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Isometric Collision Rules for the Four-Dimensional FCHC Lattice Gas

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Abstract. Collision rules are presented for the four-dimensional face-centered-hypercubic-lattice (FCHC). The velocity set after collision is deduced from the velocity set before collision by an isometry, chosen so as to preserve the momentum and minimize the viscosity. A detailed implementation recipe is given. The shear viscosity is computed; the result shows that essentially all memory of the previous velocities is lost at each collision. Another set of collision rules, based on a random choice of the output state, has similar properties. The isometric principle can also be applied to the two-dimensional square (HPP) and triangular (FHP) lattices: one recovers the usual rules with minor differences.

1. Introduction

Lattice gas automata have recently emerged as a new technique for the numerical simulation of fluid motion (see [1], and in particular [2], for an introduction to the subject). Particles move on a regular lattice. Time is divided into a sequence of equal time steps, and the evolution consists in two alternating phases: (i) *propagation*: during one time step, each particle moves from one node to another along a link of the lattice; (ii) *collision*: at the end of a time step, particles arriving at a given node collide and instantaneously acquire new velocities, which determine their motion for the next propagation step. Thus, two basic ingredients are needed: the lattice and the collision rules. Taken together, they define a *lattice gas model.*

In pioneering work, Hardy, de Pazzis, and Pomeau [3,4,5] considered a square lattice with simple collision rules (called *HPP model* in what follows). This model, however, is not sufficiently isotropic for a simulation of the full Navier-Stokes equations. A two-dimensional model with the required degree of isotropy was proposed by Frisch, Hasslacher and Pomeau *(FHP model)* [6]; it consists of a triangular lattice and appropriate collision rules. This model has already been used in a number of simulations; see [1] for examples.

The subject is much less advanced in three dimensions. It turns out that no suitable three-dimensional lattice exists [6,7,8]. One must therefore go to four dimensions. (Three-dimensional problems are then easily simulated as a particular case). A four-dimensional lattice with the required properties has been proposed by d'Humières, Lallemand, and Frisch [7,2]: the *face-centered-hypercubic* (FCHC) *lattice*. The nodes are the points with integer coordinates (x_1, x_2, x_3, x_4) such that the sum $x_1 + x_2 + x_3 + x_4$ is even. Each node is linked to its 24 nearest neighbors $\mathbf{x}'$, which lie at a distance $\sqrt{2}$, and correspond to the following values of the vector $\mathbf{x}' - \mathbf{x}$:

$$\begin{array}{lll} (\pm 1, \pm 1, 0, 0), & (\pm 1, 0, \pm 1, 0), & (\pm 1, 0, 0, \pm 1), \\ (0, \pm 1, \pm 1, 0), & (0, \pm 1, 0, \pm 1), & (0, 0, \pm 1, \pm 1). \end{array} \tag{1.1}$$

These 24 nearest neighbors form a regular polytope. We normalize the time step to 1, so that the vectors (1) are also the 24 possible velocities of particles arriving at a node or leaving it. The velocities will be called $\mathbf{c}_i$, with $i = 1$ to 24 (this numbering is arbitrary). All velocities have the same modulus $c = \sqrt{2}$.

However, no collision rules have been proposed so far for the FCHC lattice (this is why we speak of the *FCHC lattice* and not of the *FCHC model*). It is the purpose of the present paper to present one possible set of rules, which satisfies the basic conditions, is easily implemented, and results in a reasonably low value of the viscosity. The basic principle is that the velocity set after a collision derives from the velocity set before collision by a suitably chosen *isometry* (i.e. a rotation around the origin, plus an optional mirror symmetry). We refer therefore to these rules as the *isometric collision rules*, or the *isometric algorithm*. Together with the FCHC lattice, they define what might be called the *FCHC isometric model*. Rivet [9] has recently conducted numerical simulations based on this model; he has shown that its properties are in agreement with theoretical predictions, and that it can be used in practice for the simulation of three-dimensional fluids.

2. Isometric collision rules

We define G as the group of the isometries which preserve the set of velocities (1). This group will be studied in more detail in section 3. We also define the *input state* as the set of the velocities of the incoming particles (before collision). The input state is conveniently represented as a collection of 24 boolean numbers: $s = (s_1, \ldots, s_{24})$, where $s_i = 1$ if velocity $\mathbf{c}_i$ is present in the input state, 0 otherwise. Similarly, we define the *output state* as the set of the velocities of the outgoing particles (after collision), and we represent it by $s' = (s'_1, \ldots, s'_{24})$.

Collision rules must satisfy the following conditions (see, for instance, [2,10]):

1. In any particular collision, the number of particles is preserved.

2. In any particular collision, the total momentum is preserved.

3. There does not exist any other quantity which is preserved in all collisions.

4. Exclusion principle: The new velocities are different from each other.

5. The collision rules have the same symmetries as the lattice; more precisely, they are invariant under any isometry of G.

6. The collisions satisfy semi-detailed balancing.

In the two-dimensional "six-bit" FHP lattice, the number of possible input states is only $2^6 = 64$, so that the collision rules can be selected by hand. Moreover, the above conditions severely constrain the choice of the rules and only a few variations are possible [2,11]. In the present FCHC lattice, the situation is completely different; there are $2^{24} = 16\,777\,216$ input states, and it is clearly out of the question to consider them one by one. We need a guiding principle, leading to a more or less automated construction of the rules. Also, one finds that the conditions still leave room for a tremendous number of possible collision rules, and the problem is to choose among this multitude. This again points to the need for some structure in the rules. In other words, we will impose additional restrictions so as to bring down the number of possibilities.

Our first restriction is defined by the following rule:

Rule 1. *Every collision is an isometry.*

By this, we mean that in all cases, the output state is deduced from the input state by an isometry of G. Motivations for this rule are, first, that in a sense we select "simple" collisions, so that the actual computation will be easier. We note also that in the HPP and FHP lattices, all collisions are isometries. Finally, the above conditions 1 and 4 are automatically satisfied.

Condition 2, however, is not automatically satisfied: the isometry must be chosen so as to preserve the momentum. This suggests the introduction of a second rule.

Rule 2. *The isometry depends on the momentum only.*

Taken together, rules 1 and 2 lead to a considerable reduction of the number of cases to be examined. As will be seen in section 5, the number of possible values of the momentum is only 7009. By taking advantage of the symmetries, we will be able to bring down the number of cases to 37, and ultimately to 12.

Another important criterion for the choice of the collision rules is that the resulting shear viscosity of the lattice gas should be as low as possible, so that higher Reynolds numbers can be reached [2,10]. Intuitively speaking, this means that the mean free path should be as short as possible, or that the output state of a collision should be "as different as possible" from the input state. (A precise definition will be given in section 4.) In this respect, one might wonder if the above rules are not overly restrictive and if there is not a risk that the only permitted isometry will be the identity in many cases. Fortunately, it turns out that this never happens: the number of permitted isometries is always at least two (see table 2 below). In other words, there exists always at least one non-trivial isometry (distinct from the identity) which preserves the momentum.

The number of permitted isometries ranges in fact from 2 to 1152, depending on the momentum, and is larger than 2 in most cases (see Table 2). Thus, one still has much freedom in the choice of the collision rules. It will be shown in section 4 that the contribution of an isometry M to the viscosity can be characterized by a number w lying between 0 and 1. Roughly speaking, this number measures the average correlation between an input state s and the corresponding output state s' obtained by M. (In particular, $w = 1$ for the identity.) In order to minimize the viscosity, one should choose isometries with w as small as possible. We call H the subgroup of G consisting of all isometries which preserve a given momentum, and w_{min} the minimum of w on H. We call *optimal isometry* an isometry of H for which $w = w_{min}$. Our third rule, then, is

Rule 3. *The isometry is randomly chosen among all optimal isometries.*

Our collision rules are thus completely defined. For convenience we will refer to them as *the isometric algorithm*. The rules are obviously invariant under any isometry; thus, the above condition 5 is automatically satisfied. Condition 6 (semi-detailed balancing) is also satisfied; in fact, the stricter condition of detailed balancing is satisfied, because the inverse of an optimal isometry is also optimal. Finally, it is not difficult to show that condition 3 is also satisfied.

The isometric algorithm is applicable not only to the FCHC lattice, but to any "one-speed model" belonging to the general class defined in [2] and [10]. It is of interest to note that in the case of the HPP lattice, the classical collision rules are exactly recovered; this is described in Appendix A. Similarly, in the case of the FHP lattice, we recover the usual rules, including the "head-on collisions with spectator" and the dual collisions, with one minor change (see Appendix B).

3. The isometry group G

The isometries of $\mathbf{R}^4$ which preserve the set of 24 velocities, or equivalently the regular polytope formed by the 24 nearest neighbors, form a group G called *symmetry group* of the polytope, of order 1152 [12]. An isometry can be represented by a matrix:

$$M = \begin{pmatrix} a_{11} & \dots & a_{14} \\ \vdots & & \vdots \\ a_{41} & \dots & a_{44} \end{pmatrix} \tag{3.1}$$

The image of a velocity $\mathbf{c}$ in the isometry M is $M\mathbf{c}$. (By a slight abuse of language, we designate the isometry and the matrix by the same symbol M.) The composition law in the group is the ordinary matrix product. Particular examples of isometries are

1. The change of sign of one coordinate α. This will be noted S_α. For example, we have

$$S_1 = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.2}$$

2. The permutation of two coordinates α and β ($\alpha \neq \beta$). This isometry will be noted $P_{\alpha\beta}$. For example,

$$P_{12} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.3}$$

3. The isometry described in [7], equation 12, which we call Σ:

$$\Sigma = \frac{1}{2} \begin{pmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{pmatrix}. \tag{3.4}$$

Here, it will be more convenient to use two other isometries obtained by combining Σ with some S_α and $P_{\alpha\beta}$:

$$\Sigma_1 = P_{14}P_{23}S_1S_2S_3S_4\Sigma = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \end{pmatrix}, \tag{3.5}$$

$$\Sigma_2 = P_{14}P_{23}S_2S_3S_4\Sigma S_4 = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}. \tag{3.6}$$

It can be shown that the above isometries are sufficient to generate all elements of G (i.e., they form a *generating set*). In fact, a minimal generating set can be formed with five elements only; for example, $S_1, P_{12}, P_{13}, P_{14}, \Sigma_1$. In practice, however, it will be more convenient to use the redundant set of 12 elements:

$$S_1, S_2, S_3, S_4, P_{12}, P_{13}, P_{14}, P_{23}, P_{24}, P_{34}, \Sigma_1, \Sigma_2. \tag{3.7}$$

It can be shown that every isometry M has one and only one representation of the form

$$M = \begin{pmatrix} I \\ S_4 \end{pmatrix} \begin{pmatrix} I \\ S_3 \end{pmatrix} \begin{pmatrix} I \\ S_2 \end{pmatrix} \begin{pmatrix} I \\ S_1 \end{pmatrix} \begin{pmatrix} I \\ P_{34} \end{pmatrix} \begin{pmatrix} I \\ P_{23} \\ P_{24} \end{pmatrix} \begin{pmatrix} I \\ P_{12} \\ P_{13} \\ P_{14} \end{pmatrix} \begin{pmatrix} I \\ \Sigma_1 \\ \Sigma_2 \end{pmatrix} \tag{3.8}$$

where, in each parentheses, one of the factors is to be chosen. I is the identity. Equation (3.8) will be called the *normal form* of M.

It can be remarked that every element of the list (3.7) is a simple symmetry with respect to a hyperplane in the four-dimensional space. The equation of the hyperplane is $x_\alpha = 0$ for S_α, $x_\alpha = x_\beta$ for $P_{\alpha\beta}$, $x_1 + x_4 = x_2 + x_3$ for Σ_1, $x_1 = x_2 + x_3 + x_4$ for Σ_2.

4. Minimization of the viscosity

This section is written with general notations so as to be valid not only for the FCHC lattice but for all lattices satisfying the usual conditions [2,10]. As explained in the introduction, we want to select the isometry so as to minimize the viscosity of the lattice gas. The kinematic shear viscosity is given by [10], equation (102):

$$\nu = \frac{\tau c^2}{2(D+2)} \frac{\mu_4}{1-\mu_4} \tag{4.1}$$

where τ is the time step, c is the velocity modulus, D is the number of space dimensions, and μ_4 is the *viscosity index*, which is a dimensionless number lying between 0 and 1, given by (ibid., equations (101) and (87))

$$\mu_4 = 1 - \frac{D}{2(D-1)n} \sum_s \sum_{s'} A(s;s') d^{p-1}(1-d)^{n-p-1} \sum_i \sum_j s_i (s_j - s'_j) \cos^2 \theta_{ij} \tag{4.2}$$

where n is the number of velocities, $A(s;s')$ is the probability of a transition from an input state s to an output state s', d is the average probability of a particle arriving along a link, $p = \sum_i s_i$ is the number of particles, and θ_{ij} is the angle between the velocities $\mathbf{c}_i$ and $\mathbf{c}_j$. For the FCHC lattice with its usual normalization, we have $\tau = 1$, $c^2 = 2$, $D = 4$, $n = 24$, and (4.1) reduces to

$$\nu = \frac{1}{6} \frac{\mu_4}{1-\mu_4} \tag{4.3}$$

For a given isometry M, we will compute an approximate average value of (4.2), using statistical arguments to estimate $\cos^2 \theta_{ij}$. We will assume that the input velocities are arbitrary and independent. This is not strictly true, since the input states which we are considering must have a given momentum; this constrains the choice of the input velocities. However, the viscosity is controlled by the *second-order momentum* [10], which is largely decoupled from the first-order momentum. The present estimates are in fact borne out by exact computations.

We remark first that as a consequence of the lattice isotropy ([10] equation (49b)), we have for a given i

$$\sum_j \cos^2\theta_{ij} = \frac{n}{D} \tag{4.4}$$

It follows that for arbitrarily and independently chosen i and j, the average value is

$$\left\langle \cos^2\theta_{ij} \right\rangle = \frac{1}{D} \tag{4.5}$$

Next, we consider the particular case where $\mathbf{c}_j = M\mathbf{c}_i$ (i.e., the direction j is the image of the direction i by the isometry). In this case, i and j are not independent, and the average value of $\cos^2\theta_{ij}$ will depend on the isometry M. For instance, if M is the isometry, then the average value is obviously 1. We will denote this value by w:

$$\left\langle \cos^2\theta_{ij} \right\rangle_{\mathbf{c}_j = M\mathbf{c}_i} = w \tag{4.6}$$

w is easily computed from M:

$$w = \frac{1}{nc^4} \sum_i (\mathbf{c}_i \cdot M\mathbf{c}_i)^2 \tag{4.7}$$

Finally, we consider the case where $\mathbf{c}_j$ can take any value except $M\mathbf{c}_i$. Combining (4.5) and (4.6), we obtain

$$\left\langle \cos^2\theta_{ij} \right\rangle_{\mathbf{c}_j \neq M\mathbf{c}_i} = \frac{1}{n-1}\left(\frac{n}{D} - w\right) \tag{4.8}$$

We now proceed to estimate the quantity

$$Q = \sum_i s_i \sum_j s'_j \cos^2\theta_{ij} \tag{4.9}$$

This double sum contains p^2 non-vanishing terms ($s_i = 1$ and $s'_j = 1$) since there are p input velocities and p output velocities. Of these, exactly p terms correspond to $\mathbf{c}_j = M\mathbf{c}_i$, since the output state derives from the input state through M. Therefore, $p(p-1)$ terms correspond to $\mathbf{c}_j \neq M\mathbf{c}_i$. Using (4.6) and (4.8), we obtain

$$\langle Q \rangle = pw + \frac{p(p-1)}{n-1}\left(\frac{n}{D} - w\right) = \frac{p(n-p)w}{n-1} + \frac{p(p-1)n}{(n-1)D} \tag{4.10}$$

Next, we have to estimate the quantity

$$Q^* = \sum_i s_i \sum_j s_j \cos^2 \theta_{ij} \tag{4.11}$$

We observe that (4.11) is simply a particular case of (4.9), obtained when M is the identity, so its value is immediately obtained by substituting $w = 1$ in (4.10):

$$\langle Q^* \rangle = \frac{p(n-p)}{n-1} + \frac{p(p-1)n}{(n-1)D}. \tag{4.12}$$

Combining (4.10) and (4.12), we obtain

$$\left\langle \sum_i \sum_j s_i (s_j - s'_j) \cos^2 \theta_{ij} \right\rangle = \langle Q^* - Q \rangle = \frac{p(n-p)}{n-1}(1-w). \tag{4.13}$$

We recall that this relation is only approximate. It indicates, however, that in order to minimize the viscosity we should select isometries for which w is smallest.

w is given by (4.7). Its minimal value is 0; this value is reached if every velocity is perpendicular to its image. The maximal value is $w = 1$; it is reached in particular when M is the identity, and more generally if every velocity is either identical or opposite to its image.

w can be easily computed as an explicit function of the elements $a_{\alpha\beta}$ of the matrix M. Let c_{i1}, c_{i2}, c_{i3}, c_{i4} be the coordinates of $\mathbf{c}_i$. We have

$$\begin{aligned} w &= \frac{1}{nc^4} \sum_i \Big(\sum_\alpha \sum_\beta a_{\alpha\beta} c_{i\alpha} c_{i\beta}\Big)^2 \\ &= \frac{1}{nc^4} \sum_i \Big(\sum_\alpha \sum_\beta a_{\alpha\beta} c_{i\alpha} c_{i\beta}\Big)\Big(\sum_\gamma \sum_\delta a_{\gamma\delta} c_{i\gamma} c_{i\delta}\Big) \\ &= \frac{1}{nc^4} \sum_\alpha \sum_\beta \sum_\gamma \sum_\delta a_{\alpha\beta} a_{\gamma\delta} \sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta}. \end{aligned} \tag{4.14}$$

From the symmetry relations [10,8], we have

$$\sum_i c_{i\alpha}^2 c_{i\beta}^2 = \frac{nc^4}{D(D+2)} \quad (\alpha \neq \beta), \qquad \sum_i c_{i\alpha}^4 = \frac{3nc^4}{D(D+2)},$$

$$\sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} = 0 \quad \text{in all other cases,} \tag{4.15}$$

and we obtain

$$w = \frac{1}{D(D+2)} \Big[\sum_\alpha \sum_{\beta \neq \alpha} (a_{\alpha\alpha} a_{\beta\beta} + a_{\alpha\beta}^2 + a_{\alpha\beta} a_{\beta\alpha}) + 3 \sum_\alpha a_{\alpha\alpha}^2 \Big], \tag{4.16}$$

which can also be written

$$w = \frac{1}{D(D+2)}\Big[\sum_{\alpha}\sum_{\beta>\alpha}(a_{\alpha\beta}+a_{\beta\alpha})^2 + (\sum_{\alpha} a_{\alpha\alpha})^2 + 2\sum_{\alpha} a_{\alpha\alpha}^2\Big]. \tag{4.17}$$

This equation shows in particular that $w = 0$ if and only if M is antisymmetric: $a_{\alpha\alpha} = 0$, $a_{\alpha\beta} = -a_{\beta\alpha}$. For the FCHC lattice, the only isometries having this property are those which consist of two $\pi/2$ rotations, such as

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \tag{4.18}$$

and the other isometries deduced from (4.18) by permutations; there are 12 of them.

5. Normalized momenta

Let q_1, q_2, q_3, q_4 be the coordinates of the momentum. Clearly, the number and the nature of the allowed isometries will depend on the values of the q_α; for instance, if $q_1 = 0$, we can use S_1; if $q_1 = q_2$, we can use P_{12}, and so on.

A detailed enumeration shows that the momentum can take 7009 distinct values (see table 1 below). We can, however, reduce considerably the number of cases to be considered by taking advantage of the symmetries of the problem. Specifically, we will show that by using appropriate changes of coordinates we can restrict our attention to *normalized momenta*, which we define as those which satisfy the following conditions:

$$q_1 \geq q_2 \geq q_3 \geq q_4 \geq 0 \quad \text{and} \quad (q_4 = 0 \quad \text{or} \quad q_1 + q_4 < q_2 + q_3). \tag{5.1}$$

The full treatment of a collision is then as follows. (i) We make a change of coordinates as required. This is equivalent to applying to the input state an isometry Γ, belonging to G, such that the new momentum satisfies (5.1). (ii) We compute the collision by applying an isometry M which preserves the momentum. (iii) We come back to the initial coordinates by Γ^{-1}. In other words, the isometry $\Gamma^{-1}M\Gamma$ is applied to the input velocities to obtain the output velocities.

We now define the isometry Γ. It consists of three steps:

1. If one of the q_α is negative, we invert the sign of the corresponding coordinate (we apply S_α). We are thus reduced to the case where all q_α are positive or zero.

2. We use the coordinate permutations $P_{\alpha\beta}$ to sort the q_α in non-increasing order. Thus, the first half of (5.1) is already satisfied.

3. If $q_4 > 0$ and $q_1 + q_4 = q_2 + q_3$, we apply Σ_2. If $q_4 > 0$ and $q_1 + q_4 > q_2 + q_3$, we apply Σ_1; then, if the new q_4 is negative, we apply S_4. It is not difficult to show that the new momentum satisfies (5.1).

There are 37 normalized momenta; it can be shown that no further reduction of the number of cases is possible. The coordinates of the normalized momenta are listed in table 1, columns 1 to 4. Column 5 is the *class* (see below). Column 6 is the number r of momenta which reduce to a given normalized momentum. The total of this column gives the total number of momenta as 7009.

6. Optimal isometries

We determine first the subgroup H of the isometries which preserve each normalized momentum. Momenta which define the same subgroup H will be said to belong to the same *class*. A detailed study shows that there are 12 classes. They are enumerated in table 2. The first column is an arbitrary identification number. The second column is the definition of the class. The third column is the order of H (i.e., the number of isometries which preserve the momentum). (Note that the number r appearing in table 1 is the *index* of H in G, and therefore $r|H| = |G| = 1152$). The fourth column is a generating set for H.

Next, for each class we compute w for each element of the subgroup H, using its matrix representation and the formula (4.17). We note the minimal value w_{min} of w in H. The isometries for which $w = w_{min}$ will be called *optimal*. table 3 gives for each class the value of w_{min} in column 2, the number of optimal isometries in column 3, and the list of the optimal isometries (written in normal form) in column 4.

7. Recipe

We collect here as a recipe all steps of a collision computation.

1. Compute the components q_1, q_2, q_3, q_4 of the momentum.
2. Change of coordinates:
   (a) If $q_1 < 0$, apply the isometry S_1 to the input state (and of course also to the momentum). Proceed in the same way for q_2, q_3, q_4.
   (b) Apply $P_{\alpha\beta}$ so as to have the q_α in non-increasing order: $q_1 \geq q_2 \geq q_3 \geq q_4 \geq 0$.
   (c) If $q_4 > 0$ and $q_1 + q_4 = q_2 + q_3$, apply Σ_2. If $q_4 > 0$ and $q_1 + q_4 > q_2 + q_3$, apply Σ_1, and then eventually S_4 so as to have $q_4 \geq 0$.
3. Collision:
   (a) Determine the class, using the definitions of table 2, column 2.

q_1	q_2	q_3	q_4	Class	r
0	0	0	0	12	1
1	1	0	0	10	24
2	0	0	0	11	24
2	1	1	0	6	96
2	2	0	0	10	24
2	2	2	0	8	96
3	1	0	0	9	144
3	2	1	0	3	192
3	3	0	0	10	24
3	3	2	0	5	288
3	3	3	1	2	192
4	0	0	0	11	24
4	1	1	0	7	288
4	2	0	0	9	144
4	2	2	0	6	96
4	3	1	0	3	192
4	3	3	0	7	288
4	4	0	0	10	24
4	4	2	0	5	288
4	4	3	1	1	576
4	4	4	0	8	96
5	1	0	0	9	144
5	2	1	0	4	576
5	3	0	0	9	144
5	3	2	0	3	192
5	4	1	0	3	192
5	4	3	0	4	576
5	5	0	0	10	24
5	5	2	0	5	288
6	0	0	0	11	24
6	1	1	0	7	288
6	2	0	0	9	144
6	2	2	0	7	288
6	3	1	0	4	576
6	3	3	0	6	96
6	4	0	0	9	144
6	4	2	0	3	192

Table 1: FCHC lattice: normalized momenta.

Class	Definition	$\lvert H\rvert$	Generating set
1	$q_1 = q_2 > q_3 > q_4 > 0$	2	P_{12}
2	$q_1 = q_2 = q_3 > q_4 > 0$	6	P_{12}, P_{23}
3	$q_1 > q_2 > q_3 > q_4 = 0,\ q_1 = q_2 + q_3$	6	S_4, Σ_1
4	$q_1 > q_2 > q_3 > q_4 = 0,\ q_1 \neq q_2 + q_3$	2	S_4
5	$q_1 = q_2 > q_3 > q_4 = 0$	4	S_4, P_{12}
6	$q_1 > q_2 = q_3 > q_4 = 0,\ q_1 = 2q_2$	12	S_4, P_{23}, Σ_1
7	$q_1 > q_2 = q_3 > q_4 = 0,\ q_1 \neq 2q_2$	4	S_4, P_{23}
8	$q_1 = q_2 = q_3 > q_4 = 0$	12	S_4, P_{12}, P_{23}
9	$q_1 > q_2 > q_3 = q_4 = 0$	8	S_4, P_{34}
10	$q_1 = q_2 > q_3 = q_4 = 0$	48	$S_4, P_{12}, P_{34}, \Sigma_1$
11	$q_1 > q_2 = q_3 = q_4 = 0$	48	S_4, P_{23}, P_{34}
12	$q_1 = q_2 = q_3 = q_4 = 0$	1152	$S_4, P_{12}, P_{23}, P_{34}, \Sigma_1$

Table 2: FCHC lattice: the 12 classes and the corresponding subgroups H.

Class	w_{min}	Optimal isometries	
1	1/2	1	P_{12}
2	1/4	2	$P_{23}P_{12},\ P_{23}P_{13}$
3	1/4	2	$S_4\Sigma_1,\ S_4\Sigma_2$
4	1/2	1	S_4
5	1/3	1	S_4P_{12}
6	1/4	4	$S_4\Sigma_1,\ S_4\Sigma_2,\ S_4P_{23}\Sigma_1,\ S_4P_{23}\Sigma_2$
7	1/3	1	S_4P_{23}
8	1/4	4	$P_{23}P_{12},\ P_{23}P_{13},\ S_4P_{23}P_{12},\ S_4P_{23}P_{13}$
9	1/3	3	$S_4S_3,\ S_3P_{34},\ S_4P_{34}$
10	1/6	6	$S_3P_{34}P_{12},\ S_4P_{34}P_{12},\ S_4S_3\Sigma_1,$ $S_4S_3P_{34}P_{12}\Sigma_1,\ S_4S_3\Sigma_2,\ P_{34}P_{12}\Sigma_2$
11	1/6	6	$S_4S_2P_{23},\ S_4S_3P_{23},\ S_3S_2P_{24},$ $S_4S_3P_{24},\ S_3S_2P_{34},\ S_4S_2P_{34}$
12	0	12	$S_3S_1P_{34}P_{12},\ S_4S_1P_{34}P_{12},\ S_3S_2P_{34}P_{12},\ S_4S_2P_{34}P_{12},$ $S_2S_1P_{24}P_{13},\ S_4S_1P_{24}P_{13},\ S_3S_2P_{24}P_{13},\ S_4S_3P_{24}P_{13},$ $S_2S_1P_{23}P_{14},\ S_3S_1P_{23}P_{14},\ S_4S_2P_{23}P_{14},\ S_4S_3P_{23}P_{14}$

Table 3: FCHC lattice: optimal isometries.

(b) Choose at random one of the optimal isometries of table 3, column 4.

(c) Apply this isometry.

4. Apply a change of coordinates which is the inverse of the change made in step 2. Since all isometries S_α, $P_{\alpha\beta}$, Σ_α are identical with their inverses, this can be done simply in applying the same sequence of isometries as in step 2, in reverse order.

8. Viscosity

Now that the collision rules have been fully specified, the viscosity can be computed from (4.1) and (4.2). μ_4 depends on d: it is a polynomial of degree 23 in d. The computation of the coefficients of this polynomial takes about one hour on a VAX 785. Only the terms corresponding to normalized momenta need to be computed; they are then multiplied by the coefficient r given in the last column of table 1. Figure 1 shows μ_4 as a function of $24d$, which is the average number of particles per node (full line).

The collision rules are invariant under duality—i.e., when particles are replaced by "holes" ($s_i \mapsto 1 - s_i$). Therefore, $\mu_4(d) = \mu_4(1-d)$. This symmetry is apparent in figure 1. We note also that μ_4 is close to $1/2$ over a large interval of d values; this will be commented upon in section 9.

The Reynolds number in a lattice gas simulation is [2]

$$R = Ml_0R_* \tag{8.1}$$

where M is the Mach number; l_0 is the characteristic scale of the flow, expressed in units of one link length; R_* is given in the case of the FCHC lattice by

$$R_* = 2\sqrt{2}\frac{1-2d}{1-d}\frac{1-\mu_4}{\mu_4}. \tag{8.2}$$

Figure 2 shows R_* as a function of $24d$ (full line). With the isometric algorithm, the largest attainable value of R_* is approximately 2 and is reached for $24d \simeq 4$.

9. Random algorithm

We describe now another algorithm for the computation of collisions, which turns out to have properties very similar to the isometric algorithm. The basic rule is very simple:

Rule. *The output state is randomly chosen among all states which have the same particle number and the same momentum as the input state.*

This will be called the *random algorithm*. The conditions 1, 2, 4, 5, 6 (see introduction) are obviously satisfied; here, also, we have in fact detailed balancing. Condition 3 is also satisfied since all permitted collisions to

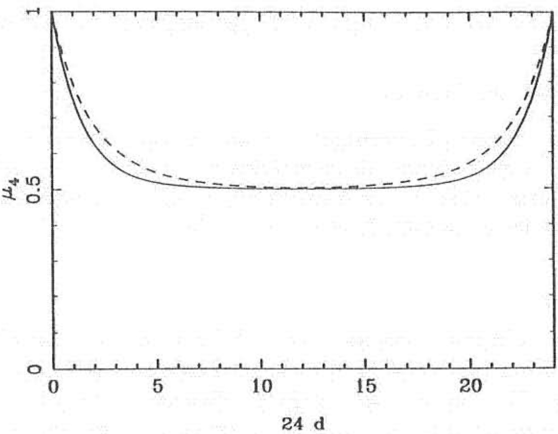

Figure 1: Viscosity index μ_4 as a function of the average number of particles per node, $24d$. Full line: isometric algorithm. Dashed line: random algorithm. The kinematic shear viscosity of the FCHC lattice is related to μ_4 by: $\nu = \mu_4/[6(1-\mu_4)]$.

This will be called the *random algorithm*. The conditions 1, 2, 4, 5, 6 (see introduction) are obviously satisfied; here, also, we have in fact detailed balancing. Condition 3 is also satisfied since all permitted collisions do happen in the random algorithm, and in particular those of the isometric algorithm.

Figures 1 and 2 show the viscosity index μ_4 and the quantity R_* for the random algorithm (dashed lines). The largest attainable value of R_* is 1.74, for $24d \simeq 4.8$. We note that here again μ_4 is close to 1/2 over a large range of values of d. A heuristic explanation can be given by estimating the quantity (4.2) in the same way as in Section 4. When the number of incoming particles is neither close to 0 nor to n, the number of permitted output states is large. We may assume then that the output state is practically uncorrelated with the input state. In estimating the quantity (4.9), we therefore use the average value (4.5) for all p^2 terms, obtaining

$$Q = \frac{p^2}{D}. \tag{9.1}$$

Combining this with (4.12), we obtain

$$\langle Q^* - Q \rangle = \frac{D-1}{D}\frac{p(n-p)}{n-1} \tag{9.2}$$

and after substitution in (4.2):

$$\mu_4 = 1 - \frac{1}{2}\sum_s \sum_{s'} A(s;s')\frac{p(n-p)}{n(n-1)}d^{p-1}(1-d)^{n-p-1} \tag{9.3}$$

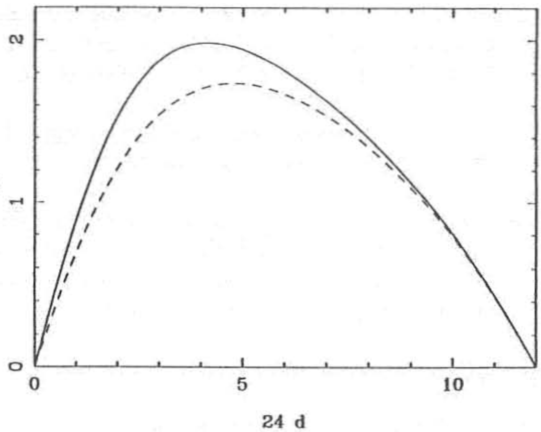

Figure 2: The quantity R_*, proportional to the Reynolds number, as a function of the average number of particles per node, $24d$. Full line: isometric algorithm. Dashed line: random algorithm. The actual Reynolds number R is related to R_* by equation (8.1).

or, summing on s':

$$\mu_4 = 1 - \frac{1}{2}\sum_s \frac{p(n-p)}{n(n-1)} d^{p-1}(1-d)^{n-p-1}. \tag{9.4}$$

The number of input states for a given p is the binomial coefficient $n!/[p!(n-p)!]$; therefore,

$$\mu_4 = 1 - \frac{1}{2}\sum_{p=1}^{n-1} \frac{(n-2)!}{(p-1)!(n-p-1)!} d^{p-1}(1-d)^{n-p-1} = \frac{1}{2}. \tag{9.5}$$

A more direct argument can be made, using the second-order tensors $Y_{\alpha\beta}$, $Y'_{\alpha\beta}$ and the quantities μ_1 to μ_4 defined in [10]. If the input and output states are uncorrelated, the quantity $\sum_\alpha \sum_\beta Y_{\alpha\beta} Y'_{\alpha\beta}$ vanishes on the average. Then μ_4 reduces to $(\mu_1 + \mu_2)/2$, which is $1/2$.

In retrospect, then, the fact that μ_4 is close to $1/2$ in the isometric algorithm for most values of d might be an indication that in that algorithm also the output state is nearly uncorrelated with the input state (at least as far as the second-order momentum is concerned).

In both algorithms, this vanishing correlation means that the particles lose all memory of their previous velocities at each collision. In other words, the mean free path (insofar as it can be defined for a lattice gas, where particles do not preserve their individuality) is smaller than one link length.

A practical implementation of the random algorithm would require that one first computes and stores tables of the states sorted by particle number and momentum. The size of these tables can be reduced by considering only the normalized momenta defined in section 5. The recipe consists then in the same steps 1, 2, and 4 as in Section 7, and a different step 3 as follows:

3. Collision: Choose at random an output state among all those which have the correct particle number and momentum.

We have described the random algorithm because its principle is very simple and because of its curious similarity to the isometric algorithm. In practice, the isometric algorithm is probably to be preferred, since its implementation is less cumbersome and its performance is somewhat better.

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Appendix A. HPP lattice

We apply here the isometric algorithm to the HPP lattice. The four velocities are

$$(1,0), \qquad (0,1), \qquad (-1,0), \qquad (0,-1). \tag{A.1}$$

The isometries form a group G of order 8. A generating set is formed by the symmetry S with respect to the line $y = 0$ and the rotation R by an angle $\pi/2$:

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{A.2}$$

The elements of G are:

$$I, R, R^2, R^3, S, RS, R^2S, R^3S. \tag{A.3}$$

w is again defined by (4.7). The HPP lattice is not isotropic at fourth order, and the equations (4.15) cannot be used; instead, we have

$$\sum_i c_{i\alpha}^4 = 2, \qquad \sum_i c_{i\alpha}c_{i\beta}c_{i\gamma}c_{i\delta} = 0 \quad \text{in all other cases.} \tag{A.4}$$

We obtain

$$w = \frac{1}{2}(a_{11}^2 + a_{22}^2). \tag{A.5}$$

The values of w for the eight elements (A.3) are respectively

q_1	q_2	Class	r
0	0	3	1
1	0	2	4
1	1	1	4

Table 4: HPP lattice: normalized momenta

Class	Definition	$\|H\|$	Generating set
1	$q_1 = q_2 > 0$	2	RS
2	$q_1 > q_2 = 0$	2	S
3	$q_1 = q_2 = 0$	8	S, R

Table 5: HPP lattice: the 3 classes and the corresponding subgroups H.

$$1, 0, 1, 0, 1, 0, 1, 0. \qquad (A.6)$$

By using an appropriate change of coordinates, we can reduce the problem to normalized momenta satisfying

$$q_1 \geq 0, \qquad 0 \leq q_2 \leq q_1. \qquad (A.7)$$

Tables 4, 5, and 6 are analogous to the tables 1, 2, and 3 and show respectively the three normalized momenta, the definitions of the three classes, and the optimal isometries.

The transition rules are found to reduce to

$$(i, i+2) \mapsto (i+1, i+3), \qquad (A.8)$$

in an obvious notation. In all other cases, the velocities are unchanged. These are exactly the usual rules for the HPP lattice.

Class	w_{min}	Optimal isometries	
1	0	1	RS
2	1	2	I, S
3	0	4	R, R^3, RS, R^3S

Table 6: HPP lattice: optimal isometries.

Appendix B. FHP lattice

We apply here the isometric algorithm to the FHP lattice. The six velocities are

$$(\frac{1}{2}, \frac{\sqrt{3}}{2}), \qquad (-\frac{1}{2}, \frac{\sqrt{3}}{2}), \qquad (-1, 0),$$

q_1	q_2	Class	r
0	0	3	1
1	0	2	6
3/2	$\sqrt{3}/2$	1	6
2	0	2	6

Table 7: FHP lattice: normalized momenta.

Class	Definition	$\lvert H\rvert$	Generating set
1	$q_1 > q_2 > 0$	2	RS
2	$q_1 > q_2 = 0$	2	S
3	$q_1 = q_2 = 0$	12	S, R

Table 8: FHP lattice: the 3 classes and the corresponding subgroups H.

$$(-\frac{1}{2}, -\frac{\sqrt{3}}{2}), \qquad (\frac{1}{2}, -\frac{\sqrt{3}}{2}), \qquad (1,0). \tag{B.1}$$

The isometries form a group G of order 12. A generating set is formed by the symmetry S with respect to the line $y = 0$ and the rotation R by an angle $\pi/3$:

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad R = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \tag{B.2}$$

The elements of G are:

$$I, R, R^2, R^3, R^4, R^5, S, RS, R^2S, R^3S, R^4S, R^5S \tag{B.3}$$

The FHP lattice is isotropic to fourth order and we can use (4.15) and (4.17), obtaining

$$w = \frac{1}{8}[(a_{12} + a_{21})^2 + (a_{11} + a_{22})^2 + 2(a_{11}^2 + a_{22}^2)] \tag{B.4}$$

The values of w for the 12 elements (B.3) are

$$1, \frac{1}{4}, \frac{1}{4}, 1, \frac{1}{4}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}. \tag{B.5}$$

By using an appropriate change of coordinates, we can reduce the problem to normalized momenta satisfying

$$q_1 \geq 0, \qquad 0 \leq q_2 \leq \frac{\sqrt{3}}{3} q_1. \tag{B.6}$$

Tables 7, 8, and 9 show respectively the four normalized momenta, the definitions of the three classes, and the optimal isometries.

Class	w_{min}	Optimal isometries	
1	1/2	1	RS
2	1/2	1	S
3	1/4	4	R, R^2, R^4, R^5

Table 9: FHP lattice: optimal isometries.

The transition rules are found to reduce to

$$\begin{aligned}
(i, i+3) &\mapsto (i+1, i+4) \text{ or } (i-1, i+2), \\
(i, i+2, i+4) &\mapsto (i+1, i+3, i+5) \text{ or } (i, i+2, i+4), \\
(i-1, i, i+2) &\mapsto (i-2, i, i+1), \\
(i+1, i+2, i+4, i+5) &\mapsto (i, i+2, i+3, i+5) \\
&\quad\ \text{or } (i, i+1, i+3, i+4).
\end{aligned} \tag{B.7}$$

In all other cases, the velocities are unchanged. (7a) is the standard rule for head-on collisions. (7d) is the rule for dual collisions. (7b) is the standard rule for symmetric triple collisions, with one small difference: here the probability that the velocities are modified is only 1/2. Finally, (7c) is the rule for the "head-on collisions with spectator". In all other cases, the velocities are unchanged. Thus, we recover the usual rules for the FHP lattice, with one minor modification.

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