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Viscosity of a Lattice Gas

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Abstract. The shear viscosity of a lattice gas can be derived in the Boltzmann approximation from a straightforward analysis of the numerical algorithm. This computation is presented first in the case of the Frisch-Hasslacher-Pomeau two-dimensional triangular lattice. It is then generalized to a regular lattice of arbitrary dimension, shape, and collision rules with appropriate symmetries. The viscosity is shown to be positive. A practical recipe is given for choosing collision rules so as to minimize the viscosity.

1. Introduction

1.1 Goal

For computational efficiency, the collision rules in a lattice gas automaton should be chosen so as to make the shear viscosity as small as possible [1]. For a given set of rules, the viscosity can be estimated through numerical simulations [2,3]. It would be much more convenient, however, to have an explicit formula through which the viscosity could be computed directly from the lattice rules. Here, I present such a formula, which is applicable when the following conditions are satisfied:

1. there is a single population of particles (all velocities have the same modulus);
2. the lattice and the collision rules are "sufficiently symmetrical", in a sense which will be made more precise below (section 3);
3. the Boltzmann approximation is valid (the probabilities of arrival of particles at a node from different directions can be assumed independent);
4. the system is not far from isotropic equilibrium (low Mach number);
5. the only quantities conserved by collisions are the number of particles and the momentum; and
6. the collisions satisfy semi-detailed balancing.

It can be shown from the formula that the viscosity is always positive. Moreover, from the structure of the formula, one can derive a simple rule for the optimization of individual collisions.

1.2 Method

The formula will be derived by a straightforward analysis of the lattice rules; apart from the basic definition of shear viscosity, nothing is borrowed from the classical theories of fluid dynamics or statistical mechanics. The derivation consists of the following steps:

1. Define a steady, homogeneous state, with linear shear velocity field.
2. Write equations for collisions.
3. Write equations for propagation.
4. Solve these equations to determine the detailed structure of the steady state.
5. Compute the momentum flux and the viscosity.

In order to show the argument more clearly, the computation is first presented in detail for a simple case: the triangular lattice introduced by Frisch, Hasslacher, and Pomeau [4] (*FHP lattice*). The five steps are described in sections 2.1 to 2.5, then the computation is generalized to arbitrary lattices in sections 3.1 to 3.5.

1.3 The FHP lattice

We recall briefly the definition of the FHP lattice. We consider a plane triangular lattice, populated by particles. At any given time, a particle is in a given node and has a velocity pointing towards one of the six neighbor nodes, with a given modulus c. At a given node, no two particles can have the same velocity (exclusion principle). Evolution proceeds in two alternating phases: (i) *collisions*: particles arriving at a node "collide" and may change their velocities, according to definite *collision rules*; and (ii) *propagation*: each particle moves to the next node in the direction of its velocity. Several variations are possible concerning the collision rules; here we will use the original rules as defined in [4], i.e. only binary head-on collisions and triple collisions (see also [1], figures 4a and b). Note that each collision preserves the number of particles and the momentum. Note also the overall symmetry of the rules: they are invariant under any rotation or symmetry which preserves the lattice.

1.4 Notation

The velocities are $\mathbf{c}_i = (c_{i1}, c_{i2})$, with $i = 1$ to 6 (figure 1). The position of a node is $\mathbf{x} = (x_1, x_2)$. $N_i(\mathbf{x})$ is the probability of a particle *arriving* at node $\mathbf{x}$ with velocity $\mathbf{c}_i$. (In general, N_i should depend on time as well as on position; here, however, we will limit our attention to a steady state). $N_i'(\mathbf{x})$ is the probability of a particle *leaving* node $\mathbf{x}$ with velocity $\mathbf{c}_i$. We will use physical units rather than dimensionless units in order to avoid any ambiguity in the use of the final formula: l is the link length, τ is

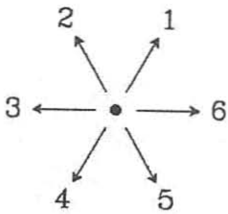

Figure 1: The six velocities of the FHP lattice.

the propagation time, and m is the mass of a particle. Thus, the velocity modulus is $c = l/\tau$, and the number of nodes per unit area is $f = 2/(\sqrt{3}\,l^2)$.

2. Computation of the viscosity for the FHP lattice

2.1 Steady state

The gas density is

$$\rho(\mathbf{x}) = fm \sum_{i=1}^{6} N_i(\mathbf{x}). \tag{2.1}$$

We will consider a homogeneous state: $\rho(\mathbf{x})$ has a constant value ρ.

In the simplest case of an isotropic velocity distribution, all N_i are equal to the same constant value d:

$$N_i(\mathbf{x}) = \frac{\rho}{6fm} = d. \tag{2.2}$$

We will consider a state which does not differ too much from isotropy:

$$N_i(\mathbf{x}) = d + \nu_i(\mathbf{x}), \qquad N_i'(\mathbf{x}) = d + \nu_i'(\mathbf{x}), \tag{2.3}$$

with

$$\nu_i(\mathbf{x}), \nu_i'(\mathbf{x}) \ll 1. \tag{2.4}$$

We have

$$\sum_{i=1}^{6} \nu_i = 0. \tag{2.5}$$

All computations will be made to first order in the ν_i.

The mean velocity $\mathbf{u}$ at a node $\mathbf{x}$ is defined by

$$\rho\mathbf{u}(\mathbf{x}) = fm \sum_{i=1}^{6} N_i(\mathbf{x})\mathbf{c}_i. \tag{2.6}$$

We will consider a state in which $\mathbf{u}$ is a shear flow:

$$u_1 = Tx_2, \qquad u_2 = 0, \tag{2.7}$$

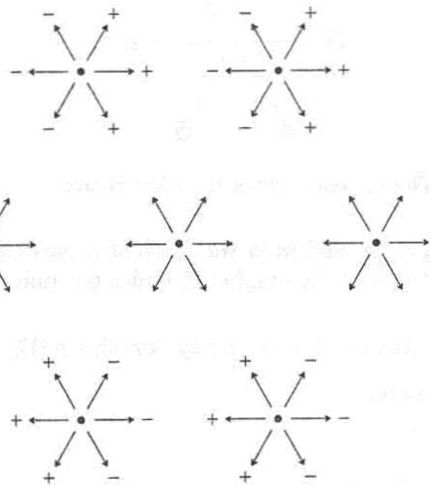

Figure 2: Deviations from equilibrium at seven neighboring nodes.

where T is a given constant. The steady state is thus defined by two constants, ρ and T. Our objective is to compute its detailed structure, i.e., the values of the $N_i(\mathbf{x})$.

It seems natural to assume that each ν_i is also a linear function of x_2:

$$\nu_i(\mathbf{x}) = k_i x_2 + \epsilon_i, \tag{2.8}$$

where the k_i and ϵ_i ($i = 1$ to 6) are 12 constants to be determined. The interpretation of the constants k_i is straightforward. Figure 2 represents the velocities at seven neighboring nodes. The central horizontal line corresponds to $x_2 = 0$: the mean velocity is $\mathbf{u} = 0$ as shown by equation (2.7). Therefore, we do not expect any systematic first-order deviation from equilibrium on that line. In the upper horizontal line, x_2 is positive, and the mean velocity $\mathbf{u}$ has a positive horizontal constant. Therefore, we expect an increase of the populations N_i for the velocities $i = 1, 5, 6$ lying in the right half-plane, and a decrease for the velocities $i = 2, 3, 4$ lying in the left half-plane, as indicated by the + and − signs (which are the signs of the ν_i). In the lower horizontal line, we have the opposite effect. For any particular velocity $\mathbf{c}_i$, then, we have a linear variation of ν_i with the ordinate x_2.

The interpretation of the ϵ_i terms is more subtle; they result from the combination of shear and propagation. Consider the situation one propagation step after figure 2. The central node receives an under-average number of particles along directions 1 and 4, and an over-average number

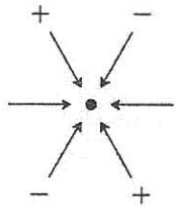

Figure 3: Shear-induced anisotropy.

along directions 2 and 5 (figure 3). Thus, a *shear-induced anisotropy* is created. This anisotropy is represented by the ϵ_i terms.

Substitution of equation (2.8) in the mass and momentum equations (2.1) and (2.6) gives three equations for the ϵ_i:

$$\sum_{i=1}^{6} \epsilon_i = 0, \qquad \sum_{i=1}^{6} \epsilon_i c_{i1} = 0, \qquad \sum_{i=1}^{6} \epsilon_i c_{i2} = 0, \tag{2.9}$$

and three equations for the k_i:

$$\sum_{i=1}^{6} k_i = 0, \qquad ,\sum_{i=1}^{6} c_{i1} k_i = 6dT, \qquad \sum_{i=1}^{6} c_{i2} k_i = 0. \tag{2.10}$$

These equations are not sufficient to determine the ϵ_i and the k_i. To complete the determination, we must write that the state of the system is invariant under collisions plus propagation. So we first establish equations for these two mechanisms.

2.2 Collisions

In this section, we consider a given node $\mathbf{x}$; to simplify, we will omit the coordinate $\mathbf{x}$ and write N_i for $N_i(\mathbf{x})$, etc.

A particular collision is defined by an *input state*, defined as a subset of the n velocities, and an *output state*, similarly defined. The input state is conveniently defined by a collection of n numbers:

$$s = (s_1, \ldots, s_6), \tag{2.11}$$

where $s_i = 1$ if velocity $\mathbf{c}_i$ is present in the input state, $s_i = 0$ otherwise. Similarly, we define

$$s' = (s'_1, \ldots, s'_6) \tag{2.12}$$

for the output state. We write a collision as $C = (s; s')$. Each collision C has an associated probability, which we write

$$A(C) \qquad \text{or} \qquad A(s; s'). \tag{2.13}$$

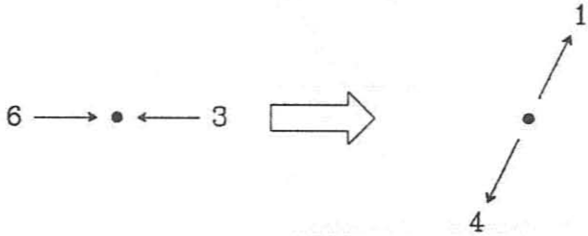

Figure 4: Example of a collision.

As an example, for the collision represented on figure 4, we have

$$s = (0,0,1,0,0,1), \qquad s' = (1,0,0,1,0,0), \tag{2.14}$$

and the associated probability is, under the classical FHP rules:

$$A(0,0,1,0,0,1;1,0,0,1,0,0) = A(s;s') = 1/2. \tag{2.15}$$

It will be convenient to formally define a *collision* for all s and s', even if the collision rules do not provide for any actual transition from s to s'; in that case, we simply write $A(s;s') = 0$. There are $2^6 = 64$ possible input states s, and 64 possible output states s'. Therefore, $A(s;s')$ can be written as a 64×64 matrix. In this way, the whole set of collision rules is neatly encoded into a single matrix. It is a very sparse matrix: most cases correspond to forbidden transitions, i.e. $A = 0$ (in particular, all cases where the number of particles or the momentum of s and s' do not agree). Note also that for an input state s which does not change, there is $A(s;s') = 1$ for $s' = s$, and $A(s;s') = 0$ for $s' \neq s$.

The sum of all A corresponding to a given input state s must of course be 1; so for any s we have

$$\sum_{s'} A(s;s') = 1. \tag{2.16}$$

We will assume that the symmetric relations are also satisfied, i.e. for any s', there is

$$\sum_{s} A(s;s') = 1. \tag{2.17}$$

This is called *semi-detailed balancing*.

In what follows, we will frequently have to sum over all collisions, and we will use the various notations

$$\sum_C A\mathcal{F} = \sum_{\mathfrak{f}} \sum_{\mathfrak{f}'} \mathcal{A}(\mathfrak{f};\mathfrak{f}')\mathcal{F} =$$

$$\sum_{s_1=0}^{1} \cdots \sum_{s_6=0}^{1} \sum_{s_1'=0}^{1} \cdots \sum_{s_6'=0}^{1} A(s_1, \ldots, s_6; s_1', \ldots, s_6')\mathcal{F}. \tag{2.18}$$

where $\mathcal{F}$ is any expression.

For any given collision $(s; s')$ with non-zero probability, the number of particles p and the momentum $\mathbf{q}$ must be preserved. In other words, if $A(s; s') \neq 0$, then

$$p = \sum_{i=1}^{6} s_i = p' = \sum_{i=1}^{6} s_i', \tag{2.19}$$

and

$$\mathbf{q} = \sum_{i=1}^{6} s_i \mathbf{c}_i = \mathbf{q}' = \sum_{i=1}^{6} s_i' \mathbf{c}_i. \tag{2.20}$$

We use now the Boltzmann approximation and we write that the probability of an input state s is

$$\prod_{j=1}^{6} N_j^{s_j} (1 - N_j)^{1-s_j}. \tag{2.21}$$

Therefore, the probability of having a particle with velocity $\mathbf{c}_i$ in the output state is:

$$N_i' = \sum_C s_i' A \prod_{j=1}^{6} N_j^{s_j} (1 - N_j)^{1-s_j}. \tag{2.22}$$

If we sum the probabilities of all input states which contain $\mathbf{c}_i$, we obtain N_i:

$$N_i = \sum_s s_i \prod_{j=1}^{6} N_j^{s_j} (1 - N_j)^{1-s_j} \tag{2.23}$$

or, using equation (2.16)

$$N_i = \sum_C s_i A \prod_{j=1}^{6} N_j^{s_j} (1 - N_j)^{1-s_j}. \tag{2.24}$$

Therefore,

$$N_i' - N_i = \sum_C (s_i' - s_i) A \prod_{j=1}^{6} N_j^{s_j} (1 - N_j)^{1-s_j}. \tag{2.25}$$

If $p = 0$, there is $s_i = s_i' = 0$ for all i, and the corresponding term in the right-hand side of equation (2.25) vanishes. Similarly, the term corresponding to $p = 6$ vanishes. Therefore, we will consider in equation (2.25) and in all subsequent equations (which derive from it) that the summation is to be made only on collisions with

$$1 \le p \le n-1. \tag{2.26}$$

Substituting $N_i = d + \nu_i$, $N_i' = d + \nu_i'$, and developing to first order in the ν_i, we obtain

$$\nu_i' - \nu_i = \sum_C (s_i' - s_i) A d^p (1-d)^{6-p} \left[1 + \frac{1}{d(1-d)} \sum_{j=1}^{6} (s_j - d)\nu_j \right]. \tag{2.27}$$

The first term can be written, using equations (2.19), (2.16), and (2.17)

$$\sum_C s_i' A d^{p'} (1-d)^{6-p'} - \sum_C s_i A d^p (1-d)^{6-p} =$$

$$\sum_{s'} s_i' d^{p'} (1-d)^{6-p'} - \sum_s s_i d^p (1-d)^{6-p}. \tag{2.28}$$

This vanishes since the two terms represent the same summation. Using also equation (2.5), we obtain the fundamental *collision equation*:

$$\nu_i' - \nu_i = \sum_C (s_i' - s_i) A d^{p-1} (1-d)^{5-p} \sum_{j=1}^{6} s_j \nu_j. \tag{2.29}$$

As an example, consider the case $i = 1$. $s_i' - s_i$ is different from zero in six cases:

$$\begin{aligned}
&s = (1,0,0,1,0,0), && s' = (0,1,0,0,1,0), && p = 2, && A = 1/2;\\
&s = (1,0,0,1,0,0), && s' = (0,0,1,0,0,1), && p = 2, && A = 1/2;\\
&s = (0,1,0,0,1,0), && s' = (1,0,0,1,0,0), && p = 2, && A = 1/2;\\
&s = (0,0,1,0,0,1), && s' = (1,0,0,1,0,0), && p = 2, && A = 1/2;\\
&s = (1,0,1,0,1,0), && s' = (0,1,0,1,0,1), && p = 3, && A = 1;\\
&s = (0,1,0,1,0,1), && s' = (1,0,1,0,1,0), && p = 3, && A = 1.
\end{aligned} \tag{2.30}$$

Therefore, the collision equation is

$$\nu_1' - \nu_1 = \frac{1}{2} d(1-d)^3 (\nu_2 + \nu_5 + \nu_3 + \nu_6 - 2\nu_1 - 2\nu_4)$$

$$+ d^2 (1-d)^2 (\nu_2 + \nu_4 + \nu_6 - \nu_1 - \nu_3 - \nu_5) \tag{2.31}$$

The other equations ($i = 2, \ldots, 6$) are deduced by rotation of indices.

2.3 Propagation

The probability of arrival of a particle at a node equals the probability of leaving the previous node:

$$N_i(\mathbf{x} + \tau\mathbf{c}_i, t + \tau) = N_i'(\mathbf{x}, t). \tag{2.32}$$

Since we assume a steady state, this equation reduces to

$$N_i(\mathbf{x} + \tau\mathbf{c}_i) = N_i'(\mathbf{x}). \tag{2.33}$$

Substituting the expressions (2.3) for N and N' and using (2.8), we obtain the fundamental *propagation equation*:

$$\nu_i(\mathbf{x}) - \nu_i'(\mathbf{x}) = -\tau k_i c_{i2}. \tag{2.34}$$

2.4 Computation of the steady state

Combining the collision and propagation equations, (2.29) and (2.34), and substituting (2.8), we obtain a set of six equations:

$$\sum_C (s_i' - s_i) A d^{p-1}(1-d)^{5-p} \sum_{j=1}^{6} s_j(k_j x_2 + \epsilon_j) - \tau k_i c_{i2} = 0$$

$$(i = 1, \ldots, 6). \tag{2.35}$$

We use now these equations, together with equations (2.9) and (2.10), to determine the steady state. We consider first the terms proportional to x_2 in equation (2.35), which give six equations:

$$\frac{1}{2} d(1-d)^3(k_2 + k_5 + k_3 + k_6 - 2k_1 - 2k_4)$$

$$+ d^2(1-d)^2(k_2 + k_4 + k_6 - k_1 - k_3 - k_5) = 0 \tag{2.36}$$

and five similar equations deduced by circular permutation. This is a set of linear homogeneous equations. But in fact, there are only three independent equations, because of the conservation of mass and momentum. Therefore, equation (2.36) has non-zero solutions, which have the general form

$$k_i = K_0 + K_1 c_{i1} + K_2 c_{i2} \tag{2.37}$$

where K_0, K_1, K_2 are arbitrary constants. Making use now of equation (2.10), we find that the K_i are uniquely determined and the k_i are

$$k_i = \frac{2dT}{c^2} c_{i1}. \tag{2.38}$$

We remark that k_i is proportional to the horizontal component of $\mathbf{c}_i$; this agrees with the intuitive description of figure 2.1.

We consider next the terms independent of x_2 in equation (2.35), which give after substitution of the solution (2.38):

$$\frac{1}{2}d(1-d)^3(\epsilon_2+\epsilon_5+\epsilon_3+\epsilon_6-2\epsilon_1-2\epsilon_4)$$

$$+d^2(1-d)^2(\epsilon_2+\epsilon_4+\epsilon_6-\epsilon_1-\epsilon_3-\epsilon_5)-\frac{2d\tau T}{c^2}c_{11}c_{12}=0 \tag{2.39}$$

and five similar equations. These are six linear inhomogeneous equations. Again, there are only three independent equations. Combining with equation (2.9), we have a system of six independent equations to solve.

It will be helpful to inquire into the physical meaning of equation (2.39). Figures 2 and 3 showed that propagation produces a deficit of particles in directions 1 and 4 and an excess in directions 2 and 5. Thus, it tends to produce an anisotropy in the ϵ_i. On the other hand, since the collision rules are symmetrical, they should tend to damp out any anisotropy. Thus, the first two terms in equation (2.39) represent the damping of the anisotropy by collisions, while the last term represents the excitation of the anisotropy by propagation. The equation is satisfied when these two processes are in equilibrium.

This suggests the following conjecture: the equilibrium anisotropy, represented by the ϵ_i, should be proportional to the excitation term in equation (2.39):

$$\epsilon_i \propto -c_{i1}c_{i2}. \tag{2.40}$$

Looking at figure 1, we see that this can be written

$$\begin{aligned} &\epsilon_1=-\epsilon, \qquad &&\epsilon_2=\epsilon, \qquad &&\epsilon_3=0,\\ &\epsilon_4=-\epsilon, \qquad &&\epsilon_5=\epsilon, \qquad &&\epsilon_6=0 \end{aligned} \tag{2.41}$$

where ϵ is a constant. The equations (2.9) are satisfied. Substituting into equation (2.39), we find that the conjecture is true: the equations are satisfied if we take

$$\epsilon=\frac{\tau T}{2\sqrt{3}\,c^2}(1-d)^{-3} \tag{2.42}$$

and the solution is

$$\epsilon_i=-\frac{2\tau T}{3c^2}(1-d)^{-3}c_{i1}c_{i2}. \tag{2.43}$$

The steady state is thus completely determined. It is given by equations (2.3), (2.8), (2.38), (2.43):

$$N_i=d+\frac{2dT}{c^2}c_{i1}x_2-\frac{2\tau T}{3c^2}(1-d)^{-3}c_{i1}c_{i2}. \tag{2.44}$$

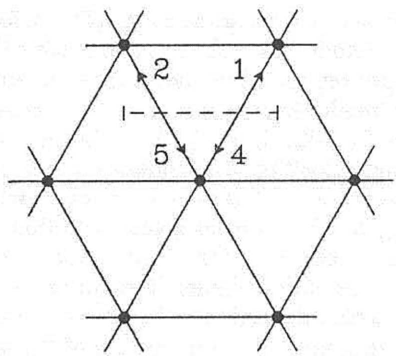

Figure 5: Computation of the momentum flux across a segment (shown as a dashed line).

2.5 Momentum flux

In view of the spatial periodicity of the lattice, it will be sufficient to compute the horizontal momentum Q transferred downwards across a horizontal segment of length l, situated above a node $\mathbf{x}$, during one propagation time τ (figure 5). The shear viscosity η is then defined by

$$Q = \eta T l \tau. \tag{2.45}$$

Contributions to Q come from four possible particle motions, corresponding to velocity directions 1, 2, 4, 5, as indicated on the figure. For instance, there is a probability $N_4(\mathbf{x})$ that a horizontal momentum mc_{41} will be transferred downwards, etc. Summing these contributions, we obtain

$$Q = m[N_4(\mathbf{x})c_{41} + N_5(\mathbf{x})c_{51} - N_1(\mathbf{x} + \tau\mathbf{c}_1)c_{11} - N_2(\mathbf{x} + \tau\mathbf{c}_2)c_{21}]. \tag{2.46}$$

Equating this to equation (2.45) and substituting the values (2.44) found for the steady state, we finally obtain the shear viscosity for the FHP lattice:

$$\eta = \rho\tau c^2 \left[\frac{1}{12d(1-d)^3} - \frac{1}{8}\right]. \tag{2.47}$$

The first term agrees with the result derived for small d in reference 5. Good agreement is found with the numerical simulation of reference 2.

3. Computation of the viscosity for a general lattice

We generalize now the computation to arbitrary lattices (subject to the conditions stated in the introduction).

We call D the number of space dimensions ($D = 2$ for the FHP lattice). Thus, the position of a node is $\mathbf{x} = (x_1, \ldots, x_D)$. We will use Greek letters α, β, ... for subscripts representing coordinates; a summation on one of these subscripts will implicitly run from 1 to D. We call n the number of velocities ($n = 6$ for the FHP lattice). We will use Latin letters i, j for subscripts representing velocities; a summation on one of these subscripts will implicitly run from 1 to n. The velocities are $\mathbf{c}_i$, with components $c_{i\alpha}$. The definitions of N_i, N_i', l, τ, and m given in section 1.4 are unchanged. The velocity modulus is still $c = l/\tau$. The quantity f is now defined as the number of nodes per unit volume; it is proportional to l^{-D}, with a numerical coefficient which depends on the lattice geometry.

We specify now the symmetry requirements of the lattice. For the purpose of the present paper, we will only need to specify symmetries for the set of n velocities $V = \{\mathbf{c}_1, \ldots, \mathbf{c}_n\}$.

1. *The set V must be isotropic to fourth order.* By this, we mean the following. For a given integer r, we define a tensor of order r

$$B_{\alpha_1\ldots\alpha_r} = \sum_i c_{i\alpha_1} \ldots c_{i\alpha_r}. \tag{3.1}$$

We require that up to order $r = 4$ these tensors are isotropic (i.e., their components are invariant in any rotation of the coordinate axes). As is easily shown, the tensors are then given by [6]:

$$B_\alpha = \sum_i c_{i\alpha} = 0,$$

$$B_{\alpha\beta} = \sum_i c_{i\alpha} c_{i\beta} = \frac{nc^2}{D}\delta_{\alpha\beta},$$

$$B_{\alpha\beta\gamma} = \sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} = 0,$$

$$B_{\alpha\beta\gamma\zeta} = \sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\zeta} = \frac{nc^4}{D(D+2)}(\delta_{\alpha\beta}\delta_{\gamma\zeta} + \delta_{\alpha\gamma}\delta_{\beta\zeta} + \delta_{\alpha\zeta}\delta_{\beta\gamma}) \tag{3.2}$$

where $\delta_{\alpha\beta}$ is the Kronecker symbol.

2. All velocities should be in a sense interchangeable. This is formalized as follows. We call G the group of the isometries of the D-dimensional space which map V on itself. Then, *for any two velocities $\mathbf{c}_i$ and $\mathbf{c}_j$, there exists an isometry of G which maps $\mathbf{c}_i$ on $\mathbf{c}_j$.*

3. We consider now a particular velocity $\mathbf{c}_i$. In addition to the symmetry around the origin, expressed by (1) above, the set V must also exhibit a definite symmetry around $\mathbf{c}_i$, which we now specify. First, we decompose each velocity $\mathbf{c}_j$ as

$$\mathbf{c}_j = \mathbf{c}_{j\parallel} + \mathbf{c}_{j\perp} , \tag{3.3}$$

where $\mathbf{c}_{j\parallel}$ is parallel to $\mathbf{c}_i$ and $\mathbf{c}_{j\perp}$ is perpendicular to $\mathbf{c}_i$. We call G_i the subgroup of G consisting of all isometries in which $\mathbf{c}_i$ is invariant. For a given j, consider the set V_{ij} of all velocities $\mathbf{c}_{I(j)}$ which can be obtained from $\mathbf{c}_j$ by an isometry $I \in G_i$. Their parallel components are equal:

$$\mathbf{c}_{I(j)\parallel} = \mathbf{c}_{j\parallel}. \tag{3.4}$$

The symmetry condition will be that *the set of perpendicular components $\mathbf{c}_{I(j)\perp}$ is isotropic to second order in the hyperplane perpendicular to $\mathbf{c}_i$.*

To translate this condition into equations, it will be convenient to temporarily redefine the coordinate system in such a way that the x_1 axis is parallel to $\mathbf{c}_i$. We have then $\mathbf{c}_{j\parallel} = (c_{j1}, 0, \ldots, 0)$, $\mathbf{c}_{j\perp} = (0, c_{j2}, \ldots, c_{jD})$, and the condition is

$$\begin{aligned} &\textstyle\sum_{I\in G_i} c_{I(j)\alpha} = 0, && (\alpha = 2, \ldots, D), \\ &\textstyle\sum_{I\in G_i} c_{I(j)\alpha} c_{I(j)\beta} = R\delta_{\alpha\beta}, && (\alpha, \beta = 2, \ldots, D), \end{aligned} \tag{3.5}$$

where R is the same for all α, β. (Note that we have summed over the isometries $I \in G_i$ rather than over the elements of V_{ij}. This is easily shown to be equivalent. Consider the subgroup G_{ij} of G_i made of the isometries which leave $\mathbf{c}_i$ and $\mathbf{c}_j$ invariant. For any velocity $\mathbf{c}_k \in V_{ij}$, the isometries which map $\mathbf{c}_j$ into $\mathbf{c}_k$ form a left coset of G_{ij}; their number is $|G_{ij}|$. Thus, summing over $I \in G_i$, we obtain each velocity the same number of times).

The constant R can be computed as follows. We call θ_{ij} the angle between $\mathbf{c}_i$ and $\mathbf{c}_j$. Then,

$$c_{I(j)1} = c_{j1} = c\cos\theta_{ij} \tag{3.6}$$

and

$$\sum_{\alpha=2}^{D} c_{I(j)\alpha}^2 = c^2 \sin^2\theta_{ij}. \tag{3.7}$$

Summing over $I \in G_i$ and using (3.2b), we obtain

$$R = \frac{|G_i| c^2 \sin^2\theta_{ij}}{D-1}. \tag{3.8}$$

Finally, we specify the symmetry requirements for the collision rules. They are quite simple:

4. *Collision rules must be invariant under any isometry of G.* In other words, for any collision $(s; s')$ and for any isotropy $I \in G$, there is

$$A[I(s); I(s')] = A(s; s'), \tag{3.9}$$

where $I(s)$ has the obvious meaning.

These conditions are satisfied by the FHP lattice, and also by the face-centered-hypercubic lattice (FCHC) introduced by d'Humières, Lallemand, and Frisch [7,1]. For the HPP lattice [1,8–10], however, relation (3.2d) is not satisfied.

3.1 Steady state

Equations (2.1) to (2.6) are still valid, with 6 replaced by n. For an isotropic velocity distribution, instead of (2.2) we have

$$N_i(\mathbf{x}) = \frac{\rho}{nfm} = d. \tag{3.10}$$

We consider a state in which the mean velocity field is an arbitrary linear function of the position $\mathbf{x}$: instead of equation (2.7), we postulate the more general form

$$u_\alpha = \sum_\beta T_{\alpha\beta} x_\beta \qquad (\alpha = 1, \ldots, D). \tag{3.11}$$

The $T_{\alpha\beta}$ are the components of a tensor, which is the velocity gradient:

$$T_{\alpha\beta} = \frac{\partial u_\alpha}{\partial x_\beta}. \tag{3.12}$$

ν_i is then assumed to be also a linear function of coordinates: instead of equation (2.8), we have

$$\nu_i = \sum_\beta k_{i\beta} x_\beta + \epsilon_i \tag{3.13}$$

where the $k_{i\beta}$ and the ϵ_i are constants to be determined.

The equations (2.9) and (2.10) become

$$\sum_i \epsilon_i = 0, \qquad \sum_i \epsilon_i c_{i\alpha} = 0, \tag{3.14}$$

and

$$\sum_i k_{i\beta} = 0, \qquad \sum_i c_{i\alpha} k_{i\beta} = ndT_{\alpha\beta}. \tag{3.15}$$

Note that α and β can take all values in these equations. Thus, equation (3.14) represents a total of $D+1$ equations, and equation (3.15) represents a total of $D(D+1)$ equations.

3.2 Collisions

The collision equation is almost the same as equation (2.29), the only difference being that 6 is replaced by n:

$$\nu_i' - \nu_i = \sum_C (s_i' - s_i) A d^{p-1} (1-d)^{n-p-1} \sum_j s_j \nu_j. \tag{3.16}$$

3.3 Propagation

The propagation equation (2.34) becomes

$$\nu_i(\mathbf{x}) - \nu_i'(\mathbf{x}) = -\tau \sum_\alpha k_{i\alpha} c_{i\alpha}. \tag{3.17}$$

3.4 Computation of the steady state

Combining these equations and substituting (3.13), we obtain a set of n equations:

$$\sum_C (s_i' - s_i) A d^{p-1} (1-d)^{n-p-1} \sum_j s_j \Big(\sum_\beta k_{j\beta} x_\beta + \epsilon_j\Big) - \tau \sum_\alpha k_{i\alpha} c_{i\alpha} = 0$$

$$(i = 1, \ldots n). \tag{3.18}$$

Considering first the terms linear in $\mathbf{x}$, we obtain a set of Dn linear homogeneous equations for the $k_{i\beta}$. Mass and momentum are conserved; we assume that the collision rules have been so chosen that there is no other conserved quantity. Then, only $D(n - D - 1)$ of these equations are independent, and solutions have the form

$$k_{i\beta} = K_{0\beta} + \sum_\alpha K_{\alpha\beta} c_{i\alpha}, \tag{3.19}$$

where the $K_{0\beta}$ and $K_{\alpha\beta}$ are arbitrary constants. Using the relations (3.15) and the symmetry conditions (3.2), we find that these constants are uniquely determined and the $k_{i\beta}$ are

$$k_{i\beta} = \frac{Dd}{c^2} \sum_\alpha c_{i\alpha} T_{\alpha\beta}. \tag{3.20}$$

Substituting equation (3.20) in equation (3.17), we obtain

$$\nu_i(\mathbf{x}) - \nu_i'(\mathbf{x}) = -\frac{\tau D d}{c^2} \sum_\alpha \sum_\beta T_{\alpha\beta} c_{i\alpha} c_{i\beta}. \tag{3.21}$$

Summing over i, and taking into account the conservation of particle number, we obtain

$$\sum_\alpha T_{\alpha\alpha} = 0. \tag{3.22}$$

Thus, the tensor $T_{\alpha\beta}$ cannot be entirely arbitrarily chosen: its trace must be zero. This is a consequence of the fact that the density has been assumed constant in space and time.

We consider next the terms independent of $\mathbf{x}$ in equation (3.18). We obtain a set of n linear inhomogeneous equations:

$$\sum_C (s'_i - s_i) A d^{p-1} (1-d)^{n-p-1} \sum_j s_j \epsilon_j - \frac{\tau D d}{c^2} \sum_\alpha \sum_\beta T_{\alpha\beta} c_{i\alpha} c_{i\beta} = 0$$

$$(i = 1, \ldots, n). \tag{3.23}$$

Only $n - D - 1$ of them are independent. Combining with equation (3.14), we have a system of n equations to solve for the n unknowns ϵ_j. It might seem at first view that this system cannot be explicitly solved in the general case. However, we can again conjecture that the anisotropy (represented by the ϵ_i) is proportional to the propagative excitation, i.e., that

$$\epsilon_i = -\lambda \frac{\tau D d}{c^2} \sum_\alpha \sum_\beta T_{\alpha\beta} c_{i\alpha} c_{i\beta} \tag{3.24}$$

where λ is a constant. It turns out that the conjecture is true and that (3.24) is indeed a solution of the equations, with λ given by

$$\frac{1}{\lambda} = \frac{D}{D-1} \sum_C (s_i - s'_i) A d^{p-1} (1-d)^{n-p-1} \sum_j s_j \cos^2 \theta_{ij}, \tag{3.25}$$

where i is an arbitrarily chosen direction and θ_{ij} is the angle between velocities $\mathbf{c}_i$ and $\mathbf{c}_j$. A detailed proof of this result is given in Appendix A. The steady state is now fully determined. It is given by equations (2.3), (3.13), (3.20), and (3.24):

$$N_i = d + \frac{Dd}{c^2} \sum_\alpha \sum_\beta T_{\alpha\beta} c_{i\alpha} x_\beta - \lambda \frac{\tau D d}{c^2} \sum_\alpha \sum_\beta T_{\alpha\beta} c_{i\alpha} c_{i\beta}. \tag{3.26}$$

The non-dimensional factor λ has a simple physical meaning. We define the post-collision anisotropy terms ϵ'_i by

$$\nu'_i = \sum_\beta k_{i\beta} x_\beta + \epsilon'_i. \tag{3.27}$$

From equations (3.21) and (3.24), we deduce

$$\epsilon'_i = (1-\lambda) \frac{\tau D d}{c^2} \sum_\alpha \sum_\beta T_{\alpha\beta} c_{i\alpha} c_{i\beta}, \tag{3.28}$$

or

$$\epsilon'_i = \left(1 - \frac{1}{\lambda}\right) \epsilon_i. \tag{3.29}$$

In other words, collisions damp a fraction $1/\lambda$ of the anisotropy.

We remark also that equation (3.26) can be written

$$N_i = d + \frac{Dd}{c^2} \sum_\alpha \sum_\beta T_{\alpha\beta} c_{i\alpha} (x_\beta - \lambda \tau c_{i\beta}), \tag{3.30}$$

which could lead to an interpretation of λ as a *mean-free path*, expressed in link lengths.

3.5 Momentum flux

We compute the momentum flux across a "surface" of dimension $D-1$, of measure σ, centered in $\mathbf{x}$, perpendicular to a unit vector $\mathbf{v}$. This surface is assumed to be large in relation to link length: $\sigma \gg l^{D-1}$. Links parallel to $\mathbf{c}_i$ which cross the surface correspond to destination nodes which lie in a volume $\sigma\tau\mathbf{c}_i \cdot \mathbf{v}$. The number of these nodes is $\sigma\tau f \mathbf{c}_i \cdot \mathbf{v}$. The average position of a destination node is $\mathbf{x} + \tau\mathbf{c}_i/2$; therefore, the probability of existence of a particle on a link crossing the surface is on the average

$$N_i(\mathbf{x} + \frac{1}{2}\tau\mathbf{c}_i) = N_i(\mathbf{x}) + \frac{1}{2}\tau\mathbf{c}_i \cdot \nabla N_i = N_i(\mathbf{x}) + \frac{1}{2}\tau\mathbf{k}_i \cdot \mathbf{c}_i, \tag{3.31}$$

according to equation (3.13). (Note that this could be written more symmetrically: $[N_i(\mathbf{x}) + N_i'(\mathbf{x})]/2$.) Thus, the number of particles crossing the surface in the direction $\mathbf{v}$ during the time τ is

$$\sigma\tau f(\mathbf{c}_i \cdot \mathbf{v}) \left[N_i(\mathbf{x}) + \frac{1}{2}\tau\mathbf{k}_i \cdot \mathbf{c}_i \right]. \tag{3.32}$$

Each particle carries a momentum $m\mathbf{c}_i$. Finally, we sum on i and we divide by τ and σ to obtain the desired flux per unit surface:

$$fm \sum_i \mathbf{c}_i(\mathbf{c}_i \cdot \mathbf{v}) \left[N_i(\mathbf{x}) + \frac{1}{2}\tau\mathbf{k}_i \cdot \mathbf{c}_i \right]. \tag{3.33}$$

Taking for $\mathbf{v}$ the axis directions, we obtain the components of the tensorial flux:

$$F_{\gamma\varsigma} = fm \sum_i c_{i\gamma} c_{i\varsigma} \left[N_i(\mathbf{x}) + \frac{1}{2}\tau\mathbf{k}_i \cdot \mathbf{c}_i) \right]. \tag{3.34}$$

We substitute the values of N_i and $\mathbf{k}_i$ given by equations (3.26) and (3.20):

$$F_{\gamma\varsigma} =$$

$$fm \sum_i c_{i\gamma} c_{i\varsigma} \left[d + \frac{Dd}{c^2} \sum_\alpha \sum_\beta T_{\alpha\beta} c_{i\alpha} x_\beta - \frac{\tau D d}{c^2} \left(\lambda - \frac{1}{2} \right) \sum_\alpha \sum_\beta T_{\alpha\beta} c_{i\alpha} c_{i\beta} \right]. \tag{3.35}$$

Using equations (3.2) and (3.10), we obtain

$$F_{\gamma\varsigma} =$$

$$\frac{\rho c^2}{D}\delta_{\gamma\varsigma} - \frac{\rho\tau c^2}{D+2}\left(\lambda - \frac{1}{2}\right)\sum_\alpha\sum_\beta T_{\alpha\beta}(\delta_{\alpha\beta}\delta_{\gamma\varsigma} + \delta_{\alpha\gamma}\delta_{\beta\varsigma} + \delta_{\alpha\varsigma}\delta_{\beta\gamma}) \quad (3.36)$$

or, using equation (3.22):

$$\begin{aligned} F_{\gamma\gamma} &= \frac{\rho c^2}{D} - \frac{2\rho\tau c^2}{D+2}\left(\lambda - \tfrac{1}{2}\right) T_{\gamma\gamma}, \\ F_{\gamma\varsigma} &= -\frac{\rho\tau c^2}{D+2}\left(\lambda - \tfrac{1}{2}\right)(T_{\gamma\varsigma} + T_{\varsigma\gamma}) \qquad (\gamma \neq \varsigma). \end{aligned} \quad (3.37)$$

Equation (3.37b) shows that the shear velocity is

$$\eta = \frac{\rho\tau c^2}{(D+2)}\left(\lambda - \frac{1}{2}\right). \quad (3.38)$$

Note that the kinematic viscosity η/ρ can be interpreted, as in classical gases, as the product of the particle velocity c by a mean-free path. This mean-free path equals the link length $l = \tau c$ multiplied by the dimensionless constant $(\lambda - 1/2)/(D+2)$.

Substituting equation (3.25), we obtain the explicit formula

$$\eta = \frac{\rho\tau c^2}{D+2}\left[\frac{D-1}{D\sum_C (s_i - s_i')Ad^{p-1}(1-d)^{n-p-1}\sum_j s_j\cos^2\theta_{ij}} - \frac{1}{2}\right]. \quad (3.39)$$

i in this formula is an arbitrarily chosen direction.

4. Minimization of the viscosity

We show now that the formula (3.39) can be written in a different way, involving a sum of squared quantities. As a consequence, the viscosity is always positive. The new formula provides also a practical recipe for choosing collision rules which minimize the viscosity.

The right-hand side of equation (3.25) is independent of the chosen i. We can therefore sum over i and divide by n:

$$\frac{1}{\lambda} = \frac{D}{(D-1)n}\sum_C Ad^{p-1}(1-d)^{n-p-1}\sum_i (s_i - s_i')\sum_j s_j\cos^2\theta_{ij}. \quad (4.1)$$

This can be written

$$\begin{aligned} \frac{1}{\lambda} &= \frac{D}{(D-1)nc^4}\sum_C Ad^{p-1}(1-d)^{n-p-1} \\ &\quad \sum_i (s_i - s_i')\sum_j s_j\sum_\alpha c_{i\alpha}c_{j\alpha}\sum_\beta c_{i\beta}c_{j\beta} \\ &= \frac{D}{(D-1)nc^4}\sum_C Ad^{p-1}(1-d)^{n-p-1}\sum_\alpha\sum_\beta \\ &\quad \sum_i (s_i - s_i')c_{i\alpha}c_{i\beta}\sum_j s_j c_{j\alpha}c_{j\beta}. \end{aligned} \quad (4.2)$$

We define

$$X_{\alpha\beta} = \sum_i s_i c_{i\alpha} c_{i\beta}. \tag{4.3}$$

The tensor $X_{\alpha\beta}$ is the *second-order momentum* of the input state. Note that it is symmetrical: $X_{\alpha\beta} = X_{\beta\alpha}$. Similarly,

$$X'_{\alpha\beta} = \sum_i s'_i c_{i\alpha} c_{i\beta} \tag{4.4}$$

is the second-order momentum of the output state. Equation (4.2) becomes

$$\frac{1}{\lambda} = \frac{D}{(D-1)nc^4} \sum_C A d^{p-1} (1-d)^{n-p-1} \sum_\alpha \sum_\beta (X_{\alpha\beta} - X'_{\alpha\beta}) X_{\alpha\beta}. \tag{4.5}$$

The trace of $X_{\alpha\beta}$ is

$$\sum_\alpha X_{\alpha\alpha} = \sum_\alpha \sum_i s_i c_{i\alpha}^2 = \sum_i s_i c^2 = pc^2. \tag{4.6}$$

We split $X_{\alpha\beta}$ into isotropic and anisotropic parts:

$$X_{\alpha\beta} = \frac{pc^2}{D} \delta_{\alpha\beta} + Y_{\alpha\beta}. \tag{4.7}$$

The tensor $Y_{\alpha\beta}$ has a null trace:

$$\sum_\alpha Y_{\alpha\alpha} = 0. \tag{4.8}$$

Similarly, we write

$$X'_{\alpha\beta} = \frac{pc^2}{D} \delta_{\alpha\beta} + Y'_{\alpha\beta}. \tag{4.9}$$

Substituting into equation (4.5) and going over to the more detailed collision notation (see equation (2.18)), we obtain

$$\frac{1}{\lambda} = \frac{D}{(D-1)nc^4} \sum_s \sum_{s'} A(s;s') d^{p-1} (1-d)^{n-p-1} \sum_\alpha \sum_\beta (Y_{\alpha\beta} - Y'_{\alpha\beta}) Y_{\alpha\beta}.$$

We introduce the quantities

$$\begin{aligned}
\mu_1 &= \frac{D}{2(D-1)nc^4} \sum_s \sum_{s'} A(s;s') d^{p-1} (1-d)^{n-p-1} \sum_\alpha \sum_\beta Y_{\alpha\beta}^2, \\
\mu_2 &= \frac{D}{2(D-1)nc^4} \sum_s \sum_{s'} A(s;s') d^{p-1} (1-d)^{n-p-1} \sum_\alpha \sum_\beta Y'^2_{\alpha\beta}, \quad (4.10) \\
\mu_3 &= \frac{D}{4(D-1)nc^4} \sum_s \sum_{s'} A(s;s') d^{p-1} (1-d)^{n-p-1} \sum_\alpha \sum_\beta (Y_{\alpha\beta} - Y'_{\alpha\beta})^2, \\
\mu_4 &= \frac{D}{4(D-1)nc^4} \sum_s \sum_{s'} A(s;s') d^{p-1} (1-d)^{n-p-1} \sum_\alpha \sum_\beta (Y_{\alpha\beta} + Y'_{\alpha\beta})^2.
\end{aligned}$$

Equation (4.10) can be written

$$\frac{1}{\lambda} = \mu_1 - \mu_2 + 2\mu_3, \tag{4.11}$$

or

$$\frac{1}{\lambda} = 3\mu_1 + \mu_2 - 2\mu_4. \tag{4.12}$$

μ_1 and μ_2 are computed in Appendix B; their values are simply

$$\mu_1 = \mu_2 = \frac{1}{2}. \tag{4.13}$$

From equations (4.12) and (4.13), we then have

$$\frac{1}{2\lambda} = \mu_3 = 1 - \mu_4. \tag{4.14}$$

Substituting in equation (3.38), we obtain

$$\eta = \frac{\rho\tau c^2}{2(D+2)} \frac{\mu_4}{1-\mu_4}. \tag{4.15}$$

μ_3 and μ_4 cannot be negative, as shown by their expressions (4.11c) and (4.11d). Therefore, from equation (4.15):

$$0 \leq \mu_4 \leq 1. \tag{4.16}$$

It follows that *the viscosity η is positive of zero.* μ_4 is a dimensionless number, lying between 0 and 1, which characterizes the viscosity of the lattice gas; it might be called the *viscosity index.*

The limiting case $\mu_4 = 1$ corresponds to an infinite viscosity. It requires $\mu_3 = 0$, or, as shown by equation (11c), $Y'_{\alpha\beta} = Y_{\alpha\beta}$ for all collisions: the second-order momentum must be invariant in collisions. This happens in particular in the trivial case where there are no proper collisions (i.e., the velocities remain unchanged during the collision phase).

The other limiting case, $\mu_4 = 0$, is more interesting: It corresponds to zero viscosity. For this, we must have for every collision:

$$Y_{\alpha\beta} + Y'_{\alpha\beta} = 0. \tag{4.17}$$

This rule has a simple geometrical interpretation. Let us call *total state* the sum of the input and output states; the rule is then: *for every collision, the second-order momentum of the total state must be isotropic.* (Note that "sum" is taken in the algebraic sense: if a velocity exists both in the input and in the output state, it must be counted twice in the computation of the second-order momentum). A collision which satisfies this condition will be called a *perfect collision.*

In practice, not all collisions can be perfect. In particular, when there is only one velocity ($p = 1$), the output state is necessarily identical to the input state since the first-order momentum must be conserved. On the other hand, the second-order momentum is anisotropic. The quantity

(4.18) is non-zero. We can therefore strengthen our result: *The viscosity is always positive.*

We remark that for any input state with $p = n/2$ (i.e., with exactly one half of the incoming links occupied by particles) a perfect collision rule can be devised as follows:

1. Take the dual of the input state (i.e. replace particles by "holes" and vice versa);
2. Effect a symmetry with respect to the origin. In other words, call $\sigma(i)$ the index corresponding to the opposite velocity (i.e., $\mathbf{c}_{\sigma(i)} = -\mathbf{c}_i$); then, the rule is: $s'_{\sigma(i)} = 1 - s_i$. It is easily seen that the number of particles and the first-order momentum are preserved, while the second-order momentum of the total state is isotropic. For instance, in the FHP lattice, we obtain the rules for triple collisions shown in figure 6. In the first two cases, the velocities are unchanged. The third case is the "head-on collision with spectator" [11].

In order to minimize the viscosity, one must first sort the states into subsets according to particle number and momentum, and then pair the states so as to minimize the quantities (4.18). Roughly speaking, each collision should replace the input state by an output state whose second-order momentum is as much as possible "symmetrical with respect to isotropy." Work is in progress to apply this recipe to the four-dimensional, 24-velocity lattice gas proposed by d'Humières, Lallemand, and Frisch [1,7]. Present results indicate that this fine-tuning of the collision rules can lower the viscosity by a factor between 3 and 4 with respect to a collision algorithm in which the output state is randomly chosen (among all states having the same particle number and momentum as the input state). More generally, it seems likely that the larger the number n of velocities, the more closely the limit $\eta = 0$ can be approached.

Appendix A.

We prove here that equation (3.24), with λ given by (3.25), is a solution of the equations (3.14) and (3.23). The first part is simple: using equations (3.2) and (3.22), we immediately find that the equations (3.14) are verified.

We introduce the abbreviated notation

$$Q_i = \sum_\alpha \sum_\beta T_{\alpha\beta} c_{i\alpha} c_{i\beta}. \tag{A.1}$$

Substituting equation (3.24) in (3.23), we find that the equations to be satisfied are

$$Q_i = \lambda \sum_C (s_i - s'_i) A d^{p-1} (1-d)^{n-p-1} \sum_j s_j Q_j$$

$$(i = 1, \dots, n). \tag{A.2}$$

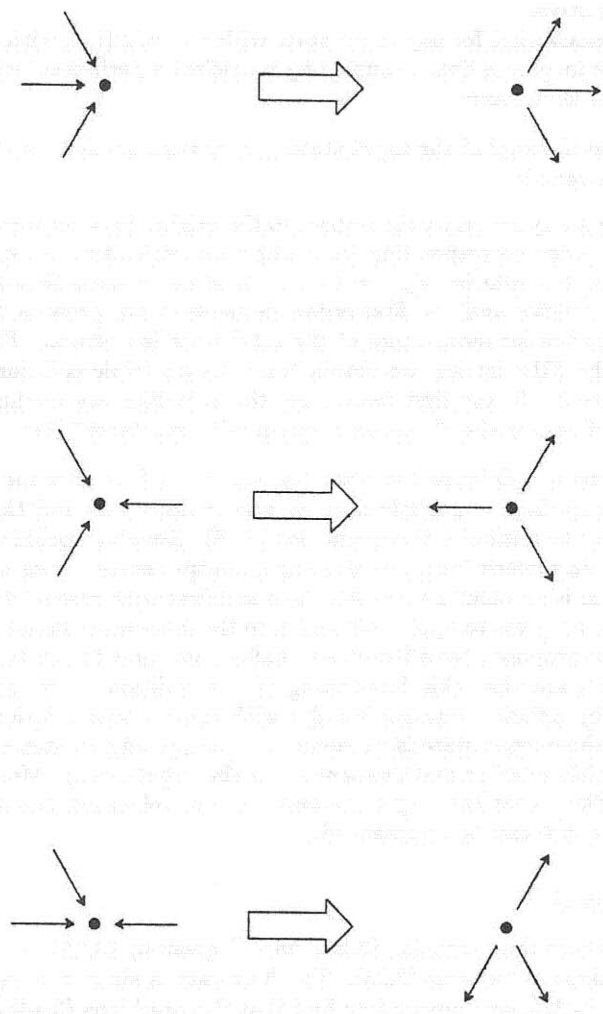

Figure 6: "Perfect" rules for triple collisions in the FHP lattice.

We consider now a particular value of i, and the subgroup G_i of G consisting of all isometries in which $\mathbf{c}_i$ is invariant. We divide the collisions into equivalence classes according to the following rule: two collisions belong to the same class W if there exists an isometry of G_i which maps one into the other. More precisely, two collisions $(s; s')$ and $(\tilde{s}; \tilde{s}')$ belong to the same class if there exists an isometry $I \in G_i$ which maps s into $\tilde{s}$ and s' into $\tilde{s}'$.

We decompose now the sum over collisions in equation (A.1): we sum first over the members of each class W, and then over the classes:

$$Q_i = \lambda \sum_W \sum_{C \in W} (s_i - s_i') A d^{p-1} (1-d)^{n-p-1} \sum_j s_j Q_j. \tag{A.3}$$

Because of symmetry assumption (4) (see beginning of section 3), A is constant inside a class W. s_i, s_i', p are also constant inside a class, and therefore equation (A.3) can be written

$$Q_i = \lambda \sum_W (s_i - s_i') A d^{p-1} (1-d)^{n-p-1} \sum_{C \in W} \sum_j s_j Q_j. \tag{A.4}$$

Consider a particular class W and a particular collision $C^* = (s^*; s^{prime*}) \in W$. We call G_i^* the subgroup of G_i made of isometries which leave C^* invariant. For any collision $C \in W$, the isometries which map C^* into C form a left coset of G_i^*; their number is $|G_i^*| = |G_i|/|W|$. So, instead of summing on collisions in W, we can sum on isometries in G_i:

$$\sum_{C \in W} \mathcal{F}(C) = \frac{|W|}{|G_i|} \sum_{I \in G_i} \mathcal{F}[I(C^*)], \tag{A.5}$$

where $\mathcal{F}$ is an arbitrary function. Thus, equation (A.4) becomes

$$Q_i = \lambda \sum_W (s_i - s_i') A d^{p-1} (1-d)^{n-p-1} \frac{|W|}{|G_i|} \sum_{I \in G_i} \sum_j s_j^* Q_{I(j)}. \tag{A.6}$$

We have used here the fact that each input velocity of C is the image of an input velocity of C^*. Substituting equation (A.1) in the right-hand side and changing the summation order, we have

$$Q_i = \lambda \sum_W (s_i - s_i') A d^{p-1} (1-d)^{n-p-1} \frac{|W|}{|G_i|} \sum_j s_j^* \sum_\alpha \sum_\beta T_{\alpha\beta} \sum_{I \in G_i} c_{I(j)\alpha} c_{I(j)\beta}. \tag{A.7}$$

We take a coordinate system such that the x_1 axis is parallel to $\mathbf{c}_i$. Then $c_{I(j)1} = c_{j1}$ and equation (A.7) takes the form

$$Q_i = \lambda \sum_W (s_i - s_i') A d^{p-1} (1-d)^{n-p-1} \frac{|W|}{|G_i|} \sum_j s_j^*$$

$$\Bigg[T_{11} c_{j1}^2 |G_i| + c_{j1} \sum_{\beta=2}^{D} T_{1\beta} \sum_{I \in G_i} c_{I(j)\beta}$$

$$+c_{j1}\sum_{\alpha=2}^{D} T_{\alpha 1} \sum_{I\in G_i} c_{I(j)\alpha} + \sum_{\alpha=2}^{D}\sum_{\beta=2}^{D} T_{\alpha\beta} \sum_{I\in G_i} c_{I(j)\alpha}c_{I(j)\beta}\Bigg]. \tag{A.8}$$

Using equations (3.5), (3.6), and (3.8), we obtain

$$Q_i = \lambda \textstyle\sum_W (s_i - s_i')Ad^{p-1}(1-d)^{n-p-1}|W| \sum_j s_j^* \left[T_{11}c^2\cos^2\theta_{ij} + \sum_{\alpha=2}^{D} T_{\alpha\alpha}\frac{c^2\sin^2\theta_{ij}}{D-1}\right] \tag{A.9}$$

or, using equation (3.22)

$$Q_i = \lambda \sum_W (s_i - s_i')Ad^{p-1}(1-d)^{n-p-1}|W| \sum_j s_j^* T_{11}c^2 \frac{D\cos^2\theta_{ij} - 1}{D-1}. \tag{A.10}$$

Summing over all collisions $C^* \in W$, dividing by $|W|$, and dropping the asterisks, we obtain

$$Q_i = \lambda \sum_W (s_i - s_i')Ad^{p-1}(1-d)^{n-p-1} \sum_{C\in W}\sum_j s_j T_{11}c^2 \frac{D\cos^2\theta_{ij} - 1}{D-1}. \tag{A.11}$$

From equation (A.1), we find

$$Q_i = T_{11}c^2. \tag{A.12}$$

We can then divide both sides by Q_i and we obtain

$$1 = \lambda \sum_C (s_i - s_i')Ad^{p-1}(1-d)^{n-p-1} \sum_j s_j \frac{D\cos^2\theta_{ij} - 1}{D-1}. \tag{A.13}$$

We remark that the tensor $T_{\alpha\beta}$ has entirely disappeared: the equation (A.13) depends only on the collision rules. As a consequence, because of symmetry assumptions (2) and (4) (section 3), this equation is the same for all directions i. The conjecture is verified, and we have found a solution for the probabilities N_i.

The rightmost term $1/(D-1)$ in equation (A.13) can be deleted because it gives a null contribution; this is easily seen by summing over i. We obtain then for λ the equation (3.25).

Appendix B.

We evaluate here μ_1 and μ_2 defined by equations (4.11a) and (4.11b). μ_1 does not depend on s'; therefore, its value is, according to equation (2.16):

$$\begin{aligned}\mu_1 &= \frac{D}{2(D-1)nc^4}\sum_s d^{p-1}(1-d)^{n-p-1}\sum_\alpha\sum_\beta\left[X_{\alpha\beta}-\frac{pc^2}{D}\delta_{\alpha\beta}\right]^2 = \\ &\frac{D}{2(D-1)nc^4}\sum_s d^{p-1}(1-d)^{n-p-1}\sum_\alpha\sum_\beta \\ &\left[\sum_i s_i\left(c_{i\alpha}c_{i\beta}-\frac{c^2}{D}\delta_{\alpha\beta}\right)\right]\left[\sum_j s_j\left(c_{j\alpha}c_{j\beta}-\frac{c^2}{D}\delta_{\alpha\beta}\right)\right] \\ &= \frac{D}{2(D-1)nc^4}\sum_\alpha\sum_\beta \\ &\sum_i\left(c_{i\alpha}c_{i\beta}-\frac{c^2}{D}\delta_{\alpha\beta}\right)\sum_j\left(c_{j\alpha}c_{j\beta}-\frac{c^2}{D}\delta_{\alpha\beta}\right)\sum_s s_is_jd^{p-1}(1-d)^{n-p-1}.\end{aligned}\tag{B.1}$$

If $i=j$, the sum over s is

$$\sum_s s_id^{p-1}(1-d)^{n-p-1} = \sum_{s_1=0}^{1}\cdots\sum_{s_n=0}^{1} s_id^{p-1}(1-d)^{n-p-1},\tag{B.2}$$

or, using $p=\sum_k s_k$:

$$\frac{1}{d(1-d)}\sum_{s_1=0}^{1} d^{s_1}(1-d)^{1-s_1}\cdots\sum_{s_n=0}^{1} d^{s_n}(1-d)^{1-s_n}s_i = \frac{1}{1-d}\tag{B.3}$$

(the sum over s_i gives d; the sums over s_k for $k\neq i$ give 1).

If $i\neq j$, the sum over s in equation (1) is

$$\sum_s s_is_jd^{p-1}(1-d)^{n-p-1} = \frac{d}{1-d},\tag{B.4}$$

by a similar computation. Equation (1) becomes

$$\mu_1 = \frac{D}{2(D-1)nc^4}\sum_\alpha\sum_\beta\left(\frac{1}{1-d}\sum_i\sum_{j=i}+\frac{d}{1-d}\sum_i\sum_{j\neq i}\right)$$

$$\left(c_{i\alpha}c_{i\beta}-\frac{c^2}{D}\delta_{\alpha\beta}\right)\left(c_{j\alpha}c_{j\beta}-\frac{c^2}{D}\delta_{\alpha\beta}\right).\tag{B.5}$$

The summations over i and j can also be written

$$\left(\sum_i\sum_{j=i}+\frac{d}{1-d}\sum_i\sum_j\right).\tag{B.6}$$

The second term vanishes, and there remains

$$\mu_1 = \frac{D}{2(D-1)nc^4} \sum_\alpha \sum_\beta \sum_i \left(c_{i\alpha} c_{i\beta} - \frac{c^2}{D} \delta_{\alpha\beta} \right)^2. \tag{B.7}$$

For $\alpha = \beta$, the sum over i is, using equation (3.2):

$$\sum_i c_{i\alpha}^4 - 2\frac{c^2}{D} \sum_i c_{i\alpha}^2 + n\frac{c^4}{D^2} = \frac{3nc^4}{D(D+2)} - \frac{nc^4}{D^2}, \tag{B.8}$$

and for $\alpha \neq \beta$:

$$\sum_i c_{i\alpha}^2 c_{i\beta}^2 = \frac{nc^4}{D(D+2)}. \tag{B.9}$$

Finally, we sum over α and β, and equation (B.5) reduces to

$$\mu_1 = \frac{1}{2}. \tag{B.10}$$

We consider now the quantity μ_2. It is independent of s. Using the assumption of semi-detailed balancing (2.17), we can sum over s and eliminate A. A computation similar to the above one gives then

$$\mu_2 = \frac{1}{2}. \tag{B.11}$$

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