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Diffusion Simulation with a Deterministic One-Dimensional Lattice-Gas Model

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A one-dimensional lattice-gas model is proposed and used to simulate diffusion processes in one dimension. Explicit forms of transport coefficients are given as a function of density and kinetic energy within the Boltzmann approximation. Without definitions of temperature and pressure, a steady nontrivial solution is given analytically in the nonconvective case when the kinetic energy is kept constant.

KEY WORDS: Lattice gas; cellular automata; diffusion.

1. INTRODUCTION

Since the work of Frisch *et al.*,[1] there has been an increasing interest in lattice-gas models for fluid mechanics and many extensions of this model have been proposed and applied to different problems, using different species or velocities and/or higher space dimension.[2] While most of the studies driven by practical applications concern two- and three-dimensional flows, little work exists on the one-dimensional case: simulations of the Burgers' equation[3] and compressible flows.[4,5] However, the one-dimensional models present very interesting theoretical properties. They are significantly simpler than their counterpart in higher dimensions and thus they give better access to analytical results. They also have specific properties such as the divergence of transport coefficients with the size of the system.[6] In this paper, we study a one-dimensional model with two particle speeds and use it to simulate diffusion processes in a much simpler way than Chopard and Droz.[7] The microscopic model and its conserved quantities are described in Section 2. The macroscopic equations and the

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transport coefficients are given in Section 3, along with a discussion of the difficulties of correctly defining a temperature scale. The details of the calculations for the complete set of known nonphysical invariants will be left for a future work. The results of the numerical simulations are presented in Section 4 for the speed of sound and the steady solution at constant kinetic energy.

2. MICROSCOPIC DESCRIPTION OF THE MODEL

We take a circle and discretize it in L sites (lattice with periodic boundary condition). There are particles which interact at the nodes of the lattice and move from node to node according to their velocities. The evolution of the system consists in two steps: collision step and propagation step. To obtain the hydrodynamic behaviors, the redistribution of particles during the collision step must satisfy three conservation laws for mass, momentum, and energy. During the propagation step, the particles move from nodes to nodes according to their velocities, the mass, momentum, and energy being globally conserved. Let $M=\{m_i\}$ and $C=\{c_i\}$ be the sets of particle masses and velocities for the four-bit model studied in this paper:

i	1	2	3	4
M	$\{m,$	$m,$	$2m,$	$2m\}$
C	$\{2c,$	$-2c,$	$c,$	$-c\}$

We add an exclusion principle for the particles, such that there is no more than one particle of the same mass and same velocity on a given site at a given time, as if all the particles were fictitious fermions. Among the $2^4=16$ possible states only 2 of them can undergo effective collisions: the head-on collisions of a fast-light (hot) particle with a slow-heavy (cold) particle leads to a reversal of their velocities (collision of particle 1 with particle 4 gives particle 2 and particle 3, and vice versa), as shown in Fig. 1.

Since there is an exclusion principle, the system can be described by four Boolean fields $\{n_i(x, t)\}$, where $n_i(x, t)$ is the presence ($n_i=1$) or the absence ($n_i=0$) of particle i at site x and time t. The exact discrete microdynamical equation for $n_i(x, t)$ is given by (for a time step equal to 1)

$$n_i(x+c_i, t+1)=n_i(x, t)-v_i T(\mathbf{n}(x, t)) \tag{2.1}$$

Fig. 1. Reversible collision laws of the model: particles $(1+4)\leftrightarrow(2+3)$.

where c_i is the velocity of particle i, v_i is the ith component of a four-component vector $\mathbf{v} = \{1, -1, -1, 1\}$, and the collision term $T(\mathbf{n})$ is a nonlinear function of n_k ($k \in \{1, 2, 3, 4\}$) given by

$$T(\mathbf{n}) = n_1(1-n_2)(1-n_3)\, n_4 - (1-n_1)\, n_2 n_3 (1-n_4) \tag{2.2}$$

The conservation laws come from the following relations derived from Eq. (2.1):

$$n_1(x+2c, t+1) + n_2(x-2c, t+1) = n_1(x, t) + n_2(x, t) \tag{2.3}$$

$$n_3(x+c, t+1) + n_4(x-c, t+1) = n_3(x, t) + n_4(x, t) \tag{2.4}$$

$$n_1(x+2c, t+1) - n_4(x-c, t+1) = n_1(x, t) - n_4(x, t) \tag{2.5}$$

Summing the appropriate linear combinations of Eqs. (2.3)–(2.5) on all the lattice nodes, it is very easy to check the conservation of the total mass, momentum, and kinetic energy. But Eqs. (2.3) and (2.4) can also be summed on sublattices when L is divisible by four, showing the existence of four nonphysical conservation laws.[8–10] Three of these "spurious" invariants are "staggered" in space and time:

$$H_{he} = (-1)^t \sum_x (-1)^x [n_1(2x, t) + n_2(2x, t)] \tag{2.6}$$

$$H_{ho} = (-1)^t \sum_x (-1)^x [n_1(2x+1, t) + n_2(2x+1, t)] \tag{2.7}$$

$$H_c = (-1)^t \sum_x (-1)^x [n_3(x, t) + n_4(x, t)] \tag{2.8}$$

and the fourth one is only staggered in space:

$$F_h = \sum_x (-1)^x [n_1(x, t) + n_2(x, t)] \tag{2.9}$$

Recently, we have found four more invariants with a period three both in space and time when L is divisible by three:

$$H_{\bar{\omega}r} = \bar{\omega}^t \sum_x \bar{\omega}^x [n_1(x, t) - n_4(x, t)] \tag{2.10}$$

$$H_{\bar{\omega}l} = \bar{\omega}^{-t} \sum_x \bar{\omega}^x [n_2(x, t) - n_3(x, t)] \tag{2.11}$$

$$H_{\omega r} = \omega^t \sum_x \omega^x [n_1(x, t) - n_4(x, t)] \tag{2.12}$$

$$H_{\omega l} = \omega^{-t} \sum_x \omega^x [n_2(x, t) - n_3(x, t)] \tag{2.13}$$

where $\omega = (-1+3\sqrt{-1})/2$ and $\bar{\omega} = (-1-3\sqrt{-1})/2$ are the complex cube roots of unity.

Then, when L is divisible by 12, the present model has 11 global invariants.

3. MACROSCOPIC EQUATIONS AND TEMPERATURE

3.1. Macroscopic Equations and Transport Coefficients

With such a large number of invariants, the derivation of the full set of macroscopic dynamical equations is very painful and will be left for future work. In what follows, we shall assume that all the spurious invariants are set to zero and their local fluctuations can be neglected. These assumptions allow us to deal only with the physical quantities and to derive their dynamical equations from the following three key points.

The first one is the Boltzmann approximation (molecular chaos assumption): the ensemble average of the collision term of Eq. (2.1) can be replaced by the collision term of the averaged local quantities $N_i(x, t) = \langle n_i(x, t) \rangle$. Then, taking the ensemble average, Eq. (2.1) can be written

$$N_i(x + c_i, t + 1) = N_i(x, t) - v_i T(\mathbf{N}(x, t)) \tag{3.1}$$

The macroscopic variables—the density ρ, the momentum J, and the energy e—are now related to the N_i by

$$\rho = \sum_{i=1}^{4} m_i N_i \tag{3.2}$$

$$J = \sum_{i=1}^{4} m_i c_i N_i \tag{3.3}$$

$$e = \sum_{i=1}^{4} \frac{1}{2} m_i c_i^2 N_i \tag{3.4}$$

The second point is the existence of an H-theorem[11] which proves the existence of an equilibrium state for the homogeneous situation obeying a Fermi–Dirac distribution, a function only of the conserved quantities assumed uniform in space and time.

The last point is the existence of different time scales for different physical processes when the homogeneous equilibrium is modified by small perturbations, slowly varying over length scales longer than $1/\varepsilon$, with $\varepsilon \ll 1$: relaxation to equilibrium with a time scale t_0 (at this level, the dynamics

is reversible), macroscopic sound propagation with a time scale $t_1 = t_0/\varepsilon$, and macroscopic diffusion with a time scale $t_2 = t_0/\varepsilon^2$, with $t_0 \ll t_1 \ll t_2$.

When ε and J/mc are much smaller than 1 (and the spurious invariants set to zero), a local expansion of the local equilibrium around $J = 0$, followed by a multiscale expansion in ε of the perturbations, can be used to derive the complete set of macroscopic hydrodynamics equations from Eq. (3.1):

$$\partial_t \rho + \partial_x J = 0 \tag{3.5}$$

$$\partial_t J + \partial_x 2e = 0 \tag{3.6}$$

$$\partial_t e + \partial_x(\tfrac{1}{2}c_s^2 J) + \partial_x(C_\rho \partial_x \rho + C_e \partial_x e) = 0 \tag{3.7}$$

where the speed of sound c_s and the coefficients C_ρ and C_e are functions of ρ and e:

$$c_s^2 = \left(\frac{4d_h(1-d_h) + d_c(1-d_c)}{\chi}\right) c^2 \tag{3.8}$$

$$C_\rho = \left(\frac{1}{\chi} - 1\right) c^4 \tag{3.9}$$

$$C_e = -\left(\frac{1}{\chi} - 1\right) \frac{5c^2 - c_s^2}{2} \tag{3.10}$$

χ, d_h, and d_c being related to ρ and e by

$$\chi = d_h(1-d_h) + d_c(1-d_c) \tag{3.11}$$

$$d_h = \frac{2e - \rho c^2}{6mc^2} \tag{3.12}$$

$$d_c = \frac{2\rho c^2 - e}{6mc^2} \tag{3.13}$$

Equations (3.5)–(3.7) are an approximation of the exact Boltzmann equation which neglects the contributions of order εJ^3, $\varepsilon^2 J^2$, $\varepsilon^3 J$, and higher. The full set of equations correct to the same order of the spurious invariants requires the addition of eight equations. Their derivation will be obtained by splitting the local distributions N_i in their slow and fast components in space and time.[12] Preliminary results for the spurious invariants of period two and four indicate that they act as passive scalars and do not interact with the physical equations up to order εI^3, where I is one of these spurious invariants. At this time, no analysis of the effects of

the spurious invariants of period three has been performed, but since they appear at the level of momentum terms, they could show up at the level of the pressure term, as in ref. 10.

3.2. Definitions of a Temperature Scale

We did not use the term "heat conduction" in the previous subsection because the temperature was not defined. It seems that the usual definition of temperature T through the kinetic energy e is not very proper in our fictitious fermion system. We want to discuss the two definitions of temperature through entropy and through kinetic energy e. The definition of entropy S is the following:

$$S = \sum_{i=1}^{4} [N_i \ln N_i + (1 - N_i) \ln(1 - N_i)] \tag{3.14}$$

which can be written for an equilibrium state as follows:

$$\begin{aligned} S = \frac{1}{3mc^2} & [(2e - \rho c^2) \ln(2e - \rho c^2) + (2\rho c^2 - e) \ln(2\rho c^2 - e) \\ & + (6mc^2 + \rho c^2 - 2e) \ln(6mc^2 + \rho c^2 - 2e) \\ & + (6mc^2 - 2\rho c^2 + e) \ln(6mc^2 - 2\rho c^2 + e) - 4 \ln 6] \end{aligned} \tag{3.15}$$

The temperature can be defined by:

1. $T_{\text{th}} = -(\partial e / \partial S)_\rho$, so that T_{th} is given by

$$T_{\text{th}} = 3c^2 \left(\ln \frac{2\rho c^2 - e}{6mc^2 - 2\rho c^2 + e} + 2 \ln \frac{6mc^2 + \rho c^2 - 2e}{2e - \rho c^2} \right)^{-1} \tag{3.16}$$

which varies over $(-\infty, +\infty)$,

2. Definition through kinetic energy:

$$T_k = \frac{2e}{\rho} \tag{3.17}$$

which varies between 1 and 4, while T_k varies between 1 and 2 in the case studied by Chopard and Droz.[7]

Figure 2 shows the temperature as a function of the density for $e = 3.0$ according to Eqs. (3.16) and (3.17). The thermodynamic temperature T_{th} is negative for $\rho < 3m$, which corresponds to the situation of a two-level system with more particles in the excited state than in the fundamental one.

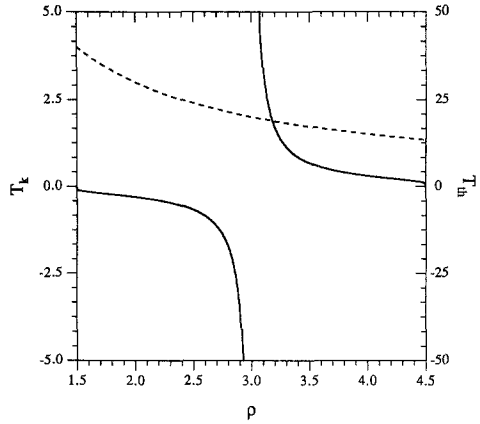

Fig. 2. Temperature as a function of density; the solid lines come from Eq. (3.16) and the dashed line from Eq. (3.17).

For $\rho > 3$, T_{th} is positive, corresponding to the physical situation of more cold particles than hot ones. Around $\rho = 3$, T_{th} changes its sign, going from $-\infty$ to ∞. As stated by Ernst,[13] from a thermodynamic point of view, the only valid definition of the temperature is given by (3.16), which must be used to derive the related coefficients, such as the heat conduction or heat capacities.

In addition, in the same paper Ernst pointed out that the Droz model and ours describe more a diffusive process than a thermal one: the populations of slow and fast particles are constant. However, the formal derivation of the dynamical equations is exactly the same for the two approaches and, in our opinion, this point remains quite academic without a blind test to distinguish them, a test which has not yet been found.

4. NUMERICAL SIMULATIONS

4.1. Speed of Sound Measurements

The speed of sound is measured from the period of oscillation of a small periodic perturbation of the velocity for given average density and energy.[14] The statistical noise is kept to a reasonable level by averaging 2048 independent lines with a length $L = 1024$ and periodic boundary conditions. Figures 3 and 4 show the results of simulations for two different energies e compared to the values predicted by Eq. (3.8). Note that this method gives access to C_ρ and C_e, but these quantities diverge for long wavevectors and comparisons between simulations and theory require very lengthy calculations beyond the scope of this paper.[6]

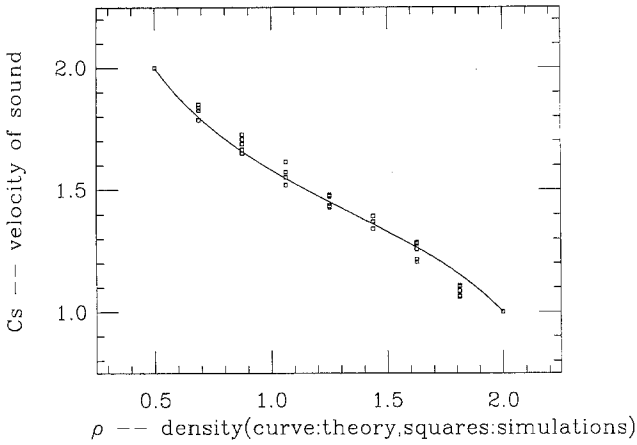

Fig. 3. Speed of sound c_s as a function of density ρ for energy $e = 1.0$, square points are the numerical results, the solid line is from Eq. (3.8).

4.2. Steady Solutions

When $J = 0$, ρ is steady and e constant, as a consequence of Eqs. (3.5) and (3.6), while it results from Eq. (3.7) that e is also steady and ρ is the solution of

$$\partial_x(C_\rho \partial_x \rho) = 0 \tag{4.1}$$

Integrating twice Eq. (4.1), we obtain the analytical solution for a given kinetic energy e:

$$\rho + \frac{6m^2c^2}{(m^2c^4 + 6mc^2e - e^2)^{1/2}} \ln\left(\frac{\rho_1 - \rho}{\rho - \rho_2}\right) = K_1 x + K_2 \tag{4.2}$$

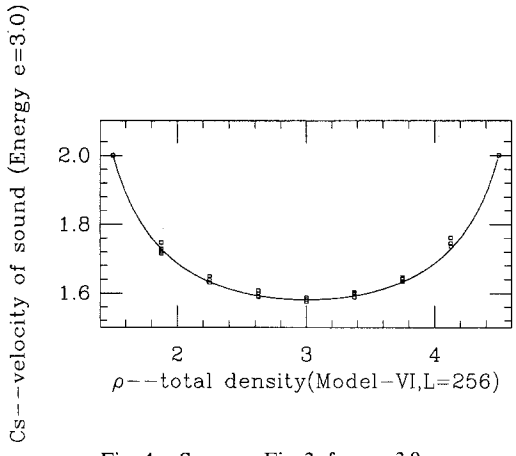

Fig. 4. Same as Fig. 3, for $e = 3.0$.

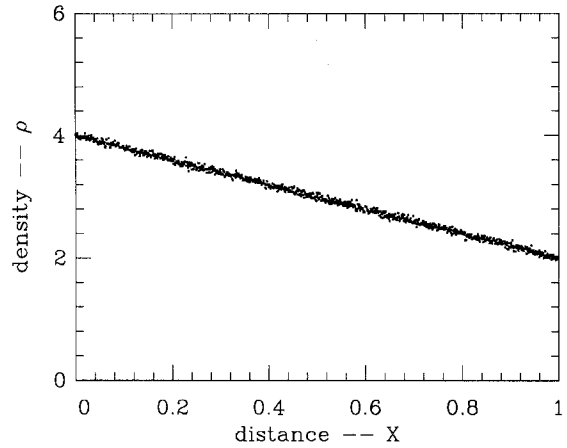

Fig. 5. Steady solution of density ρ as a function of the distance x; points are the numerical results, the solid line is the analytical solution.

where K_1 and K_2 are two integration constants which depend on the boundary conditions, while ρ_1, ρ_2 are the two roots of the following equation:

$$\rho^2 - \frac{6mc^2 + 8e}{5c^2}\rho + \frac{5e^2 - 6mc^2 e}{5c^4} = 0 \tag{4.3}$$

with $\rho_1 > \rho_2$. We see from Eq. (4.2) that the density ρ is almost a linear function of x.

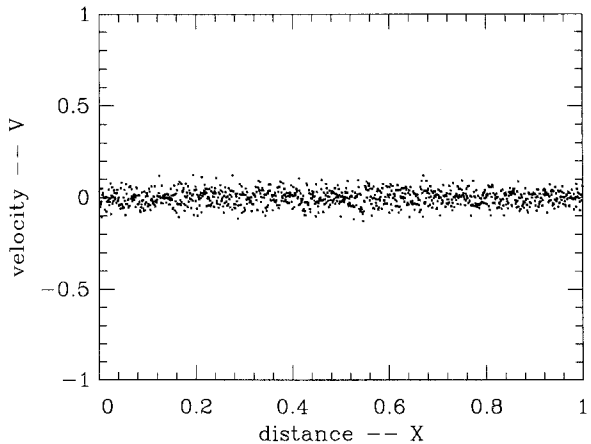

Fig. 6. Velocity fluctuations showing the amplitude of the statistical noise.

For the simulations, the initial configuration is chosen such that $J=0.0$, $e=3.0$, and $\rho(x)$ is a linear function of x, with $\rho(0)=4.0$ and $\rho(L)=2.0$. In this case, K_1 and K_2 are respectively equal to $2.448/L$ and 1.776 ($L=1023$). Using fixed boundary conditions, the values of e, $\rho(0)$, and $\rho(L)$ are kept constant. The simulation is then run 1000 time steps to reach an equilibrium. Figure 5 gives the final density distribution; note the nearly linear dependence on x of this distribution, which prevents any measurement of size effects on C_ρ from such a noisy simulation. Figure 6 shows the velocity fluctuation resulting from the statistical noise, due to the microdynamics and the Monte Carlo method used to set up the initial configuration and the boundary conditions. Since these fluctuations remain small and bounded, there is no production of a macroscopic flow and the hypotheses of steady states and negligible spurious invariants hold during the time evolution.

5. CONCLUSION

This very simple, and apparently harmless, lattice-gas model can be used not only to simulate one-dimensional unsteady flows, but also to investigate both numerically and theoretically difficult problems appearing in lattice gases, such as the effects of spurious invariants or the thermal properties of these models. Various boundary and initial conditions can easily be inserted in the numerical program (this is one of the advantages of lattice-gas models). We have derived the three hydrodynamic equations and the corresponding transport coefficients through a Chapman–Enskog expansion. Since the submission of the first version of this paper, an exhaustive search for linear invariants has been performed which guarantees that all of them are now known.[9] However, the derivation of the eight macroscopic dynamical equations for the eight linear spurious invariants has not yet been finished due to the complexity of the calculations. Numerical simulations do confirm the theoretical predictions for the speed of sound c_s and the analytical steady solution of density ρ. Numerical measurements for the transport coefficients are under investigation and their divergence will be studied by the renormalization group theory.[6] Exact solutions have been obtained for the corresponding model of the standard discrete kinetic theory without exclusion principle.[15,16]

We have also shown that this gas is not an ideal one, as stated by Chopard and Droz.[7] However, a complete thermodynamic description remains to be done. Especially, the pressure and the sound speed have to be derived within this frame and the results compared to those obtained by the kinetic theory. In our opinion, these points are of particular importance in order to retain enough control on the simulations of thermal processes.

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