invariance, is independent of j .

Let us consider now two examples for which Eq. (5.2) has traveling front solutions with different degrees of stability. In both cases $c_j^-(\eta) = 0$,

so we have only creations and the ultimate stable steady state is one with all sites occupied. The creation rate is $\varepsilon^2 c_j^+(\eta)$ with

$$c_j^+(\eta) = \frac{1}{2}\lambda[\eta(j-1) + \eta(j+1)][1 - \eta(j)] \quad (\text{case I}) \quad (5.3)$$

and

$$c_j^+(\eta) = \frac{1}{2}\lambda[\eta(j-2)\eta(j-1) + \eta(j+1)\eta(j+2)][1 - \eta(j)] \quad (\text{case II}) \quad (5.4)$$

In words, case I corresponds to a particle “giving birth” on a neighboring empty site with macroscopic rate $\lambda/2$, while in case II it is necessary to have two particles on adjacent sites either to their right or left to produce a new particle on an empty site (binary production^(1,23)). Substituting the corresponding values of $F(\rho)$ computed from (5.2) into (5.1) gives

$$\frac{\partial}{\partial t} \rho(q, t) = \frac{a^2}{\tau} \frac{\partial^2}{\partial q^2} \rho(q, t) + \lambda\rho(1 - \rho), \quad 0 \leq \rho \leq 1 \quad (5.5)$$

$$\frac{\partial}{\partial t} \rho(q, t) = \frac{a^2}{\tau} \frac{\partial^2}{\partial q^2} \rho(q, t) + \lambda\rho^2(1 - \rho), \quad 0 \leq \rho \leq 1 \quad (5.6)$$

Equations (5.5) and (5.6) are classical reaction-diffusion-type equations first studied by Fisher⁽²⁴⁾ as models of genetic trait diffusion and investigated further by Kolmogorov *et al.*⁽²⁵⁾ (KPP) and many others in many contexts; see ref. 1. We refer to the first of these equations as the KPP equation and to the second as the binary production equation.

It is clear that in both cases the macroscopic equations (5.5) and (5.6) have exactly two stationary spatially uniform solutions, $\rho = 1$ and $\rho = 0$. These correspond of course to translation-invariant stationary states of the microscopic model: all sites occupied or all sites empty. The solution $\rho = 1$ is stable, while $\rho = 0$ is unstable against perturbations. We are interested in the time evolution of initial densities $\rho(q, 0)$ that connect stable to unstable fixed points, i.e.,

$$\rho(x, 0) \rightarrow \begin{cases} 1 & \text{as } x \rightarrow -\infty \\ 0 & \text{as } x \rightarrow +\infty \end{cases} \quad (5.7)$$

It was shown in ref. 25 (see also ref. 26) that both equations have traveling front solutions of the form $\rho(q, t) = u(q - ct)$ with $u(q)$ a smooth, monotone-decreasing function of q , $u(-\infty) = 1$, $u(\infty) = 0$. Such solutions exist for all values of c greater than some minimal speed $c^* > 0$, $c_I^* = c_{II}^* = 2(\lambda a^2/\tau)^{1/2}$. (There are of course also solutions moving in the opposite direction.)

The traveling front solutions $u(q)$ all decay exponentially with q —the larger the speed, the slower the decay. This can be understood in terms of the rate of particle production $F(\rho)$. Integrating (5.1) over q , one obtains the speed of a stationary front as $c = \int_{-\infty}^{\infty} F(u(q)) dq$, which, using (5.5) or (5.6), clearly increases with the size of the transition region. The existence of a minimum speed is not so obvious—it is connected with the fact that $\rho(q, t)$ must be in the interval $[0, 1]$. KPP further showed that given any initial $\rho(q, 0)$ that decays “rapidly enough” to zero as $q \rightarrow \infty$, e.g., $\rho(q, 0) = 0$ for $q > q_0$, then $\rho(q, t)$ “converges” as $t \rightarrow \infty$ to the traveling front solution $u^*(q - c^*t)$. The front with smallest speed thus has as its basin of attraction all rapidly decaying initial density profiles. This can be thought of as a “velocity selection principle”⁽²⁷⁾ and we may naturally ask whether this can be understood from the microscopic model.

The question was answered affirmatively in ref. 28 for the KPP case. It was shown there that for the creation rate (5.3), starting with initial states of the system for which the average density decays, as $j \rightarrow \infty$, in an integrable way so that there is, with probability one, a *last* particle, the state as seen from that particle converges to a stationary state with a *unique* velocity $v(\varepsilon)$. Furthermore, this velocity (properly scaled) converges to c^* , i.e., $\varepsilon^{-1}v(\varepsilon) \rightarrow c^*$ as $\varepsilon \rightarrow 0$. The same result presumably holds also for the binary production.

6. LONG-TIME DYNAMICS AND AMPLIFICATION OF FLUCTUATIONS

So far we have tried to show how hydrodynamic equations emerge as the microscopic and macroscopic scales become separated, i.e., as $\varepsilon \rightarrow 0$. These results hold for fixed macroscopic times and imply that for small but fixed ε the particles follow “closely” the solution of the macroscopic equation for microscopic times of order $\varepsilon^{-1}\tau$ or $\varepsilon^{-2}\tau$, depending on the model. More precisely, the derivations prove that the deviation from the solution of the hydrodynamic equation, call it the remainder $R(\varepsilon, t)$, goes to zero for fixed macroscopic time t when $\varepsilon \rightarrow 0$. They leave open the question of how $R(\varepsilon, t)$ grows with t for fixed ε . This is the problem we want to study now for the models discussed before. For example, for the weakly asymmetric lattice gas with an initially sharp step our theorem tells us that, when $\varepsilon \rightarrow 0$, the (microscopic) density profile follows, when looked at on a macroscopic scale, the solution of Burgers’ equation with step initial conditions. We want to know what happens to the particles for microscopic times larger than $\varepsilon^{-2}\tau$.

To address the question of deviations from hydrodynamic behavior, it is natural to ask whether the macroscopic solution under consideration is

stable against small perturbations, i.e., whether all the eigenvalues of the linearization have negative real parts. If so, one may argue that the noise of the microscopic dynamics can be considered as such a small perturbation and hence the actual density profile should have only small deviations from the macroscopic solution. (We ignore here highly improbable fluctuations to some other stable solution.) If, on the other hand, the solution is unstable, the dynamical mechanism of amplification of intrinsic microscopic fluctuations has to be investigated, a task outside the realm of the macroscopic equation.

In Section 1, Equations (1.2) and (1.3), we noted how a refinement of the law of large numbers is provided by the central limit theorem. Since the macroscopic equation is such a law of large numbers, here there also will be such corrections, except that, instead of a single variable x_j , we have to consider now all macroscopic variables simultaneously. There is in fact a quasimacroscopic theory, known as hydrodynamic fluctuation theory, where, on a more or less heuristic basis, small Gaussian noise terms are added to the deterministic hydrodynamic equation. We now briefly describe this theory in the context of the models we have introduced, where it can in fact be proven rigorously, albeit again only for fixed macroscopic times when fluctuations are indeed small. Nevertheless, as we shall see, these fluctuations provide clues to the actual long-time behavior, to which we return afterward.

Let $n^\varepsilon([q, q + \delta], t)$ be the actual number of particles in the macroscopic interval $[q, q + \delta]$ at the macroscopic time $t (\cong \varepsilon^{-1}\tau, \varepsilon^{-2}\tau, \text{ depending on the model})$. Our derivations assert that with probability one

$$\lim_{\varepsilon \rightarrow 0} (\varepsilon a) n^\varepsilon([q, q + \delta], t) = \int_q^{q+\delta} dq' \rho(q', t) \quad (6.1)$$

where $\rho(q, t)$ is the solution of the macroscopic equation. This is the law of large numbers. We now write the number of particles in $[q, q + \delta]$ as its average value plus a (small) deviation,

$$\varepsilon a n^\varepsilon([q, q + \delta], t) = \varepsilon a \langle n^\varepsilon([q, q + \delta], t) \rangle + \varepsilon^{1/2} \int_q^{q+\delta} dq' \xi^\varepsilon(q', t) \quad (6.2)$$

Since $n^\varepsilon([q, q + \delta], t)$ is a sum over roughly ε^{-1} terms, typical fluctuations should be of the order $1/\sqrt{\varepsilon}$. We therefore normalized the second term on the right-hand side of (6.2) so as to have $\xi^\varepsilon(q, t)$ of order one. Of course, (6.2) is a mere tautology. The crux is that in the limit $\varepsilon \rightarrow 0$ the statistics of the fluctuations simplify and become *Gaussian*.

More precisely, one proves that

$$\lim_{\varepsilon \rightarrow 0} \xi^\varepsilon(q, t) = \xi(q, t) \quad (6.3)$$

in the sense that joint distributions of the left-hand side converge to those of the right-hand side,^(20,29-32) where the $\xi(q, t)$ are Gaussian random variables governed by a Langevin equation of the form

$$\frac{\partial}{\partial t} \xi(q, t) = L_t \xi(q, t) + W(q, t) \tag{6.4}$$

Here L_t is the linear operator obtained by linearizing the macroscopic equation around the solution $\rho(q, t)$ under consideration. $W(q, t)$ are Gaussian fluctuating forces with mean zero. Their covariance is of the general form

$$\langle W(q, t) W(q', t') \rangle = \delta(t - t') R_t(q, q') \tag{6.5}$$

where the noise covariance $R_t(q, q')$ has to be computed from the microscopic dynamics. For conservative-type equations $R_t(q, q')$ may also be obtained through a time-dependent generalization of the fluctuation-dissipation theorem. Physically, $W(q, t)$ represents the instantaneous noisiness of the system. Since the noise is small (of order $\sqrt{\varepsilon}$), it will in the course of time be either damped or amplified, according to the linearized equation.

Applying the above scheme to the weakly asymmetric lattice gas [cf. Eq. (4.4)], one obtains the linearized operator

$$L_t \xi(q) = -\frac{\partial}{\partial q} \{ \alpha [1 - 2\rho(q, t)] \xi(q) \} + v \frac{\partial^2}{\partial q^2} \xi(q) \tag{6.6}$$

and the noise covariance

$$R_t(q, q') = 2v \frac{\partial}{\partial q} \left\{ \rho(q, t) [1 - \rho(q, t)] \frac{\partial}{\partial q} \right\} \delta(q - q') \tag{6.7}$$

For the reaction-diffusion equation (5.1) one finds the linearized operator

$$L_t \xi(q) = v \frac{\partial^2}{\partial q^2} \xi(q) + F'(\rho(q, t)) \xi(q) \tag{6.8}$$

and the covariance of the fluctuating forces

$$\begin{aligned} R_t(q, q') = & 2v \frac{\partial}{\partial q} \left\{ \rho(q, t) [1 - \rho(q, t)] \frac{\partial}{\partial q} \right\} \delta(q - q') \\ & + 2 [\langle c_0^+(\eta) \rangle_{\rho(q,t)} + \langle c_0^-(\eta) \rangle_{\rho(q,t)}] \delta(q - q') \end{aligned} \tag{6.9}$$

see (5.2) for the definition of $\langle \cdot \rangle_\rho$. We note that the first terms of (6.7) and (6.9) are the same. This is the instantaneous noise due to the diffusive exchange. The jump bias produces no extra noise (on this scale), whereas the creation and annihilation of particles are noisy, yielding the second term in (6.9).

The hydrodynamic fluctuation theory does not improve on the time domain of the macroscopic description. It only refines its resolution. However, on that finer scale, the precursor of the long-time dynamics already may be recognized. We explain how this works by applying the fluctuation theory to three examples, starting with the shock front of Burgers' equation.

(i) The stationary solution of the viscous Burgers equation is of the form $\rho_s(q - v_s t)$, $\rho_s(-\infty) = \rho_-$, $\rho_s(\infty) = \rho_+$, $\rho_- < \rho_+$. In (6.6) and (6.7) we then set $\rho(q, t) = \rho_s(q - vt)$. Including now the fluctuations of order $\sqrt{\varepsilon}$ as governed by the Langevin equation (6.4), we can write the time evolution of the shock as

$$\rho_s(q - v_s t) + \varepsilon^{1/2} \left[\frac{\partial}{\partial q} \rho_s(q - v_s t) \xi(t) + (\text{noise bounded in time}) \right] + O(\varepsilon) \quad (6.10)$$

$\xi(t)$ is a Gaussian random variable with covariance

$$\langle \xi(t)^2 \rangle = \text{const} \cdot t \quad (6.11)$$

It is suggestive to rewrite (6.10) as

$$\rho_s(q - vt - \varepsilon^{1/2} \xi(t)) + \varepsilon^{1/2} (\text{noise bounded in time}) + O(\varepsilon) \quad (6.12)$$

Thus, besides the inevitable noise, the shock picks up a random-walk-like displacement. Note that this is in accordance with the observation made in Section 3. We expect then that for times of the order $\varepsilon^{-3}\tau$ the statistics of the microscopic particle configurations is well approximated by

$$\rho_s(q - \varepsilon^{-1} v_s t - \xi(t)) \quad (6.13)$$

Each individual configuration resembles a shock profile, whose position is given by $\varepsilon^{-1} v_s t + \xi(t)$, where $\xi(t)$ is a Gaussian random variable of order one on the *macroscopic* spatial scale; cf. ref. 33 for a partial proof.

(ii) Another example of the power of the fluctuation theory is the escape from an unstable equilibrium point.⁽³⁴⁾ Here the nonlinearity of the reaction-diffusion equation is $F(\rho) = -V'(\rho)$, with V a double-well poten-

tial symmetric around $1/2$. Initially, each site, on some bounded macroscopic interval, is independently occupied with probability $1/2$. On the macroscopic scale, the system is then at the unstable point, $\rho_0(q) = 1/2$. Density fluctuations grow exponentially in time and furnish the random initial data for the deterministic evolution into either one of the two potential minima.

(iii) The long-time dynamics of traveling fronts for reaction–diffusion equations depends on the precise form of the production term. Let us first study the KPP equation. The stability of the equation, linearized around the traveling front, is determined by the decay of the perturbation at infinity. Perturbations that decay faster than the traveling front die out in the course of time. If the decay is the same as that of the traveling front, the perturbation causes a finite displacement for long times. More slowly decaying perturbations blow up in the course of time. If we add noise to the linearized equation, then, according to (6.4) and (6.9), the density fluctuations diverge exponentially in time. There is no distinction, from this point of view, among fronts with different velocities: while the minimal velocity can be selected microscopically by observing the drift of the first particle, no similar *selection principle* comes from the analysis of the density fluctuations.

The exponential growth can be understood by considering the initial fluctuations. Let us take the state at time zero to be given by the product measure with the probability that site j is occupied set equal to $\rho(ej)$, with $\rho(q)$ being a traveling front for the KPP equation. Then the density fluctuations have the time-zero covariance

$$\langle \xi(q, 0) \xi(q', 0) \rangle = \delta(q - q') \rho(q) [1 - \rho(q)] \quad (6.14)$$

so that the typical deviations decay for $q \rightarrow \infty$ as $[\rho(q)]^{1/2}$. Since $\rho(q)$ decays exponentially, these typical deviations from $\rho(q)$ decay much more slowly than $\rho(q)$ itself (only one-half of the exponent). The fluctuations propagate according to the linearized KPP equation, which, as already noted, is unstable for such slowly decaying perturbations. Thus, they will grow exponentially in time.

The microscopic origin of this behavior is presumably due, like the macroscopic one, to small density fluctuations close to where the edge of the front is, i.e., infinitely far, in macroscopic units (when the hydrodynamic scaling is considered), from the bulk of the front. Such fluctuations have time to grow and become macroscopic before the bulk of the front reaches the region where they were initially produced, and thus total density fluctuations grow very rapidly (a mechanism that might be similar to that observed for dendritic growth⁽²⁷⁾). Unfortunately, a quantitative

microscopic analysis of such phenomena is technically very complicated and so far there are no results.

The binary case considered in Section 5, Eq. (5.6), is much simpler. This can be easily understood microscopically: to create a new particle at j , two particles are needed adjacent to j . Hence, the fluctuations in the reaction rate will be very much decreased in the low-density region. In fact, one can compute the asymptotic behavior of the covariance for the density fluctuation field in the case of the traveling front with minimal velocity. One then finds a behavior like (6.12), ρ_s now being the traveling wave solution of the binary production. As for Burgers' equation, this indicates that the shape of the traveling front is microscopically stable, so that in the long-time regime only random rigid shifts of the profile will be observed.

It is quite surprising, at least for us, that the asymmetric exclusion shocks and the traveling fronts in the binary reaction equation have similar stability properties from a *microscopic* viewpoint. In the exclusion process the particle number is conserved in the microscopic evolution and the only dynamical fluctuations are in the current. From this we can understand why there is a random change in the velocity of the shock. For diffusion-reaction equations, on the other hand, the reactive part does not conserve the particle number. One would therefore expect weaker stability properties. We find, however, that because the limiting macroscopic equations have in both cases the same stability properties with respect to local perturbations, this is also the case at the microscopic level: the shape of the front is stable. This argues strongly in favor of the "completeness" of the information contained in the macroscopic equation.

7. SUMMARY

We investigated the behavior of some stochastic particle models with emphasis on how the macroscopic description emerges from the microscopic dynamics in a scaling limit. While our choice of models, particularly the restriction to one dimension, was dictated primarily by the desire for simplicity of exposition, it must be admitted that even the most complicated models that can be treated with mathematical rigor are fairly primitive when compared to the complexity of even the simplest fluids governed by Newtonian dynamics. However, the main point we wanted to make and wish to emphasize again is that in these models particles move in a microscopic time over microscopic distances and interact with neighboring particles only. Therefore, the *spatial* degrees of freedom have the "right physics." In this sense these models capture, we believe, the essential features of real systems. They play the same role for hydro-

dynamics as the Ising model does for phase transitions: they show, by explicit analysis, the essential microscopic ingredients responsible for macroscopic behavior.

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