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Edited by

ERROL (ASHER) GOTSMAN
School of Physics and Astronomy
Raymond and Beverly Sackler Faculty of Exact Sciences
Tel Aviv University

YUVAL NE'EMAN
Wolfson Chair Extraordinary in Theoretical Physics,
Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University
and Center for Particle Theory, University of Texas, Austin

ALEXANDER VORONEL
School of Physics and Astronomy
Raymond and Beverly Sackler Faculty of Exact Sciences
Tel Aviv University

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On the Rigorous Derivation of Hydrodynamical Equations from Stochastic Lattice Gas Models*

JOEL L. LEBOWITZ

Department of Mathematics and Physics, Rutgers University, New Brunswick, NJ 08903, USA

Abstract
The emergence of deterministic macroscopic equations from microscopic dynamics is analysed for some simple models. Fluctuations about the macroscopic behaviour – which can be large in some cases – are also discussed.

1. Introduction

Landau made fundamental contributions to both microscopic and macroscopic physics. It is therefore appropriate that this conference covers phenomena occurring on scales ranging from the Planck length to the size of the universe. In this talk I shall be concerned with the connection between the motions of atoms or molecules whose mean free paths are typically measured in Angstroms, and hydrodynamic behaviour usually observed on scales of millimetres or larger; a ratio of macro to micro scales of about 10^6–10^7.

By hydrodynamic behaviour I mean collective phenomena described by macroscopic space–time fields obeying deterministic laws. These laws generally take the form of nonlinear partial differential equations,

$$\frac{\partial}{\partial t} M_\alpha(\mathbf{r}, t) = F_\alpha(\mathbf{M}(\mathbf{r}, t), \text{grad } \mathbf{M}(\mathbf{r}, t), \ldots), \tag{1}$$

where $\mathbf{M}(\mathbf{r}, t) = \{M_\alpha(\mathbf{r}, t)\}$ denotes a "full" set of macroscopic fields depending on space and time. When M_α is conserved by the microscopic interactions, as is the case for the density and momentum in the Euler and Navier–Stokes equations, then F_α in (1) has the form of a divergence, $F_\alpha = -\nabla \cdot \mathbf{J}_\alpha$, where J_α is the current associated to M_α. 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

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general small. The details of microscopic structure generally enter in F only through the numerical value of some parameters, e.g. heat conductivity and viscosity in the Navier–Stokes equations.

The origin of this structure lies in the fact that the hydrodynamic laws are a consequence solely of the existence of 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 behaviour. All that is necessary is that the models contain the essential features responsible for the phenomena of interest. Direct visual evidence for this has come recently from computer simulations implementing microscopic dynamics for "large" numbers of particles. These have shown dramatically how similar indeed are self-organized macroscopic evolutions resulting from very different microscopic models – including Ising-like cellular automata.[1]

The utility of simple models, e.g. the Ising spin system, is well established for equilibrium behaviour and in this paper I wish to describe some recent progress in the mathematical derivation of hydrodynamic-type laws of form (1) for similarly simple dynamical models. I believe, and hope to convince you, that these models capture the essential features of the transition from microscopic to macroscopic evolutions, involving the appearance of collective modes and self-organization phenomena, in real physical systems. For more details on the general principles underlying this approach the reader is referred to the article by Lebowitz, Presutti and Spohn[3] on which this talk is mainly based.

Before discussing specific models I wish to focus attention on the fact that deterministic equations like (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. In fact one of the main practical motivations for studying the micro–macro connection comes from situations where the hydrodynamic laws fail, partially or entirely, to describe all the phenomena of interest. This can happen in cases where the solution of the macroscopic equations leads to shocks or other instabilities. (The phenomenon of cell formation in the Bénard problem described by Gunther Ahlers in his paper here may be such an example where "microscopic noise" is relevant – but this is still an open question.)

I should also note here that in computer simulations of steady-state situations one can apparently make the ratio of macro to micro scales as small as 10–10^2 and still obtain hydrodynamic behaviour.[2] This

"persistence of macroscopic behaviour" down to almost the microscopic level for stationary non-uniform states as in the Bénard convection regime and in flow around an obstacle is reminiscent of what happens in equilibrium systems, away from critical points. Why this should be so is something important to understand. Before we can do that, however, in a reliable manner we need to develop a consistent mathematical theory of the emergence of macroscopic laws like (1) from microscopic dynamics in an idealized limiting case, i.e. when the ratio of macroscopic to microscopic scales goes to infinity. This is analogous to – but mathematically considerably harder than – the theory of infinite volume Gibbs states, which plays the corresponding role for equilibrium systems.

1.1. The Formulation of Macroscopic Laws

The essential element in the transition from microscopic to macroscopic evolutions is the summing over a large number of elementary events. This brings in the "law of large numbers" which is crucial for obtaining deterministic autonomous macroscopic equations, like (1), *not just for ensemble averages*, but for the *almost sure value* of quantities which fluctuate on the microscopic scale, i.e. macroscopic equations which describe the actual evolution of a single 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 phenomenon 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 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–Bénard problem may yield a zero velocity field which really corresponds to a superposition of states with different 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.

We can illustrate some aspects of the micro–macro relation by considering the simplest example of independent identically distributed random variables $x_1, x_2, \ldots$. Let $f(x_i)$ 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

$$X_N = \frac{1}{N} \sum_{i=1}^{N} x_i \tag{2}$$

approaches m with probability one, as $N \to \infty$, i.e. in the macroscopic limit we have deterministic behaviour. 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

$$\xi_N = \sqrt{N}[X_N - m] = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} (x_i - m). \tag{3}$$

Then as $N \to \infty$, ξ_N tends to a Gaussian *random variable* ξ with mean zero and variance σ^2. We thus have here both a deterministic behaviour and fluctuations about it, which depend very little on the details of the microscopic distribution $f(x)$. We didn't 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 produce "local equilibrium" states parameterized 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) about a given solution $\mathbf{M}(\mathbf{r}, t)$ with a "random source term". In fact such fluctuations are often added in a purely heuristic way to the macroscopic equations – we justify them in some cases. In particular when the solutions of (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 them to significant deviations between the actual behaviour of the system and that predicted by (1) over "long" times.

2. Microscopic Models for the Burgers' Equation

After this long introduction let me illustrate the type of models used and results obtained, by describing some recent work on the derivation of the one-dimensional Burgers' equation. This equation, which I write in the form,

$$\frac{\partial \rho(q, t)}{\partial t} = -\frac{\partial}{\partial q}\left[c\rho(1-\rho) - \nu \frac{\partial \rho}{\partial q}\right], \quad q \in \mathbb{R}, \tag{4}$$

is one of the simplest conservative nonlinear equations of the form (1). It has only one scalar field, $\rho(q, t)$, and the equation can be readily integrated

for a variety of initial conditions. The non-negative parameters c and ν have the dimension of velocity and kinematic viscosity.

I shall describe here two microscopic models[4] which, depending on the microscopic dynamics, give rise to (4) with either c, ν or both being different from zero. The last case will involve, in addition to the appropriate scalings of space–time, also some scaling of the dynamics. The microscopic models and dynamics are those of stochastic lattice gases and $\rho(q, t)$ represents the macroscopic particle density (divided by its maximum value) so that $0 \leqslant \rho(q, t) \leqslant 1$, a condition preserved by the evolution (4). There are various transformations which one can make on (4) with a corresponding variety of interpretations of the field variable and the parameters. A favourite one is to put (4) in a form which suggests a one-dimensional version of the Navier–Stokes equations or, when $\nu = 0$, the Euler equations.

In the first model I discuss time will be continuous also on the microscopic scale, while in the second model microscopic time will be discrete – our system is then a probabilistic cellular automaton. As expected, this distinction is lost when going over to a macroscopic description.

Model 1

We consider a one-dimensional lattice with (microscopic) spacing a. Each site can be occupied by at most one particle. A microscopic configuration of the system is specified by $\boldsymbol{\eta} = \{\eta(x)\}$, $x \in Z$, $\eta(x) = 0, 1$. The dynamics consists of each particle deciding independently to jump to its right with a rate p/τ and to its left with a rate $(1-p)/\tau$; τ is a microscopic time unit and $\frac{1}{2} \leqslant p \leqslant 1$. The bias in attempted jumps to the right is $p-(1-p) = 2p-1$. I say attempted jumps because the rule is that when a particle finds the site it wishes to jump to already occupied, it stays in place. This corresponds to a hard-core interaction between the particles.

The stationary measures for this dynamics are simple: they are a one-parameter family of translation-invariant product (Bernoulli) measures ν_n in which each site is independently occupied with a probability $n \in [0,1]$; we have $\langle \eta(x) \rangle_{\nu_n} = n$ and $\langle \eta(x_1) \ldots \eta(x_k) \rangle_{\nu_n} = n^k$ for $x_1, \ldots x_k$ distinct sites.

Remarks

1. The reason there is a whole family of measures is, of course, due to the conservative nature of the dynamics. We are free to choose our microscopic density per site, n, as we wish.
2. For $p \neq \frac{1}{2}$ the measure ν_n is not reversible, i.e. does not satisfy detailed balance. There are in fact in this case non-translation invariant product

measures in which $\langle\eta(x)\rangle$ goes to zero as $x\to-\infty$ and to one as $x\to\infty$. These will, however, not play any role in our analysis.

The net current J across the bond connecting sites x and $x+a$ is in any state μ, given by

$$J_\mu(x)=p/\tau\langle\eta(x)[1-\eta(x+a)]\rangle_\mu-(1-p)/\tau<\eta(x+a)[1-\eta(x)]\rangle_\mu. \quad (5)$$

In the stationary state ν_n, J is constant; it is equal to $(2p-1)n(1-n)/\tau$ for all x.

Now let us assume that at some initial time, $t=0$, our system has a non-uniform 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 $\rho_0(q)$, $0\leqslant\rho_0(q)\leqslant 1$, and assuming that, as in the stationary state, each site has at time $t=0$ an independent probability of being occupied equal to $n_0^\varepsilon(x)$ given by

$$n_0^\varepsilon(x)=\rho_0(\varepsilon x) \quad (6)$$

i.e. we take the ratio of macroscopic to microscopic units of length to be ε^{-1}. Clearly the density gradient, measured on the microscopic scale (units of a), is of order ε and vanishes as $\varepsilon\to 0$. 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, $p\neq\frac{1}{2}$, 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 $\varepsilon\tau$.

Let now $n^\varepsilon([q, q+\delta], t)$ be the actual number of particles at a macroscopic time t (micro time t/ε) 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 $\varepsilon\to 0$ is that this random variable converges with probability one to a number

$$\frac{\varepsilon a}{\delta}n^\varepsilon([q, q+\delta], t)\to\frac{1}{\delta}\int_q^{q+\delta}\mathrm{d}q'\rho(q', t), \quad (7)$$

where $\rho(q, t)$ is the solution of the *inviscid* Burgers' equation

$$\frac{\partial\rho(q, t)}{\partial t}=-\frac{\partial}{\partial q}[c\rho(q, t)[1-\rho(q, t)]] \quad (8)$$

with $c=(a/\tau)(2p-1)$. Equation (8) is to be solved with the initial condition $\rho(q, 0)=\rho_0(q)$.

Equation (8) is analogous to the Euler equations of hydrodynamics; it is invariant, as it must be from its derivation, under the scaling $t\to\lambda t$, $q\to\lambda q$.

It tells us that on the time scale ε^{-1} the macroscopic particle current on the right side of (4) is dominated by the driving force c. The dissipation, containing an extra space derivative, is of order ε and disappears when $\varepsilon \to 0$. To see it, for ε small but unequal to zero, we have to either look for corrections to the macroscopic equation (8) or go to times of order ε^{-2} microscopically, i.e. of order ε^{-1} macroscopically.

Before discussing such corrections to hydrodynamical behaviour we consider the case $p = \frac{1}{2}$. In this case there is no driving force, $c = 0$, and the right side of (8) vanishes. To see any change in the macroscopic particle density we have to wait for times which are of order τ/ε^2. In fact scaling space as before and time as ε^{-2} we get the macroscopic diffusion equation

$$\frac{\partial \rho(q, t)}{\partial t} = -\nu \frac{\partial^2 \rho(q, t)}{\partial q^2} \tag{9}$$

where $\nu = \frac{1}{2}(a^2/\tau)$ and the equation is again to be solved subject to the initial condition $\rho(q, 0) = \rho_0(q)$. The fact that (9) is linear is somewhat accidental: there are other models which under the same kind of space–time scaling lead to a nonlinear diffusion equation. What is not accidental is that (8) is invariant under the scale, $q \to \lambda q$, $t \to \lambda^2 t$.

It is now easy to guess how to modify the dynamics of our model to yield (4). We make the driving force $(2p-1)$ itself of order ε so that under the scalings ε^{-1} for space and ε^{-2} for time all terms of (9) are of the same order. This is the weakly asymmetric process and is in fact right: setting $2p - 1 = \varepsilon$ and scaling as for (9) we obtain the Burgers' equation (4) with c and ν as in (8) and (9).

There is no physical significance to this change of dynamics with ε. In a real system the dynamics is fixed – independent of the scale on which we view it. In fact for real systems there is no ε, and we are simply saying that the driving force is of the same magnitude as the ratio of micro to macro scales.

Model 2

This is the cellular automaton model invented by Boghosian and Levermore.[5] It has a structure similar to that of the Frisch, Hasslacher and Pomeau (FHP) cellular automata used for modelling the Navier–Stokes equations in two and three dimensions,[1] in that particles have velocities and the updating is done synchronously. Unlike the FHP models which are entirely (or predominantly) deterministic – this makes the computation fast – the present model has a very strong stochastic element. We need this, at the present stage of our mathematical abilities, for proving rigorous results.

We again consider a system of particles on the one-dimensional lattice but now each particle has a "velocity" $\sigma = \pm 1$. There is an exclusion rule

that two particles at the same site cannot have the same velocity. Therefore each site x may have at most two particles (with different velocities). At each integral multiple of the unit time τ there is an updating of the automaton. This consists of two steps, the first is stochastic, the second one deterministic:

Step 1 – Velocity flips: This updating rule acts independently at each site x. If there are two or no particles at x then nothing happens. If, on the other hand, there is one particle at x with velocity $\sigma(x)$ then its new velocity $\sigma'(x)$ takes the vaue $+1$ with probability p and -1 with probability $(1-p)$, i.e. the $\sigma'(x)$ are independent random variables with mean 2ε.
Step 2 – Advection: Every particle at site x moves to $x+a\sigma'(x)$, keeping its velocity.

Boghosian and Levermore argued convincingly, and demonstrated numerically, that the density profile of their model does indeed follow the solution of Burgers' equation over a macroscopic time period of order unity. Their main difficulty in actually proving this involved controlling the correlations which may build up in the microscopic system – a problem which, as already mentioned, is central to all models of this kind. Note that there is an effective interaction, "collisions", among the particles. The fact that a particle cannot flip its velocity if another one is present at the same site causes non trivial space–time correlations in the process.

In work with Orlandi and Presutti[4] we solved this problem and proved for this model the same results as for Model 1. The microscopic state is now specified by the variables $\{\eta(x;\sigma)=0,1\}$ and the initial distribution is one in which the different sites, and also the two velocities at each site x, are independent. If the occupation probabilities $\langle\eta(x;\sigma)\rangle$ were independent of x, $\langle\eta(x;\sigma)\rangle=n$ we would again have an equilibrium state with density per site equal to $2n$. Instead we start initially with $\langle\eta(x;\sigma)\rangle=\rho_0(\varepsilon x)$, where $\rho_0(q)$ is as before. Note, however, that $\rho(q,t)$ is now half the density per site; the maximal density is equal to two since there can now be two particles at each lattice site.

The proof for this model is very similar to that of Model 1. In both cases the transition from the microscopic variables to the macroscopic density, defined by (7), goes via local equilibrium. In fact what is proven is that the joint distribution of particles at any fixed set of lattice sites $\{\varepsilon^{-1}q+j_1,\ldots,\varepsilon^{-1}q+j_m\}$ is, in the limit $\varepsilon\to 0$, the same as in any uniform equilibrium system with average density $\rho=\rho(q,t)$.

3. Propagation of Shocks and Deviations from Macroscopic Behaviour

The inviscid Burgers' equation (8) 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 equation is supplemented with the condition that the entropy has to increase. This agrees with the solution obtained from the full equation (4) when we let $\nu \to 0$ in the solution. There is of course no room for such extra conditions in our microscopic model. The dynamics of particles are sufficient now to produce a unique evolution. In fact the theorem asserts that as $\varepsilon \to 0$ 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

$$\rho_0(q) = \begin{cases} \rho_- & \text{for } q<0, \\ \rho_+ & \text{for } q>0, \end{cases} \tag{10}$$

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

$$v_x = \frac{a}{\tau}(2p-1)(1-\rho_- - \rho_+), \tag{11}$$

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 $\varepsilon \to 0$, 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 solution of (4), when $\nu \neq 0$, for the initial conditions (10). The discontinuity is now smoothed out, but there is still a front with a shape that remains fixed, connecting the density ρ_- and ρ_+ travelling at the speed v_s. The thickness of this front is of $0(\nu/c)$. This suggests that on the microscopic scale too we should see a transition region connecting the low- and high-density regions of finite width D, in lattice units, travelling with a (mean) velocity v_s. That is, if we follow the evolution of our microscopic system with $p > \frac{1}{2}$ and with initial conditions (6) and (10) the interface should reach a fixed shape and should not keep on broadening. There are very strong hints, but no full proof as yet, that this is in fact the case: there is a stationary state of the lattice gas which has a front

of finite width D which moves with mean velocity v_s. There are fluctuations in the location of this front which behave like a Brownian motion. Evidence for this comes from both analytic and numerical computations and a full proof may be forthcoming soon. What one can show at present is that this is what happens in the weakly asymmetric process where $1-2p=\varepsilon$, and the macroscopic behaviour is dominated for times of order ε^{-2} by the Burgers' equation (4). The dominant deviation from this behaviour when one considers longer times of order ε^{-3} is then proven to be fluctuation in the location of the front.

The above picture is consistent with that obtained from fluctuating hydrodynamics. In the framework of that theory one assumes 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 $v(t)=v_x+\sqrt{\varepsilon}\xi(t)$, where t is macroscopic time $\xi(t)$ is white noise with a strength depending on ρ_+ and ρ_-. Thus the shock makes a random walk with mean square displacement 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 in the derivation of the deterministic equation,i.e. of order ε^{-1} macroscopic time units.

4. Summary

I have described the behaviour of some stochastic particle models with emphasis on how the macroscopic description emerges from the microscopic dynamics in a scaling limit. While even the most complicated models which can be treated with mathematical rigour at the present time are fairly primitive, the main point I 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 neighbouring particles only. Therefore the *spatial* degrees of freedom have the "right physics". In this sense these modes capture the essential features of real systems. They play the same role for hydrodynamics as the Ising model does for phase transitions: they show, by explicit analysis, the essential microscopic ingredients responsible for macroscopic behaviour.

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