Shock wave structure in a lattice gas

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The motion and structure of shock and expansion waves in a simple particle system, a lattice gas and cellular automaton, are determined in an exact computation. Shock wave solutions, also exact, of a continuum description, a model Boltzmann equation, are compared with the lattice results. The comparison demonstrates that, as proved by Caprino \textit{et al.} [“A derivation of the Broadwell equation,” Commun. Math. Phys. \textbf{135}, 443 (1991)] only when the lattice processes are stochastic is the model Boltzmann description accurate. In the strongest shock wave, the velocity distribution function is the bimodal function proposed by Mott-Smith. © 2007 American Institute of Physics. [DOI: 10.1063/1.2723156]

I. INTRODUCTION

Discrete velocity and lattice gases have become tools for clarifying the Boltzmann equation\textsuperscript{1-3} and for fluid mechanics.\textsuperscript{4-6} The paper of Benzi \textit{et al.}\textsuperscript{7} is an interesting general discussion of these ideas. In this paper the aim is to illustrate ideas and concepts in both areas. To this end, the lattice gas results are initially viewed as experimental and the model Boltzmann equation as the corresponding theory. For these purposes the two-dimensional lattice gas of Hardy and Pomeau\textsuperscript{8} is appropriate. It is sufficiently simple to allow a large number of particles to be followed exactly and yet has properties that lead to the formation of shock and expansion waves and to the formation of an equilibrium state. In addition the model Boltzmann equations for shock waves can be solved exactly.

II. PROBLEM FORMULATION

The Hardy-Pomeau model, a lattice version of a discrete velocity gas,\textsuperscript{9,10} consists of indistinguishable articles moving on a two-dimensional lattice with four fixed velocities. Particles move and collide according to the following rules. In each time step, all particles move to the adjacent site and then some collide. Collisions, which turn the collision partners through 90°, take place if and only if two particles with oppositely directed velocities occupy the same site and the collision destination velocity locations are empty. Mass and momentum are conserved in the moves and collisions. Particles pass through each other between sites. The system is reversible so that from any initial condition, an isolated system develops a long-term Poincaré cycle and returns to the initial state after sufficient time. This model has been used previously to demonstrate how thermodynamically irreversible processes can arise in microscopically reversible systems.\textsuperscript{11}

It is emphasized that the model is not intended to represent a real gas. With only a single speed, the thermodynamics is not realistic. Further, the model solutions are not Galilean invariant. The value of the model is in the availability of exact model Boltzmann solutions for comparison with the lattice gas results.

III. SHOCK AND EXPANSION WAVE GENERATION

The model and the arrangement for generating the waves are as follows. Consider a square lattice with reflective boundaries at $y=0$ and $y=L$, and those at $x=0$ and $x=L$ at first periodic so that east and west moving particles leaving at one boundary enter at the other. In the following, particles moving north (N), east (E), south (S), and west (W) will sometimes be denoted by the numerals 1 to 4. The gas has a mean velocity to the right when there are more E (2) particles than W (4) particles. This velocity $u$ is $c[n(2)−n(4)]/n$, where $c$ is the particle velocity and $n(i)$ the particle number density, i.e., the number per side or area, and $n=\Sigma n(i)$. For zero $y$-velocity, $n(1)=n(3)$. After the gas equilibrates, the boundaries at $x=0$ and $L$ are made reflective (as if walls were inserted) and the gas comes to rest at each wall with a shock generated at the right boundary and an expansion wave at the left.

This arrangement for generating the shock waves is that used by Cafflisch in his investigation of shock wave structure in a similar discrete velocity gas\textsuperscript{12} and by Nadiga \textit{et al.}\textsuperscript{13} studying shocks in a nine-velocity cellular automaton. It may be noted that the shocks cannot be generated by piston motion. Particles reflected from a moving piston have the full range of velocities, a process not describable by discrete velocity models.

Density distributions $n(i)$ averaged over the $y$-columns and five adjacent times, and normalized by the free stream value, are shown in Figs. 1 and 2 for $u/c=0.5$ and 1, respectively. In the computations, the particle velocity, the lattice spacing, and the time step are unity.

IV. MODEL BOLTZMANN EQUATION

The model equation for the distribution function is derived following the Boltzmann procedure. This function,
Probability of this occurrence and, for dimensional consistency, is the collision cross section. Since particles move on grid lines and collide only when particles of oppositely directed velocity occupy the same site, the collision rate depends only on the number densities of the colliding particles and their relative velocity. Thus, the loss \( L_i \) is \( 2\sigma n(1)n(3) \), where \( 2\sigma \) is the relative velocity and \( \sigma \), in the usual derivation, is the collision cross section. Since particles move on grid lines and collide only when particles of oppositely directed velocity occupy the same site, \( \sigma \) is taken to be the probability of this occurrence and, for dimensional consistency, \( n(i) \) is viewed as the particles per unit horizontal length divided by the number of horizontal lines. In this way, \( n(i) \) can continue to be viewed as the particle number per unit area. Particles are thrown into the velocity cell 1 by collisions between the 2 and 4 particles. Thus, with \( \sigma \) taken to be \( \frac{1}{2} \) (an assumption to be checked later), the equations become:

\[
\begin{align*}
\frac{\partial n(i)}{\partial t} + c_x \frac{\partial n(i)}{\partial x} + c_y \frac{\partial n(i)}{\partial y} &= G(i) - L(i).
\end{align*}
\]

For north (1) moving particles loss occurs only when these particles collide with the south (3) particles. With the Boltzmann Stosszahlansatz—the assumption that there are no correlations in the particle motions—the collision rate depends only on the number densities of the colliding particles and their relative velocity. Thus, the loss \( L_1 \) is \( 2\sigma n(1)n(3) \), where \( 2\sigma \) is the relative velocity and \( \sigma \), in the usual derivation, is the collision cross section. Since particles move on grid lines and collide only when particles of oppositely directed velocity occupy the same site, \( \sigma \) is taken to be the probability of this occurrence and, for dimensional consistency, \( n(i) \) is viewed as the particles per unit horizontal length divided by the number of horizontal lines. In this way, \( n(i) \) can continue to be viewed as the particle number per unit area. Particles are thrown into the velocity cell 1 by collisions between the 2 and 4 particles. Thus, with \( \sigma \) taken to be \( \frac{1}{2} \) (an assumption to be checked later), the equations become:

\[
\begin{align*}
\frac{\partial n(1)}{\partial t} + c_x \frac{\partial n(1)}{\partial x} + c_y \frac{\partial n(1)}{\partial y} &= G_1 - L_1 = c[n(2)n(4) - n(1)n(3)], \\
\frac{\partial n(2)}{\partial t} + c_x \frac{\partial n(2)}{\partial x} + c_y \frac{\partial n(2)}{\partial y} &= G_2 - L_2 = c[n(1)n(3) - n(2)n(4)], \\
\frac{\partial n(3)}{\partial t} + c_x \frac{\partial n(3)}{\partial x} + c_y \frac{\partial n(3)}{\partial y} &= G_3 - L_3 = c[n(2)n(4) - n(1)n(3)], \\
\frac{\partial n(4)}{\partial t} + c_x \frac{\partial n(4)}{\partial x} + c_y \frac{\partial n(4)}{\partial y} &= G_4 - L_4 = c[n(1)n(3) - n(2)n(4)].
\end{align*}
\]

These equations are put in nondimensional form by defining \( n_i = n(i)/n_a \), where \( n_a \) is the average field density; i.e., the total number of particles divided by the field area. For one-dimensional flow in the x direction, \( n(1) = n(3) \), and the equations become:

\[
\begin{align*}
\frac{\partial n_1}{\partial \tau} &= (n_2 n_4 - n_1^2), \\
\frac{\partial n_2}{\partial \tau} + \frac{\partial n_2}{\partial \eta} &= (n_1^2 - n_2 n_4), \\
\frac{\partial n_4}{\partial \tau} - \frac{\partial n_4}{\partial \eta} &= (n_1^2 - n_2 n_4),
\end{align*}
\]

where \( \tau = n_a c \tau, \eta = n_a x \).

This system of equations constitutes the Boltzmann description of the lattice gas. The populations \( n_i \) make up the distribution function as they do for the discrete velocity gas.

### A. Shock wave propagation and structure

In Fig. 1, where \( u/c = 0.50 \) and \( n_a = 0.20 \), the lattice is 2000 units long and 2000 units high. The number of particles at each site fluctuates between 0 and 4. The shock propagates with a fixed shape while the expansion wave becomes less steep, as is the case in real gases. In Fig. 2 the initial condition is a stream of particles all with unit velocity to the right. In this case the gas separates from the left wall and a shock of density ratio three emerges at the right. The propagation speeds, structure, and distribution functions of the shock waves are discussed in the following and the results compared with the model Boltzmann equations approximations.

### B. Euler equation and shock jump conditions

To study the shock wave structure, it is convenient to work in the coordinate system in which the shock is stationary. The shock speed and density jump are independent of the wave structure and can be determined from the inviscid Euler equation. This equation is obtained by sequentially multiplying Eqs. (1)–(3) by the collisional invariants, the...
molecular weight and particle velocities, and summing. The right-hand sides vanish because the particle number and momentum are conserved in the collisions. The results are:

\[
\frac{\partial \rho}{\partial \tau} + \frac{\partial \rho u}{\partial \eta} = 0, \tag{4}
\]

\[
\frac{\partial \rho u}{\partial \tau} + \frac{\partial (n_2 + n_4)}{\partial \eta} = 0, \tag{5}
\]

where

\[
\rho = m \sum n_i,
\]

\[
u = \frac{m(n_2 - n_4)}{\rho},
\]

and \(m\) is the molecular weight (taken to be unity in the following).

The equations describe nonviscous adiabatic flows and thus flows in equilibrium; in the lattice gas this condition is \(n_2 = n_1 = n_4\).

With this condition, Eq. (5) can be written, following Caflisch,

\[
\frac{\partial \rho u}{\partial \tau} + \frac{\partial F(u)}{\partial \eta} = 0,
\]

where

\[
F(u) = (1/2)(1 + u^2).
\]

For the shocks in Figs. 1 and 2 moving to the left at velocity \(s\) in a rightward flowing stream of velocity \(u\), the jump conditions from the Euler equations are:

\[
\rho_1(u_{r} - s) = \rho_1(u_{l} - s),
\]

\[
\rho_1(F_{r} - u_{r}s) = \rho_1(F_{l} - u_{l}s),
\]

where the subscripts \(l\) and \(r\) denote conditions upstream and downstream of the shock wave, respectively.

Noting that \(F_{r} = F(u_{r}) = 1/2\), we find the shock speed in terms of \(u\) to be

\[
s = \frac{1}{2}\sqrt{u^2 + \sqrt{u^4/4} + 2}. \tag{6}
\]

From the continuity equation (6), the density ratio is

\[
\frac{\rho_r}{\rho_l} = \frac{(u - s)}{s}. \tag{7}
\]

From the results in Figs. 1 and 2, and for other speeds, Figs. 3 and 4 compare the density ratio and speed from these equations with those in the lattice. That the flow is in equilibrium entering and leaving the shock is shown later.

C. Speed of sound

Equations (6) and (7) indicate that as the density jump falls to zero, the wave speed is \(1/\sqrt{2}\). This is the speed of a wave in equilibrium. The structure of weak or acoustic waves not in equilibrium is described by linearized versions of Eqs. (1)–(3) for perturbations about the condition \(u=0\), \(n_1=n_2=n_3=n_4\). Denote the perturbations \(n_i'\). Equations (1)–(3) then lead to a single equation for \(n_1'\), for \(n_4'\), say:

\[
\frac{\partial}{\partial t} \left( \frac{\partial^2 n_4'}{\partial x^2} - \frac{c^2 \partial^2 n_4'}{2 \partial x^2} \right) - \frac{\partial}{\partial x} \left( \frac{\partial n_4'}{\partial x} - c^2 \frac{\partial^2 n_4'}{2 \partial x^2} \right) = 0.
\]

Moore and Gibson\(^{14}\) discuss equations of this form for gases out of vibrational or dissociation equilibrium, in which case \(c\) is called the frozen speed and \(c/\sqrt{2}\) the equilibrium speed. Whitham\(^{15}\) showed that for equations of this type the wave propagating at speed \(c\) decays exponentially and the low speed wave diffuses. (Similar results are demonstrated by Nadiga \textit{et al.}\(^{13}\) for the nine-velocity gas.) Here, particles leaving the wall at speed \(c\) (=1 in the model) begin, with every collision, to form the equilibrium state. Hence, the perturbation propagates only at \(c/\sqrt{2}\). Detailed results for a wave in a flow with \(u/c = 0.10\) are shown in Fig. 5. The relative fluctuations are large, but it is clear that no significant disturbance propagates at the speed \(c\) and that the speed of the main disturbance is consistent with \(c/\sqrt{2}\).

D. Shock wave structure

As was noted above, the model is not Galilean invariant; consequently, Eqs. (1)–(3) are different in this coordinate system. In a system moving with speed \(s\), they are

\[
-s \frac{dn_1}{d\eta} = (n_2 - n_1^2), \tag{8}
\]
Consider first $u_i = 1$ in which all the free stream particles are moving east and $(n_2)_i = 1$. From Eq. (6) $s = -1/2$. From these equations, $n_1$ and $n_3$ are functions of $n_2$, so that Eq. (9) can be written

\[(1 - s) \frac{dn_3}{d\eta} = (n_1^2 - n_2 n_3), \tag{9}\]

\[- (1 + s) \frac{dn_3}{d\eta} = (n_2 n_4 - n_3^2). \tag{10}\]

The degree of departure from equilibrium is the magnitude of $k = n_2 n_4 - n_1^2$, the collision term in Eqs. (8)–(10). This function, together with the Boltzmann $H$-function, i.e., $H = \sum n_i \ln n_i$, are shown in Fig. 10, where they are plotted on an

...
arbitrary scale. There are small departures from equilibrium and fall in the $H$-function in the expansion wave and large changes in the shock.

E. Velocity distribution function

The velocity distribution function for the $u/c=1.0$ shock wave was discussed above and is given in Eqs. (12) and (13) as follows:

$$n_2 = \frac{(1 - 3Ae^{2\eta})}{(1 - 4Ae^{2\eta})},$$

where

$$A = \frac{[n_2(0) - 1]}{[4n_2(0) - 3]}$$

and $n_1 = n_3 = 3(1 - n_2)$.

For the $u/c=0.5$ shock, this function was found by numerical integration of Eqs. (8)–(10). These solutions are compared with the stochastic lattice values in Figs. 11 and 12.

Mott-Smith was one of the first investigators to apply the Boltzmann equation in the study of shock wave structure. 18 He postulated a binomial velocity distribution function in high Mach number waves that consists of a combination of the upstream and downstream Maxwellian functions. Narasimha and Das19 present an analytical solution of the Boltzmann equation for the infinitely strong shock that has precisely this form. That work suggested the following re-examination of the distribution function for the $u/c=1.0$ shock wave discussed above. That function can be put in the form proposed by Mott-Smith by subtracting $n_1$ from $n_2$, leaving $1/(1 - 4Ae^{2\eta})$ to be denoted $n_L$, an incoming particle beam of declining strength. The subtracted term then becomes part of the rising strength exit equilibrium function $n_R$, consisting of $n_1 + n_2 + n_3 + n_4$, all equal. These functions are compared with the lattice gas values in Fig. 13.

Narasima and Das describe their spectral method as reducing the Boltzmann equation to an equivalent infinite order nonlinear dynamical system. The functions in Fig. 13 are remarkably similar to those in their Fig. 5(a), the solution with a single mode. This solution describes the shock process as the scattering of an incoming particle beam into an exiting distribution function.

Such distributions are also observed in high Mach number shock waves. See Pham-Van-Diep et al.20 and Alsmeyer21 for a further discussion.

V. DISCUSSION AND CONCLUDING REMARKS

The lattice results for the deterministic lattice gas have been considered experimental and compared to the model Boltzmann solutions as theory; the corresponding situation in real gases would be a comparison of Boltzmann equation solutions to experiments. In that case, of course, the collisions cannot be made probabilistic and general solutions to the Boltzmann equations are not available. However, the Bird direct simulation Monte Carlo (DSMC) method produces solutions to the Boltzmann equation.22,23 Thus, the remarkable agreement between the experiments and the DSMC solutions in, for instance, Pham-Van-Diep et al.20 and Alsmeyer,21 suggests that correlations do not develop in real gases.

Shock waves are simple examples of thermodynamically irreversible processes taking place in a microscopically reversible system. Confusion in this subject comes from a failure to distinguish between macroscopic and microscopic ir-
reversibility. In this model the difference is clear: the particle collisions and motions are reversible and the change in the $H$-function across the shock is a property of the collection of particles.

Finally, the departure from equilibrium and fall in the $H$-function in the expansion wave are reminders that in fluid mechanics such waves are treated as isentropic, usually without any remark about the approximation.

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