

A Cellular-Automaton Fluid Model with Simple Rules in Arbitrarily Many Dimensions

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A new cellular-automaton model for fluid dynamics is introduced. Unlike the conventional FHP-type models, the model uses easily implementable, deterministic pair interaction rules which work on arbitrary-dimensional orthogonal lattices. The statistical and hydrodynamic theory of the model is developed, and the Navier–Stokes-like hydrodynamic equations that describe the macroscopic behavior of the model are derived. It turns out that the unwanted anisotropic convection behavior can be eliminated in the incompressible limit by suitable choice of the mass density. An explicit expression for the viscosity tensor is calculated from a Boltzmann-type approximation. Unfortunately, the viscosity turns out to be anisotropic, which is a drawback as against the conventional FHP and FCHC models. Nevertheless, the new model could become interesting for fluid dynamic problems with additional variables (e.g., free surfaces), especially in two dimensions, since its simple rules could relatively easily be extended for such cases.

KEY WORDS:

1. INTRODUCTION

A “cellular automaton” (CA) is a set of regularly arranged elements, called “cells,” with a discrete dynamics generated by an iteration rule giving the state of a cell at time $t + 1$ as a function of the state of a few neighboring cells at time t , where the state of a cell can assume only a small finite number of different values. CAs can serve as maximally discretized computer models for various types of collective phenomena. It is even possible to simulate fluid dynamics by suitably defined CAs, as has recently been

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demonstrated by Frisch *et al.*⁽¹⁾ (FHP). The CA model of FHP represents a gas consisting of particles that move around and collide with each other on certain discrete trajectories on a two-dimensional, hexagonally symmetric lattice, according to certain simple rules, which conserve the number of particles and their total momentum. Although the microscopic motion of the FHP particles is unrealistically simplified, the macroscopically averaged local densities of mass and momentum of the FHP gas can be shown to obey a set of partial differential equations which, under certain asymptotic conditions, are dynamically equivalent to the incompressible Navier–Stokes equations,⁽²⁾

$$\nabla \cdot \mathbf{u} = 0, \quad (\partial_t + \mathbf{u} \cdot \nabla) \mathbf{u} + \nabla \phi = \nu \nabla^2 \mathbf{u} \quad (1)$$

This means that the FHP model can serve as a tool for numerical simulations of fluid dynamics^(3–8); it thus provides an interesting alternative to the usual finite-difference and finite-element methods. By suitable modifications of various kinds, the application range of the FHP model can be extended from “simple” Navier–Stokes flow to more complex hydrodynamic problems, such as passive scalar transport, surface tension, or even magnetohydrodynamics.^(9–18)

Why does the FHP model need a hexagonal lattice? Actually, the FHP model arose as a modification of an earlier, very simple model with a square lattice, introduced by Hardy *et al.*⁽¹⁹⁾ (HPP). The HPP lattice gas behaves in many respects like a physical fluid, but in contrast to the FHP model, it cannot simulate the Navier–Stokes equations quantitatively because of the anisotropic structure of the convection and viscosity term in the hydrodynamic equations of the HPP gas. The HPP gas is hydrodynamically equivalent to a physical gas or fluid only in some relatively uninteresting hydrodynamic limiting cases in which these terms are unimportant, such as undamped sound waves or linear potential flow. The FHP model overcomes this anisotropy problem in a very elegant way: Roughly speaking, it can be shown that the hexagonal symmetry guarantees the isotropy of all tensors up to and including fourth order in the hydrodynamic equations of the lattice gas,⁽²⁾ so that in particular the convection and viscosity terms, whose coefficients are fourth-order tensors, automatically become isotropic. A quadratic or cubic symmetry (such as in the HPP model), however, implies isotropy of tensors up to third order only.

Its hexagonal structure restricts the FHP model to two dimensions. However, d’Humières *et al.*⁽²⁰⁾ have discovered that one can construct in *four* dimensions a CA model with a face-centered hypercubic symmetry, which, like the hexagonal symmetry in 2D, guarantees the isotropy of

tensors up to fourth order. By projecting this so-called FCHC (“face-centered hypercubic”) model down to three dimensions, one obtains a CA with a cubic lattice that can simulate incompressible Navier–Stokes flow in 3D. The FCHC model can also be projected to two dimensions, which leads to a 2D Navier–Stokes-simulating CA with a square lattice.

An unsatisfactory feature of the FCHC model is the large number of different possible collision configurations, which complicates the definition of suitable collision rules and the formulation of an efficient algorithm without resorting to huge lookup tables.^(22–24) For the modeling of pure Navier–Stokes flow, these technical problems can be overcome and the FCHC performs quite well. However, the unhandiness of its rules makes it extremely difficult to extend the FCHC model for fluid dynamic problems with additional variables, such as magnetohydrodynamics or surface tension.⁽²⁵⁾

Now, the FCHC method is not the only possible way to obtain Navier–Stokes-simulating CAs with square or cubic lattices; the desired isotropy properties can also be established by various other tricks.^(17,20,21) However, in 3D there seems to be no serious alternative to the FCHC model (see ref. 20, where an alternative 3D model is considered).

These considerations motivated me to devise the new model⁽²⁹⁾ which I discuss here. Its special structure, which differs slightly from the conventional models (such as the FHP or the FCHC), makes it possible to use relatively simple rules on a simple (square or cubic) lattice with in principle arbitrary space dimension d (e.g., $d=2$ or $d=3$). The rules are composed of elementary deterministic cell pair interactions, which are easy to implement and could be easily modified for more complex cases with additional variables.

The purpose of this paper is to present the definition and statistical theory of the model. The development of the theory follows standard methods⁽²⁾ and leads to a characterization of the macroscopic near-equilibrium behavior by equations of state and hydrodynamic equations which characterize the dynamics of the local macroscopic order parameters. It turns out that the Navier–Stokes-like hydrodynamics of our model is anisotropic, which is not surprising, as there are no symmetries guaranteeing the isotropy of fourth-order tensors. The first approximation of the hydrodynamic equations, which does not include friction effects and can be derived relatively easily from the equilibrium distribution, shows that the anisotropy of the nonlinear convection term ($\sim \mathbf{u} \nabla \mathbf{u}$) can be eliminated by a suitable choice of the mean density in the incompressible limit. We also tackle the slightly less trivial second approximation in order to compute the viscosity, which unfortunately turns out to be anisotropic.

The anisotropy of the viscosity is clearly a drawback of the model in

comparison to the conventional models, i.e., FHP for 2D, and FCHC for 3D, particularly in view of the considerable progress which has been made in the technical optimization of the latter models; e.g., in refs. 26 and 27 an efficient implementation of the FHP model is presented; in ref. 28, the FCHC model is used to investigate 3D flow through porous media, etc. (further material in this direction can be found in the January 1991 issue of *Physica D*, Vol. 47). Nevertheless, I think the new model remains interesting, maybe not for the simulation of *pure* Navier–Stokes flow, where the conventional models can do the job better, but possibly as a starting point for future models for 3D fluid dynamic situations in which additional variables appear, such as the above-mentioned free surfaces, magnetohydrodynamics, and the like. The construction of corresponding extensions of the FCHC model is extremely difficult because of its complicated rules. Here, the simple, easy-to-extend rules of my model could open new perspectives.

The paper is organized as follows. Sections 2 and 3 are concerned with the detailed definition of the model and its rules. In Section 4, the statistical equilibrium is discussed with the help of the Gibbs formalism. In Section 5, we begin the derivation of hydrodynamic equations by means of a Chapman–Enskog expansion, and obtain explicitly the first (frictionless) approximation. In Section 6, various hydrodynamic limiting cases are discussed. In Sections 7 and 8, we discuss the second approximation and calculate explicitly the friction (diffusion) coefficients from a Boltzmann-type approximation. In Section 9, the anisotropy of the viscosity tensor is demonstrated in a simple example. In Section 10, we take a brief look at what computer experiments with the new model have produced so far.

2. THE MODEL

The basic ideas for the construction of our CA model are the same as those used in the classical models, i.e., the HPP, FHP, FCHC, and similar models: One imagines a gas consisting of individual particles, flying around in a d -dimensional space ($d=2$ or $d=3$, usually). In our model, d is arbitrary. The velocity \mathbf{v} of a model particle can take only a finite number b of possible discrete values:

$$\mathbf{v} \in \mathbf{V} = \{\mathbf{v}_1, \dots, \mathbf{v}_b\} \quad (2)$$

e.g., the velocity set \mathbf{V} used in the HPP and FHP models is shown in Figs. 1 and 2, respectively. In our model, \mathbf{V} consists of the $b = 2^d$ possible different vectors $\mathbf{v} = (v_1, \dots, v_d)$ with components

$$v_j \in \{\pm 1\} \quad (3)$$

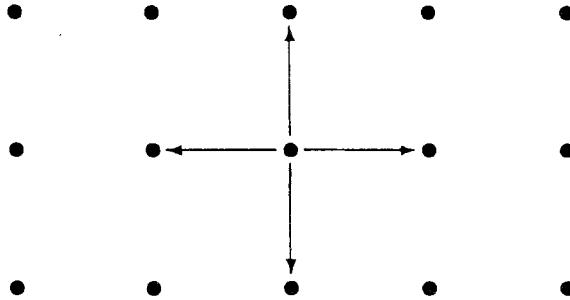


Fig. 1. Lattice and discrete velocities v_a ($a = 1, 2, 3, 4$) in the HPP model.

(Fig. 3). A particle can change its velocity only in collisions with other particles. Collisions occur only at the special instants of time

$$t \in \mathbf{Z} \equiv \{ \dots, -1, 0, 1, 2, \dots \} \tag{4}$$

and at certain special locations,

$$\mathbf{x} \in \mathbf{X}(t) \tag{5}$$

where $\mathbf{X}(t)$ is a suitable set of lattice points, which in our model is defined by $\mathbf{x} = (x_1, \dots, x_d)$ with

$$x_j \in \mathbf{Z}_e \quad \text{if} \quad t \in \mathbf{Z}_e \equiv \{ \dots, -2, 0, 2, 4, \dots \} \tag{6}$$

$$x_j \in \mathbf{Z}_o \quad \text{if} \quad t \in \mathbf{Z}_o \equiv \{ \dots, -1, 1, 3, 5, \dots \} \tag{7}$$

See Fig. 3 (cf. Figs. 1 and 2 for the HPP and FHP models). All particles are assumed to be located at lattice points $\mathbf{x} \in \mathbf{X}(t)$ whenever $t \in \mathbf{Z}$. The collisions at $t \in \mathbf{Z}$ and $\mathbf{x} \in \mathbf{X}(t)$ are accomplished by a suitable rule for

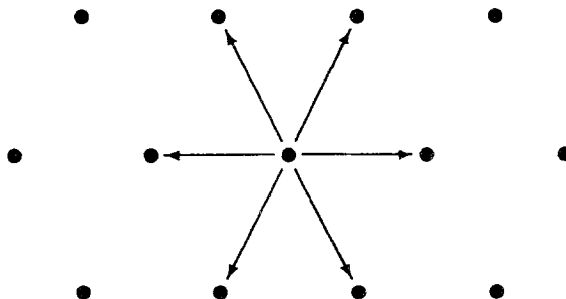


Fig. 2. Hexagonal lattice and discrete velocities v_a ($a = 1, \dots, 6$) of the FHP model.

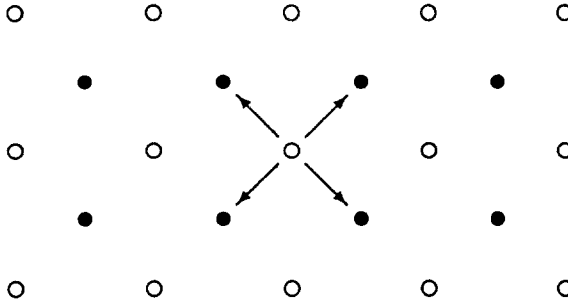


Fig. 3. Lattice structure of our model (in two dimensions). Particle positions at even and odd times are shown as white and black circles, respectively; the arrows indicate the possible particle velocities.

transforming a local configuration of incoming particles into a corresponding configuration of outgoing particles. The collision rule is usually chosen such that the total *mass* (number of particles) and the total *momentum* of a local configuration do not change in the collision. These collision invariants are essential for the model to produce on a macroscopic scale the desired Navier–Stokes-like hydrodynamic behavior. One could also introduce a CA analog of *energy* conservation (as in ref. 17), but normally this is not done, since for most interesting hydrodynamic limiting cases, such as incompressible flow, energy conservation is irrelevant, so an additional modeling of energy conservation would only further complicate the CA model unnecessarily.

In order to formulate the dynamics of such a model in CA form, one views each of the possible discrete one-particle phase space points (\mathbf{x}, \mathbf{v}) as a “cell,” whose state can be characterized by its occupation number $n(t, \mathbf{x}, \mathbf{v})$. To keep the model as simple as possible, one additionally postulates an “exclusion principle” which prevents that two particles simultaneously occupy the same cell, so that

$$n(t, \mathbf{x}, \mathbf{v}) \in \{0, 1\} \quad (8)$$

In the conventional models, the occupation number specifies the state of a cell completely, and in particular the momentum $\mathbf{m}(t, \mathbf{x}, \mathbf{v})$ of a cell is defined by the usual formula “mass times velocity,” i.e., $\mathbf{m}(t, \mathbf{x}, \mathbf{v}) = \mathbf{v}n(t, \mathbf{x}, \mathbf{v})$. In our model, however, the momentum is defined differently: We postulate that each particle carries with it a vector-valued quantity $\mathbf{n} = (n_1, \dots, n_d)$, which we call “absolute momentum,” with components

$$n_j \in \{0, 1\} \quad (9)$$

and we define the “momentum” \mathbf{m} of a particle with velocity \mathbf{v} and absolute momentum \mathbf{n} componentwise by

$$m_j := n_j v_j \tag{10}$$

In other words, momentum \mathbf{m} and velocity \mathbf{v} agree only in the signs of their components, while the magnitudes of the momentum components, which according to (10), (9), and (3) are

$$|m_j| = n_j \in \{0, 1\} \tag{11}$$

play the role of additional Boolean degrees of freedom [the equality sign in (11) also explains the name “absolute momentum” for \mathbf{n}]. With our momentum definition, the characterization of the state of a cell merely by its occupation number $n(t, \mathbf{x}, \mathbf{v})$ would be incomplete; rather, we have to specify for each cell $1 + d$ Boolean quantities

$$n_J(t, \mathbf{x}, \mathbf{v}) \in \{0, 1\} \quad (J=0, 1, \dots, d) \tag{12}$$

where $n_0 \equiv n$ is the number of particles in the cell, and $(n_1, \dots, n_d) \equiv \mathbf{n}$ is the total amount of absolute momentum contained in the cell (see Fig. 4). Note that these quantities cannot take arbitrary Boolean values independently of each other: Since empty cells ($n_0 \equiv n = 0$) always have zero absolute momentum ($\mathbf{n} = 0$), there is the restriction

$$n_j(t, \mathbf{x}, \mathbf{v}) \leq n_0(t, \mathbf{x}, \mathbf{v}) \tag{13}$$

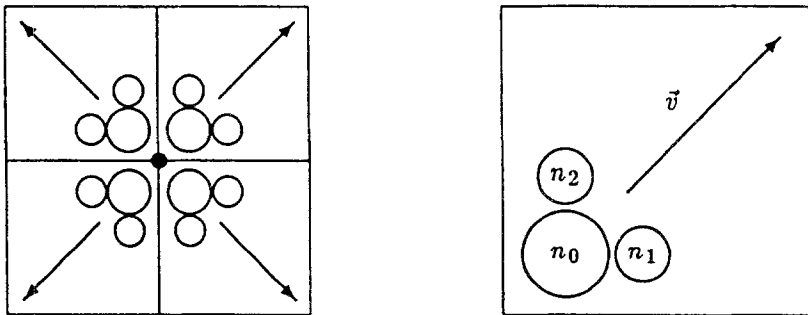


Fig. 4. Local structure of our model. The left picture shows the local cells (indicated by the small squares) with different velocities (the arrows) at a lattice point (the dot in the middle); the right picture shows one of the cells in more detail. Each circle corresponds to a bit in the computer. The bit n_0 indicates the presence or absence of a particle in a cell, while the bits n_1 and n_2 indicate the presence or absence of a momentum component in the x_1 and x_2 directions, respectively.

For brevity, it is from now on always implicitly assumed that

$$j, k, \dots \in \{1, \dots, d\} \quad (14)$$

$$J, K, \dots \in \{0, 1, \dots, d\} \quad (15)$$

whenever these letters occur as indices, and the notation

$$\begin{aligned} \mathbf{a} &:= (a_1, \dots, a_d) \\ a_* &:= (a_0, \mathbf{a}) = (a_0, a_1, \dots, a_d) \end{aligned} \quad (16)$$

is used for d -tuples and $(1+d)$ -tuples of quantities a_J , where \mathbf{a} is called a “vector” and a_* a “hypervector.” Thus, the state of a cell is characterized by the hypervector

$$n_*(t, \mathbf{x}, \mathbf{v}) \in \mathbf{S} \quad (17)$$

where the set of admissible values is

$$\mathbf{S} = \{n_* : n_J \in \{0, 1\}, n_J \leq n_0\} \quad (18)$$

We define the “hypermomentum” m_* of a cell by

$$m_J(t, \mathbf{x}, \mathbf{v}) := v_J n_J(t, \mathbf{x}, \mathbf{v}) \quad (19)$$

where v_1, \dots, v_d are the ordinary components of the cell velocity \mathbf{v} and

$$v_0 := 1 \quad (20)$$

The vectorial part \mathbf{m} of the hypermomentum $m_* = (m_0, \mathbf{m})$ then is the momentum of the cell in the sense of our definition, while the scalar part $m_0 = n_0$ specifies the mass of the cell.

The dynamics of the CA model now has to be specified as an iteration rule for transforming the state at time t into the state at time $t+1$. Each step of the iteration consists of two substeps: the collision at time t and the subsequent free motion during the time from t to $t+1$. The free motion leads to the following “shift rule” for transforming the state immediately after the collision at time t into the state immediately before the next collision at time $t+1$:

$$n_J(t+1, \mathbf{x} + \mathbf{v}, \mathbf{v}) = n'_J(t, \mathbf{x}, \mathbf{v}) \quad (21)$$

The collision transitions

$$n_J(t, \mathbf{x}, \mathbf{v}) \rightarrow n'_J(t, \mathbf{x}, \mathbf{v}) \quad (22)$$

are generated by a local rule of the form

$$n'_{\mathbf{v}J} = f_{\mathbf{v}J}(n_{**}) \quad (23)$$

where

$$n_{\mathbf{v}J}(t, \mathbf{x}) \equiv n_J(t, \mathbf{x}, \mathbf{v}) \quad (24)$$

and

$$n_{**} \equiv (n_{\mathbf{v}J} : \forall(\mathbf{v}, J)) \quad (25)$$

i.e., n_{**} represents a local collision configuration. We require the “collision function” $f_{\mathbf{v}J}$ in (23) to have two essential properties: First, it has to preserve the total hypermomentum (i.e., both mass and momentum) of the cells that take part in a collision:

$$\sum_{\mathbf{v}} v_J n'_{\mathbf{v}J} = \sum_{\mathbf{v}} v_J n_{\mathbf{v}J} \quad (26)$$

This ensures that the hypermomentum density becomes a local macroscopically relevant, i.e., hydrodynamic, quantity. The second important property is that

$$f_{**} : n_{**} \mapsto n'_{**} \quad \text{is one-to-one} \quad (27)$$

i.e., we require that the local state n_{**} before the collision can always be uniquely reconstructed from knowledge of the state n'_{**} after the collision. As will be seen later, this “reversibility” property plays a similar role as does the Hamiltonian form of the equations of motion in classical mechanics: it allows us to apply the Gibbs formalism, which yields important information about the statistical equilibrium state.

3. THE COLLISION MECHANISM

The simplest possible collision rule consistent with our requirements of hypermomentum conservation and reversibility would be, of course, the identity transformation: $n'_{\mathbf{v}J} = n_{\mathbf{v}J}$. However, this would give rise to a whole bunch of unwanted additional conservation laws and therefore is out of the question. Instead, a “good” rule, loosely stated, should try to redistribute the hypermomentum among the local cells as well as possible.

An easily implementable algorithm that deals systematically with the huge number of different possible collision configurations can be

constructed as follows. We accomplish the local transformation $n_{\mathbf{v}J} \rightarrow n'_{\mathbf{v}J}$ in d successive steps:

$$n_{\mathbf{v}J} = n_{\mathbf{v}J}^1 \rightarrow n_{\mathbf{v}J}^2 \rightarrow \dots \rightarrow n_{\mathbf{v}J}^{d+1} = n'_{\mathbf{v}J} \tag{28}$$

i.e., in the first step, the original state just before the collision, $n_{\mathbf{v}J} \equiv n_{\mathbf{v}J}^1$, gets transformed into an intermediate state, $n_{\mathbf{v}J}^2$, which in turn then gets transformed into $n_{\mathbf{v}J}^3$, etc., until after d steps the final state $n_{\mathbf{v}J}^{d+1} \equiv n'_{\mathbf{v}J}$ is reached, whereupon by definition the collision process is finished and the particles start flying apart in free motion (remember that the whole collision process occurs “infinitely fast” in the model, although of course the actual performance of the transformations will consume valuable computer time). At the k th step ($n_{\mathbf{v}J}^k \rightarrow n_{\mathbf{v}J}^{k+1}$), we let each velocity \mathbf{v} interact with a single partner velocity $R_k \mathbf{v}$ whose value differs from \mathbf{v} only in that the sign of its k th component is reversed:

$$\begin{aligned} R_1 \mathbf{v} &:= (-v_1, +v_2, \dots, +v_d) \\ R_2 \mathbf{v} &:= (+v_1, -v_2, \dots, +v_d) \\ &\vdots \\ R_d \mathbf{v} &:= (+v_1, +v_2, \dots, -v_d) \end{aligned} \tag{29}$$

Thus,

$$(R_k \mathbf{v})_j = (-1)^{\delta_{jk}} v_j \tag{30}$$

Figure 5 illustrates the so-defined interaction pairs. Our pairs transformation rule for the k th step has the form

$$n_{\mathbf{v}J}^{k+1} = f_J^k(n_{\mathbf{v}^*}^k, n_{(R_k \mathbf{v})^*}^k) \tag{31}$$

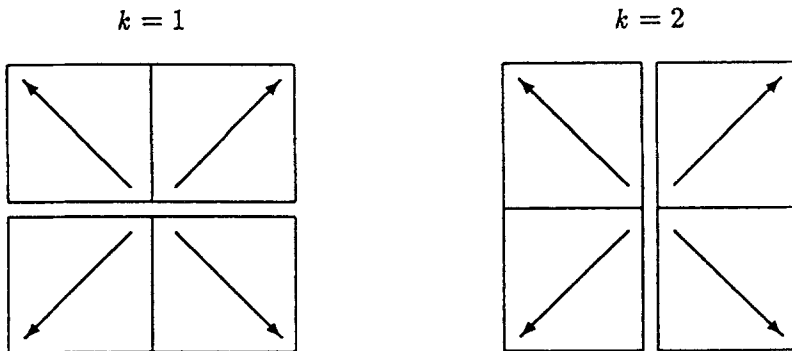


Fig. 5. Local pairs of interacting cells in subsequent collision steps (each square represents a cell; their velocity vectors are indicated by the arrows).

where

$$f_*^k = (f_0^k, \dots, f_d^k): \mathbf{S} \times \mathbf{S} \rightarrow \mathbf{S} \quad (32)$$

with \mathbf{S} given by (18). We define $f_j^k(n_*, n_*^+)$ for arbitrary $n_* \in \mathbf{S}$ and $n_*^+ \in \mathbf{S}$ explicitly as follows:

$$f_0^k(n_*, n_*^+) = \begin{cases} 1 & \text{if } n_0 = 0 \text{ and } n_0^+ = 1 \text{ and } n_k^+ = 0 \\ 0 & \text{if } n_0^+ = 0 \text{ and } n_0 = 1 \text{ and } n_k = 0 \\ n_0 & \text{otherwise} \end{cases}$$

$$f_k^k(n_*, n_*^+) = \begin{cases} 1 & \text{if } n_0 = n_0^+ = 1 \text{ and } n_k = n_k^+ = 0 \\ 0 & \text{if } n_0 = n_0^+ = 1 \text{ and } n_k = n_k^+ = 1 \\ n_0 & \text{otherwise} \end{cases} \quad (33)$$

$$f_j^k(n_*, n_*^+) = \begin{cases} n_j^+ & \text{if } \begin{cases} n_0 = 0 \text{ and } n_0^+ = 1 \text{ and } n_k^+ = 0 \\ n_0^+ = 0 \text{ and } n_0 = 1 \text{ and } n_k = 0 \\ n_0 = n_0^+ = 1 \end{cases} \\ n_j & \text{otherwise} \end{cases}$$

for $j \neq k$; here n_j and n_j^+ are abbreviations for $n_{\mathbf{v}J}^k$ and $n_{(R_k\mathbf{v})J}^k$, respectively [cf. (31)].

The transformation of an interacting cell pair $(\mathbf{v}, R_k\mathbf{v})$ according to (31) can then be characterized by the mapping

$$F_k: \mathbf{S} \times \mathbf{S} \rightarrow \mathbf{S} \times \mathbf{S}, \quad (n_*, n_*^+) \mapsto (f_*^k(n_*, n_*^+), f_*^k(n_*^+, n_*)) \quad (34)$$

By inspecting Fig. 6, which illustrates F_k , one recognizes the following important properties:

$$f_j^k(n_*, n_*^+) + (-1)^{\delta_{jk}} f_j^k(n_*^+, n_*) = n_j + (-1)^{\delta_{jk}} n_j^+ \quad (35)$$

and

$$F_k \circ F_k = \text{id} \quad (36)$$

where “ \circ ” symbolizes concatenation of mappings, and “id” is the identity mapping.

From (35) it follows that the total hypermomentum of each interacting cell pair is conserved:

$$m_{\mathbf{v}J}^{k+1} + m_{(R_k\mathbf{v})J}^{k+1} = m_{\mathbf{v}J}^k + m_{(R_k\mathbf{v})J}^k \quad (37)$$

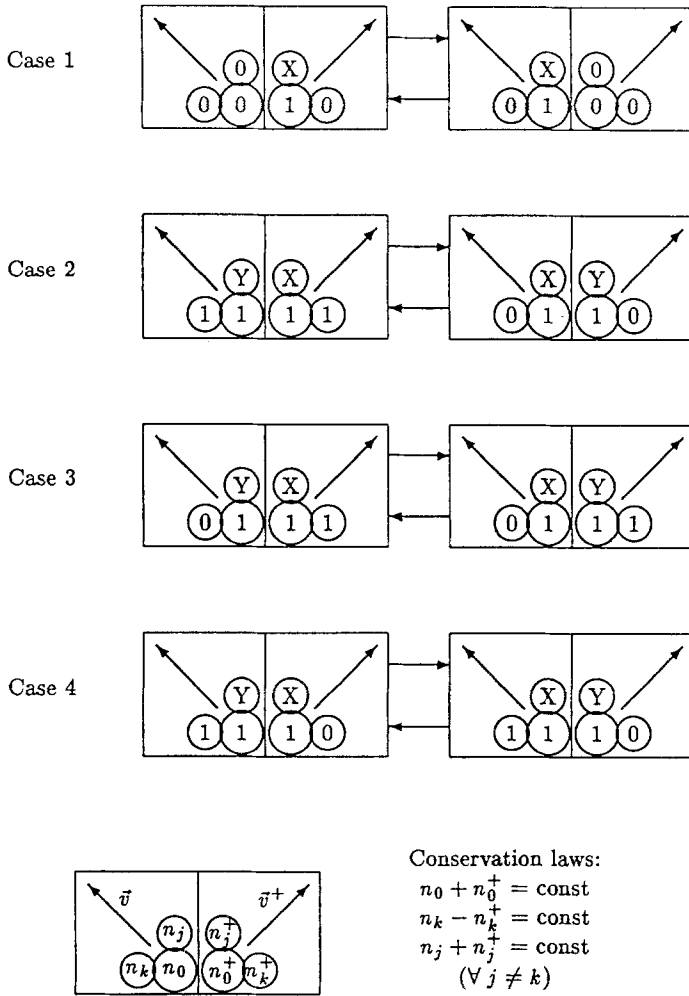


Fig. 6. Collision rule for a pair of interacting cells (\mathbf{x}, \mathbf{v}) and $(\mathbf{x}, \mathbf{v}^+)$. The partner cell's velocity $\mathbf{v}^+ = R_k \mathbf{v}$ is \mathbf{v} with sign-reversed k th component. $k \in \{1, \dots, d\}$ is the number of the step and corresponds to the "interaction direction." Shown are all the possible nontrivial transitions, i.e., all other configurations remain unchanged. Note that each arrow (symbolizing a transition) has a partner that points in the reverse direction, which means that the pair rule is self-inverse. Also notice that case 1 is a "one-particle collision," i.e., one particle changes its velocity without changing its momentum, while cases 2, 3, and 4 are "two-particle collisions," where either particle retains its velocity, but not its momentum. The diagram at the bottom of the picture explains the various symbols; next to it, the conservation laws are indicated. The index j ($\neq k$) represents collectively all space directions orthogonal to the interaction direction k .

where

$$m_{\mathbf{v}J}^k(t, \mathbf{x}) \equiv v_J n_{\mathbf{v}J}^k(t, \mathbf{x}) \quad (38)$$

is the hypermomentum of cell \mathbf{v} at step k . Thus, our collision rule, being entirely composed of hypermomentum-conserving pair transitions, satisfies indeed the desired local conservation law (26). From Eq. (36), which states that each pair transformation rule is self-inverse, it is also clear that our collision rule has the postulated reversibility property: The state $n_{**} \equiv n_{**}^1$ before the collision can be uniquely reconstructed from the state $n_{**}' \equiv n_{**}^{d+1}$ after the collision by simply applying the pair rules in reverse order, i.e., by computing

$$n_{\mathbf{v}J}^k = f_J^k(n_{\mathbf{v}*}^{k+1}, n_{(R_k\mathbf{v})*}^{k+1}) \quad (39)$$

successively for $k = d, d-1, \dots, 1$.

We finally mention that the special form (33) of f_J^k is fixed by the additional requirement that as many bits as possible should be changed in an elementary pair interaction without violating the hypermomentum conservation.

4. EQUILIBRIUM STATISTICS

Let us now investigate the statistical properties of our model. To this end, we write the dynamics of our CA in the form

$$n_{**}(t+2, \cdot) = \hat{F}n_{**}(t, \cdot) \quad (40)$$

Here

$$\begin{aligned} n_{**}(t, \cdot) &\equiv (n_{**}(t, \mathbf{x}): \forall \mathbf{x} \in \mathbf{X}(t)) \\ &\equiv (n_{\mathbf{v}J}(t, \mathbf{x}): \forall (\mathbf{x}, \mathbf{v}, J)) \end{aligned} \quad (41)$$

is the complete set of lattice state variables, and the operator \hat{F} describes the evolution of the system over a time interval $\Delta t = 2$ according to our rules. We consider $\Delta t = 2$ rather than $\Delta t = 1$, since the set $\mathbf{X}(t)$ of lattice points alternates with each timestep according to (7), so it would not make sense to compare lattice states at times t and $t+1$ with each other. Furthermore, we assume periodic boundary conditions in all space directions and restrict \mathbf{x} to the periodicity volume, so the number of possible lattice states is finite, albeit very large. Let

$$P(t, n_{**}(\cdot)) := \text{prob}\{n_{**}(t, \cdot) = n_{**}(\cdot)\} \quad (42)$$

which is the probability for the occurrence of lattice state $n_{**}(\cdot)$ at time t in a statistical ensemble of automata. The evolution law for these probabilities is

$$P(t+2, \hat{F}n_{**}(\cdot)) = P(t, n_{**}(\cdot)) \quad (43)$$

because \hat{F} is one-to-one due to the reversibility of our dynamics.

The ‘‘Gibbs distribution’’ $P^E(\cdot)$ for our model is defined by

$$\begin{aligned} P^E(n_{**}(\cdot)) &= \frac{1}{Z} W(n_{**}(\cdot)) \\ W(n_{**}(\cdot)) &= \exp \left[- \sum_J \mu_J M_J(n_{**}(\cdot)) \right] \\ Z &= \sum_{n_{**}(\cdot)} W(n_{**}(\cdot)) \end{aligned} \quad (44)$$

where the μ_J are arbitrary real parameters, and

$$M_J(n_{**}(\cdot)) := \sum_{\mathbf{x}, \mathbf{v}} v_J n_{\mathbf{v}J}(\mathbf{x}) \quad (45)$$

are the components of the total hypermomentum M_* of the lattice state $n_{**}(\cdot)$. As is well known, such a Gibbs distribution can be uniquely characterized by the fact that it maximizes the statistical entropy (Boltzmann’s H -function)

$$- \sum_{n_{**}(\cdot)} P^E(n_{**}(\cdot)) \ln P^E(n_{**}(\cdot)) = \max \quad (46)$$

under the constraint of fixed expectation values

$$\sum_{n_{**}(\cdot)} P^E(n_{**}(\cdot)) M_J(n_{**}(\cdot)) = \bar{M}_J \quad (47)$$

Since our dynamics conserves the total hypermomentum, $M_*(\cdot)$ has the property

$$M_J(\hat{F}n_{**}(\cdot)) = M_J(n_{**}(\cdot)) \quad (48)$$

from which it follows immediately that

$$P^E(\hat{F}n_{**}(\cdot)) = P^E(n_{**}(\cdot)) \quad (49)$$

This in turn means that $P^E(\cdot)$ is a stationary solution of (43), i.e., $P^E(\cdot)$ represents an equilibrium distribution. Its parameters μ_J are the intensive

thermodynamic quantities corresponding to the extensive dynamical invariants M_J .

Of course, the Gibbs distributions $P^E(\cdot)$ represents only a particular class of stationary distributions, and the question arises whether there are possibly other macroscopically relevant distributions. That would be the case, for instance, if there were additional extensive dynamical invariants independent of the M_J , which could then be included in the Gibbs formulas, giving rise to additional parameters analogous to the μ_J . Such a case has recently been discussed for the FHP and similar models by Zanetti⁽³⁰⁾ (the Zanetti invariants do not appear in our model due to our alternating lattice).

Since the hypermomentum (45) is additive over the cells (\mathbf{x}, \mathbf{v}) , the Gibbs probability (44) splits into a product of cell probabilities:

$$P^E(n_{**}(\cdot)) = \prod_{\mathbf{x}, \mathbf{v}} P_{\mathbf{v}}(n_{\mathbf{v}*}(\mathbf{x})) \quad (50)$$

where

$$P_{\mathbf{v}}(n_{\mathbf{v}*}) = \text{prob}\{n_{\mathbf{v}*}(t, \mathbf{x}) = n_{\mathbf{v}*}\} \quad (51)$$

(the probability for the occurrence of a given cell state $n_{\mathbf{v}*} \in \mathbf{S}$) is given by

$$\begin{aligned} P_{\mathbf{v}}(n_{\mathbf{v}*}) &= W_{\mathbf{v}}(n_{\mathbf{v}*})/Z_{\mathbf{v}} \\ W_{\mathbf{v}}(n_{\mathbf{v}*}) &= \exp\left(-\sum_{J=0}^d \mu_J v_J n_J\right) \\ Z_{\mathbf{v}} &= \sum_{n_{\mathbf{v}*} \in \mathbf{S}} W_{\mathbf{v}}(n_{\mathbf{v}*}) \end{aligned} \quad (52)$$

Equation (50) means that there are no statistical correlations between different cells.

Taking into account the restricted set (18) of possible values for $n_{\mathbf{v}*}$, we have

$$P_{\mathbf{v}}(0, \mathbf{0}) = 1 - \rho_{\mathbf{v}}, \quad P_{\mathbf{v}}(1, \mathbf{n}) = \rho_{\mathbf{v}} Q_{\mathbf{v}}(\mathbf{n}) \quad (53)$$

with

$$\rho_{\mathbf{v}} = \text{prob}\{n_{\mathbf{v}0} = 1\} = \langle n_{\mathbf{v}0} \rangle \quad (54)$$

$$(55)$$

and

$$Q_{\mathbf{v}}(\mathbf{n}) = \rho_{\mathbf{v}} \text{prob}\{\mathbf{n}_{\mathbf{v}} = \mathbf{n} \mid n_{\mathbf{v}0} = 1\} \quad (56)$$

where “|” means “under the condition that.” Here $\rho_{\mathbf{v}}$ is the occupation probability of a cell with velocity \mathbf{v} , while $Q_{\mathbf{v}}(\mathbf{n})$ is the probability that a particle ($n_0 = 1$) with velocity \mathbf{v} has absolute momentum \mathbf{n} . Using (52), one finds that the joint probability for the absolute momentum components (n_1, \dots, n_d) of a particle splits into a product:

$$Q_{\mathbf{v}}(\mathbf{n}) = \prod_{j=1}^d Q_{\mathbf{v}j}(n_j) \quad (57)$$

where

$$Q_{\mathbf{v}j}(n_j) = \text{prob}\{n_{\mathbf{v}j} = n_j \mid n_{\mathbf{v}0} = 1\} \quad (n_j \in \{0, 1\}) \quad (58)$$

is the probability that the j th absolute momentum component of a particle with velocity \mathbf{v} has a given value n_j . Thus, (57) states that the momentum components of a particle are not statistically correlated with each other.

In (57), we have $n_j \in \{0, 1\}$ and thus

$$Q_{\mathbf{v}j}(1) = \sigma_{\mathbf{v}j}, \quad Q_{\mathbf{v}j}(0) = 1 - \sigma_{\mathbf{v}j} \quad (59)$$

with

$$\sigma_{\mathbf{v}j} = \text{prob}\{n_{\mathbf{v}j} = 1 \mid n_{\mathbf{v}0} = 1\} = \langle n_{\mathbf{v}j} \mid n_{\mathbf{v}0} = 1 \rangle \quad (60)$$

As shown in Appendix B, evaluation of (52) yields

$$\rho_{\mathbf{v}} = f\left(\mu_0 + \sum_{j=1}^d \ln f(-\mu_j v_j)\right), \quad \sigma_{\mathbf{v}j} = f(\mu_j v_j) \quad (61)$$

with

$$f(\xi) := \frac{1}{1 + e^{\xi}} \quad (62)$$

Equations (61) give the probabilities $\rho_{\mathbf{v}}$ and $\sigma_{\mathbf{v}j}$ as functions of the set of distribution parameters, $\mu_{\star} = (\mu_0, \dots, \mu_d)$. Different values of μ_{\star} correspond to different values of the spatial hypermomentum density $q_{\star} = (q_0, \dots, q_d)$. The hypermomentum density is defined by

$$q_J := 2^{-d} \sum_{\mathbf{v}} v_J p_{\mathbf{v}J} \quad (63)$$

where

$$p_{\mathbf{v}J} := \langle n_{\mathbf{v}J} \rangle \quad (64)$$

The normalization factor 2^{-d} in (63) gives q_* the desired meaning of “hypermomentum per unit volume” [note that each lattice point according to (7) “occupies” a volume of 2^d in d dimensions]. In particular,

$$\mathbf{q} = (q_1, \dots, q_d) \quad (65)$$

is the momentum density, and

$$\rho := q_0 \quad (66)$$

is the mass density. Note that $\rho = 1$ if the lattice is completely occupied.

The $p_{\mathbf{v},j}$ can be expressed by $\rho_{\mathbf{v}}$ and $\sigma_{\mathbf{v},j}$:

$$p_{\mathbf{v},0} = \rho_{\mathbf{v}}, \quad p_{\mathbf{v},j} = \rho_{\mathbf{v}} \sigma_{\mathbf{v},j} \quad (67)$$

and Eqs. (63) become

$$\rho = 2^{-d} \sum_{\mathbf{v}} \rho_{\mathbf{v}}, \quad q_j = 2^{-d} \sum_{\mathbf{v}} v_j \rho_{\mathbf{v}} \sigma_{\mathbf{v},j} \quad (68)$$

This set of equations, together with (61), can be used to solve for the μ_j in terms of the q_j ; the result inserted back into (61) then gives $\rho_{\mathbf{v}}$ and $\sigma_{\mathbf{v},j}$ as functions of q_* . Although a closed-form solution of this nonlinear equation set is not possible, one can obtain an asymptotic solution for small $|\mathbf{q}|$ (Appendix B). The result is

$$\begin{aligned} \rho_{\mathbf{v}} &= \rho + 2 \frac{1-\rho}{2-\rho} \mathbf{v} \cdot \mathbf{q} + 2 \frac{(1-\rho)(1-2\rho)}{(2-\rho)^2 \rho} [(\mathbf{v} \cdot \mathbf{q})^2 - q^2] + O(q^3) \\ \sigma_{\mathbf{v},j} &= \frac{1}{2} + \frac{v_j q_j}{(2-\rho)\rho} + O(q^3) \end{aligned} \quad (69)$$

where $q := |\mathbf{q}| \ll 1$.

5. HYDRODYNAMICS—FIRST APPROXIMATION

Our knowledge of the equilibrium distribution now constitutes the starting point for the derivation of hydrodynamic equations. The hydrodynamic description of the CA is based on the assumption that a local near-equilibrium situation has established, where all local statistical quantities are entirely determined by a few local macroscopic order parameters, namely the components $q_j(t, \mathbf{x})$ of the local hypermomentum density. In particular, the local expectation values $p_{\mathbf{v},j} = \langle n_{\mathbf{v},j} \rangle$ and

$p'_{vJ} = \langle n'_{vJ} \rangle$ immediately before and after the collisions become local functionals of the hypermomentum density:

$$p_{vJ} = \tilde{p}_{vJ}(q_*, \nabla q_*, \nabla\nabla q_*, \dots) \quad (70)$$

$$p'_{vJ} = \tilde{p}'_{vJ}(q_*, \nabla q_*, \nabla\nabla q_*, \dots) \quad (71)$$

where \tilde{p}_{vJ} and \tilde{p}'_{vJ} are certain continuously differentiable functions, which in the special case of exact equilibrium ($\mathbf{V} = 0$) must reduce to

$$\tilde{p}_{vJ}(q_*, 0, 0, \dots) = \tilde{p}'_{vJ}(q_*, 0, 0, \dots) = \tilde{p}_{vJ}^0(q_*) \quad (72)$$

with

$$p_{v0}^0 = p'_{v0}{}^0 = \rho_v^0(q_*) \quad (73)$$

$$p_{vj}^0 = p'_{vj}{}^0 = \rho_v^0(q_*) \sigma_{vj}^0(q_*)$$

where $\rho_v^0(q_*)$ and $\sigma_{vj}^0(q_*)$ are given by Eqs. (69) according to our equilibrium theory. The hydrodynamic equations we are looking for then are a closed set of local evolution equations for the order parameters q_J :

$$\partial_t q_J = \dot{q}_J(q_*, \nabla q_*, \nabla\nabla q_*, \dots) \quad (74)$$

As the q_J are densities of conserved quantities, the right-hand side of (74) must be of the form

$$\dot{q}_J(q_*, \nabla q_*, \dots) = - \sum_k \nabla_k Q_{Jk}(q_*, \nabla q_*, \dots) \quad (75)$$

where Q_{Jk} is the ‘‘hypermomentum flux density.’’

In order to determine the local functionals p_{vJ} , \tilde{p}'_{vJ} , and Q_{Jk} , one can formally expand them in Chapman–Enskog series of the form $O(1) + O(\nabla) + O(\nabla^2) + \dots$:

$$p_{vJ} = p_{vJ}^0(q_*) + r_{vJ} + O(\nabla^2) \quad \text{with} \quad r_{vJ} = \sum_{Lm} R_{vJLm}(q_*) \nabla_m q_L \quad (76)$$

$$p'_{vJ} = p'_{vJ}{}^0(q_*) + r'_{vJ} + O(\nabla^2) \quad \text{with} \quad r'_{vJ} = \sum_{Lm} R'_{vJLm}(q_*) \nabla_m q_L \quad (77)$$

$$Q_{Jk} = Q_{Jk}^0(q_*) + Q_{Jk}^\nabla + O(\nabla^2) \quad \text{with} \quad Q_{Jk}^\nabla = - \sum_{Lm} T_{JLkm}(q_*) \nabla_m q_L \quad (78)$$

[the minus sign in (78) is just a convention], with

$$O(\nabla^2) := O(\nabla\nabla q_*) + O(\nabla q_* \nabla q_*) + O(\nabla\nabla\nabla q_*) + \dots \quad (79)$$

This sort of expansion is justified if the characteristic length scale Δx of the hydrodynamic fields is sufficiently small, so that

$$O(\nabla^k) = O((\Delta x)^{-k}), \quad (k = 0, 1, 2, \dots) \quad (80)$$

One obtains a first approximation for the hydrodynamics by putting $Q_{Jk} \approx Q_{Jk}^0$; this gives $\partial_i q_J = \sum_k \nabla_k Q_{Jk}^0(q_*)$, which is time-reversal symmetric and therefore cannot describe friction effects, such as viscosity. In order to capture friction effects, one must proceed to the second approximation $Q_{Jk} \approx Q_{Jk}^0 + Q_{Jk}^V$, which leads to additional diffusive terms, where the quantities T_{JLkm} in (78) play the role of diffusion coefficients.

The unknown terms in (76)–(78) must be determined from the requirement to be consistent with the discrete microdynamics of our CA. Taking the local expectation value of (21), we have

$$[\exp(\partial_i + \mathbf{v} \cdot \nabla)] p_{vJ} = p'_{vJ} \quad (81)$$

where $p_{vJ} = \langle n_{vJ} \rangle$ and $p'_{vJ} = \langle n_{vJ} \rangle$ refer to the state before and after the collision, respectively. The exponential in (81) symbolizes a space-time shift operator, with

$$\exp(\partial_i + \mathbf{v} \cdot \nabla) = 1 + (\partial_i + \mathbf{v} \cdot \nabla) + \frac{1}{2}(\partial_i + \mathbf{v} \cdot \nabla)^2 + \dots \quad (82)$$

when the space-time derivatives of the operand are small. Applying $2^{-d} \sum_{\mathbf{v}} v_J$ to (81), we get

$$2^{-d} \sum_{\mathbf{v}} v_J [(\partial_i + \mathbf{v} \cdot \nabla) + \frac{1}{2}(\partial_i + \mathbf{v} \cdot \nabla)^2 + \dots] p_{vJ} = 0 \quad (83)$$

Here, we have used the definition (63) of q_J and the fact that

$$2^{-d} \sum_{\mathbf{v}} v_J p'_{vJ} = 2^{-d} \sum_{\mathbf{v}} v_J p_{vJ} \quad (84)$$

due to the local conservation law (26). We now make the formal ansatz

$$\partial_i = \partial_{i1} + \partial_{i2} + \dots, \quad \partial_{i1} = O(\nabla), \quad \partial_{i2} = O(\nabla^2), \dots \quad (85)$$

If we insert (85) and (76) into (83) and then collect terms of equal order of magnitude, respectively, we obtain

$$\begin{aligned} 0 &= 2^{-d} \sum_{\mathbf{v}} v_J (\partial_{i1} + \mathbf{v} \cdot \nabla) p_{vJ}^0 \\ &\quad + 2^{-d} \sum_{\mathbf{v}} v_J [\partial_{i2} p_{vJ}^0 + \frac{1}{2}(\partial_{i1} + \mathbf{v} \cdot \nabla)^2 p_{vJ}^0 + (\partial_{i1} + \mathbf{v} \cdot \nabla) r_{vJ}] \\ &\quad + O(\nabla^3) \end{aligned} \quad (86)$$

Each order of magnitude must vanish separately; in particular, the $O(\nabla)$ terms give

$$2^{-d} \sum_{\mathbf{v}} v_J (\partial_{t1} + \mathbf{v} \cdot \nabla) p_{\mathbf{v}J}^0 = 0 \quad (87)$$

This can be written as

$$\partial_{t1} q_J + \sum_k \nabla_k Q_{Jk}^0 = 0 \quad (88)$$

with

$$Q_{Jk}^0 := 2^{-d} \sum_{\mathbf{v}} v_J v_k p_{\mathbf{v}J}^0 \quad (89)$$

where the identity

$$2^{-d} \sum_{\mathbf{v}} v_J p_{\mathbf{v}J}^0(q_*) = q_J \quad (90)$$

has been used. Thus, we have found that the first term in (78) is given by (89). Inserting (73) and (69) into (86), we obtain with the help of Appendix A

$$\begin{aligned} \mathbf{g}^0 &= 2 \frac{1-\rho}{2-\rho} \mathbf{q} + O(q^3) \quad (g_k^0 \equiv Q_{0k}^0) \\ Q_{jk}^0 &= \left(\frac{\rho}{2} - 2 \frac{(1-\rho)(1-2\rho)}{(2-\rho)^2 \rho} q_j^2 \right) \delta_{jk} + 4 \frac{(1-\rho)^2}{(2-\rho)^2} q_j q_k + O(q^3) \end{aligned} \quad (91)$$

Here we have introduced the notation

$$\mathbf{g} := (g_1, \dots, g_d), \quad g_k := Q_{0k} \quad (92)$$

for the mass components of the hypermomentum tensor Q_{Jk} . Note that, according to our index convention, Q_{jk} denotes the ordinary (nonhyper) momentum flux tensor.

With the above formulas (91), we have determined the $O(1)$ approximation for the flux, $Q_{Jk} = Q_{Jk}^0 + O(\nabla)$, and thus obtained the $O(\nabla)$ terms of the hydrodynamic equations,

$$\begin{aligned} \partial_t \rho + \nabla \cdot \mathbf{g}^0(\rho, \mathbf{q}) &= O(\nabla^2) \\ \partial_t q_j + \sum_k \nabla_k Q_{jk}^0(\rho, \mathbf{q}) &= O(\nabla^2) \end{aligned} \quad (93)$$

Even if both the still unknown diffusive $O(\nabla^2)$ terms in (93) and the $O(q^3)$ terms in (91) were negligible, the resulting hydrodynamics would be anisotropic due to the term proportional to $q_j^2 \delta_{jk}$ in (91). For the purpose of fluid-dynamics simulation, an at least approximately hydrodynamic behavior of the CA would of course be desirable. Note, however, that the coefficient of the anisotropic $q_j^2 \delta_{jk}$ term in (91) vanishes for $\rho = 1/2$; therefore the case $\rho \approx 1/2$ is of special interest.

6. HYDRODYNAMIC LIMITING CASES

The information we have collected about the hydrodynamic equations up to now enables us to investigate various important hydrodynamic limiting cases, even without explicit knowledge of the diffusive $O(\nabla^2)$ terms, which we will return to later.

Let us first make the specific assumption that the hydrodynamic variables and their space-time scales have the following relative orders of magnitude:

$$\partial_t = O(\varepsilon^2), \quad \nabla = O(\varepsilon^2), \quad \rho = \frac{1}{2} + O(\varepsilon), \quad \mathbf{q} = O(\varepsilon) \quad (94)$$

with $\varepsilon \ll 1$. Here, $\partial_t = O(\varepsilon^2)$ means $1/\Delta t = O(\varepsilon^2)$ where Δt is the smallest typical hydrodynamic time scale, etc. Then Eqs. (93) with (91) become, up to negligible terms,

$$\begin{aligned} \partial_t \rho + \nabla \cdot \left[\left(\frac{10}{9} - \frac{8}{9} \rho \right) \mathbf{q} \right] &= 0 \\ \partial_t q_j + \sum_k \nabla_k \left[\frac{\rho}{2} \delta_{jk} + \frac{8}{9} q_j q_k \right] &= 0 \end{aligned} \quad (95)$$

The analog of (95) for a physical fluid is the compressible Euler equations

$$\begin{aligned} \partial_t \rho + \nabla \cdot \mathbf{q} &= 0 \\ \partial_t q_j + \sum_k \nabla_k \left[p(\rho) \delta_{jk} + \frac{1}{\rho} q_j q_k \right] &= 0 \end{aligned} \quad (96)$$

where $p(\rho)$ is the pressure (for simplicity we here assume that the temperature dependence is unimportant or has been eliminated), and $\mathbf{q} = \rho \mathbf{u}$, with \mathbf{u} being the hydrodynamic velocity. Comparison of (95) with (96) shows that the automaton's hydrodynamics is not equivalent to that of a physical fluid even in this special isotropic limiting case, because the convection term $O(q \nabla q)$ in (95) has an "unphysical" ρ dependence, which is an effect arising from the absence of Galilei invariance in the automaton.

Another important limiting case is the “acoustic limit”

$$\partial_t \rho = O(\varepsilon), \quad \mathbf{V} = O(\varepsilon), \quad \rho = \rho_0 + O(\varepsilon), \quad \mathbf{q} = O(\varepsilon) \quad (97)$$

(here the mean density ρ_0 is arbitrary), which leads to the linear equations of sound

$$\partial_t \rho + 2 \frac{1 - \rho_0}{2 - \rho_0} \nabla \cdot \mathbf{q} = 0, \quad \partial_t \mathbf{q} + \frac{1}{2} \nabla \rho = 0 \quad (98)$$

Eliminating \mathbf{q} , one gets

$$(\partial_t^2 + c^2 \nabla^2) \rho = 0 \quad (99)$$

where the (isotropic) speed of sound is

$$c = \left(\frac{1 - \rho_0}{2 - \rho_0} \right)^{1/2} \quad (100)$$

For the special value $\rho_0 = 1/2$, we have

$$c = 1/\sqrt{3} \quad (101)$$

More interesting for the purpose of flow simulation, however, is the “inviscid incompressible” case with $\rho_0 = 1/2$,

$$\partial_t \rho = O(\varepsilon^3), \quad \mathbf{V} = O(\varepsilon^2), \quad \rho = \frac{1}{2} + O(\varepsilon^2), \quad \mathbf{q} = O(\varepsilon) \quad (102)$$

which leads to

$$\nabla \cdot \mathbf{q} = 0, \quad (\partial_t + \frac{8}{9} \mathbf{q} \cdot \nabla) \mathbf{q} + \frac{1}{2} \nabla \rho = 0 \quad (103)$$

These equations closely resemble the incompressible Euler equations for an ideal physical fluid:

$$\nabla \cdot \mathbf{u} = 0, \quad (\partial_t + \mathbf{u} \cdot \nabla) \mathbf{u} + \nabla \phi = 0 \quad (104)$$

where $\phi = p/\rho_0$ is the kinematic pressure. Equations (103) and (104) are easily seen to be equivalent; they can be transformed into each other with

$$\phi = \frac{4}{9} \rho, \quad \mathbf{u} = \frac{8}{9} \mathbf{q} \quad (105)$$

This means that in the inviscid incompressible case, the CA can simulate a physical fluid obeying the incompressible Euler equations, where Eqs. (105) define the observables “kinematic pressure” and “hydrodynamic

velocity” in the CA model. Note that the so-defined hydrodynamic velocity \mathbf{u} has to be interpreted as a momentum convection velocity, and must not be confused with the mean velocity \mathbf{w} of the CA particles, which is

$$\mathbf{w} = \frac{\langle \sum_{\mathbf{v}} \mathbf{v} n_{\mathbf{v}0} \rangle}{\langle \sum_{\mathbf{v}} n_{\mathbf{v}0} \rangle} = \frac{\sum_{\mathbf{v}} \mathbf{v} \rho_{\mathbf{v}}}{\sum_{\mathbf{v}} \rho_{\mathbf{v}}} \approx \frac{\sum_{\mathbf{v}} \mathbf{v} \rho_{\mathbf{v}}^0}{\sum_{\mathbf{v}} \rho_{\mathbf{v}}^0} = \frac{\mathbf{g}^0}{\rho} \approx \frac{2(1-\rho)}{(2-\rho)\rho} \mathbf{q} \quad (106)$$

so that for $\rho \approx 1/2$,

$$\mathbf{w} = \frac{4}{3} \mathbf{q} = \frac{3}{2} \mathbf{u} \quad (107)$$

The peculiar fact that $\mathbf{u} \neq \mathbf{w}$ is typical of CAs, and can be explained as follows: In a physical fluid, Galilean invariance forces both macroscopic velocities to be the same. The CA model, however, does not contain any discrete equivalent of Galilei invariance; rather, the situation is loosely analogous to a copper wire in an electric circuit, where the mean velocity of the electrons is much smaller than the velocity of the information which they transport. In both cases, there is obviously a well-defined “rest” frame of reference, so there is no reason why the two macroscopic velocities should agree. The phenomenon that the mass and momentum convection velocities differ by a nontrivial factor also appears in the FHP, FCHC, and all other similar models; the proportionality factor (which in our special case is 2/3) in general depends on the mass density ρ ; it is usually denoted by $g(\rho)$ in the literature (often briefly called the “ g -factor”), after the notation introduced by FHP in their pioneering paper⁽¹⁾ (e.g., $g \approx 1/2$ for small ρ in the FHP-I model⁽²⁾).

The idea to obtain the desired isotropic form $(\mathbf{u} \cdot \nabla) \mathbf{u}$ of the convection term in the CA hydrodynamics by suitable choice of an adjustable statistical parameter (the mean density ρ_0 in our case) is not new, and has already been proposed and applied in other CA fluid models.^(9,16,17,20) Unfortunately, this trick does not work for the simple HPP model: Although one can eliminate the anisotropic terms in the HPP model by a suitable choice of ρ_0 , it is of not much use there because then also the isotropic part of the convective contribution [analogous to the $q_j q_k$ term our Eq. (91)] vanishes simultaneously.

For most hydrodynamic problems, the inviscid incompressible approximation is too much idealized, and one uses instead of (104) the incompressible Navier–Stokes equations, which contain an additional friction term:

$$\nabla \cdot \mathbf{u} = 0, \quad (\partial_t + \mathbf{u} \cdot \nabla) \mathbf{u} + \nabla \phi = \nu \nabla^2 \mathbf{u} \quad (108)$$

where ν is the kinematic (shear) viscosity coefficient. An analogous set of

incompressible hydrodynamic equations with viscosity for our CA model is obtained in the limiting case

$$\partial_t = O(\varepsilon^2), \quad \nabla = O(\varepsilon), \quad \rho = \frac{1}{2} + O(\varepsilon^2), \quad \mathbf{q} = O(\varepsilon) \quad (109)$$

Using (74), (75), (78), and (91), and dropping negligible terms, one finds

$$\nabla \cdot \mathbf{q} = 0, \quad (\partial_t + \frac{8}{9} \mathbf{q} \cdot \nabla) q_j + \frac{1}{2} \nabla_j \rho = \sum_{klm} T_{jklm} \nabla_l \nabla_m q_k \quad (110)$$

where the viscosity tensor T_{jklm} is defined by the function $T_{JLkm}(q_*)$ introduced in (78), evaluated at $\rho = 1/2$ and $\mathbf{q} = 0$. If one could show that T_{jklm} were isotropic, then (110) would be equivalent to (108) by means of the transformation (105). Unluckily, though, our model does not have symmetries that force T_{jklm} to be isotropic; we therefore have to explicitly consider the second approximation in order to get more detailed information about the friction terms in our model.

7. THE SECOND-ORDER CORRECTION TERMS

For the next-higher-order approximation of the hydrodynamic equations, we have to extract the $O(\nabla^2)$ terms from (86), obtaining

$$2^{-d} \sum_{\mathbf{v}} v_J [\partial_{t2} p_{\mathbf{v}J}^0 + \frac{1}{2} (\partial_{t1} + \mathbf{v} \cdot \nabla)^2 p_{\mathbf{v}J}^0 + (\partial_{t1} + \mathbf{v} \cdot \nabla) r_{\mathbf{v}J}] = 0 \quad (111)$$

With (87), this becomes

$$2^{-d} \sum_{\mathbf{v}} v_J [\partial_{t2} p_{\mathbf{v}J}^0 + \frac{1}{2} \mathbf{v} \cdot \nabla (\partial_{t1} + \mathbf{v} \cdot \nabla) p_{\mathbf{v}J}^0 + (\partial_{t1} + \mathbf{v} \cdot \nabla) r_{\mathbf{v}J}] = 0 \quad (112)$$

Using again (90), we find

$$\partial_{t2} q_J + \sum_k \nabla_k Q_{Jk}^{\nabla} = 0 \quad (113)$$

with

$$Q_{Jk}^{\nabla} = 2^{-d} \sum_{\mathbf{v}} v_J v_k (r_{\mathbf{v}J} + \frac{1}{2} s_{\mathbf{v}J}) \quad (114)$$

where

$$s_{\mathbf{v}J} := (\partial_{t1} + \mathbf{v} \cdot \nabla) p_{\mathbf{v}J}^0 \quad (115)$$

The latter quantity can be explicitly computed, since $p_{v_J}^0$ is a known function of q_* , and $\partial_{i1} q_L$ is given by (88) and (89), so that we obtain for (115) an expression of the form

$$s_{v_J} = \sum_{Lm} S_{v_JLm}(q_*) \nabla_{mqL} \tag{116}$$

with well-defined coefficients S_{v_JLm} . The desired friction coefficients can then be written as

$$T_{JLkm} = -2^{-d} \sum_v v_J v_k (R_{v_JLm} + \frac{1}{2} S_{v_JLm}) \tag{117}$$

according to (76), (78), (114), and (116).

The only open unknowns in (116) now are the R_{v_JLm} , which are defined as the coefficients of the $O(\nabla)$ term r_{v_J} in the series (76) for p_{v_J} . In order to gain more information about r_{v_J} , we expand Eq. (81) in powers of ∇ , and obtain for the $O(\nabla)$ terms

$$s_{v_J} = r'_{cJ} - r_{cJ} \tag{118}$$

where we have used (82), (85), (76), and (77). However, this new relation does not yet solve our problem to determine r_{v_J} , because we are now confronted with the additional unknowns r'_{v_J} .

One possibility to resolve this dilemma is to postulate a Boltzmann-type ‘‘collision equation,’’ i.e., a local functional relation between p_{v_J} and p'_{v_J} of the form

$$p'_{v_J} = f_{v_J}(p_{**}) \tag{119}$$

with $p_{**} \equiv (p_{uK}; \forall(\mathbf{u}, K))$. The postulated relation (119) is a sort of macroscopic generalization of the exactly valid microscopic collision equation (23). Forming the expectation value of the microscopic equation (23) and taking into account that $n_{v_J} \in \{0, 1\}$, we find

$$p'_{v_J} = \left\langle \sum_{n_{**}} n'_{v_J} P(f_{**}^{-1}(n_{**})) \right\rangle \tag{120}$$

Here, the sum extends over all possible local states n_{**} ; f_{**}^{-1} is the (well-defined!) inverse of the collision transformation $f_{**}: n_{**} \mapsto n'_{**}$, and

$$P(n_{**}) := \text{prob}\{n_{**}(t, \mathbf{x}) = n_{**}\} \tag{121}$$

is the probability for the occurrence of a given local state. Note that the above $P(\cdot)$ contains information not only about single-bit probabilities

$p_{\mathbf{v}J} = \langle n_{\mathbf{v}J} \rangle$, but also about correlations between different local bits, e.g., between $n_{\mathbf{v}J}$ and $n_{\mathbf{u}K}$ for $(\mathbf{v}, J) \neq (\mathbf{u}, K)$. Therefore, the macroscopic collision equation (119) contains implicitly an assumption analogous to Boltzmann's Stosszahl-Ansatz, namely that all local correlations are determined solely by the single-bit probabilities alone, so that $P(\cdot)$ becomes a well-defined function of p_{**} . The special structure of our equilibrium distribution now suggests the following ansatz:

$$P(n_{**}) = \prod_{\mathbf{v}} P_{\mathbf{v}}(n_{\mathbf{v}*}) \quad (122)$$

where $P_{\mathbf{v}}(n_{\mathbf{v}*})$ is defined by (53), (57), and (59), with

$$\rho_{\mathbf{v}} := p_{\mathbf{v}0}, \quad \sigma_{\mathbf{v}J} := p_{\mathbf{v}J}/p_{\mathbf{v}0} \quad (123)$$

In other words, we neglect in our nonequilibrium distribution all those correlations which would vanish in the equilibrium case. This prescription makes $P(\cdot)$ a function of p_{**} , which in turn, by way of (120), defines the desired macroscopic collision function $f_{\mathbf{v}J}(\cdot)$ for (119).

The $O(\nabla)$ terms of the ∇ expansion of (119) with (76) and (77) yield

$$r'_{\mathbf{v}J} = \sum_{\mathbf{u}K} A_{\mathbf{v}J\mathbf{u}K} r_{\mathbf{u}K} \quad (124)$$

with

$$A_{\mathbf{v}J\mathbf{u}K} := \frac{\partial f_{\mathbf{v}J}(p_{**}^0)}{\partial p_{\mathbf{u}K}} - \delta_{\mathbf{v}\mathbf{u}} \delta_{JK} \quad (125)$$

Together, (118) and (124) constitute a set of linear equations for an equal number of unknowns ($r_{\mathbf{v}J}$ and $r'_{\mathbf{v}J}$), but the so-defined linear problem is degenerate because the collision equation (119) satisfies the conservation relation (84), which implies

$$2^{-d} \sum_{\mathbf{v}} v_J r'_{\mathbf{v}J} = 2^{-d} \sum_{\mathbf{v}} v_J r_{\mathbf{v}J} \quad (126)$$

for $J=0, 1, \dots, d$; therefore, $1+d$ of the equations (124) are linearly dependent of the others. On the other hand, the definition of q_* , Eq. (63), and the identity (90) yield an additional set of $1+d$ equations:

$$2^{-d} \sum_{\mathbf{v}} v_J r_{\mathbf{v}J} = 0 \quad (127)$$

so that Eqs. (118), (124), and (127) taken together should fix the unknowns $r_{\mathbf{v}J}$ (and $r'_{\mathbf{v}J}$) uniquely. Once $r_{\mathbf{v}J}$ is known, we can insert it into

(114) and thus obtain the desired explicit expression for the frictional part Q_{Jk}^{\vee} of the hypermomentum flux.

8. THE FRICTION COEFFICIENTS

We will now explicitly calculate the friction coefficients $T_{JLkm}(q_*)$ for $\rho = 1/2$ and $\mathbf{q} = 0$ by actually carrying out the program just sketched.

First, the macroscopic collision equation (119) has to be found. In analogy to the microscopic collision rule, (28) and (31), we make the ansatz

$$p_{\vee J}^{k+1} = f_J^k(p_{\vee*}^k, p_{(R_k \vee)*}^k) \tag{128}$$

where $p_{\vee J}^k = \langle n_{\vee J}^k \rangle$ refers to the k th partial step of the transformation. The microscopic version of the functions $f_J^k(\cdot, \cdot)$ is given by (33), which can also be written in algebraic form as

$$\begin{aligned} f_J^k(n_*, n_*^+) &= n_J + \Delta n_J^k(n_*, n_*^+) \\ \Delta n_0^k(n_*, n_*^+) &= (1 - n_0)(n_0^+ - n_k^+) - (1 - n_0^+)(n_0 - n_k) \\ \Delta n_k^k(n_*, n_*^+) &= (n_0 - n_k)(n_0^+ - n_k^+) - n_k n_k^+ \\ \Delta n_j^k(n_*, n_*^+) &= [(1 - n_k)(n_0^+ - n_k^+) + n_k n_k^+] n_j^+ \\ &\quad - [(1 - n_k^+)(n_0 - n_k) + n_k^+ n_k] n_j \quad \text{for } j \neq k \end{aligned} \tag{129}$$

As can be easily verified, this is equivalent to (33) for all possible discrete values, $n_* \in \mathbf{S}$ and $n_*^+ \in \mathbf{S}$, with \mathbf{S} given by (18). In order to obtain the macroscopic version of $f_J^k(\cdot, \cdot)$ we take the expectation value of (129) and make use of the Boltzmann-type assumptions that:

- (i) n_* and n_*^+ are uncorrelated.
- (ii) If $n_0 = 1$, then n_j and n_k ($j \neq k$) are uncorrelated (for $n_0 = 0$, we have always $n_j = n_k = 0$); the same applies to n_*^+ .

These assumptions (which would be strictly satisfied in the equilibrium case) imply

$$\begin{aligned} \langle n_J n_K^+ \rangle &= \langle n_J \rangle \langle n_K^+ \rangle, & \langle n_J n_K n_L^+ \rangle &= \langle n_J n_K \rangle \langle n_L^+ \rangle, & \dots \\ \frac{\langle n_j n_k \rangle}{\langle n_0 \rangle} &= \frac{\langle n_j \rangle}{\langle n_0 \rangle} \times \frac{\langle n_k \rangle}{\langle n_0 \rangle} & (j \neq k), & \dots \end{aligned} \tag{130}$$

Additionally, we can use trivial relations like

$$n_0 n_j = n_j, \quad (n_j)^2 = n_j, \quad \dots \tag{131}$$

which follow from the mere fact that n_* , $n_*^+ \in \mathbf{S}$. In this way, we get from (129) by averaging the desired transformation function for the expectation values $p_J = \langle n_J \rangle$ and $p_J^+ = \langle n_J^+ \rangle$:

$$\begin{aligned}
 f_J^k(p_*, p_*^+) &= p_J + \Delta p_J^k(p_*, p_*^+) \\
 \Delta p_0^k(p_*, p_*^+) &= (1 - p_0)(p_0^+ - p_k^+) - (1 - p_0^+)(p_0 - p_k) \\
 \Delta p_k^k(p_*, p_*^+) &= (p_0 - p_k)(p_0^+ - p_k^+) - p_k p_k^+ \\
 \Delta p_j^k(p_*, p_*^+) &= [(1 - p_k)(p_0^+ - p_k^+) + p_k p_k^+] \frac{p_j^+}{p_0^+} \\
 &\quad - [(1 - p_k^+)(p_0 - p_k) + p_k^+ p_k] \frac{p_j}{p_0} \quad \text{for } j \neq k
 \end{aligned} \tag{132}$$

Since we are only interested in a linear approximation for $\rho \approx 1/2$ and $\mathbf{q} \approx 0$, we set

$$p_{vJ}^k = p_{vJ}^0 + r_{vJ}^k \tag{133}$$

with

$$p_{v0}^0 = \frac{1}{2}, \quad p_{vJ}^0 = \frac{1}{4} \tag{134}$$

for $\rho = 1/2$ and $\mathbf{q} = 0$ according to (73) and (69). Linearizing (132) for small r_{vJ}^k then gives

$$r_{vJ}^{k+1} = L_J^k(r_{v*}^k, r_{(R_k v)*}^k) \tag{135}$$

with

$$\begin{aligned}
 L_J^k(r_*, r_*^+) &= r_J + \Delta r_J^k(r_*, r_*^+) \\
 \Delta r_0^k(r_*, r_*^+) &= -\frac{3}{4}(r_0 - r_0^+) + \frac{1}{2}(r_k - r_k^+) \\
 \Delta r_k^k(r_*, r_*^+) &= \frac{1}{4}(r_0 + r_0^+) - \frac{1}{2}(r_k + r_k^+) \\
 \Delta r_j^k(r_*, r_*^+) &= -\frac{1}{8}(r_0 - r_0^+) + \frac{1}{4}(r_k - r_k^+) - \frac{1}{2}(r_j - r_j^+) \quad \text{for } j \neq k
 \end{aligned} \tag{136}$$

Equations (135) with (136), iterated according to the scheme

$$r_{vJ} = r_{vJ}^1 \rightarrow \dots \rightarrow r_{vJ}^{d+1} = r'_{vJ} \tag{137}$$

then define the coefficients $A_{vJ uK}$ in the linearized collision equation (124).

Fortunately, we need not directly calculate the $A_{vJ uK}$ and then solve the coupled set of equations (118), (124), and (127) for r_{vJ} , which would

be hopelessly complicated. The problem can be simplified by symmetry considerations. To this end, we set

$$r_{\mathbf{v}J}^k = \sum_{Lm} R_{\mathbf{v}JLm}^k \nabla_{mqL} \quad (138)$$

with yet unknown coefficients $R_{\mathbf{v}JLm}^k$. The symmetry of our model with respect to reversal of the x_h axis, where $h \in \{1, \dots, d\}$ is arbitrary, then implies

$$r_{(R_h\mathbf{v})J}^k = \sum_{Lm} R_{\mathbf{v}JLm}^k (-1)^{\delta_{hm}} (-1)^{\delta_{hL}} \nabla_{mqL} \quad (139)$$

where $R_h\mathbf{v}$ means \mathbf{v} with sign-reversed h th component according to (29). Comparison of (138) with (139) yields the symmetry relation

$$R_{(R_h\mathbf{v})JLm}^k = (-1)^{\delta_{hL}} (-1)^{\delta_{hm}} R_{\mathbf{v}JLm}^k \quad (140)$$

Now, an arbitrary \mathbf{v} with components $v_j \in \{\pm 1\}$ can always be transformed into the vector

$$\mathbf{1} := (1, \dots, 1) \quad (141)$$

by applying an appropriate sequence of sign-reversal operators R_h . In this manner, we obtain by repeated application of (140)

$$R_{\mathbf{v}JLm}^k = v_L v_m R_{JLm}^k \quad \text{with} \quad R_{JLm}^k := R_{\mathbf{1}JLm}^k \quad (142)$$

Consequently,

$$\begin{aligned} r_{\mathbf{v}J}^k &= \sum_{Lm} R_{JLm}^k v_L v_m \nabla_m q_L \\ r_{\mathbf{v}J}^k \pm r_{(R_k\mathbf{v})J}^k &= \sum_{Lm} [1 \pm (-1)^{\delta_{kL}} (-1)^{\delta_{km}}] R_{JLm}^k v_L v_m \nabla_m q_L \end{aligned} \quad (143)$$

Substituting this into (135) with (136), we find

$$R_{JLm}^{k+1} = R_{JLm}^k + \Delta R_{JLm}^k \quad (144)$$

where

$$\begin{aligned} \Delta R_{kLm}^k &= \frac{1}{2} R_{0Lm}^k - R_{kLm}^k \\ \Delta R_{JLm}^k &= 0 \quad \text{for } J \neq k \\ &\text{if } L \neq k \neq m \quad \text{or } L = k = m \end{aligned} \quad (145)$$

and

$$\begin{aligned}
 \Delta R_{0Lm}^k &= -\frac{3}{2}R_{0Lm}^k + R_{kLm}^k \\
 \Delta R_{kLm}^k &= 0 \\
 \Delta R_{jLm}^k &= -\frac{1}{4}R_{0Lm}^k + \frac{1}{2}R_{kLm}^k - R_{jLm}^k \quad \text{for } j \neq k \\
 &\quad \text{if } L \neq k = m \quad \text{or } L = k \neq m
 \end{aligned} \tag{146}$$

Iterating (144) with (145) and (146), we find, after some calculation (Appendix C), the following expression for $R'_{JLm} \equiv R_{JLm}^{d+1}$ in terms of $R_{JLm} \equiv R_{JLm}^1$:

$$\begin{aligned}
 R'_{00m} &= -\frac{1}{2}R_{00m} + R_{m0m} \\
 R'_{0im} &= R_{0imm} \delta_{im} \\
 R'_{j0m} &= R_{m0m} \delta_{jm} + (-\frac{1}{4}R_{00m} + \frac{1}{2}R_{m0m})(1 - \delta_{jm}) \\
 R'_{jim} &= \frac{1}{2}R_{0imm} \delta_{im} + (-\frac{1}{4}R_{0im} + \frac{1}{2}R_{ilm}) \delta_{jm} \gamma_{mi} \\
 &\quad + (-\frac{1}{4}R_{0im} + \frac{1}{2}R_{iml}) \delta_{jl} \gamma_{lm}
 \end{aligned} \tag{147}$$

where

$$\gamma_{jk} := \begin{cases} 1 & \text{if } j > k \\ 0 & \text{if } j \leq k \end{cases} \tag{148}$$

The side condition (127), with $r_{vJ} = \sum_{Lm} v_L v_m R_{JLm} \nabla_m q_L$, yields

$$R_{JLm} \sum_v v_J v_L v_m = 0 \tag{149}$$

from which we obtain, with the help of Appendix A,

$$R_{0mm} = 0, \quad R_{m0m} = 0 \tag{150}$$

(note that we use no implicit summation convention). Finally, we have to consider Eq. (118). In order to evaluate the term (115), we first note that, for $\rho \approx 1/2$, (73) and (69) give

$$\begin{aligned}
 p_{v0}^0 &= \rho + \frac{2}{3} \mathbf{v} \cdot \mathbf{q} + \dots \\
 p_{vj}^0 &= \frac{\rho}{2} + \frac{1}{3} \mathbf{v} \cdot \mathbf{q} + \frac{2}{3} v_j q_j + \dots
 \end{aligned} \tag{151}$$

while (88) and (91) yield

$$\partial_{t_1} \rho = -\frac{2}{3} \nabla \cdot \mathbf{q} + \dots, \quad \partial_{t_1} \mathbf{q} = -\frac{1}{2} \nabla \rho + \dots \tag{152}$$

where

$$\dots := O((|\rho - \frac{1}{2}| + |\mathbf{q}|)^2) \quad (153)$$

Therefore (115) becomes (the “+ ...” is omitted from now on)

$$\begin{aligned} s_{v_0} &= \frac{2}{3}\mathbf{v} \cdot \nabla \rho + \frac{2}{3}(\mathbf{v} \cdot \nabla)\mathbf{q} \cdot \mathbf{v} - \frac{2}{3}\nabla \cdot \mathbf{q} \\ s_{v_j} &= \frac{1}{3}\mathbf{v} \cdot \nabla \rho - \frac{1}{3}v_j \nabla_j \rho + \frac{1}{3}(\mathbf{v} \cdot \nabla)\mathbf{q} \cdot \mathbf{v} - \frac{1}{3}\nabla \cdot \mathbf{q} + \frac{2}{3}(\mathbf{v} \cdot \nabla) q_j v_j \end{aligned} \quad (154)$$

Thus, the coefficients in (116) can be written in a form analogous to (142):

$$S_{\mathbf{v}JLm} = v_L v_m S_{JLm} \quad (155)$$

(which is not surprising, because the same symmetry arguments apply), with

$$\begin{aligned} S_{00m} &= \frac{2}{3} \\ S_{0lm} &= \frac{2}{3}(1 - \delta_{lm}) \\ S_{j0m} &= \frac{1}{3}(1 - \delta_{jm}) \\ S_{jlm} &= \frac{1}{3}(1 + 2\delta_{jl} - \delta_{lm}) \end{aligned} \quad (156)$$

according to (154). Equation (118) now states that

$$S_{JLm} = R'_{JLm} - R_{JLm} \quad (157)$$

Inserting (156), (147), and (150), and solving for R_{JLm} , we find

$$\begin{aligned} R_{00m} &= -\frac{4}{9} \\ R_{0lm} &= -\frac{2}{3}(1 - \delta_{lm}) \\ R_{j0m} &= -\frac{4}{9}(1 - \delta_{jm}) \\ R_{jlm} &= -\frac{1}{3}(1 + 2\delta_{jl} - \delta_{lm} + \delta_{jm}\gamma_{ml}) \end{aligned} \quad (158)$$

The friction coefficients can then be computed as

$$T_{JLkm} = -2^{-d} \sum_{\mathbf{v}} v_J v_L v_k v_m (R_{JLm} + \frac{1}{2}S_{JLm}) \quad (159)$$

according to (117), (142), and (155). Inserting (158) and (156), and consulting again Appendix A, we obtain

$$D_{km} := T_{00km} = \frac{1}{9}\delta_{kl} \quad (160)$$

$$T_{jlk m} = \frac{1}{6}(3\delta_{jl}\delta_{km} + \delta_j\delta_{lk}(1 + \gamma_{mk}) - 2\delta_{jlk m}) \quad (161)$$

for the mass diffusion tensor D_{km} and the kinematic viscosity tensor T_{jklm} , respectively (the mass-momentum cross diffusion coefficients T_{0lkm} and T_{j0km} vanish by symmetry).

9. THE ANISOTROPY OF THE VISCOSITY

It would be nice if our CA model could simulate the viscosity of a fluid correctly. Unfortunately, however, the viscosity tensor we have just derived is anisotropic. To see this explicitly, let us consider the simple example of a two-dimensional shear flow in the direction of the x_1 axis, with

$$q_1 = q_1(t, x_2), \quad q_2 \equiv 0 \quad (162)$$

The incompressible Navier–Stokes-type equations (108) then reduce to

$$\partial_t q_1 = \nu (\nabla_2)^2 q_1 \quad \text{with} \quad \nu = T_{1122} \quad (163)$$

Here, ν is the effective kinematic shear viscosity coefficient. For the slightly more general case that the flow direction makes an angle α with the x_1 axis, Eq. (163) must be replaced with

$$\partial_t q'_1 = \nu' (\nabla'_2)^2 q'_1 \quad \text{with} \quad \nu' = T'_{1122} \quad (164)$$

where the primed quantities refer to the rotated coordinate system. They are related to their unprimed counterparts by

$$\mathbf{x} = R\mathbf{x}', \quad \mathbf{V} = R\nabla', \quad \mathbf{q} = R\mathbf{q}' \quad (165)$$

$$T'_{j'k'l'm'} = \sum_{jklm} T_{jklm} R_{jj'} R_{kk'} R_{ll'} R_{mm'} \quad (166)$$

with the orthogonal matrix

$$R = (R^{-1})^T = \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix} \quad (167)$$

Consequently,

$$\begin{aligned} \nu' &= T'_{1122} \\ &= T_{1122} \cos^4 \alpha + T_{2211} \sin^4 \alpha \\ &\quad + (T_{1111} + T_{2222} - T_{1212} - T_{2121} - T_{1221} - T_{2112}) \cos^2 \alpha \sin^2 \alpha \end{aligned} \quad (168)$$

Now (161) yields

$$\begin{aligned} T_{1122} = T_{2211} = \frac{1}{2}, \quad T_{1111} = T_{2222} = \frac{1}{3} \\ T_{1212} = T_{2121} = 0, \quad T_{1221} = \frac{1}{6}, \quad T_{2112} = \frac{1}{2} \end{aligned} \quad (169)$$

which inserted into (168) give

$$v(\alpha) \equiv v' = \frac{1}{2}(\cos^4 \alpha + \sin^4 \alpha) \quad (170)$$

We see that the effective viscosity coefficient depends on the angle α , with values in the range

$$\frac{1}{4} \leq v(\alpha) \leq \frac{1}{2} \quad (171)$$

where the maximum is at $\alpha = 0$ and the minimum at $\alpha = 45^\circ$ (plus arbitrary multiples of 90° , respectively). This is, of course, in sharp contrast to a physical fluid, for which the viscosity would be angle-independent.

10. COMPUTER EXPERIMENTS

There are several weak points in the our hydrodynamic theory. The first is the notorious implicit "ergodic hypothesis," which in our case is the assumption that ρ and \mathbf{q} are the *only* macroscopically relevant variables. It is always difficult to rule out the possible appearance of additional "hidden variables" by strict mathematical arguments.⁽³⁰⁾ The second weak point is the Boltzmann-type assumption about the absence of various correlations, which was needed for the explicit calculation of the friction coefficients.

In order to test our theory, computer experiments are necessary. Some simulations with the two-dimensional version of our model have been performed meanwhile.⁽³¹⁾ They seem to confirm the validity of the hydrodynamic description of the lattice gas. For example, an attempt to simulate a van Karman vortex street produced the pictures shown in Figs. 7–9 (run on a Convex C2, with $\approx 10^6$ site updates per second). They prove that our CA model behaves at least qualitatively like a physical fluid. Furthermore, observation of the evolution of a shear flow in the x_1 direction leads to an experimental value of $v = 0.46 \pm 0.02$ for the effective kinematic viscosity coefficient; this is quite close to the value $v = 1/2$ predicted by our theory [Eq. (170) with $\alpha = 0$]. Also, the measured value for the speed of sound, $c = 0.58 \pm 0.02$ for $\rho = 1/2$, agrees well with the theoretical prediction $c = 1/\sqrt{3} \approx 0.577$ [Eq. (101)].

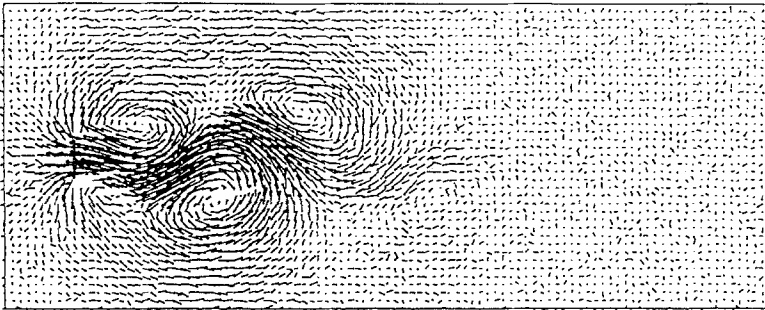


Fig. 7. Vortex street simulated with the 2D version of our model. The width of the obstacle is 800, and the in-stream velocity is $u = 0.1$. The mean flow has been subtracted in the picture. Shown is the flow pattern which has evolved from our initial setup after $t = 60,000$ time steps.

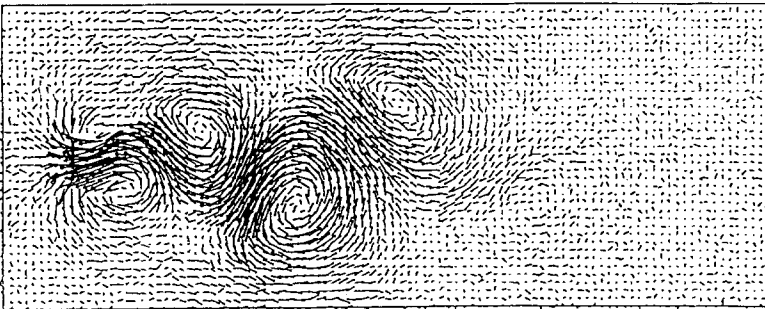


Fig. 8. The same vortex street as in Fig. 7, at $t = 70,000$.

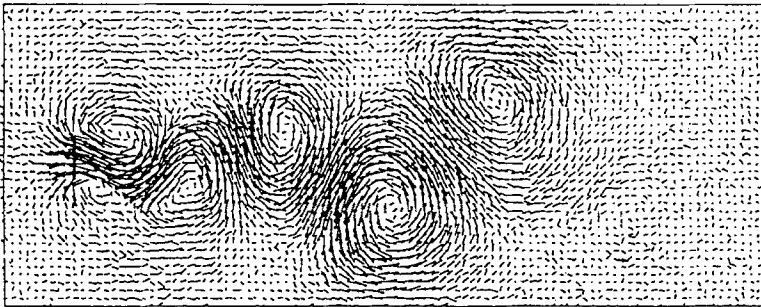


Fig. 9. The same vortex street as in Fig. 7, at $t = 80,000$.

11. CONCLUSIONS

As we have seen, our model simulates nearly all terms of the Navier–Stokes equations in two and three dimensions correctly, except that the viscosity in the model displays an unphysical anisotropy. This viscosity anisotropy is clearly a drawback as against the conventional FHP and FCHC models, in which the isotropy is enforced by built-in discrete symmetries. However, our model is better than, say, the HPP model, which is technically much simpler than ours, since in our model the unphysical anisotropy of the convection term can be eliminated (by taking $\rho \approx 1/2$), which is impossible with the HPP model. On the other hand, there are “conventional” models, such as those discussed in refs. 17, 20, and 21, in which the unhandiness imposed by the special discrete isotropy-enforcing symmetries is avoided by the same trick as in our model, namely to achieve the desired isotropy of the convection term by a suitable choice of an adjustable parameter. At first glance, these “quasi-isotropic” conventional models look more attractive than ours, because they are easy to visualize (see e.g., Fig. 1 in ref. 17), while our model is a little hard to explain, mainly because of its peculiar momentum definition, which (to the author’s knowledge) has no analogy in the physical world. From the programmer’s viewpoint, however, our model is very advantageous: Our rule (in 2D as well as 3D) is defined completely by Eqs. (33), which admittedly look ugly, but are easy to translate into computer code. The rules of comparable conventional models generally do not admit such a compact systematic algorithmic formulation (e.g., note that Fig. 1 in ref. 17 shows only a very small fraction of all possible nontrivial collision configurations). This applies to a much stronger extent to the 3D case (e.g., the “quasi-isotropic” 3D model presented in ref. 20 has not been pursued any further by the authors, with good reason; another example of a non-FCHC 3D model can be found in ref. 32).

In summary, one can say that for the case of pure Navier–Stokes flow (including things such as flow through porous media), our model is no satisfactory alternative to the conventional FHP and FCHC models, because of its anisotropic viscosity. However, for applications where additional hydrodynamic variables appear (free boundaries, etc.), the conventional models might turn out as too specialized, since the introduction of additional variables into the model, especially when they are to obey additional conservation laws, always blows up the complexity of the rules to a considerable extent (e.g., compare the rules of the magnetohydrodynamic CA presented in ref. 15 with those of the simple FHP model on which it is based). This poses a real problem especially in 3D, where the rules of the standard model (FCHC) are already very intricate in its basic version.

Here our model offers an interesting starting point, since our pair-interaction method effectively reduces the huge number of possible collision configurations to a small number of possible configurations in each of the elementary pair interactions.

APPENDIX A. MOMENT RELATIONS

One easily verifies by simple calculation the following “moment relations” for the set of discrete velocities $\mathbf{v} = (v_1, \dots, v_d)$ with $v_j = \pm 1$:

$$2^{-d} \sum_{\mathbf{v}} 1 \equiv v^{(0)} = 1 \quad (\text{A1})$$

$$2^{-d} \sum_{\mathbf{v}} v_j \equiv v_j^{(1)} = 0 \quad (\text{A2})$$

$$2^{-d} \sum_{\mathbf{v}} v_j v_k \equiv v_{jk}^{(2)} = \delta_{jk} \quad (\text{A3})$$

$$2^{-d} \sum_{\mathbf{v}} v_j v_k v_l \equiv v_{jkl}^{(3)} = 0 \quad (\text{A4})$$

$$2^{-d} \sum_{\mathbf{v}} v_j v_k v_l v_m \equiv v_{jklm}^{(4)} = \delta_{jk} \delta_{lm} + \delta_{jl} \delta_{km} + \delta_{jm} \delta_{kl} - 2\delta_{jklm} \quad (\text{A5})$$

where the Kronecker deltas δ_{jk} and δ_{jklm} are = 1 if all indices take the same value, and = 0 otherwise. Note that δ_{jklm} and hence also $v_{jklm}^{(4)}$ is an anisotropic tensor.

APPENDIX B. EQUILIBRIUM FORMULAS

Equations (61) arise as follows. From (52), we find

$$\begin{aligned} 1 - \rho_{\mathbf{v}} &= \text{prob}\{n_0(t, \mathbf{x}, \mathbf{v}) = 0\} \\ &= P_{\mathbf{v}}(0, \mathbf{0}) = W_{\mathbf{v}}(0, \mathbf{0})/Z_{\mathbf{v}} \\ &= 1/Z_{\mathbf{v}} \end{aligned} \quad (\text{B1})$$

and

$$\begin{aligned} Z_{\mathbf{v}} &= W_{\mathbf{v}}(0, \mathbf{0}) + \sum_{\mathbf{n}} W_{\mathbf{v}}(1, \mathbf{n}) \\ &= 1 + e^{-\mu_0} \prod_{j=1}^d \sum_{n_j=0}^1 e^{-\mu_j v_j n_j} \\ &= 1 + e^{-\mu_0} \prod_j (1 + e^{-\mu_j v_j}) \end{aligned} \quad (\text{B2})$$

Consequently,

$$\begin{aligned} \rho_v &= 1 - \frac{1}{Z_v} = \frac{Z_v - 1}{Z_v} \\ &= \frac{1}{1 + e^{\mu_0} / \prod_j (1 + e^{-\mu_j v_j})} \\ &= f\left(\mu_0 + \sum_{j=1}^d \ln f(-\mu_j v_j)\right) \end{aligned} \tag{B3}$$

with

$$f(\xi) := \frac{1}{1 + e^\xi} \tag{B4}$$

Thus we have shown the first of Eqs. (61). Furthermore, we have

$$\begin{aligned} Q_v(\mathbf{n}) &= \text{prob}\{\mathbf{n}(t, \mathbf{x}, \mathbf{v}) = \mathbf{n} \mid n_0(t, \mathbf{x}, \mathbf{v}) = 1\} \\ &= \frac{P_v(1, \mathbf{n})}{\rho_v} = \frac{W_v(1, \mathbf{n})}{Z_v - 1} \\ &= \prod_{j=1}^d Q_{v_j}(n_j) \end{aligned} \tag{B5}$$

with

$$\begin{aligned} Q_{v_j}(n_j) &= W_{v_j}(n_j) / Z_{v_j} \\ W_{v_j}(n_j) &= \exp(-\mu_j v_j n_j) \\ Z_{v_j} &= \sum_{n_j=0}^1 W_{v_j}(n_j) \end{aligned} \tag{B6}$$

This leads to the second of Eqs. (61):

$$\sigma_{v_j} = Q_{v_j}(1) = \frac{1}{1 + \exp(\mu_j v_j)} \equiv f(\mu_j v_j) \tag{B7}$$

In order to derive (69), we first expand (61) in Taylor series for $|\boldsymbol{\mu}| =: \mu \ll 1$. Using for (62) the expansion formula

$$\begin{aligned} f(\xi + \eta) &= f(\xi) + f'(\xi)[f(\xi) - 1]\eta \\ &\quad + f''(\xi)[f(\xi) - 1][f(\xi) - \tfrac{1}{2}]\eta^2 + \dots \end{aligned} \tag{B8}$$

we obtain from (61)

$$\begin{aligned} \rho_{\mathbf{v}} = & \phi + \phi(\phi - 1) \left(\frac{\boldsymbol{\mu} \cdot \mathbf{v}}{2} - \frac{\mu^2}{8} \right) \\ & + \phi(\phi - 1) \left(\phi - \frac{1}{2} \right) \frac{(\boldsymbol{\mu} \cdot \mathbf{v})^2}{4} + O(\mu^3) \end{aligned} \quad (\text{B9})$$

$$\sigma_{v_j} = \frac{1}{2} - \frac{\mu_j v_j}{4} + O(\mu^3) \quad (\text{B10})$$

with

$$\phi := f(\mu_0 - d \ln 2) \quad (\text{B11})$$

Inserting this into (68), we find with the help of Appendix A,

$$\rho = 2^{-d} \sum_{\mathbf{v}} \rho_{\mathbf{v}} = \phi + \phi(\phi - 1)^2 \frac{\mu^2}{4} + O(\mu^3) \quad (\text{B12})$$

$$q_j = 2^{-d} \sum_{\mathbf{v}} v_j \rho_{\mathbf{v}} \sigma_{v_j} = [\phi(\phi - 1) - \rho] \frac{\mu_j}{4} + O(\mu^3) \quad (\text{B13})$$

This suggests the ansatz

$$\phi = \rho + \alpha q^2 + P(q^3) \quad (\text{B14})$$

$$\boldsymbol{\mu} = \beta \mathbf{q} + O(q^3) \quad (\text{B15})$$

which leads to

$$\alpha = -\frac{4(1-\rho)^2}{\rho(2-\rho)^2}, \quad \beta = -\frac{4}{\rho(2-\rho)} \quad (\text{B16})$$

and hence to (69).

APPENDIX C. THE LINEARIZED COLLISION EQUATION

In order to obtain Eqs. (147) from the recursion formulas (144)–(146), we consider four possible cases for the indices L and m in R_{JLm}^k :

- (i) $L = 0$.
- (ii) $0 < L \equiv l < m$.
- (iii) $L \equiv l = m$.
- (iv) $L \equiv l > m$.

(i) $L = 0$. Here, Eqs. (144)–(146) yield, for $J = 0$:

$$\begin{aligned} R_{00m}^m &= R_{00m}^{m-1} = \dots = R_{00m}^1 \equiv R_{00m} \\ R'_{00m} &\equiv R_{00m}^{d+1} = R_{00m}^d = \dots = R_{00m}^{m+1} = -\frac{1}{2}R_{00m}^m + R_{m0m}^m \end{aligned} \quad (C1)$$

for $j < m$:

$$\begin{aligned} R_{j0m}^j &= \dots = R_{j0m}^1 \equiv R_{j0m} \\ R_{j0m}^m &= \dots = R_{j0m}^{j+1} = \frac{1}{2}R_{00m}^j \\ R'_{j0m} &\equiv R_{j0m}^{d+1} = \dots = R_{j0m}^{m+1} = -\frac{1}{4}R_{00m}^m + \frac{1}{2}R_{m0m}^m \end{aligned} \quad (C2)$$

for $j = m$:

$$R'_{m0m} \equiv R_{m0m}^{d+1} = \dots = R_{m0m}^m = \dots = R_{m0m}^1 \equiv R_{m0m} \quad (C3)$$

and for $j > m$:

$$\begin{aligned} R_{j0m}^m &= \dots = R_{j0m}^1 \equiv R_{j0m} \\ R_{j0m}^j &= \dots = R_{j0m}^{m+1} = -\frac{1}{4}R_{00m}^m + \frac{1}{2}R_{m0m}^m \\ R'_{j0m} &\equiv R_{j0m}^{d+1} = \dots = R_{j0m}^{j+1} = \frac{1}{2}R_{j0m}^j \end{aligned} \quad (C4)$$

Eliminating the intermediate values (with upper index 2, ..., d), we get

$$\begin{aligned} R'_{00m} &= -\frac{1}{2}R_{00m} + R_{m0m} \\ R'_{m0m} &= R_{m0m} \\ R'_{j0m} &= -\frac{1}{4}R_{00m} + \frac{1}{2}R_{m0m} \quad (j \neq m) \end{aligned} \quad (C5)$$

(ii) $l < m$. Here we obtain, for $J = 0$:

$$\begin{aligned} R'_{0lm} &= \dots = R'_{0lm}^1 \equiv R_{0lm} \\ R_{0lm}^m &= \dots = R_{0lm}^{l+1} = -\frac{1}{2}R'_{0lm} + R'_{llm} \\ R'_{0lm} &\equiv R_{0lm}^{d+1} = \dots = R_{0lm}^{m+1} = -\frac{1}{2}R_{0lm}^m + R_{mlm}^m \end{aligned} \quad (C6)$$

for $j < l$:

$$\begin{aligned} R_{jlm}^j &= \dots = R_{jlm}^1 \equiv R_{jlm} \\ R'_{jlm} &= \dots = R_{jlm}^{j+1} = \frac{1}{2}R_{0lm}^j \\ R_{jlm}^m &= \dots = R_{jlm}^{l+1} = -\frac{1}{4}R'_{0lm} + \frac{1}{2}R'_{llm} \\ R'_{jlm} &\equiv R_{jlm}^{d+1} = \dots = R_{jlm}^{m+1} = -\frac{1}{4}R_{0lm}^m + \frac{1}{2}R_{mlm}^m \end{aligned} \quad (C7)$$

for $j = l$:

$$\begin{aligned} R_{llm}^m &= \dots = R_{llm}^l = \dots = R_{llm}^1 \equiv R_{llm} \\ R'_{llm} &\equiv R_{llm}^{d+1} = \dots = R_{llm}^{m+1} = -\frac{1}{4}R_{0lm}^m + \frac{1}{2}R_{mlm}^m \end{aligned} \quad (C8)$$

for $l < j < m$:

$$\begin{aligned} R_{jlm}^l &= \dots = R_{jlm}^1 \equiv R_{jlm} \\ R_{jlm}^j &= \dots = R_{jlm}^{l+1} = -\frac{1}{4}R_{0lm}^l + \frac{1}{2}R_{llm}^l \\ R_{jlm}^m &= \dots = R_{jlm}^{j+1} = \frac{1}{2}R_{0lm}^j \\ R'_{jlm} &\equiv R_{jlm}^{d+1} = \dots = R_{jlm}^{m+1} = -\frac{1}{4}R_{0lm}^m + \frac{1}{2}R_{mlm}^m \end{aligned} \quad (C9)$$

for $j = m$:

$$\begin{aligned} R_{mlm}^l &= \dots = R_{mlm}^1 \equiv R_{mlm} \\ R'_{mlm} &\equiv R_{mlm}^{d+1} = \dots = R_{mlm}^m = \dots = R_{mlm}^{l+1} = -\frac{1}{4}R_{0lm}^l + \frac{1}{2}R_{llm}^l \end{aligned} \quad (C10)$$

and for $j > m$:

$$\begin{aligned} R_{jlm}^l &= \dots = R_{jlm}^1 \equiv R_{jlm} \\ R_{jlm}^m &= \dots = R_{jlm}^{l+1} = -\frac{1}{4}R_{0lm}^l + \frac{1}{2}R_{llm}^l \\ R_{jlm}^j &= \dots = R_{jlm}^{m+1} = -\frac{1}{4}R_{0lm}^m + \frac{1}{2}R_{mlm}^m \\ R'_{jlm} &\equiv R_{jlm}^{d+1} = \dots = R_{jlm}^{j+1} = \frac{1}{2}R_{0lm}^j \end{aligned} \quad (C11)$$

Elimination of the intermediate values then leads to

$$R'_{Jlm} = \left(-\frac{1}{4}R_{0lm} + \frac{1}{2}R_{llm}\right) \delta_{Jlm} \quad (l < m) \quad (C12)$$

(iii) $l = m$. Here we have, for $J = 0$:

$$R'_{0mm} \equiv R_{0mm}^{d+1} = \dots = R_{0mm}^m = \dots = R_{0mm}^1 \equiv R_{0mm}$$

and for $J \equiv j > 0$:

$$\begin{aligned} R_{jmm}^j &= \dots = R_{jmm}^1 \equiv R_{jmm} \\ R'_{jmm} &\equiv R_{jmm}^{d+1} = \dots = R_{jmm}^m = \dots = R_{jmm}^{j+1} = \frac{1}{2}R_{0mm}^j \end{aligned} \quad (C13)$$

(both for $j = m$ and $j \neq m$). Thus

$$\begin{aligned} R'_{0mm} &= R_{0mm} \\ R'_{jmm} &= \frac{1}{2}R_{0mm} \end{aligned} \quad (C14)$$

(iv) $l > m$. This case differs from case (ii) only in that the roles of l and m must be interchanged. Therefore the result is

$$R'_{lm} = (-\frac{1}{4}R_{0lm} + \frac{1}{2}R_{mim}) \delta_{jl} \quad (l > m) \quad (\text{C15})$$

Taken together, Eqs. (197), (204), (206), and (207) constitute the set of Eqs. (147).

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