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Nonlinear Lattice Gas Hydrodynamics

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Starting from a microdynamical description, we derive the equations governing the evolution of the hydrodynamic variables in a lattice gas automaton. The essential features are: (i) the local collision rules satisfy semi-detailed balance; this condition guarantees that a factorized local equilibrium distribution of the Fermi–Dirac form is invariant under the collision step, but not under propagation; (ii) particles entering a collision are uncorrelated (Boltzmann hypothesis); and (iii) the system can be arbitrarily far from global equilibrium; we do not not assume linear response, as usually imposed, to obtain the dissipative contributions. Linearization of the resulting hydrodynamic equations leads to Green–Kubo formulas for the transport coefficients. The main result is the set of fully nonlinear hydrodynamic equations for the automaton in the lattice Boltzmann approximation; these equations have a validity domain extending beyond the region close to equilibrium.

KEY WORDS: Hydrodynamic equations; lattice gas automata; nonlinear response; Boltzmann hypothesis; Green–Kubo transport coefficients.

One of the main objectives of statistical mechanics is to provide a connection between the microscopic dynamics of a system with many degrees of freedom and its macroscopic behavior. In this context, we propose the derivation of the fully nonlinear hydrodynamic equations that describe the macroscopic evolution of a lattice gas automaton. Previous derivations of hydrodynamic equations from the automaton microdynamics[1–5] are restricted to regions close to global equilibrium, thus limiting the validity of the results obtained in this way to a regime in which linear response and simple fluctuation-dissipation relations are valid. The present treatment does not make use of this hypothesis. Instead, it is assumed that the system is close to a local equilibrium state, where the space and time variation of

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the thermodynamic potentials occurs on a hydrodynamic scale (i.e., gradients are small). This is the usual Chapman–Enskog picture for a nonequilibrium system, which is necessary to derive the hydrodynamic equations from the microscopic dynamics.

A lattice gas automaton consists of a collection of particles moving on a regular d-dimensional lattice $\mathscr{L}$ at discrete time steps. A particle on a given node (with position denoted by $\mathbf{r}$) has a velocity chosen from a discrete set of values $\{\mathbf{c}_i\}_{i=1}^{b}$ corresponding to the particle being at rest, or to the particle propagating in one time step to sites which are the nearest neighbors, next nearest neighbors, etc. Each of these velocity states (labeled by Latin indices i, j,...), corresponds to a channel associated to a lattice node. We require that there be a maximum of one particle per channel. This *exclusion principle* is important because it allows a symbolic representation of the state of the system in terms of a given set of bits, and of its dynamics in terms of operations over sets of bits, which are easily implemented on a computer. The state of the automaton at time t is thus described by specifying the *configuration* on each and every node, i.e., the set of bits $\{n_i(\mathbf{r}, t)\}_{i=1}^{b}$ before collision, or the set of bits $\{n_i^*(\mathbf{r}, t)\}_{i=1}^{b}$ after collision.

The evolution of the automaton takes place in two stages: First, a propagation step, in which particles are moved according to their velocity; second, a local collision step, during which at each node a new configuration is chosen in a prescribed fashion as a function of the precollisional configuration. This second step is crucial to determine the type of physics the automaton will exhibit at the macro- and mesoscopic levels. In particular, the collision step should preserve the quantities that are invariant under the dynamics of the model system. The microdynamics of the automaton can then be summarized by the equation

$$n_i(\mathbf{r}, t+1) = n_i^*(\mathbf{r}-\mathbf{c}_i, t) \tag{1}$$

which means that the occupation of channel i on node $\mathbf{r}$ at a given time $t+1$ is equal to the postcollisional configuration of channel i on node $\mathbf{r}-\mathbf{c}_i$ at time t. Time and space are measured in automaton units.

Observables of the automaton are defined as averages over a nonequilibrium ensemble: $f_i(\mathbf{r}, t) = \langle n_i(\mathbf{r}, t)\rangle_{\mathrm{NE}}$ and $f_i^*(\mathbf{r}, t) = \langle n_i^*(\mathbf{r}, t)\rangle_{\mathrm{NE}}$. In particular, the hydrodynamic variables, that is, the densities of conserved quantities, are given by

$$\langle \underline{A}(\mathbf{r}, t)\rangle_{\mathrm{NE}} \equiv \{\langle A_\alpha(\mathbf{r}, t)\rangle\}_{\alpha=0}^{N_{\mathrm{hydro}}-1} = \sum_{i=1}^{b} f_i(\mathbf{r}, t)\,\underline{a}_i = \sum_{i=1}^{b} f_i^*(\mathbf{r}, t)\,\underline{a}_i \tag{2}$$

where $\underline{a}_i$ is a vector whose elements are the collisional invariants. In a thermal automaton whose collision rules preserve the number of particles, the momentum, and the kinetic energy per node, $\underline{a}_i = \{1, \mathbf{c}_i, e_i = c_i^2/2\}$ for the collisional invariants and $\langle \underline{A}(\mathbf{r}, t) \rangle = \{\rho(\mathbf{r}, t), \rho \mathbf{u}(\mathbf{r}, t), e(\mathbf{r}, t)\}$ for the hydrodynamic variables. In this case, the number of hydrodynamic fields is $N_{\text{hydro}} = D + 2$, where D is the space dimension of the automaton universe (we ignore effects related to spurious global invariants[6]).

The average of Eq. (1) over the nonequilibrium ensemble yields

$$f_i(\mathbf{r}, t+1) = f_i^*(\mathbf{r} - \mathbf{c}_i, t) = \exp\{-\mathbf{c}_i \cdot \nabla_{\mathbf{r}}\} f_i^*(\mathbf{r}, t) \tag{3}$$

With the assumption that particles entering a collision are decorrelated, Eq. (3) becomes the lattice Boltzmann equation

$$f_i(\mathbf{r}, t+1) = \exp\{-\mathbf{c}_i \cdot \nabla_{\mathbf{r}}\} \sum_{\{s\}\{\sigma\}} \sigma_i \langle \xi \rangle_{\{s\} \to \{\sigma\}} \times \prod_{k=1}^{b} (f_k(\mathbf{r}, t))^{s_k} (1 - f_k(\mathbf{r}, t))^{(1-s_k)} \tag{4}$$

where $\langle \xi \rangle_{\{s\} \to \{\sigma\}}$ is the collision matrix. The entries of this matrix are the probabilities having a configuration $\{\sigma\}$ as the outcome of a collision starting from a configuration $\{s\}$.

In automata with semi-detailed balance, $\sum_{\{s\}} \langle \xi \rangle_{\{s\} \to \{\sigma\}} = 1$, it can be shown[2] that an arbitrary distribution of the Fermi–Dirac form for the single-particle distribution

$$f_i = \frac{1}{1 + \exp\{-\underline{b} * \underline{a}_i\}} \tag{5}$$

without correlations between fluctuations in different channels, is invariant under the collision step. The quantities $\underline{b}$ are the thermodynamic fields conjugate to the conserved quantities (e.g., in a thermal automaton $\underline{b} \equiv \{\alpha, \gamma, -\beta\}$, where β is inversely proportional to the absolute temperature, α/β is the chemical potential, and γ is the thermodynamic potential conjugate to the momentum). The scalar product denoted by $*$ is a contraction of the indices labeling the conserved quantities. We define a local equilibrium ensemble

$$f_i^{\text{LE}}(\mathbf{r}, t) = \frac{1}{1 + \exp\{-\underline{b}(\mathbf{r}, t) * \underline{a}_i\}} \tag{6}$$

such that

$$\langle \underline{A}(\mathbf{r}, t)\rangle_{\mathrm{LE}} = \sum_{i=1}^{b} f_i^{\mathrm{LE}}(\mathbf{r}, t)\, \underline{a}_i$$
$$= \sum_{i=1}^{b} \frac{1}{1+\exp\{-\underline{b}(\mathbf{r}, t) * \underline{a}_i\}}\, \underline{a}_i \equiv \langle \underline{A}(\mathbf{r}, t)\rangle_{\mathrm{NE}} \tag{7}$$

Equation (7) defines the thermodynamic potentials implicitly in terms of the local values of the densities of conserved quantities: $\underline{b}(\mathbf{r}, t) = \underline{b}(\langle \underline{A}(\mathbf{r}, t)\rangle)$. For densities of conserved quantities, since the local equilibrium ensemble has been defined in such a way that $\langle \underline{A}(\mathbf{r}, t)\rangle_{\mathrm{LE}} = \langle \underline{A}(\mathbf{r}, t)\rangle_{\mathrm{NE}}$, we may omit the label indicating the ensemble over which the average is taken. For an arbitrary vector $\{B_l(\mathbf{r}, t)\}_{l=1}^{b}$, the local equilibrium average is given by

$$\langle B(\mathbf{r}, t)\rangle_{\mathrm{LE}} \equiv \sum_{i=1}^{b} B_l(\mathbf{r}, t)\, f_l^{\mathrm{LE}}(\mathbf{r}, t) \tag{8}$$

Multiplying Eq. (3) by $\underline{a}_i$, summing over i, and making use of the conservation laws, we obtain

$$\langle \underline{A}(\mathbf{r}, t+1)\rangle - \langle \underline{A}(\mathbf{r}, t)\rangle = \sum_{i=1}^{b} (\exp\{-\mathbf{c}_i \cdot \nabla_{\mathrm{r}}\} - 1)\, f_i^*(\mathbf{r}, t)\, \underline{a}_i \tag{9}$$

The microscopic evolution equations (9) are finite-difference equations containing the full dynamics of the automaton susceptible to describe its behavior at all scales. In order to derive hydrodynamic-type equations from (9), we introduce the parameter ε, which represents the ratio between characteristic microscopic and hydrodynamic length scales. This ratio is assumed to be small, a fact which allows us to perform a multiple-scale analysis. Thus, we anticipate the scales of physical interest in the solution of (9) and introduce the following variables[2]: a space variable $\mathbf{r}_1 = \varepsilon \mathbf{r}$ and two time variables $t_1 = \varepsilon t$, which is of order ε^0 in the regime where Euler equations are valid, and $t_2 = \varepsilon^2 t$, which is of order ε^0 in the dissipative regime. Hence, the substitutions $\nabla_{\mathrm{r}} \to \varepsilon \nabla_{\mathrm{r}_1}$ and $\partial_t \to \varepsilon\, \partial_{t_1} + \varepsilon^2\, \partial_{t_2}$ in Eq. (9) lead to the hierarchy of equations labeled by the different powers of ε:

$$\varepsilon^1: \quad \partial_{t_1} \langle \underline{A}(\mathbf{r}, t)\rangle + \nabla_{\mathbf{r}_1} \cdot \langle \underline{\mathbf{J}}(\mathbf{r}, t)\rangle_{\mathrm{LE}} = 0 \tag{10}$$

$$\varepsilon^2: \quad \left(\partial_{t_2} + \frac{1}{2}\partial_{t_1}^2\right) \langle \underline{A}(\mathbf{r}, t)\rangle = \frac{1}{2} \nabla_{\mathbf{r}_1} \nabla_{\mathbf{r}_1} : (\langle \mathbf{c}\underline{\mathbf{J}}(\mathbf{r}, t)\rangle_{\mathrm{LE}})$$
$$+ \frac{1}{\varepsilon^2} \sum_{i=1}^{b} (\exp\{-\mathbf{c}_i \cdot \nabla_{\mathbf{r}_1}\} - 1)\, \underline{a}_i (f_i^*(\mathbf{r}, t) - f_i^{\mathrm{LE}}(\mathbf{r}, t)) \tag{11}$$

The definition of the currents associated to the conserved fields is

$$\langle \underline{\mathbf{J}}(\mathbf{r}, t)\rangle_{\mathrm{LE}} \equiv \sum_{i=1}^{b} \underline{\mathbf{J}}_i f_i^{\mathrm{LE}}(\mathbf{r}, t) = \sum_{i=1}^{b} \mathbf{c}_i \underline{a}_i f_i^{\mathrm{LE}}(\mathbf{r}, t) \tag{12}$$

with $\underline{\mathbf{J}}_i \equiv \mathbf{c}_i \underline{a}_i$, and

$$\langle \mathbf{c}\mathbf{J}(\mathbf{r}, t)\rangle_{\mathrm{LE}} = \sum_{i=1}^{b} \mathbf{c}_i \underline{\mathbf{J}}_i f_i^{\mathrm{LE}}(\mathbf{r}, t) = \sum_{i=1}^{b} \mathbf{c}_i \mathbf{c}_i \underline{a}_i f_i^{\mathrm{LE}}(\mathbf{r}, t) \tag{13}$$

Equations (10) are the Euler equations describing the streaming part of the dynamics, and Eqs. (11) contain the dissipative contributions.

In order to perform the averages we choose an initial local-equilibrium ensemble in which the values of the thermodynamic variables vary significantly only over a hydrodynamic length scale. This corresponds to the Chapman–Enskog picture of a nonequilibrium state[7] where the deviations from local equilibrium are of the order of the gradients of the conserved quantities [i.e., both $\delta f_i(\mathbf{r}, t) = f_i(\mathbf{r}, t) - f_i^{\mathrm{LE}}(\mathbf{r}, t)$ and $\delta f_i^*(\mathbf{r}, t) = f_i^*(\mathbf{r}, t) - f_i^{\mathrm{LE}}(\mathbf{r}, t)$ are of order ε]. In case the initial state does not satisfy this condition, there should be an initial transient regime where the hydrodynamic equations are not valid. The duration of this regime is of the order of τ_m, the time necessary to relax to local equilibrium. Hence, to lowest order in ε, the lattice Boltzmann equation (4) can be linearized around the local equilibrium distribution,

$$\delta f_i^*(\mathbf{r}, t) = \sum_j \mathscr{L}_{ij}^{\mathrm{LE}}(\mathbf{r}, t)\, \delta f_j(\mathbf{r}, t) + \mathcal{O}(\varepsilon^2) \tag{14}$$

with

$$\mathscr{L}_{ij}^{\mathrm{LE}}(\mathbf{r}, t) = \sum_{\{s\}\{\sigma\}} \sigma_i \frac{s_j - f_j^{\mathrm{LE}}(\mathbf{r}, t)}{\kappa_j^{\mathrm{LE}}(\mathbf{r}, t)} \langle \xi \rangle_{\{s\}\to\{\sigma\}} \times \prod_{k=1}^{b} (f_k^{\mathrm{LE}}(\mathrm{r}, t))^{s_k} (1 - f_k^{\mathrm{LE}}(\mathbf{r}, t))^{(1-s_k)} \tag{15}$$

The matrix $\mathscr{L}^{\mathrm{LE}}(\mathbf{r}, t)$ can be separated into two parts

$$\mathscr{L}_{ij}^{\mathrm{LE}}(\mathbf{r}, t) = \mathscr{P}_{ij}^{\mathrm{LE}}(\mathbf{r}, t) + \tilde{\mathscr{L}}_{ij}^{\mathrm{LE}}(\mathbf{r}, t) \tag{16}$$

where $\mathscr{P}_{ij}^{\mathrm{LE}}(\mathbf{r}, t) = \kappa_i^{\mathrm{LE}}(\mathbf{r}, t)\, \underline{a}_i * \langle \underline{A} \,|\, \underline{A} \rangle_{\mathrm{LE}}^{-1}(\mathbf{r}, t) * \underline{a}_j$ is an operator projecting onto the set of constants of motion, with $\langle \underline{A} \,|\, \underline{A} \rangle_{\mathrm{LE}}(\mathbf{r}, t) = \sum_i \kappa_i^{\mathrm{LE}}(\mathbf{r}, t)\, \underline{a}_i \underline{a}_i$, the local equilibrium susceptibility matrix, and $\kappa_i^{\mathrm{LE}} = f_i^{\mathrm{LE}}(1 - f_i^{\mathrm{LE}})$. The

matrix $\tilde{\mathscr{L}}^{\mathrm{LE}}(\mathbf{r}, t)$ has the same set of eigenvectors as $\mathscr{L}^{\mathrm{LE}}(\mathbf{r}, t)$. The eigenvalues of $\tilde{\mathscr{L}}^{\mathrm{LE}}(\mathbf{r}, t)$ corresponding to the set of collisional invariants are zero. The remaining eigenvalues (i.e., the *kinetic* eigenvalues) coincide with those of $\mathscr{L}^{\mathrm{LE}}(\mathbf{r}, t)$ and have an absolute value strictly smaller than one.[8] Using these properties, we can solve Eq. (14) with the specified initial conditions [i.e., $\delta f_i(\mathbf{r}, t) = 0$]; the result reads (the technical details of the derivation will be presented elsewhere)

$$\delta f_i^*(\mathbf{r}, t) = -\sum_{\tau=1}^{t} \sum_{j=1}^{b} \{[\tilde{\mathscr{L}}^{\mathrm{LE}}(\mathbf{r}, t)]^{\tau}\}_{ij} (\mathbf{c}_j \cdot \nabla_{\mathbf{r}} + \partial_t) f_j^{\mathrm{LE}}(\mathbf{r}, t) + \mathcal{O}(\varepsilon^2 \tau_m) \tag{17}$$

Within the same level of approximation we can further replace in (17) the upper limit in the summation over τ by infinity for $t \gg \tau_m$.

Recombining Eqs. (10) and (11) and inserting the result (17), we can rewrite the equations of motion for the hydrodynamic variables as a set differential equations (valid up to order ε^2) in terms of the variables $\mathbf{r}$, t, which are now taken as continuous,

$$\partial_t \langle \underline{A}(\mathbf{r}, t) \rangle + \nabla_{\mathbf{r}} \cdot \langle \underline{\mathbf{J}}(\mathbf{r}, t) \rangle_{\mathrm{LE}} = \nabla_{\mathbf{r}} \cdot \left[\sum_{i,j,l} \underline{\mathbf{J}}_i \sum_{\tau=0}^{\infty}{}' \{[\mathscr{L}^{\mathrm{LE}}(\mathbf{r}, t)]^{\tau}\}_{ij} \mathscr{Q}_{jl}^{\mathrm{LE}}(\mathbf{r}, t)\, \mathbf{c}_l \cdot \nabla_{\mathbf{r}} f_l^{\mathrm{LE}}(\mathbf{r}, t) \right] \tag{18}$$

where $\mathscr{Q}_{ij}^{\mathrm{LE}}(\mathbf{r}, t) = \delta_{ij} - \mathscr{P}_{ij}^{\mathrm{LE}}(\mathbf{r}, t)$ is the local equilibrium projector onto the space orthogonal to the set of collisional invariants. We have replaced the matrix $\tilde{\mathscr{L}}^{\mathrm{LE}}(\mathbf{r}, t)$ by $\mathscr{L}^{\mathrm{LE}}(\mathbf{r}, t)$, given that the quantity upon which it acts contains no projections onto the conserved quantities. The prime in the summation indicates that the first term of the sum ($\tau = 0$) is multiplied by 1/2; this factor appears as a consequence of the discreteness of time in the automaton.

Equation (18) is the most general form of the hydrodynamic equations in the lattice Boltzmann approximation. They can be used to explore nonequilibrium phenomena such as far-from-equilibrium steady states and hydrodynamic instabilities. The main novelty with respect to previous derivations is that the expression of the dissipative term [on the right hand side of Eq. (18)] is valid even far from global equilibrium.

We can linearize Eq. (18) assuming small deviations from a global equilibrium state $\langle \delta \underline{A}(\mathbf{r}, t) \rangle = \langle \underline{A}(\mathbf{r}, t) \rangle - \langle \underline{A} \rangle_{\mathrm{eq}}$ to obtain the usual linear response result[3, 4, 9, 10]

$$\partial_t \langle \delta \underline{A}(\mathbf{r}, t) \rangle + \nabla_{\mathbf{r}} \cdot [\langle \underline{\mathbf{J}} | \underline{A} \rangle_{\mathrm{eq}} * \langle \underline{A} | \underline{A} \rangle_{\mathrm{eq}}^{-1} * \langle \delta \underline{A}(\mathbf{r}, t) \rangle] = \nabla_{\mathbf{r}} \nabla_{\mathbf{r}} : [\underline{\Lambda}_{\mathrm{eq}} * \langle \underline{A} | \underline{A} \rangle_{\mathrm{eq}}^{-1} * \langle \delta \underline{A}(\mathbf{r}, t) \rangle] \tag{19}$$

where $\langle \underline{\mathbf{J}} \,|\, \underline{A} \rangle_{\mathrm{eq}} = \sum_i \kappa_i^{\mathrm{eq}} \underline{\mathbf{J}}_i \underline{a}_i$, and the matrix of linear transport coefficients is given by the expression

$$\underline{\Delta}_{\mathrm{eq}} = \sum_{\tau=0}^{\infty\prime} \langle \hat{\underline{\mathbf{J}}} \,|\, \hat{\underline{\mathbf{J}}}(\tau) \rangle_{\mathrm{eq}} = \sum_{\tau=0}^{\infty\prime} \left[\sum_{i,j} \hat{\underline{\mathbf{J}}}_i \hat{\underline{\mathbf{J}}}_j \{ [\underline{\mathscr{L}}^{\mathrm{eq}}]^{\tau} \}_{ij} \kappa_j^{\mathrm{eq}} \right]$$

$$= \sum_{\tau=0}^{\infty\prime} \left[\frac{1}{V} \sum_{\mathbf{r}\mathbf{r}'} \sum_{i,j} \langle (\hat{\underline{\mathbf{J}}}_i \delta n_i(\mathbf{r}, t))(\hat{\underline{\mathbf{J}}}_j \delta n_j(\mathbf{r}', 0)) \rangle_{\mathrm{eq}}^{\mathrm{B}} \right] \tag{20}$$

where $\hat{\underline{\mathbf{J}}}_i = \sum_l \underline{\mathscr{Q}}_{jl}^{\mathrm{eq}} \underline{\mathbf{J}}_l$ is the part of the current with no projections onto the linear constants of motion, and V is the number of nodes of the lattice. The superscript B indicates that the time-correlation function is evaluated in the Boltzmann approximation (i.e., mode-coupling effects are neglected).

In summary, we have given a derivation of the nonlinear hydrodynamic equations for a lattice gas automaton satisfying the semi-detailed balance condition. This condition implies that a factorized distribution with a Fermi–Dirac form for each channel is a stable global equilibrium distribution, invariant under the automaton dynamics. The derivation makes use of the fact that a local-equilibrium distribution for each node in the lattice is invariant under the collision step of the automaton dynamics, but not under the propagation step. The deviations from local equilibrium are therefore of the order of the gradients of the densities of the conserved fields, which are small in a hydrodynamic regime. The automaton thus lends itself naturally to a Chapman–Enskog description in which the nonequilibrium distribution is obtained perturbatively from the local-equilibrium one. The present derivation ignores modifications of the probability distribution arising from the presence of spurious invariants, and neglects mode-coupling effects.

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