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Lattice Gas with a Liquid-Gas Transition

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We discuss a new momentum-conserving lattice-gas model in which particles are allowed to exchange momentum between distant sites. The interactions may be tuned so that a first-order transition occurs between a dense and a light phase. An equation of state may be predicted with the assumption that the lattice is in a factorized state just after the particles have propagated. This method accurately predicts the pressure of the stable and unstable states.

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The determination of the flow of a mixture of several phases is a difficult and complex task. It is important in many areas of science and engineering. For instance, the study of critical phenomena in fluids involves the hydrodynamics of such a mixture. Interestingly, it is possible to obtain a model of great simplicity on the microscopic scale which has both a phase transition and hydrodynamic behavior. This paper is devoted to the definition and a preliminary description of the properties of such a model. The latter is a lattice gas akin to the hexagonal lattice gas of Frisch, Hasslacher, and Pomeau,[1,2] which has already been shown to obey large-scale equations similar to the Navier-Stokes equations.[3] Such lattice-gas models with phase transitions have already been proposed in certain cases, such as separation transitions in binary fluid mixtures.[4-7] These models are remarkably realistic despite their simplicity.[5] Ising-like models have also been suggested.[8]

In our model, particles live on a hexagonal lattice $\mathcal{L}$ as in Ref. 2,

$$\mathcal{L}=\{\mathbf{x}_{ij}\,|\,\mathbf{x}_{ij}=(i+\tfrac{1}{4}(-1)^j,\tfrac{1}{2}\sqrt{3}j),\ (i,j)\in Z^2\},$$

and are allowed to have a number of velocities $\mathbf{c}_i$. There are rest particles with $\mathbf{c}_0=0$ and particles with unit velocity $\mathbf{c}_j=(\cos[2\pi(j-1)/6],\sin[2\pi(j-1)/6])$ for $0<j\leq 6$. There is at most one particle for each velocity. Thus the configuration s of a site $\mathbf{x}\in\mathcal{L}$ is defined by $s=(s_0,s_1,\ldots,s_6)$, where s_i is a Boolean variable. The rules are designed so that particles may move about in the lattice while preserving their momentum. The evolution of the lattice during one time step is obtained by the composition of several operators. As usual[2] we define a streaming operator $\mathcal{S}$ and a local collision operator $\mathcal{C}$. In what follows $\mathcal{C}$ is the "FHP III" collision operator.[2] In addition, we define several nonlocal *interaction operators* $\mathcal{I}_n,\mathcal{I}'_n$. These operators exchange momentum between pairs of sites at a distance r. They are designed to mimic a long-range attractive force between particles. This is realized by selecting ensembles of pairs in $\mathcal{L}$. At each end of a pair, the directions of particles are changed so that particles point towards each other. This is done in several steps which we now proceed to describe more precisely. The evolution of the lattice from time n to time $n+1$ is obtained by an operator $\mathcal{E}_n$:

$$\mathcal{E}_n=\mathcal{C}\circ\mathcal{I}_n\circ\mathcal{I}'_n\circ\mathcal{S}. \tag{1}$$

(In $\mathcal{I}_n$, $\mathcal{I}'_n$, etc., the index n is meant to be modulo 3.) The interaction operators act on pairs of sites taken in a partition $\mathcal{P}_n$ of the lattice. $\mathcal{P}_1$ is the set of pairs $p_{kl}=(\mathbf{x}_a,\mathbf{x}_b)=(\mathbf{x}_{2k,l},\mathbf{x}_{2k+r,l})$ and r is an odd number called the range of the interaction. $\mathcal{P}_n$ is deduced from $\mathcal{P}_1$ by a $(n-1)\pi/3$ rotation. The operator $\mathcal{I}_1$ is defined as

$$\mathcal{I}_1=\mathcal{I}_1^{(a)}\circ\mathcal{I}_1^{(b)}\circ\cdots\circ\mathcal{I}_1^{(e)}.$$

Each operator $\mathcal{I}_1^{(x)}$ above acts on each side of a pair p and attempts to perform permutations of particles between the various directions $\mathbf{c}_i$. Thus $\mathcal{I}_1^{(a)}$, for instance, tries to take particles in the directions given by solid lines

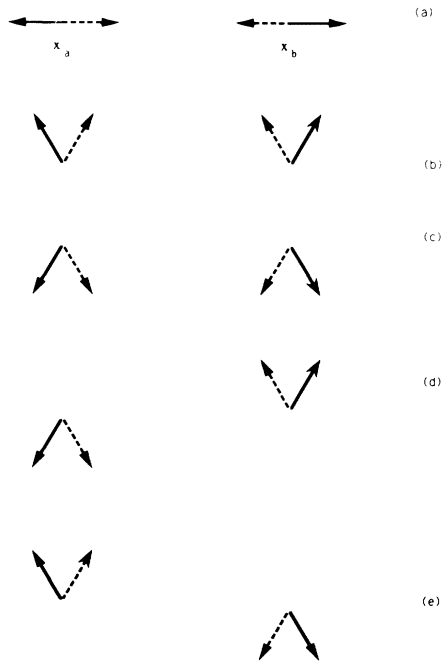

FIG. 1. The action of the interaction operators $\mathcal{I}_1^{(x)}$ represented schematically. Each operator takes particles in the directions indicated by the solid lines and puts them in the directions indicated by the dashed lines. The directions not indicated may be in an arbitrary state.

in Fig. 1(a) and put them in the directions given by dashed lines. If a direction given by solid lines is empty or if a direction given by dashed lines is occupied, $\mathcal{I}_1^{(a)}$ reduces to the identity operator. The operators $\mathcal{I}_n$ are deduced from $\mathcal{I}_1$ by a $(n-1)\pi/3$ rotation, and $\mathcal{I}_n'$ is deduced from $\mathcal{I}_n$ by a π rotation. In three time steps each pair of sites at a distance r has been processed. A momentum $\mathbf{t}_n$ is exchanged between the sites of a pair: $\mathbf{t}_n = \mathbf{g}_b' - \mathbf{g}_b = \mathbf{g}_a - \mathbf{g}_a'$, where $\mathbf{g}_a = \sum_i s_{ai}\mathbf{c}_i$ is the momentum on site $\mathbf{x}_a$ before the interaction and $\mathbf{g}_a'$ is the momentum after the interaction. The definitions above imply $\mathbf{t}_n = -|\mathbf{t}_n|\mathbf{c}_n = -|\mathbf{t}_n|(\mathbf{x}_b - \mathbf{x}_a)/r$, which means that the force is attractive.

Numerical simulation of these models is straightforward, using table-lookup algorithms for the $\mathcal{I}_n$ operators.[2] In Fig. 2 we display typical results. When the range of the interaction is large enough, and for certain values of the density, the lattice gas separates into two phases, a dense and a light one. The growth of the bubbles continues until an equilibrium state is reached where the two phases are entirely separated and the interface length is minimized. At low densities a single bubble or band of liquid is observed while a gas bubble is seen at higher densities. It is possible to observe metastable states typical of a first-order phase transition. An interesting feature of the observed patterns is the asymmetry between high- and low-density regions. Another interesting effect is that momentum-conserving models such as ours seem to yield faster separation than non-momentum-conserving lattice gases such as the Ising model.[9] One of the reasons for this is that the surface-tension effects yield faster domain growth in momentum-conserving systems.[10,11] The mechanisms of growth are described in these papers. A specific one we observed involves bubbles undergoing Brownian motion, colliding, and being rapidly squeezed into a bigger, rounder bubble by surface tension. However, at densities close to those of Fig. 2 few round bubbles are observed because the new bubbles collide again with each other. The morphology of the pattern and the mechanisms of growth depend on the density. Rounder liquid bubbles are observed at low density, while gas bubbles are observed at higher densities. In between, coalescence of liquid bubbles and expansion of gas bubbles creates the patterns of Fig. 2.

It is important to be able to predict the range r above which a phase transition will be seen, as well as the densities of the two phases. In many models of statistical physics, this may be obtained from the partition function, but this approach may not be followed here because in our model interactions do not involve forces which may be derived from a Hamiltonian. But it is still possible to make predictions using a Boltzmann-like approach. We start by defining as usual a momentum-transfer tensor as the amount of momentum transferred across a unit length per unit time. Now let $\pi_j = \langle |\mathbf{t}_j| \rangle$ be the average momentum transferred by an interaction operator $\mathcal{I}_j$. π_j' will correspond to $\mathcal{I}_j'$. The total momentum-transfer tensor for the first time evolution $\mathcal{E}_1$ is

$$P_{\alpha\beta}^1 = \sum_i N_i^1 c_{i\alpha}c_{i\beta} - \tfrac{1}{2}r\pi_1 c_{1\alpha}c_{1\beta} - \tfrac{1}{2}r\pi_1' c_{4\alpha}c_{4\beta}.$$

$N_i^t = \langle s_i \rangle_t$ is the average number of particles in direction i at time t. The momentum transfer is anisotropic. We shall attempt to predict the momentum transfer when the average momentum $\langle \mathbf{g} \rangle$ vanishes. It is then still possible to assume isotropy and time independence of N_i^t.[12] We indeed observed both in the simulations. Similarly we assume that the π_i are all equal to $\pi(\rho)$, where $\rho = \sum_{i=0}^{6} N_i$ is the density. We then obtain after time averaging

$$P_{\alpha\beta} = p\delta_{\alpha\beta},$$

and

$$p = 3\rho/17 - \tfrac{1}{2}r\pi(\rho). \qquad (2)$$

It is interesting to notice that the correction to the equation of state for the noninteracting gas pressure is proportional to the range r. On the other hand, as we shall see below $\pi(\rho)$ varies little with r far from the critical point. Thus it is always possible to increase r until an unstable region appears, where $dp/d\rho < 0$. To predict $\pi(\rho)$ we assumed that after streaming the lattice was close to a factorized state. We also consider only those

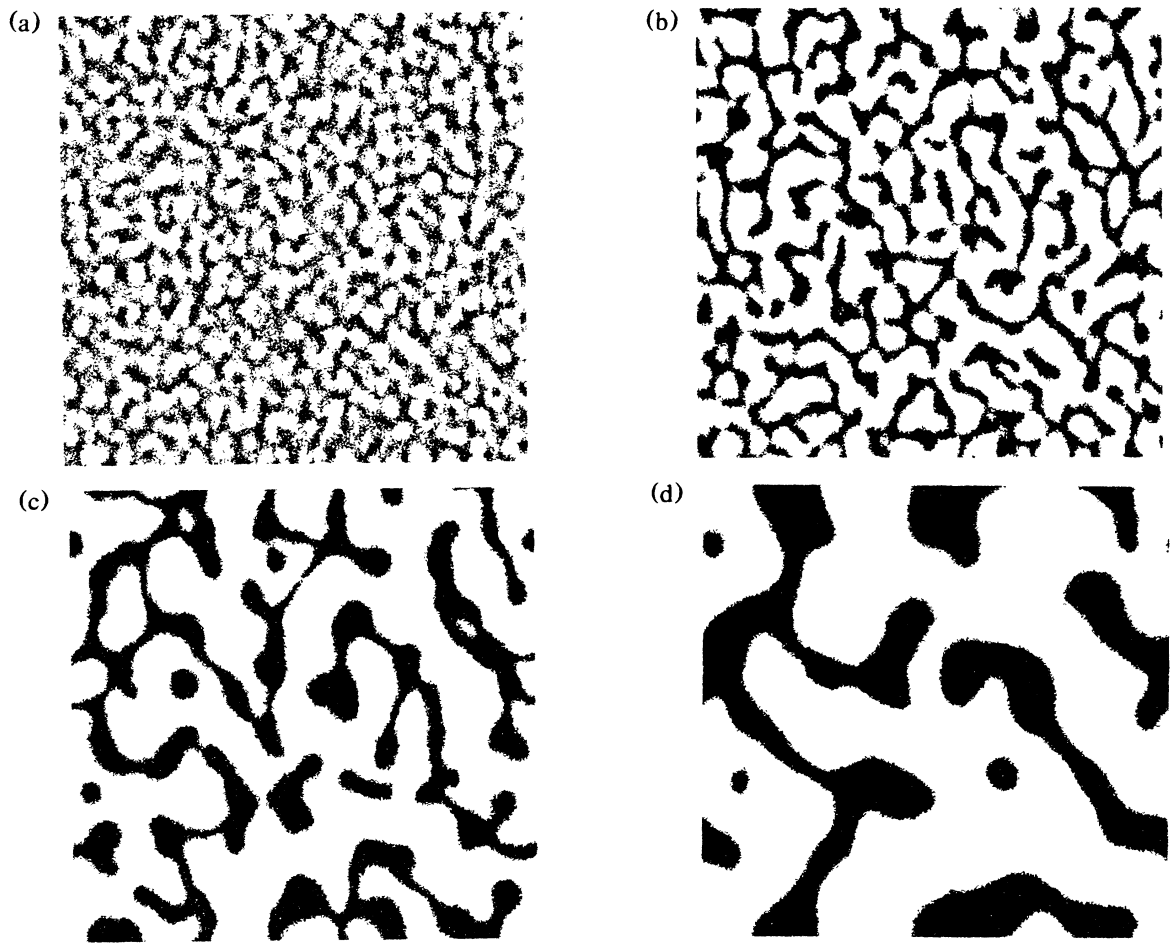

FIG. 2. The evolution of a 480×480 lattice starting from a homogeneous and randomly generated initial condition. (a) $t=8$, (b) $t=27$, (c) $t=125$, and (d) $t=729$. Grey levels are roughly proportional to density: dark areas represent high-density regions, while clear areas are not empty but of low density. Eventually an equilibrium state is reached where the phases are entirely separated.

states for which the average momentum of the lattice vanishes. This implies that the probability of having a site in configuration s in

$$W_0(s)=d^m(1-d)^{(7-m)}, \tag{3}$$

where $m=\sum_{i=0}^{6}s_i$ and $d=\rho/7$ is the reduced density. Sites are assumed to be independent from each other. This is obviously wrong near the critical point but may yield a satisfactory theory away from it. After the first interaction step, i.e., $\mathcal{I}_1$, the probability of a state s_a' will be

$$W_{1a}(s_a')=\sum_{\sigma,s_b'}A(\sigma,\sigma';1)W_0(s_a)W_0(s_b), \tag{4}$$

where $\sigma=(s_a,s_b)$, $\sigma'=(s_a',s_b')$, and $A(\sigma,\sigma';j)$ is the transition rate from the pair σ to σ' from interaction $\mathcal{I}_j$. A symmetric expression is obtained for the probability W_{1b} of observing s_b after the interaction. After the interaction, members of a pair are correlated with each other but not with other sites. Thus when we apply the operator $\mathcal{I}_1'$ to pair (s_a',s_b'), members of this new pair are uncorrelated. This makes it easy to compute the average transferred momentum:

$$\pi(\rho)=\tfrac{1}{2}\left[\sum_{\sigma}A(\sigma,\sigma';1)(\xi_b-\xi_b')d^k(1-d)^{(14-k)}+\sum_{\sigma'}A(\sigma',\sigma'';4)(\xi_b'-\xi_b'')W_{1b}(s_a')W_{1a}(s_b')\right], \tag{5}$$

where k stands for $\sum_{i=0}^{6}s_{ai}+\sum_{i=0}^{6}s_{bi}$ and $\xi_b=\mathbf{g}_b\cdot\mathbf{c}_1$, $\xi_b'=\mathbf{g}_b'\cdot\mathbf{c}_1$, etc. Because of the rotational invariance of our model, the same expression is obtained for the other interaction sequences in (1). From (2)–(5) our full equation of state is obtained. We notice that, as advertised, $\pi(\rho)$ does not depend on r.

We measured the pressure of the lattice at various densities and for several values of r. Care was taken to eliminate transients except for the very robust metastable states. In Fig. 3 we display the resulting equation of state in the p-d di-

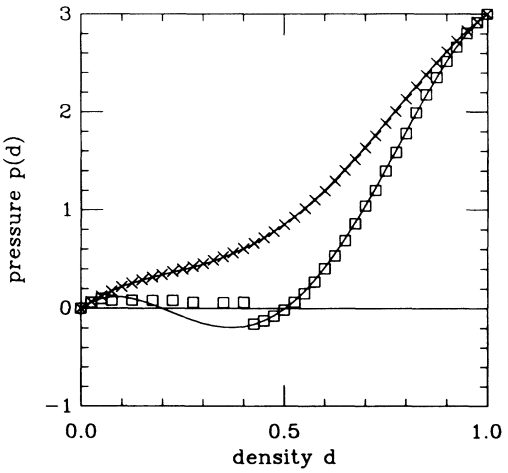

FIG. 3. The theoretical equation of state (solid lines) and the numerical results for $r=3$ (squares) and $r=7$ (crosses). A transition is seen for $r=7$ but not for $r=3$. When the two phases coexist the pressure is constant but for finite-size effects.

agram. The theoretical and numerical values of p agree well except in the unstable region. There a constant pressure is observed as expected in a first-order liquid-gas or solid-gas transition. An interesting fact is the existence of a negative-pressure region in Fig. 3. Actually, the pressure may dip arbitrary low when r is increased. These low-pressure states are metastable. If a small empty bubble is created, it expands until two coexisting states of positive pressure appear. Thus cavitation might be studied with our model.

Several remarks can be made concerning the present model and its future extensions and applications. (i) The control parameter in our model is not a temperature but the range r of the interaction. While we have varied this parameter only by discrete amounts, it is possible to replace it with a continuously varying parameter. Indeed interactions may be realized only with an arbitrary probability α, for instance, by drawing a random number before processing each pair. The equation of state is then

$$p=3\rho/7-\beta\pi(\rho)\,, \tag{6}$$

with $\beta=\alpha r/2$. The minimum range for the appearance of an interaction is $r=5$, but it can be reduced if optimized interaction operators are used. These will be described in further papers. This allows one to reach a critical state when $dp/d\rho=d^2p/d\rho^2=0$.

(ii) It is possible to alter somewhat the equation of state. This may be interesting, for instance, if one wants to change the equilibrium densities in the two phases. This is possible if one performs the interactions at a rate depending on the local number of particles. For such models the agreement with experiment is also excellent.

(iii) It is clear that arguments identical to those of Ref. 1 can be used here to predict fluid behavior on the large scale. These arguments rely only on the isotropy of fourth-order tensors on hexagonal lattices which holds also for our model. Thus hydrodynamic behavior on the large scale is necessarily isotropic. Other features of large-scale behavior such as the presence of other invariants, memory effects, Galilean invariance, etc., are under investigation.

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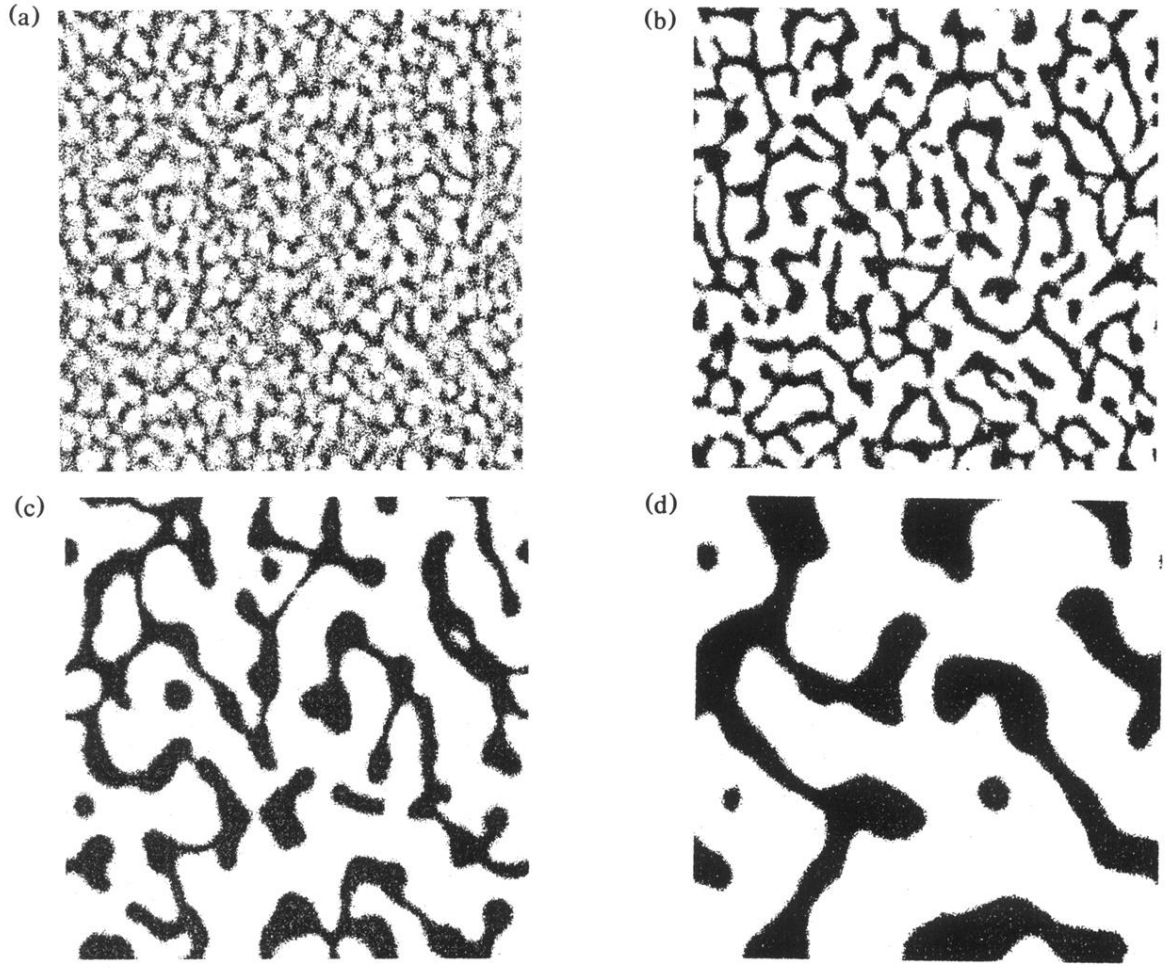
[12]This and other measurements of isotropy made with D. H. Rothman will be reported in a further paper.



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