

## MICROSCOPIC ORIGIN OF HYDRODYNAMIC EQUATIONS: DERIVATION AND CONSEQUENCES\*

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We describe some recent progress in deriving autonomous hydrodynamic type equations for macroscopic variables from model stochastic microscopic dynamics of particles on a lattice. The derivations also yield the microscopic fluctuations about the deterministic macroscopic evolution. These grow, with time, to become infinite when the deterministic solution is unstable. A form of microscopic pattern selection is also found.

### 1. Introduction

It is no secret that there does not exist at present anything resembling a rigorous derivation of the hydrodynamic equations governing the time evolution of macroscopic variables from the laws governing the dynamics of their microscopic constituents. These are generally autonomous equations of the form

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

where  $\mathbf{M}(\mathbf{r}, t)$  denotes a “full set” of macroscopic variables such as the particle, momentum and energy, density of a fluid.  $\mathbf{F}$  depends on the type of problems considered (and contains parameters specific to the system considered). Examples include the Euler and Navier–Stokes equations for fluids and diffusion-reaction type equations for chemically reacting mixtures<sup>1</sup>).

The essential mathematical element involved in the transition from microscopic to macroscopic evolution equations involves the suitable rescaling of space and time. 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 number of elementary events. This brings in the “law of large

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numbers" which is crucial for obtaining deterministic autonomous macroscopic equations, like (1.1), *not just for averages*, but for the *almost sure value* of quantities which fluctuate on the microscopic scale. Controlling the fluctuations is clearly important if the deterministic equations are to describe what is actually observed in an experiment.

The question of fluctuations is unfortunately often overlooked in discussions of this subject. This may lead then to the erroneous conclusion that the origin of the macroscopic hydrodynamical equations is directly attributable to the highly irregular behavior of trajectories of nonlinear dynamical systems. This behavior, which occurs already in systems with a *few* degree of a freedom, does not however have any intrinsic mechanism for suppression of fluctuations. The time evolution of such a nonlinear system consisting of a few particles will therefore not exhibit the kind of deterministic behavior associated with macroscopic variables discussed here; cf. van Kampen's book<sup>2</sup>).

The mathematical difficulties encountered in carrying out the derivations from realistic microscopic dynamics are enormous – possibly insurmountable. It is only in very special cases, when the dynamics is essentially trivial (hard rods in one dimension, long range forces, harmonic crystals), that hydrodynamical type equations can be derived for nonequilibrium systems evolving via Hamiltonian dynamics. Things are a little better when we consider quasi-equilibrium situations, such as the time evolution of the relative concentrations in a fluid mixture whose components are mechanically identical, but differ in their "color", e.g., some chemical isomers or spin up and down <sup>3</sup>He atoms: the system, ignoring color, is in true thermal equilibrium. Unfortunately, even for these intrinsically linear nonequilibrium phenomena, the problem is too difficult to solve completely. All we can do in general is reduce the problem to that of the behavior of "test particles" in an equilibrium fluid<sup>3</sup>).

## 2. Lattice systems with stochastic dynamics

The main progress which has been made in recent years concerns systems whose microscopic dynamics involve some stochastic elements, e.g., particles (or spins) on a lattice with stochastic dynamics. What I shall describe now is joint work with Anna de Masi and Pablo Ferrari<sup>4</sup>) and some very recent extensions of it<sup>5,6</sup>).

In this work we study interacting particle (spin) systems on a lattice under the combined influence of general Glauber (spin flip) and simple exclusion (spin exchange) dynamics. We prove that when the conserving exchanges occur on a microscopic time scale, with rate  $\varepsilon^{-2}$ ,  $\varepsilon \ll 1$ , while the Glauber rate is of order unity the magnetization  $m$  looked at on a macroscopic spatial scale of  $\varepsilon^{-1}$ ,

evolves according to an autonomous nonlinear diffusion-reaction equation,

$$\frac{\partial m(\mathbf{r}, t)}{\partial t} = \nabla^2 m + F(m), \quad \mathbf{r} \in \mathbb{R}^d, \quad (2.1)$$

where  $F(m)$  is a polynomial which can be “adjusted” by choosing suitable Glauber rates. Note that while  $m$  is no longer conserved on the macroscopic scale, it is conserved by the “fast” exchanges and so still serves as a good macroscopic variable.

The proof involves showing that the microscopic state is in fact close to “local equilibrium”. The deviations from local equilibrium produce fluctuations about the deterministic solutions of (2.1). These fluctuations form a Gaussian field with an amplitude  $\varepsilon^{d/2}$  around stable solutions of (2.1), but grow (exponentially or like some power of  $t$ ) around unstable solutions.

We believe that despite their very special (and arbitrary) microscopic dynamics these models capture the essential features of the mechanism leading to hydrodynamical laws in real systems. They may also describe, at least qualitatively, the microscopic influence on fluctuations and on pattern selection, cf. examples in section 4.

### 3. Microscopic formulation

Our system is a simple cubic lattice in  $d$ -dimensions, at each site of which there is a spin  $\sigma(\mathbf{x}) = \pm 1$ . The configuration of the lattice  $\sigma = \{\sigma(\mathbf{x}), \mathbf{x} \in \mathbb{Z}^d\}$ , changes with time via two mechanisms; a Glauber dynamics in which a spin flips at a site  $\mathbf{x}$ , with a rate  $c(\mathbf{x}; \sigma)$  and a Kawasaki dynamics in which unequal spins at neighboring sites exchange, with a rate  $\varepsilon^{-2}$ . In particle language,  $\sigma(\mathbf{x}) = \pm 1$  denotes empty and occupied sites. Glauber dynamics then corresponds to creation or annihilation of particles while exchanges correspond to particles jumping to empty sites.

There are very few restrictions on  $c(\mathbf{x}; \sigma)$ . In particular Glauber dynamics can, but need not, be chosen to satisfy detailed balance for the equilibrium state of an Ising model with specified interactions at some reciprocal temperature  $\beta$ . The exchange process on the other hand, being independent of the spin configuration on neighboring sites, acts *as if* the system were at an infinite temperature,  $\beta = 0$ . It is very fast compared to the flip rate taking place on a macroscopic time scale.

We now define the macroscopic magnetization density by rescaling space by  $\varepsilon^{-1}$ . Let  $\Delta_\varepsilon^c$  be a cubical box with sides of length  $\varepsilon^{-1}$  centered on  $\mathbf{r} \in \mathbb{R}^d$ . The

magnetization density on this scale is

$$m^\varepsilon(\mathbf{r}, t; \boldsymbol{\sigma}) = \varepsilon^d \sum_{x \in \Lambda_r^\varepsilon} \sigma(x; t), \tag{3.1}$$

where  $\sigma(x; t)$  is the value of the (random) spin variable at site  $x$  at time  $t$ .  $m^\varepsilon(\mathbf{r}, t; \cdot)$  is thus a random variable whose probability distribution depends on the initial state of the system. We shall assume the latter to have good cluster properties and that as  $\varepsilon \rightarrow 0$ ,

$$\varepsilon^{-d} |\langle \sigma(\mathbf{x}) \rangle_\varepsilon - m_0(\varepsilon \mathbf{x})| \rightarrow 0, \quad \mathbf{x} \in \mathbb{Z}^d,$$

where  $m_0(\mathbf{r})$  is a smooth function of  $\mathbf{r}$ ,  $|m_0(\mathbf{r})| \leq 1$ ,  $\mathbf{r} \in \mathbb{R}^d$ .

*Theorem.* In the limit  $\varepsilon \rightarrow 0$ ,  $m^\varepsilon(\mathbf{r}, t; \boldsymbol{\sigma}) \rightarrow \int_{\Lambda_r} m(\mathbf{r}', t) d\mathbf{r}'$ , where the integration is over the unit cube centered at  $\mathbf{r}$  and  $m(\mathbf{r}, t)$  is a *deterministic* (non-fluctuating) function of  $\mathbf{r}$  and  $t$  satisfying eq. (2.1) with initial condition  $m(\mathbf{r}, 0) = m_0(\mathbf{r})$  and  $F(m) = -2 \langle \sigma(\mathbf{x}) c(\mathbf{x}; \boldsymbol{\sigma}) \rangle_m$  – the average being taken with respect to the Bernoulli product measure, in which  $\langle \sigma(\mathbf{x}) \rangle = m$  for all  $\mathbf{x}$ . This measure is the same as the local equilibrium state for a system at infinite temperature with macroscopic magnetization  $m(\mathbf{r}, t)$ .

To see the microscopic fluctuations in the magnetization – corresponding to the deviations of the probability distribution at time  $t$  from a product measure – we must magnify them in an appropriate way.

Let

$$\phi^\varepsilon(\mathbf{r}, t; \boldsymbol{\sigma}) = \varepsilon^{-d/2} \left[ m^\varepsilon(\mathbf{r}, t; \boldsymbol{\sigma}) - \int_{\Lambda_r} m(\mathbf{r}', t) d\mathbf{r}' \right],$$

then  $\phi^\varepsilon(\mathbf{r}, t; \cdot) = \int_{\Lambda_r} \phi(\mathbf{r}', t) d\mathbf{r}'$ ;  $\phi(\mathbf{r}, t)$  a random Gaussian field satisfying an Ornstein–Uhlenbeck type stochastic equation. The equal time correlations of the fluctuation field  $\phi$ ,  $c(\mathbf{r}, \mathbf{r}'; t)$ , satisfy a linear inhomogeneous equation whose coefficients depend on the solution of (2.1).

#### 4. Examples

We shall illustrate the above analysis with two one dimensional examples, i.e., choices of Glauber rates  $c(x; \boldsymbol{\sigma})$ ,  $x$  a site on the 1-d lattice. The first example will exhibit the effect of microscopic fluctuations about an unstable solution while the

second will show a microscopic pattern selection. We expect this behavior to be typical also for higher dimensional cases:

Case I.

$$c(x; \sigma) = 1 - \gamma \sigma(x) [\sigma(x+1) + \sigma(x-1)] + \gamma^2 \sigma(x+1) \sigma(x-1). \quad (4.1)$$

For  $\gamma$  between  $-1$  and  $1$  this Glauber rate satisfies detailed balance for a one dimensional Ising model with n.n. interaction  $J$ ,  $\gamma = \tanh \beta J$ . Calling  $q$  the coordinate along the line, eq. (2.1) now takes the form

$$\frac{\partial m(q, t)}{\partial t} = \frac{\partial^2 m}{\partial q^2} - \frac{d}{dm} \left[ \frac{\gamma^2}{2} m^4 - (2\gamma - 1) m^2 \right]. \quad (4.2)$$

Eq. (4.2) has a unique solution for any initial magnetization  $m_0(q)$  in the interval  $[-1, 1]$ . In particular it has the time independent spatially homogeneous solution  $m(q, t) = m_0(q) = 0$ . This solution is stable for  $\gamma < \frac{1}{2}$ , i.e., when  $J$  is antiferromagnetic ( $J < 0$ ) or when  $0 \leq \gamma \leq \gamma_c = \frac{1}{2}$  (a "mean field" critical temperature). It becomes unstable at  $\gamma = \gamma_c$  and for  $\gamma > \gamma_c$  there exist two stable uniform solutions with spontaneous magnetizations  $\pm \gamma^{-1}(1 - \gamma/\gamma_c)^{1/2}$ . The equal time covariance of the fluctuation field  $c(q, q'; t)$  for the  $m_0(q) = 0$  solution has the form<sup>4)</sup>

$$\begin{aligned} c(q, q'; t) &= [1 - m^2(q, t)] \delta(q - q') \\ &= 8\gamma \int_0^t ds \frac{\exp \left\{ \left[ -(q - q')^2 / 8s \right] - 4(1 - \gamma/\gamma_c) s \right\}}{\sqrt{8\pi s}} \\ &\xrightarrow[\gamma < \gamma_c]{t \rightarrow \infty} \frac{\gamma}{(\gamma_c - \gamma)^{1/2}} \exp [-2(\gamma_c - \gamma)|q - q'|]. \end{aligned} \quad (4.3)$$

For  $\gamma > \gamma_c$  the fluctuations grow exponentially with time around this unstable solution while for  $\gamma = \gamma_c$  they grow like  $\sqrt{t}$ . To understand the long time behavior of this systems for  $\gamma \geq \gamma_c$  one has to go beyond linear Gaussian fluctuations. This has been done by De Masi, Presutti and Vares<sup>5)</sup>. They prove that at long times, before taking the hydrodynamical limit, the evolution departs from that predicted by (4.2), i.e.,  $m(q, t) = 0$ . Instead the microscopic state becomes a nontrivial mixture of states with different magnetizations.

Case II.

$$c(x; \sigma) = \frac{1}{8}[1 - \sigma(x)][2 + \sigma(x-1) + \sigma(x+1)]. \quad (4.4)$$

This corresponds in particle language to a particle creating a new particle (giving birth) on an adjacent empty site with a rate  $\frac{1}{2}$  (compared to the rate of jumping to such a site  $\varepsilon^{-2}$ ). It can also be interpreted in terms of a one dimensional cross section of a flame front with convection<sup>7</sup>;  $\sigma(x) = 1$  or  $-1$  represents a burned or unburned cell (or region). Equation (1.1) expressed in terms of the macroscopic density  $p(q, t) = \frac{1}{2}[1 + m(q, t)] \in [0, 1]$  has the form

$$\frac{\partial p(q, t)}{\partial t} = \frac{\partial^2 p}{\partial q^2} + p(1 - p). \quad (4.5)$$

This is a classical diffusion-reaction (D.R.) equation studied by Kolmogorov, Petrovsky and Piscounov (KPP) and others<sup>1</sup>.

An important feature of this type of D.R. equation is that it admits travelling front solutions:  $p(q, t) = u_c(q - ct)$ , where  $u_c(q)$  satisfies the equation

$$\begin{aligned} u_c''(q) + cu_c'(q) + u_c(1 - u_c) &= 0, \\ u_c(q) \rightarrow 1 \quad \text{as } q \rightarrow -\infty, \quad u_c(q) \rightarrow 0 \quad \text{as } q \rightarrow \infty, \quad \text{for } c > 0, \end{aligned} \quad (4.6)$$

which has solutions for all speeds  $|c| \geq c^*$ . The marginal speed  $c^*$  which equals 2 for our case is singled out in the sense that for all initial conditions such that  $\rho_0(q) \rightarrow 1$  as  $q \rightarrow -\infty$ ,  $\rho_0(q) = 0$  as  $q \rightarrow \infty$  converges as  $t \rightarrow \infty$  to  $u_{c^*}(q - \lambda(t))$  for appropriate  $\lambda(t)$  where  $\lambda(t)/t \rightarrow c^{* - 1}$ .

This "selection principle" was investigated from a physical point of view by Langer and coworkers<sup>8</sup>. Their interest in this problem stems from a desire to understand pattern selection principles for equations describing dendritic growth of a solid front moving into a melt.

We show in ref. 6 that as seen from the rightmost particle, our microscopic model has precisely one invariant distribution and that the average velocity,  $V(\varepsilon)$ , of this particle satisfies  $\varepsilon V(\varepsilon) \rightarrow 2$ , as  $\varepsilon \rightarrow 0$ .

The significance of this result for other pattern selection problems is not clear to us at the present time. We are currently studying the fluctuations about these travelling solutions.

## 5. Discussion

Let me discuss now briefly the case where the dynamics is exclusively of the Kawasaki type. When the jump rates are spatially symmetric the resulting hydrodynamical equation for the macroscopic density  $\rho(q, t)$  is just (2.1) with  $F = 0$ , i.e., a linear diffusion equation. When the rates are asymmetric, then in

one dimension with  $p > \frac{1}{2}$  the probability of right jumps, one obtains in the now appropriate scaling limit, in which both time and space scale like  $\varepsilon^{-1}$ , the inviscid Burger's equation<sup>9)</sup>

$$\frac{\partial \rho(q, t)}{\partial t} = (1 - 2p) \frac{\partial}{\partial q} [\rho(1 - \rho)]. \quad (5.1)$$

This is the analogue of the Euler equations for fluids. To obtain also the viscosity term  $\sim \partial^2 \rho / \partial q^2$  on the right side of (5.1) (analogous to the Navier–Stokes equations) one needs to make the asymmetry  $p - \frac{1}{2}$  small, of order  $\varepsilon$  and go to the scaling of time like  $\varepsilon^{-2}$  appropriate for dissipation<sup>9)</sup>.

This difference in scalings needed for the nondissipative and dissipative cases occurs also in the real fluid equations. Without the asymmetry parameter  $p - \frac{1}{2}$  to play with we can only expect to get the Euler equations as scaling limits. The Navier–Stokes equations should then be seen as the leading correction in some asymptotic series. This situation arises also in recent work using cellular automata dynamics (which can be thought of as a deterministic limit of stochastic particle dynamics, or vice versa) to solve the Navier–Stokes equations<sup>10)</sup>. It also occurs if one starts with the Boltzmann equation rather than with a microscopic particle system. The Boltzmann equation is itself of form (1.1) describing the autonomous evolution of quasi-macroscopic variables; instead of  $M(\mathbf{r}, t)$  we have  $f(\mathbf{r}, \mathbf{v}, t)$ ,  $\mathbf{v}$  a velocity variable, as our basic set. Once the Boltzmann equation is accepted the derivation from it of hydrodynamical equations for the appropriate set of  $M(\mathbf{r}, t)$  proceeds, with some measure of success, via Chapman–Enskog type expansion methods. These yield the Euler equations in the leading order, which is in fact the scaling limit mentioned earlier. The Navier–Stokes, Burnett and other higher order equations are then expected to form some kind of asymptotic series in the gradients.

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