Counting Lattice-Gas Invariants

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October 31, 1993

Abstract

Summarized is a method to count the number of invariants in a lattice-gas automata. A simple calculation proves that a deterministic FHP lattice-gas with a definite chirality, possesses only three invariants: the total mass and the two components of momentum. This model in somewhat simpler than FHP and is time reversible.

1 Introduction

The discovery that a very simple cellular automaton model, the Frisch, Hasslacher, and Pomeau (FHP) model [1], using only six bits of memory at each point in space reproduces hydrodynamics in its macroscopic limit has stimulated many investigations of the new domain of discrete kinetic equations. This domain, broadly termed lattice-gas dynamics, has to date expanded its scope beyond incompressible hydrodynamics to thermodynamics, multiphase phenomena, magnetohydrodynamics, reaction-diffusion systems, and seems to be continuing its growth. Given the conceptual importance of a simple lattice-gas model with its ability to simulate so many, the question arises if their exists a lattice-gas cellular automaton model even simpler than FHP that yet has no more than three invariants: the total mass and the two components of momentum. A very simple calculation, similar to that previous done [2], shows there indeed exists a simpler model.

It is well known that symmetric 3-body collisions must be included along with the FHP model's even and odd chirality 2-body collisions to achieve the correct macroscopic limit[1]. However, the fact that both even and odd 2-body collision possibilities are present, dictates when a 2-body collision occurs, a coin toss must also occur to determine the outgoing state. This coin toss makes the FHP model irreversible. Clearly if the model is constrained to have a definite chirality, say for example 2-body collisions generated by $\frac{\pi}{3}$ rotations are retained while $\frac{2\pi}{3}$ collisions are discarded, then the lattice-gas would be strictly reversible. But does this additional constraint of a fixed chirality engender any spurious invariants? The answer is no, see the results given in §3.2 for the proof.

[1]Anitsymmetric 3-body collisions, 2-body collision with a spectator particle, could also be included but this is not necessary.

2 Some Preliminaries

Symbols used

$$
\begin{array}{rcl}
\textit{Spatial Unit} & : & l \\
\textit{Temporal Unit} & : & \tau \\
\textit{Particle Speed} & : & c = \dfrac{l}{\tau} \\
\#\ \textit{Momentum Directions} & : & B \\
\textit{Lattice Vectors} & : & \hat{\mathbf{e}}_a \\
a & = & 1, 2, \ldots, B \\
\textit{Distribution Function} & : & f_a \\
\textit{Collision Operator} & : & \Omega_a \\
\textit{Jacobian Matrix} & : & J_{ab}
\end{array}
$$

It should be understood that whenever the single particle distribution function is written, its subscripted index is taken modulo B

$$f_{a+b} = f_{\text{ mod } B(a+b)}. \tag{1}$$

The lattice Boltzmann equation is

$$\partial_t f_a + c e_{ai} \partial_i f_a = \Omega_a. \tag{2}$$

A general collision operator is constructed as follows

$$\Omega_a = \sum_{\{\zeta_i\}} \alpha Q_a(\{\zeta_i\}), \tag{3}$$

where $\{\zeta_i\}$ is a set of occupied particle states and $\alpha = \pm 1$ is a scalar coefficient and where each term in the sum is written in factorized form as

$$Q_a(i_1, \ldots, i_k) = \frac{f_{a+i_1}}{1 - f_{a+i_1}} \cdots \frac{f_{a+i_k}}{1 - f_{a+i_k}} \prod_{j=1}^{B} (1 - f_{a+j}). \tag{4}$$

We expand the distribution function about its equilibrium value, f^{eq}

$$f_a = f^{\text{eq}} + \delta f_a \tag{5}$$

so that, to first order, we have

$$\Omega_a(f^{\text{eq}}) = \sum_b \frac{\partial \Omega_a}{\partial f_b} \delta f_b. \tag{6}$$

The l.h.s. of (6) must vanish, since the particle distribution is non-changing under equilibrium conditions. The eigenvalues of the Jacobian of the collision operator,

$$J_{ab} = \frac{\partial \Omega_a}{\partial f_b}, \tag{7}$$

can be calculated and the number of these that vanish must equal the number of invariant quantities in the lattice-gas dynamics. Because of the finite-point group symmetry of the spatial lattice, the Jacobian matrix will be circulant and therefore its elements can be specified by the difference of their indices, $J_{ab} = J_{a-b}$. This property of the Jacobian simplifies the solution of the eigenvalue equation

$$\sum_b J_{a-b}\xi_b^k = \lambda^k \xi_a^k, \tag{8}$$

where $k = 1, \ldots, B$. Let us make the ansatz that the eigenvectors have the following form

$$\xi_a^k = e^{2\pi iak/B}. \tag{9}$$

Then inserting (9) into (8) and taking $m = a - b$, gives

$$\lambda^k = \sum_m J_m e^{2\pi imk/B}. \tag{10}$$

3 Triangular Lattice: B=6

3.1 Eigenvectors

Using (9), the eigenvectors of the Jacobian matrix are

$$\begin{aligned}
\xi_0 &= (1,1,1,1,1,1) && (11)\\
\xi_1 &= (\epsilon,\epsilon^*,-1,\epsilon,\epsilon^*,1) && (12)\\
\xi_2 &= (\epsilon^*,\epsilon,1,\epsilon^*,\epsilon,1) && (13)\\
\xi_3 &= (-1,1,-1,1,-1,1) && (14)\\
\xi_4 &= (\epsilon,\epsilon^*,1,\epsilon,\epsilon^*,1) && (15)\\
\xi_5 &= (\epsilon^*,\epsilon,-1,\epsilon^*,\epsilon,1), && (16)
\end{aligned}$$

where $\epsilon = e^{i\frac{\pi}{3}}$.

3.2 Definite Chirality Models

Even chirality:

$$\Omega_a = Q_a(1,4) - Q_a(0,3) + Q_a(1,3,5) - Q_a(0,2,4) \tag{17}$$

$$\begin{aligned}
\Omega_0 = \; & -(f_0\ (1-f_1)\ (1-f_2)\ f_3\ (1-f_4)\ (1-f_5)) + \\
& (1-f_0)\ f_1\ (1-f_2)\ (1-f_3)\ f_4\ (1-f_5) - \\
& f_0\ (1-f_1)\ f_2\ (1-f_3)\ f_4\ (1-f_5) + \\
& (1-f_0)\ f_1\ (1-f_2)\ f_3\ (1-f_4)\ f_5
\end{aligned}$$

$$\begin{aligned}
J = \; & \mathrm{circ}[(-1+f)^2 f^2, -\left((-1+f)^2 f^2\right), (-1+f)^2 f^3 \\
& (1-2f)\ (-1+f)^2 f^2, (-1+f)^2 f^2\ (-1+2f), -\left((-1+f)^2 f^3\right)]
\end{aligned}$$

$$\begin{aligned}
\lambda_0 &= 0 \\
\lambda_1 &= 0 \\
\lambda_2 &= 2\,\epsilon\,(1+\epsilon)\,(-1+f)^3\,f^2 \\
\lambda_3 &= -6\,(-1+f)^2\,f^3 \\
\lambda_4 &= 2\,\epsilon\,(1+\epsilon)\,(1-f)^3\,f^2 \\
\lambda_5 &= 0
\end{aligned}$$

There are only three zero eigenvalues, so this even chirality model is sufficient.

Odd chirality:

$$\Omega_a = Q_a(2,5) - Q_a(0,3) + Q_a(1,3,5) - Q_a(0,2,4) \tag{18}$$

$$\begin{aligned}
\Omega_0 = {} & -\left(f_0\,(1-f_1)\,(1-f_2)\,f_3\,(1-f_4)\,(1-f_5)\right) - \\
& f_0\,(1-f_1)\,f_2\,(1-f_3)\,f_4\,(1-f_5) + \\
& (1-f_0)\,(1-f_1)\,f_2\,(1-f_3)\,(1-f_4)\,f_5 + \\
& (1-f_0)\,f_1\,(1-f_2)\,f_3\,(1-f_4)\,f_5
\end{aligned}$$

$$\begin{aligned}
J = {} & \mathrm{circ}[(-1+f)^2\,f^2, -\left((-1+f)^2\,f^3\right), (-1+f)^2\,f^2\,(-1+2\,f)\,, \\
& (1-2\,f)\,(-1+f)^2\,f^2, (-1+f)^2\,f^3, -\left((-1+f)^2\,f^2\right)]
\end{aligned}$$

$$\begin{aligned}
\lambda_0 &= 0 \\
\lambda_1 &= 0 \\
\lambda_2 &= 2\,(1+\epsilon)\,(-1+f)^3\,f^2 \\
\lambda_3 &= -6\,(-1+f)^2\,f^3 \\
\lambda_4 &= 2\,(1+\epsilon)^2\,(-1+f)^3\,f^2 \\
\lambda_5 &= 0
\end{aligned}$$

There are only three zero eigenvalues, so this odd chirality model is sufficient.

3.3 FHP

$$\Omega_a = \frac{1}{2}Q_a(1,4) + \frac{1}{2}Q_a(2,5) - Q_a(0,3) + Q_a(1,3,5) - Q_a(0,2,4) \tag{19}$$

$$\begin{aligned}
\Omega_0 = {} & -\left(f_0\,(1-f_1)\,(1-f_2)\,f_3\,(1-f_4)\,(1-f_5)\right) + \\
& \frac{(1-f_0)\,f_1\,(1-f_2)\,(1-f_3)\,f_4\,(1-f_5)}{2} - \\
& f_0\,(1-f_1)\,f_2\,(1-f_3)\,f_4\,(1-f_5) + \\
& \frac{(1-f_0)\,(1-f_1)\,f_2\,(1-f_3)\,(1-f_4)\,f_5}{2} + \\
& (1-f_0)\,f_1\,(1-f_2)\,f_3\,(1-f_4)\,f_5
\end{aligned}$$

$$
\begin{aligned}
J &= \mathrm{circ}[(-1+f)^2 f^2, \frac{-\left((-1+f)^2 f^2\ (1+f)\right)}{2}, \frac{(-1+f)^2 f^2\ (-1+3f)}{2}, \\
&\quad (1-2f)\ (-1+f)^2 f^2, \frac{(-1+f)^2 f^2\ (-1+3f)}{2}, \frac{-\left((-1+f)^2 f^2\ (1+f)\right)}{2}]
\end{aligned}
$$

$$
\begin{aligned}
\lambda_0 &= 0 \\
\lambda_1 &= 0 \\
\lambda_2 &= (1+\epsilon)^2 (-1+f)^3 f^2 \\
\lambda_3 &= -6\,(-1+f)^2 f^3 \\
\lambda_4 &= (1+\epsilon)\ (1+2\,\epsilon)\ (-1+f)^3 f^2 \\
\lambda_5 &= 0
\end{aligned}
$$

There are only three zero eigenvalues, so as is well known the FHP model is sufficient.

3.4 FHP Without 3-Body Collisions

$$
\Omega_a = \frac{1}{2} Q_a(1,4) + \frac{1}{2} Q_a(2,5) - Q_a(0,3) \tag{20}
$$

$$
\begin{aligned}
\Omega_0 &= -\left(f_0\ (1-f_1)\ (1-f_2)\ f_3\ (1-f_4)\ (1-f_5)\right) + \\
&\quad \frac{(1-f_0)\ f_1\ (1-f_2)\ (1-f_3)\ f_4\ (1-f_5)}{2} - \\
&\quad \frac{(1-f_0)\ (1-f_1)\ f_2\ (1-f_3)\ (1-f_4)\ f_5}{2}
\end{aligned}
$$

$$
J = \mathrm{circ}[(1-f)^3 f^2, \frac{(-1+f)^3 f^2}{2}, \frac{(-1+f)^3 f^2}{2}, (1-f)^3 f^2, \frac{(-1+f)^3 f^2}{2}, \frac{(-1+f)^3 f^2}{2}]
$$

$$
\begin{aligned}
\lambda_0 &= 0 \\
\lambda_1 &= 0 \\
\lambda_2 &= (1+\epsilon)^2 (-1+f)^3 f^2 \\
\lambda_3 &= 0 \\
\lambda_4 &= (1+\epsilon)\ (1+2\,\epsilon)\ (-1+f)^3 f^2 \\
\lambda_5 &= 0
\end{aligned}
$$

There are four zero eigenvalues, one to many, so as is well known the FHP model without 3-body collisions is insufficient.

4 Conclusion

A simpler model than the original two-dimensional FHP lattice-gas automaton for simulating subsonic, viscous hydrodynamics does exist. It is interesting that although the chirality of its collisions is definite, no spurious invariants appear in the macroscopic limit and, furthermore, that this lattice-gas automaton is time reversible invariant. The observation that a fixed chirality lattice-gas model can have the correct macroscopic limit is interesting for the two-dimensional hexagonal lattice. However, in the case of the three-dimensional face-centered hypercubic (fchc) lattice [3], this observation should have more practical value in helping to reduce the number of collisions. The are 24 nearest neighbors in fchc, so a full collision table has 2^{24} entries. For parallel computers such as the CAM-8 and CM-5, implementing such a large collision table is inefficient. Compression of the fchc collision table has been explored[4]. Fixing the fchc collision table chirality should allow additional compression.

I would like to thank Dr Bruce Boghosian of Thinking Machines Corporation for a related discussion.

References

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