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Propagating staggered waves in cellular automata fluids

R Brito† and M H Ernst

Institute for Theoretical Physics, University of Utrecht, PO Box 80.006, 3508 TA Utrecht, The Netherlands

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Abstract. The majority of lattice gases have, apart from the physical conserved quantities of particle number, momentum and energy, spurious ones, usually staggered in space and time. At the level of linear excitations these staggered modes may be purely diffusive or damped propagating waves. In the eight- and nine-bit model on the square lattice we find a large number of new spurious modes and we derive Green–Kubo relations for the diffusivities and damping constants and calculate them in Boltzmann approximation.

1. Introduction

Recently, Frisch *et al* [1] have proposed a new technique to simulate the incompressible Navier–Stokes equations in two dimensions, the *lattice gas cellular automata* (LGCA). This technique has been widely applied to numerical simulation both in two- and three-dimensional fluids [2]. The idea of the method is simple: it is a collection of 'molecules' with a finite number of velocities which can be at the nodes of a regular lattice at integer times. The collisions occur only at the sites of the lattice and conserve mass, linear momentum and possibly energy. Based on the idea that the macroscopic behaviour is only dominated by the conservation laws, LGCAs could have the same hydrodynamics as real fluids. However, the majority of models have, apart from the usual conserved quantities, new spurious ones. The physical set is conserved on account of properly chosen collision rules, but the unphysical or spurious set is an artifact of the discrete structure of space and time in which the cellular automaton is defined. The spurious conservation laws have no physical analogue in the continuum case.

The best known spurious invariant is the *total staggered momentum*, discovered by Kadanoff *et al* [3] in the FHP-model on the triangular lattice. Similar staggered momentum invariants occur in the eight-bits and nine-bit LGCAs [4–6], defined on a square lattice, and in the FCHC model [5], defined on the four-dimensional FC hypercubic lattice. Also *staggered number invariants* are known to occur in LGCAs with random static scatterers and cubic symmetry [7, 8] and in several one-dimensional models [9]. We will also discuss invariants that are only staggered in space, but not in time. They are related to the geometric and checker board invariants discussed by d'Humières *et al* [10].

† Permanent address: Facultad Ciencias Físicas. Universidad Complutense, 28040 Madrid, Spain.

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The motivation for this investigation is that these staggered invariants give rise to new modes that are slowly varying on hydrodynamic space and time scales, and appear to be purely diffusive in all cases studied so far. The evolution equations for these modes have to be added to the Navier–Stokes equations, including the proper non-linear couplings between those and the physical ones. In general, the existence of these new modes will change the macroscopic behaviour of the CA-fluid. For instance, the non-linear Euler equation for the FHP fluid will not only contain the usual convective term $\boldsymbol{u}\cdot\nabla\boldsymbol{u}$, where $\boldsymbol{u}(\boldsymbol{r},t)$ is the macroscopic flow velocity, but also analogous terms with $\rho\boldsymbol{u}$ replaced by the averaged staggered momentum density [11, 8].

Furthermore an understanding of the spurious modes is of great importance to properly analyse any type of simulations of LGCA-fluids, where non-linear hydrodynamic effects are present, and to relate the results eventually to the behaviour in actual fluid dynamics. Therefore one needs to understand the complete set of non-linear macroscopic equations, including the spurious ones, and all new transport coefficients related to this spurious thermodynamics and hydrodynamic variables. Once the spurious slow variables have been identified and new transport coefficients have been computed from linear response theory—which is essentially the program of this paper—the corresponding non-linear terms in the full set of fluid dynamic equations can be constructed for general LGCAs along the lines of [3, 8, 11].

In order to minimize the influence of spurious invariants in the fluid dynamic equations, it is advantageous [3] to prepare constraint equilibrium or non-equilibrium ensembles in which *all total staggered momentum vanishes exactly.*

The modified structure of the non-linear terms in the fluid dynamic equations directly modifies the mode coupling theories, and determines which pairs of slow modes are contributing to the long time behaviour of correlation functions [12].

The novel feature of this paper is the discovery of propagating staggered modes in the well-studied eight-bit square lattice model [4–6]. The staggered sound waves are soft modes with a dispersion relation like ordinary sound waves, but with a different propagation velocity. It should be stressed that the eight-bit square lattice model is not a serious candidate for large-scale simulations of two-dimensional flow problems. However, it can be viewed as a LGCA with a *temperature*, which is not the case for any of the models discussed previously. The systematic analysis of the eight-bit model should therefore be considered mostly as a prototype, that is applicable to any LGCAs.

In order to analyse the linear excitations of a CA fluid out of equilibrium, it is necessary to identify the complete set of conservation laws. By construction, the collision rules in LGCAs that qualify as fluids, conserve number, momentum and possibly energy. In terms of the occupation numbers $n(\boldsymbol{c},\boldsymbol{r},t)$ these conserved quantities are:

$$\begin{aligned} N &= \sum_{\boldsymbol{r}}\sum_{\boldsymbol{c}} n(\boldsymbol{c},\boldsymbol{r},t) = \sum_{\boldsymbol{r}} \rho(\boldsymbol{r},t) \\ \boldsymbol{P} &= \sum_{\boldsymbol{r}}\sum_{\boldsymbol{c}} \boldsymbol{c}n(\boldsymbol{c},\boldsymbol{r},t) = \sum_{\boldsymbol{r}} \boldsymbol{g}(\boldsymbol{r},t) \\ E &= \sum_{\boldsymbol{r}}\sum_{\boldsymbol{c}} \tfrac{1}{2}c^2 n(\boldsymbol{c},\boldsymbol{r},t) = \sum_{\boldsymbol{r}} e(\boldsymbol{r},t) \end{aligned} \tag{1.1}$$

with $\rho(\boldsymbol{r},t)$, $\boldsymbol{g}(\boldsymbol{r},t)$ and $e(\boldsymbol{r},t)$ the associated conserved densities. Here $n(\boldsymbol{c},\boldsymbol{r},t)=1$ if the site $\boldsymbol{r}$ and the velocity channel $\boldsymbol{c}$ is occupied at time t, and 0 otherwise.

In addition most LGCAs have spurious invariants. In the dynamic and geometric staggered invariants, that will be considered later, the discrete lattice structure

is essential. However, one can easily construct LGCAs with over-simplified collision rules, that have, in addition to the physical ones of number, momentum and energy, unphysical collisional invariants like the HPP model [13, 14], that are neither staggered in space nor time.

Unfortunately, no methods seem to exist to systematically find all conserved quantities, including the spurious ones (see however section 6). In the LGCAs considered in the literature, there exists a great variety of spurious conservation laws [10], such as staggered, geometric or checker board invariants. In this paper we focus on invariants and corresponding modes, that are staggered in space and time (dynamic staggered modes), or that are only staggered in space (geometric staggered modes). The corresponding densities may give rise to purely diffusive modes or to damped propagating ones. Possible spurious modes, which are neither staggered in space nor in time, can be treated in exactly the same manner as the physical densities in equation (1.1). They will not be considered in this paper.

The typical form of the most common spurious invariant, the total staggered momentum, is [3]:

$$\sum_{r} g_{\theta}(r,t) = \sum_{rc}(-)^{t+\theta\cdot r}(\theta\cdot c)n(c,r,t) \tag{1.2}$$

where the integer $\theta \cdot r$ being even or odd characterizes a division of the total lattice into two specific sublattices. The set of allowed values of θ depends on the model under consideration. There are *three* of these staggered momenta in the FHP models, *two* in the eight-bit and nine-bit square lattice model and *twelve* in the FCHC model. However there may be many more staggered invariants, as we shall illustrate for the eight-bit square lattice model.

At the level of linear excitations, these staggered modes do not couple to the hydrodynamic modes, nor to modes characterized by different sublattice divisions. If for a given sublattice characterization θ, only staggered modes exist with the *same vectorial character*, then these modes are purely diffusive. This situation occurs in CA-fluids, such as the FHP model, the nine-bit model and the FCHC-model, or in CA Lorentz gases [7, 15]. For these models, the staggered momentum density $g_{\theta}(k,t)$ satisfies the following equation after Fourier transformation,

$$\partial_t g_{\theta}(k,t) = -k^2 \Lambda_{\theta}(\hat{k}) g_{\theta}(k,t) \tag{1.3}$$

with an anisotropic diffusivity $\Lambda_{\theta}(\hat{k})$, where $\hat{k}$ is a unit vector parallel to k. Green–Kubo relations for the staggered momentum diffusivities [11, 16] can be put into the form [17] $\Lambda_{\theta}(\hat{k}) = (\hat{k}\cdot\hat{\theta})^2\xi_{\|} + (\hat{k}\cdot\hat{\theta}_{\perp})^2\xi_{\perp}$ with

$$\begin{aligned} \xi_{\perp} &= \frac{1}{\chi_g} c_{\perp} c_{\|} \gamma(\theta,1)\kappa c_{\perp} c_{\|} \\ \xi_{\|} &= \frac{1}{\chi_g} c_{\|}^2 \gamma(\theta,1)\kappa c_{\|}^2 \end{aligned} \tag{1.4}$$

where $c_{\|} = \hat{\theta}\cdot c$, $c_{\perp} = \hat{\theta}_{\perp}\cdot c$, and $\gamma(\theta,1)\kappa$ is the kinetic propagator. Its precise definition will be given in section 3 and an explicit expression for γ in the Boltzmann approximation is calculated in section 5. However, if there exist for a given sublattice

division two or more staggered invariants with a different vectorial character, then the staggered modes may become propagating with a propagation speed and a damping constant. This occurs in the eight-bit model [4].

The paper is organized as follows: in section 2 we present the model and discuss its conserved quantities (physical and staggered). In section 3 the diffusivities for diffusive staggered and non-staggered modes are given. In section 4 the propagating staggered modes appear. Section 5 is devoted to the calculation of diffusivities and damping constants in the Boltzmann approximation. Finally, we include some comments in section 6.

2. Square lattice models

We focus mainly on the eight-bit model, introduced by Chopard and Droz [4]. It consists of a superposition of two interacting HPP lattice gases. There are eight velocity states: four 'slow' ones with velocities $(\pm 1, 0)$ and $(0, \pm 1)$ and four 'fast' ones: $(\pm 1, \pm 1)$. Collisions between like velocities and unlike velocities are allowed and chosen in such a way that particle number N, momentum $\boldsymbol{P}$ and energy H, are conserved, as illustrated in figure 1. An equivalent set of physical conservation laws is the total momentum, the number of slow particles N_s and the number of fast particles N_f with $N = N_s + N_f$ and $H = \frac{1}{2}N_s + N_f$. In the first interpretation the model is a *thermal* lattice gas for a single component system, with a temperature and *heat conductivity*. In the second interpretation the model is an *athermal* lattice gas (without temperature) of a *binary mixture* with a *diffusion coefficient* D. We shall be using the binary mixture picture. A proper linear combination of $\rho_f(\boldsymbol{r}, t)$ and $\rho_s(\boldsymbol{r}, t)$ constitutes the diffusion mode.

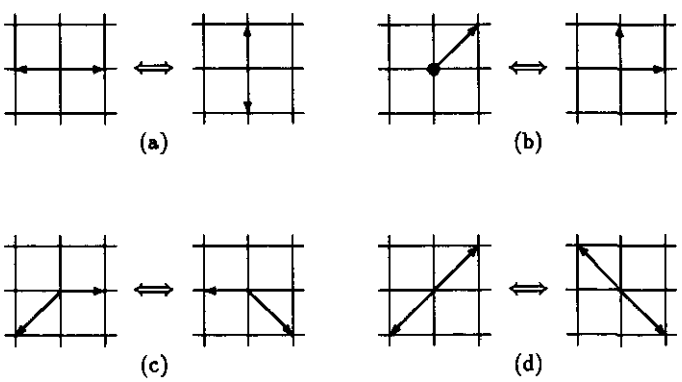

Figure 1. Collision rules for eight- and nine-bit models. Symmetry related collisions (successive rotations of $\pi/2$ and reflections on x and y) are also allowed. The ● in (b) represents a rest particle. Collision rule (b) is absent in the eight-bit model.

In addition to the physical conservation laws there exist in this model unphysical ones. Consider first a sublattice division characterized by the vector $\boldsymbol{\theta} = (1, 1)$. For the (+) or (−) sublattice the quantity $\boldsymbol{\theta} \cdot \boldsymbol{r} = r_x + r_y$ is respectively an even or odd integer. There are in fact two different types of invariants connected with this sublattice division: *geometric* and *dynamic staggered invariants*. Examples of geometric invariants are the number of fast particles on the (+)- and (−)-sublattice,

where N_{f+} and N_{f-} are separately conserved. Their sum, $N_f = N_{f+} + N_{f-}$, represents the physically relevant conservation law; their difference $\tilde{N}_{\theta f} = N_{f+} - N_{f-} = \sum_r \sum_{|c|=1} (-)^{\theta \cdot r} n(c, r, t)$ is a geometric invariant. This invariant is only staggered in space, but not in time. Examples of dynamic staggered invariants are the number of slow particles on the even and odd sublattice, N_{s+} and N_{s-} respectively. They satisfy the relations $N_{s+}(t) = N_{s-}(t+1)$ and $N_{s-}(t) = N_{s+}(t+1)$. Consequently $N_{\theta s} \equiv (-)^t [N_{s+}(t) - N_{s-}(t)] = \sum_r \sum_{|c|=1} (-)^{t+\theta \cdot r} n(c, r, t)$ is a constant of the motion (note that the c-sum is restricted to slow particles). This is the only conserved quantity associated with the vector $\theta = (1,1)$ that is staggered in both space and time. We follow the convention that a subscript θ denotes dynamic staggered modes, whereas a subscript θ in combination with a tilde denotes geometric staggered modes.

To summarize, associated with the sublattice division $\theta = (1,1)$, there exists a geometric staggered invariant $\tilde{N}_{\theta f}$ and a dynamic staggered invariant $N_{\theta s}$. The corresponding spurious densities are:

$$\tilde{\rho}_{\theta f}(r,t) = (-)^{\theta \cdot r} \sum_c a_f(c) n(c,r,t) \qquad \rho_{\theta s}(r,t) = (-)^{t+\theta \cdot r} \sum_c a_s(c) n(c,r,t) \tag{2.1}$$

where the collisional invariants are

$$a_\mu(c) = \{a_f(c), a_s(c)\} = \{\delta_{c\sqrt{2}}, \delta_{c1}\}. \tag{2.2}$$

Both densities are staggered in space. The geometric one becomes constant in time in the long wavelength limit, and is caused by the discrete lattice structure only. The dynamic one represents in the long wavelength limit an undamped oscillation, $(-1)^t$, and is caused by the combined effects of collision rules and discrete lattice structure.

Next we consider two different sublattice divisions, characterized by $\theta = (1,0)$ or $\theta = (0,1)$. Here not only the total staggered θ-momenta, defined in equation (1.2) are constants of the motion, but also the staggered number of fast particles in either of these θ-directions, defined as $N_{\theta f} = \sum_{rc} (-)^{t+\theta \cdot r} a_f(c) n(c,r,t)$.

Associated with each of the two θ-vectors, $(1,0)$ and $(0,1)$, there exist the locally conserved densities being both staggered in space and time,

$$\rho_{\theta f}(r,t) = (-)^{t+\theta \cdot r} \sum_c a_f(c) n(c,r,t) \qquad g_\theta(r,t) = (-)^{t+\theta \cdot r} \sum_c (\hat{\theta} \cdot c) n(c,r,t). \tag{2.3}$$

As we have a scalar- and vector-type conserved density per θ-vector, the corresponding elements of the Euler matrix may be non-vanishing, giving propagating modes with an anisotropic speed of sound, as we shall see later.

3. Diffusive modes

3.1. Geometric staggered modes

For the sublattice division with $\theta = (1,1)$ there are two modes (2.1) of scalar character. They behave purely diffusive according to the general method of [16]. We consider first the geometric mode, given by

$$\tilde{\rho}_{\theta f}(k,t) = \sum_c a_f(c) n(c, k + \pi\theta, t) \tag{3.1}$$

where $n(\boldsymbol{c},\boldsymbol{k},t)$ is the Fourier transform of the fluctuation out of equilibrium in the occupation number, defined as $\delta n(\boldsymbol{c},\boldsymbol{r},t) = n(\boldsymbol{c},\boldsymbol{r},t) - \langle n(\boldsymbol{c},\boldsymbol{r})\rangle$.

Once we have identified the slow mode $\tilde{\rho}_{\theta f}(\boldsymbol{k},t)$ it is straightforward to apply the method of [16] and show that $\tilde{\rho}_{\theta f}(\boldsymbol{k},t)$ satisfies a diffusion equation of the form (1.3) with $\Lambda_\theta(\hat{\boldsymbol{k}})$ replaced by a diffusivity $\tilde{D}_\theta(\hat{\boldsymbol{k}})$. The corresponding Green–Kubo formula is given by

$$\tilde{D}_\theta(\hat{\boldsymbol{k}}) = \lim_{z\to 0}\lim_{k\to 0}\frac{1}{\chi_f}\left\{\sum_{t=0}^{\infty} e^{-zt}\langle \tilde{J}_{\theta f}|\tilde{J}_{\theta f}(t)\rangle - \tfrac{1}{2}\langle \tilde{J}_{\theta f}|\tilde{J}_{\theta f}\rangle\right\} \tag{3.2}$$

provided the limits exist [16]. The inner product is defined in terms of an equilibrium average $\langle\ldots\rangle$ over a grand ensemble with a phase space density $\exp(\mathbf{b}\cdot\mathbf{A})$. Here $\mathbf{A} = \{N_s, N_f, \boldsymbol{P}, \tilde{N}_{\theta f}, N_{\theta s}, N_{\theta f}, P_\theta\}$ includes [18] the normal conserved quantities *and* all staggered invariants, and $\mathbf{b} = \{\nu_s, \nu_f, \cdots\}$ is the set of associated Lagrange multipliers, where ν_s and ν_f are the chemical potentials of slow and fast particles. The inner product between Fourier components is defined as

$$\langle A|B\rangle \equiv V^{-1}\langle A(\boldsymbol{k})B^*(\boldsymbol{k})\rangle \tag{3.3}$$

where V is the number of sites in the lattice. The susceptibility χ_f is

$$\chi_f = \langle \rho_{\theta f}|\rho_{\theta f}\rangle = \langle \rho_f|\rho_f\rangle = \sum_c a_f(c)\kappa(c) \tag{3.4}$$

with

$$\begin{aligned}\kappa(c) &= \langle n(\boldsymbol{c},\boldsymbol{k})|n(\boldsymbol{c},\boldsymbol{k})\rangle = f(c)(1-f(c))\\ f(c) &= \langle n(\boldsymbol{c},\boldsymbol{r})\rangle.\end{aligned} \tag{3.5}$$

In models without energy conservation $f(c) = f = \rho/b$ is the reduced density ($0 \leqslant f \leqslant 1$) with b the number of velocity states per site. If energy is non-trivially conserved, $f(c) = [1+\exp(-\nu+\frac{1}{2}\beta c^2)]^{-1}$ is the Fermi distribution in a system where the average invariants $\langle \boldsymbol{P}\rangle = \langle N_{\theta s}\rangle = \langle N_{\theta f}\rangle = \langle P_\theta\rangle = \langle \tilde{N}_{\theta f}\rangle = 0$. In our picture of the model as a binary mixture, $f(c) = [1+\exp(\nu_s a_s(c) + \nu_f a_f(c))]^{-1}$, or $f(1) \equiv f_1 = \rho_s/4$ and $f(\sqrt{2}) \equiv f_2 = \rho_f/4$, where ρ_s and ρ_f are the concentration of slow and fast particles respectively. The staggered current of fast particles in equation (3.2) is

$$\begin{aligned}\tilde{J}_{\theta f}(\boldsymbol{k},t) &= \sum_c j_f(c)n(c,\boldsymbol{k}+\pi\boldsymbol{\theta},t)\\ j_f(c) &= (\hat{\boldsymbol{k}}\cdot\,)a_f(c).\end{aligned} \tag{3.6}$$

The basic quantity to calculate any Green–Kubo expressions is the kinetic propagator:

$$\begin{aligned}\tilde{\Gamma}_{cc'}(\boldsymbol{k},z)\kappa(c') &= \sum_{t=0}^{\infty} e^{-zt}\sum_r e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\langle \delta n(\boldsymbol{c},\boldsymbol{r},t)\delta n(\boldsymbol{c}',0,0)\rangle\\ &= \langle \tilde{n}(\boldsymbol{c},\boldsymbol{k},z)|\tilde{n}(\boldsymbol{c}',\boldsymbol{k})\rangle\end{aligned} \tag{3.7}$$

where the labels c, c' denote the b-different velocity states.

In order to have a more convenient notation we introduce the $b \times b$ matrix

$$\gamma_{cc'}(\theta, \alpha) \equiv \lim_{z \to 0} \lim_{k \to 0} \{\tilde{\Gamma}_{cc'}(k + \pi\theta, z + \alpha\pi i) - \tfrac{1}{2}\delta_{cc'}\}. \tag{3.8}$$

The effect of the factors $(-)^{\theta \cdot r}$ in the geometric staggered modes (2.1) and $(-)^{t+\theta \cdot r}$ in the dynamic staggered modes (2.1) and (2.3) is a shift in the arguments k and z by an amount $\pi\theta$ and $\alpha\pi i$, where $\alpha = 0$ for geometric and $\alpha = 1$ for dynamic modes. Using a matrix notation, the diffusivity (3.2) can be written as,

$$\tilde{D}_\theta(\hat{k}) = \frac{1}{\chi_f} j_f \gamma(\theta, 0) \kappa j_f \tag{3.9}$$

where $j_f(c) = (\hat{k} \cdot c)\delta_{c\sqrt{2}}$ is considered a b-vector with components $j_f(c)$ and $\kappa_{cc'}$ as a diagonal matrix. These results are summarized in table 1, together with the explicit values of $\tilde{D}_\theta$ in the Boltzmann approximation.

Table 1. Summary of transport coefficients in the eight-bit model. The θ-vectors characterizes the sublattice divisions with $\alpha = 1$ for an oscillating dynamic mode and $\alpha = 0$ for a geometric mode. The current $j(c)$ enters in the Green–Kubo formulas $j\gamma(\theta, \alpha)\kappa j$ for the transport coefficients. Some symbols used are: $\chi_g = 2\kappa_1 + 4\kappa_2$, $c_l = \hat{k} \cdot c$, $c_t = \hat{k}_\perp \cdot c$, $c_\parallel = \hat{\theta} \cdot c$ and $c_\perp = \hat{\theta}_\perp \cdot c$.

Mode	θ, α	Propagation speed	Diffusivity	
			Current $j(c)$	Boltzmann value
Diffusion				
$\frac{a_s}{\chi_s} - \frac{a_f}{2\chi_f}$	(0,0),0	0	$c_l(\frac{a_s}{\chi_s} - \frac{a_f}{2\chi_f})$	$D = \frac{\kappa_1}{c_0^2}\tilde{D}_\theta$
Sound waves			$c_l(\frac{1}{2}c^2 - c_0^2)$	$\Gamma_o = \frac{2\kappa_1\kappa_2}{\chi_g^2} D$
$p + \sigma c_0 g_l$	(0,0),0	c_0	$c_x c_y$	$\nu = \frac{4\kappa_2}{\chi_g}\left(\frac{\kappa_2}{\lambda_5} - \frac{1}{2}\right)$
			$\frac{1}{2}(c_x^2 - c_y^2)$	$\nu' = \frac{\kappa_1}{\chi_g}\left(\frac{\kappa_1}{\lambda_6} - \frac{1}{2}\right)$
Geometric stagg				
$\tilde{\rho}_{\theta f}$	(1,1),0	0	$c_l a_f$	$\tilde{D}_\theta = \frac{3\kappa_2}{\lambda_8} - \frac{\kappa_2}{\kappa_1} - \frac{1}{2}$
Dynamic stagg				
$\rho_{\theta s}$	(1,1),1	0	$c_l a_s$	$D_\theta = \frac{\kappa_1}{4\kappa_2}\tilde{D}_\theta$
			$c_\perp c_\parallel$	$\Lambda_{\perp e} = \frac{1}{2}\nu$
Propagating	(1,0),1	$\lvert\hat{\theta} \cdot \hat{k}\rvert \times c_s$	$c_\perp a_f$	$\Lambda_{\perp o} = \frac{1}{2}\tilde{D}_\theta$
$\rho_{\theta f} + \sigma c_s g_\theta$	(0,1),1		$c_\parallel^2 - a_f$	$\Lambda_{\parallel e} = 2\nu'$
			$c_\parallel(a_f - c_s^2)$	$\Lambda_{\parallel o} = \frac{2\kappa_1^2}{\chi_g^2}\tilde{D}_\theta$

The diffusivity $\tilde{D}_\theta(\hat{k}) = \tilde{D}_\theta$ is isotropic, i.e. it does not depend on the direction of k. This can be seen by writing $\tilde{D}_\theta(\hat{k})$ as:

$$\begin{aligned} &\tilde{D}_\theta(\hat{k}) = \hat{k}_\alpha \hat{k}_\beta T_{\alpha\beta} \\ &T_{\alpha\beta} = c_\alpha \delta_{c\sqrt{2}} \gamma(\theta, 0) \kappa c_\beta \delta_{c\sqrt{2}}. \end{aligned} \tag{3.10}$$

Here $T_{\alpha\beta}$ is a second-rank tensor which depends on θ *only* through the factor $(-1)^{\theta\cdot r} = (-1)^{r_x+r_y}$. So it is invariant under all symmetry operations of the cubic group, i.e. sign changes of x or y and permutations x and y. However, a second-rank tensor with this symmetry is isotropic [19], $T_{\alpha\beta} = \tilde{D}_\theta \delta_{\alpha\beta}$, giving an isotropy diffusion coefficient. Similar arguments can be applied to show that $D_\theta(\hat{k})$ in the next subsection is also isotropic.

3.2. Dynamic staggered modes

For the same sublattice division with $\theta = (1,1)$ the mode $\rho_{\theta s}(k,t)$ exists. It is of dynamic origin and staggered in space and time. This mode is also purely diffusive and the method of [16] yields a Green–Kubo relation like equation (3.2) with $\tilde{J}_{\theta f}(k,t)$ in equation (3.6) replaced by

$$J_{\theta s}(k,t) = (-)^t \sum_c j_s(c) n(c, k+\pi\theta, t)$$
$$j_s(c) = (\hat{k}\cdot c) a_s(c) = (\hat{k}\cdot c)\delta_{c1}. \tag{3.11}$$

It can be reduced to a form similar to equation (3.9), i.e.

$$D_\theta(\hat{k}) = \frac{1}{\chi_s} j_s \gamma(\theta,1)\kappa j_s \tag{3.12}$$

with a susceptibility given by

$$\chi_s = \langle \rho_{\theta s} | \rho_{\theta s}\rangle = \langle \rho_s | \rho_s\rangle = \sum_c a_s(c)\kappa(c) \tag{3.13}$$

and $D_\theta(\hat{k}) = D_\theta$ is independent of $\hat{k}$ (see previous subsection).

3.3. Diffusion mode

For later comparison, we also consider the diffusion mode, which is a linear combination of $\rho_f(k,t)$ and $\rho_s(k,t)$. The general theory of fluctuations in fluids [20] suggest the linear combinations,

$$p(k,t) = \sum_c \tfrac{1}{2}c^2 n(c,k,t) = \tfrac{1}{2}\rho_s(k,t) + \rho_f(k,t)$$
$$u(k,t) = \frac{1}{\chi_s}\rho_s(k,t) - \frac{1}{2\chi_f}\rho_f(k,t). \tag{3.14}$$

Here $p(k,t)$ is the pressure fluctuation, which determines the standard sound modes (see section 4.2) and $u(k,t)$ is the concentration fluctuation, which is chosen to be independent of (or orthogonal to) the pressure fluctuation, i.e. $\langle p(k)|u(k)\rangle = 0$. The concentration fluctuation satisfies a diffusion equation of the form (1.3) with $\Lambda_\theta(\hat{k})$ replaced by D. A more systematic way to construct the proper linear combinations is given in section 4.1.

According to the method of [16] D is given by the Green–Kubo formula,

$$D = \lim_{z\to 0}\lim_{k\to 0}\frac{1}{\chi}\left\{\sum_{t=0}^{\infty} e^{-zt}\langle J|J(t)\rangle - \tfrac{1}{2}\langle J|J\rangle\right\} = \frac{1}{\chi}j\gamma(0,0)\kappa j \tag{3.15}$$

where the currents are defined by

$$\begin{aligned} J(t) &= \sum_c j(c)n(c,\boldsymbol{k},t) \\ j(c) &= c_l\left(\frac{a_s}{\chi_s} - \frac{a_f}{2\chi_f}\right) \end{aligned} \tag{3.16}$$

and the susceptibility is:

$$\chi = \langle u|u\rangle = \frac{1}{\chi_s} + \frac{1}{4\chi_f} = \frac{\langle p|p\rangle}{\chi_s\chi_f}. \tag{3.17}$$

The value of D in Boltzmann approximation is given in table 1.

4. Propagating modes

4.1. Propagating staggered modes

The novelty of the eight-bit model is that it has propagating staggered modes, being linear combinations of the vectorial staggered momentum density $g_\theta(\boldsymbol{k},t)$ and the scalar staggered number density $\rho_{\theta f}(\boldsymbol{k},t)$ for sublattices, characterized by $\boldsymbol{\theta} = (0,1)$ or $(1,0)$.

These staggered densities satisfy microscopic local conservation laws. Since we are interested here in large spatial and temporal scales we write only their continuous version, i.e.

$$\begin{aligned} \partial_t\rho_{\theta f}(\boldsymbol{k},t) &= -ikJ_{\theta f}(\boldsymbol{k},t) \\ \partial_t g_\theta(\boldsymbol{k},t) &= -ikJ_{\theta g}(\boldsymbol{k},t) \end{aligned} \tag{4.1}$$

and diagonalize them to $\mathcal{O}(k)$ in order to determine the proper linear combination of g_θ and $\rho_{\theta f}$. The currents $J_{\theta g}$ and $J_{\theta f}$ are defined through (3.11) with $j_s(c)$ replaced by $j_g(c) = (\hat{k}\cdot\boldsymbol{c})(\hat{\theta}\cdot\boldsymbol{c})$ and $j_f(c) = (\hat{k}\cdot\boldsymbol{c})a_f(c)$ respectively. Following the method of [18] the currents can be split into a local equilibrium current, $\mathcal{P}J_\theta$, and a dissipative current $\hat{J}_\theta = (1-\mathcal{P})J_\theta$, where $\mathcal{P}$ is a projection operator onto the hydrodynamic subspace, spanned by the complete set **A** of normal and staggered slow modes, as discussed in later equation (3.2). We first consider only the local equilibrium or *Euler part* of the conservation law (4.1), which is found by projecting the current on the complete set **A** of slow modes and yields for the present case in the long wavelength limit,

$$\begin{aligned} \partial_t\rho_{\theta f} &= -ikg_\theta\frac{\langle g_\theta|J_{\theta f}\rangle}{\langle g_\theta|g_\theta\rangle} = -ikg_\theta(\hat{k}\cdot\hat{\theta})c_s^2 \\ \partial_t g_\theta &= -ik\rho_{\theta f}\frac{\langle\rho_{\theta f}|J_{\theta g}\rangle}{\langle\rho_{\theta f}|\rho_{\theta f}\rangle} = -ik\rho_{\theta f}(\hat{k}\cdot\hat{\theta}) \end{aligned} \tag{4.2}$$

where

$$c_s^2 = \chi_f/\chi_g$$
$$\chi_g = \langle g_\theta | g_\theta \rangle = \tfrac{1}{2}\chi_s + \chi_f. \tag{4.3}$$

The solution to (4.2) represents two propagating staggered waves ($\sigma = \pm$),

$$\psi_\theta^\sigma(k,t) = \rho_{\theta f}(k,t) + \sigma c_s g_\theta(k,t) = (-)^t \sum_c [a_f(c) + \sigma c_s(\hat{\theta}\cdot c)] n(c, k+\pi\theta, t) \tag{4.4}$$

with a speed of propagation $c_\theta(\hat{k}) = |\hat{k}\cdot\hat{\theta}|c_s$ that depends on the direction of propagation $\hat{k}$. For the staggered waves the speed of propagation is maximal in the direction of the vector θ, and vanishes in the direction perpendicular to θ. Having established the proper linear combinations of staggered modes ψ_θ^σ that diagonalize the Euler equations (4.2), we simply follow the method of [16] to obtain the complete time dependence of the staggered excitations, including the damping, i.e.

$$\psi_\theta^\sigma(k,t) = \psi_\theta^\sigma(k,0)\exp[-\omega_\theta^\sigma(k)t]$$
$$\omega_\theta^\sigma(k) = \mathrm{i}\sigma(k\cdot\hat{\theta})c_s + k^2\Lambda_\theta^\sigma(\hat{k}). \tag{4.5}$$

After some algebra the Green–Kubo formula for the damping constant is found to be

$$\Lambda_\theta^\sigma(\hat{k}) = \lim_{z\to 0}\lim_{k\to 0}\frac{1}{\langle\psi_\theta^\sigma|\psi_\theta^\sigma\rangle}\left\{\sum_{t=0}^{\infty} \mathrm{e}^{-zt}\langle \hat{J}_\theta^\sigma | \hat{J}_\theta^\sigma(t)\rangle - \tfrac{1}{2}\langle \hat{J}_\theta^\sigma|\hat{J}_\theta^\sigma\rangle\right\} = \frac{1}{2\chi_f} j_\theta^\sigma \gamma(\theta,1)\kappa j_\theta^\sigma \tag{4.6}$$

where the staggered subtracted current $\hat{J}_\theta^\sigma = (1-\mathcal{P})J_\theta^\sigma$ is given by an expression similar to (3.11) with j_f replaced by

$$\hat{j}_\theta^\sigma(c) = [\hat{k}\cdot c - \sigma c_s(\hat{k}\cdot\hat{\theta})][a_f(c) + \sigma c_s(\hat{\theta}\cdot c)]. \tag{4.7}$$

By further exploiting the symmetries the anisotropic damping constant $\Lambda_\theta^\sigma(\hat{k})$ can be written as

$$\Lambda_\theta^\sigma(\hat{k}) = (\hat{k}\cdot\hat{\theta})^2\Lambda_\parallel + (\hat{k}\cdot\hat{\theta}_\perp)^2\Lambda_\perp \tag{4.8}$$

where each Λ is the sum of an even part Λ_e and an odd part Λ_o, with

$$\Lambda_{\perp e} = \frac{1}{2\chi_g} c_\perp c_\parallel \gamma(\theta,1)\kappa c_\perp c_\parallel$$
$$\Lambda_{\perp o} = \frac{1}{2\chi_f} c_\perp a_f(c)\gamma(\theta,1)\kappa c_\perp a_f(c)$$
$$\Lambda_{\parallel e} = \frac{1}{2\chi_g}(c_\parallel^2 - a_f(c))\gamma(\theta,1)\kappa(c_\parallel^2 - a_f(c)) \tag{4.9}$$
$$\Lambda_{\parallel o} = \frac{1}{2\chi_f} c_\parallel (a_f(c) - c_s^2)\gamma(\theta,1)\kappa c_\parallel (a_f(c) - c_s^2).$$

Recall that the shorthands $c_\parallel = \hat{\theta}\cdot c$ and $c_\perp = \hat{\theta}_\perp \cdot c$ are being used. These relations are the Green–Kubo formulas for the damping constant of the propagating staggered modes in models supporting both staggered number as well as momentum invariants. Their values in Boltzmann approximation are listed in table 1. Propagating staggered modes do not exist in the nine-bit version [21] of the model.

4.2. Sound waves

It is interesting to compare the propagating staggered waves with the usual sound waves. The latter are linear combinations of pressure fluctuations $p(\boldsymbol{k},t)$ and longitudinal momentum fluctuations $g_l(\boldsymbol{k},t)$. For the eight- and nine-bit square lattice model the usual sound modes ($\sigma = \pm$) are

$$\psi^\sigma(\boldsymbol{k},t) = p(\boldsymbol{k},t) + \sigma c_0 g_l(\boldsymbol{k},t). \tag{4.10}$$

where

$$g_l(\boldsymbol{k},t) = \sum_c (\hat{\boldsymbol{k}}\cdot\boldsymbol{c}) n(\boldsymbol{c},\boldsymbol{k},t). \tag{4.11}$$

Following the steps (4.1)–(4.9) one can also derive expressions for the speed of sound c_0 [21] and for the damping constant. In this case, the speed of propagation c_0 is given by $c_0^2 = \chi_p/\chi_g$ with $\chi_p = \langle p|p\rangle = \frac{1}{4}\sum_c c^4\kappa(c)$. The damping constant of these modes is given by

$$\begin{aligned}\Gamma^\sigma(\hat{k}) &= \lim_{z\to 0}\lim_{k\to 0}\frac{1}{\langle\psi^\sigma|\psi^\sigma\rangle}\left\{\sum_{t=0}^{\infty} e^{-zt}\langle\hat{J}^\sigma|\hat{J}^\sigma(t)\rangle - \tfrac{1}{2}\langle\hat{J}^\sigma|\hat{J}^\sigma\rangle\right\}\\ &= \frac{1}{2c_0^2\chi_g} j^\sigma\gamma(0,0)\kappa j^\sigma\end{aligned} \tag{4.12}$$

where the current $\hat{J}^\sigma = (1-\mathcal{P})J^\sigma$ is

$$\begin{aligned}\hat{J}^\sigma(\boldsymbol{k},t) &= \sum_c \hat{j}^\sigma(c) n(\boldsymbol{c},\boldsymbol{k},t)\\ \hat{j}^\sigma(c) &= [\hat{\boldsymbol{k}}\cdot\boldsymbol{c} - \sigma c_0][\tfrac{1}{2}c^2 + \sigma c_0\hat{\boldsymbol{k}}\cdot\boldsymbol{c}].\end{aligned} \tag{4.13}$$

The complete time dependence of these modes is (compare with equation (4.5)):

$$\begin{aligned}\psi^\sigma(\boldsymbol{k},t) &= \psi^\sigma(\boldsymbol{k},0)\exp[-\omega^\sigma(\boldsymbol{k})t]\\ \omega^\sigma(\boldsymbol{k}) &= \mathrm{i}k\sigma c_0 + k^2\Gamma^\sigma(\hat{k}).\end{aligned} \tag{4.14}$$

In contrast with the staggered speed of propagation, the speed of sound is independent of the direction of propagation. However, c_0 and c_s are not independent. Inspection shows that the relation $c_s^2 = 2c_0^2 - 1$ holds.

The sound damping constant $\Gamma^\sigma(\hat{k})$ *depends on the direction of propagation.* Following (4.9) we split $\Gamma^\sigma = \Gamma_e + \Gamma_o$ into an even and odd part with

$$\begin{aligned}\Gamma_e(\hat{k}) &= \frac{1}{2\chi_g}(c_l^2 - \tfrac{1}{2}c^2)\gamma(0,0)\kappa(c_l^2 - \tfrac{1}{2}c^2)\\ \Gamma_o(\hat{k}) &= \Gamma_o = (2c_0^2\chi_g)^{-1}c_l(\tfrac{1}{2}c^2 - c_0^2)\gamma(0,0)\kappa c_l(\tfrac{1}{2}c^2 - c_0^2)\\ &= D\chi_s\chi_t/(8\chi_g^2)\end{aligned} \tag{4.15}$$

where $c_l = \hat{k} \cdot c$. In the last equality the relation,

$$j(c) = -\frac{\chi_g}{\chi_f \chi_s}(c^2 - 2c_0^2)c_l \tag{4.16}$$

has been used as can be deduced from (3.16) and (3.17). The even part involves the non-isotropic viscosity tensor [18]

$$\begin{aligned}\nu_{\alpha\beta\gamma\delta} &= \chi_g^{-1}(c_\alpha c_\beta - \tfrac{1}{2}\delta_{\alpha\beta}c^2)\gamma(0,0)\kappa(c_\gamma c_\delta - \tfrac{1}{2}\delta_{\gamma\delta}c^2) \\ &= \nu\{\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma} - 2\delta^{(4)}_{\alpha\beta\gamma\delta}\} + \nu'\{2\delta^{(4)}_{\alpha\beta\gamma\delta} - \delta_{\alpha\beta}\delta_{\gamma\delta}\}.\end{aligned} \tag{4.17}$$

Greek subscripts label Cartesian components $\alpha, \beta, \gamma, \delta, \ldots = (x, y)$ and $\delta^{(4)}_{\alpha\beta\gamma\delta}$ equals 1 if all subscripts are equal and vanishes otherwise. The fourth rank viscosity tensor with square symmetry has in general three independent viscosity coefficients. However, as (4.17) is traceless in the indices $(\alpha\beta)$ and $(\gamma\delta)$, the bulk viscosity vanishes. The two remaining viscosities are given by the Green–Kubo relations

$$\begin{aligned}\nu &= \nu_{xyxy} = \chi_g^{-1} c_x c_y \gamma(0,0)\kappa c_x c_y \\ \nu' &= \nu_{xxxx} = (4\chi_g)^{-1}(c_x^2 - c_y^2)\gamma(0,0)\kappa(c_x^2 - c_y^2).\end{aligned} \tag{4.18}$$

With the help of (4.15) and (4.17) the even part of the sound damping constant can then be expressed in the viscosity coefficients,

$$\Gamma_e(\hat{k}) = \tfrac{1}{2}\nu_{llll} = \tfrac{1}{2}\nu \sin^2(2\phi) + \tfrac{1}{2}\nu' \cos^2(2\phi) \tag{4.19}$$

where the subscript l denotes a longitudinal component, parallel to the propagation direction $\hat{k} = (\cos\phi, \sin\phi)$. In isotropic LGCAs both viscosities are equal and $\Gamma_e(\hat{k}) = \frac{1}{2}\nu$ is isotropic.

5. Boltzmann approximation

5.1. Kinetic propagator

In this section we will explicitly calculate the kinetic propagator $\gamma(\theta, \alpha)$ in the Boltzmann approximation. The time evolution of the occupation numbers $n(c, r, t)$ is given by:

$$n(c, r + c, t + 1) = n(c, r, t) + I(c|n) \tag{5.1}$$

where the first term of the left hand side of this equation is the *free streaming term* and $I(c|n)$ represents the *collision term*. In general, $I(c|n)$ is non-linear in the occupation numbers, i.e., in a b-bit model, $I(c|n)$ contains at most b ns, each referring to a different velocity channel. By iterating equation (5.1) t times, one obtains the exact series for $n(c, r, t)$ expressed as a polynomial of degree b^t in the occupation numbers $n(c, r', 0)$. In the approximation of uncorrelated collisions, the so-called Boltzmann approximation, the recollisions between particles are neglected and one can resum the series as a tth power of a single step evolution.

In practice, this calculation is carried out by introducing the collision operators Ω by Taylor expanding $n(c,r,t)$ around $f(c) = \langle n(c,r,t)\rangle$ and using the relation $I(f) = 0$. This yields

$$I(c|n) = \sum_{c'} \Omega_{cc'} \delta n(c',r,t) + \sum_{c'c''} \Omega_{cc'c''} \delta n(c',r,t)\delta n(c'',r,t) + \cdots \tag{5.2}$$

If correlated collisions are neglected, the third and higher order Ω-operators do not contribute to the average occurring in the kinetic propagator (3.7). So, we neglect all non-linear terms in (5.2) and the time evolution equation for the occupation number becomes in the Boltzmann approximation,

$$\delta n(c,r+c,t+1) = \delta n(c,r,t) + \sum_{c'} \Omega_{cc'} \delta n(c',r,t). \tag{5.3}$$

After Fourier–Laplace transformation we obtain the solution

$$\tilde{n}(c,k,z) = \sum_{c'} \left(\frac{1}{e^{z+ik\cdot c} - 1 - \Omega} \right)_{cc'} e^{z+ik\cdot c'} n(c',k,0) \tag{5.4}$$

where $n(c,k,t)$ and $\tilde{n}(c,k,z)$ are the Fourier and Fourier–Laplace transform of $\delta n(c,r,t)$. When inserting equation (5.4) into equation (3.7) we obtain with the help of equation (3.5):

$$\tilde{\Gamma}_{cc'}(k,z) = \left(\frac{1}{e^{z+ik\cdot c} - 1 - \Omega} \right)_{cc'} e^{z+ik\cdot c'}. \tag{5.5}$$

By combining equations (5.5) into (3.8) the final form of the kinetic propagator $\gamma(\theta,\alpha)$ in *Boltzmann approximation follows*

$$\gamma(\theta,\alpha) = -\left[\frac{1}{\Delta(\theta,\alpha) + \Omega} + \frac{1}{2} \right] \tag{5.6}$$

where the sublattice matrix Δ is diagonal

$$\Delta_{cc'}(\theta,\alpha) = \delta_{cc'}[1 - (-1)^{\theta\cdot c + \alpha}] \qquad (\alpha = 0,1). \tag{5.7}$$

In deriving equation (5.6) we have used that the factor $\exp[i\pi\theta\cdot c' + i\pi\alpha]$, occurring to the right of equation (5.5), can be replaced by unity. The reason is that this factor occurs in all expressions of interest (1.4), (3.9), (3.12), (3.15) and (4.9) in combination with a current $j(c) = (\hat{k}\cdot c)a(c)$, that contains the proper collisional invariant $a(c)$. Therefore the relation,

$$e^{i\pi\alpha + i\pi\theta\cdot c} a(c) = a(c) \tag{5.8}$$

derived in (A.5) of appendix A, allows us to replace this factor by unity. In fact one does not really need appendix A to explicitly verify this relation. For the staggered invariants of the eight-bit model $a(c) = c_{\|}$ and $\delta_{c\sqrt{2}}$ with $\theta = (0,1),(1,0)$ and $\alpha = 1$ and $a(c) = \delta_{c1}$ for $\theta = (1,1)$ with $\alpha = 1$, and for $a(c) = \delta_{c\sqrt{2}}$ for $\theta = (1,1)$ with $\alpha = 0$.

5.2. Standard transport coefficients

The diffusion coefficient D in (3.15) and the viscosities ν and ν' in (4.18) belong to this class. In Boltzmann approximation they have the general form, $L = -j(\Omega^{-1} + \frac{1}{2})\kappa j$. It can be evaluated by combining the methods of [17, 21]. The transport coefficients can be calculated most conveniently in terms of eigenfunctions and eigenvalues of the 8×8 collision matrix Ω, i.e.

$$\Omega\kappa\psi_n = -\omega_n\kappa\psi_n. \tag{5.9}$$

They are orthogonal with respect to a weighted inner product

$$\langle\psi_n|\psi_m\rangle = \sum_c \kappa(c)\psi_n(c)\psi_m(c) \tag{5.10}$$

where $\kappa(c)$ is a weight factor defined in (3.5). For an explicit determination of the *eigenvalues* it is more convenient to consider a slightly different eigenvalue problem,

$$\Omega\kappa u_n = -\lambda_n u_n \tag{5.11}$$

where the matrix $\Omega\kappa$ is symmetric as can be verified by explicit construction of Ω from the collision rules in figure 1. Now eigenfunctions are orthogonal with respect to the inner product

$$u_n \cdot u_m = \sum_c u_n(c)u_m(c). \tag{5.12}$$

The four zero-eigenfunctions ($\omega_n = \lambda_n = 0$) are the collisional invariants,

$$\begin{aligned} &\psi_1(c) = u_1(c) = \delta_{c1} \qquad \psi_2(c) = u_2(c) = \delta_{c\sqrt{2}} \\ &\psi_3(c) = u_3(c) = c_x \qquad \psi_4(c) = u_4(c) = c_y. \end{aligned} \tag{5.13}$$

The remaining four eigenfunctions can be constructed using the symmetry considerations of [17] and orthogonalizing with the appropriate inner products,

$$\begin{aligned} &\psi_5(c) = u_5(c) = c_x c_y \\ &\psi_6(c) = u_6(c) = \tfrac{1}{2}(c_x^2 - c_y^2) \\ &\psi_7(c) = (c^2 - 2c_0^2)c_x \qquad u_7(c) = (c^2 - \tfrac{5}{3})c_x \\ &\psi_8(c) = (c^2 - 2c_0^2)c_y \qquad u_8(c) = (c^2 - \tfrac{5}{3})c_y \end{aligned} \tag{5.14}$$

where c_0 is the velocity of sound, defined below equation (4.11). The eigenfunctions with $n = 7, 8$ are degenerate because of the square symmetry. The eigenvalues in (5.9) and (5.11) satisfy the relation

$$\lambda_n = \omega_n \frac{\langle u_n|\psi_n\rangle}{u_n \cdot \psi_n} = \omega_n \frac{\langle\psi_n|\psi_n\rangle}{u_n \cdot u_n}. \tag{5.15}$$

In the last equality we have used that $u_n = \psi_n + Au_{n-4}$, valid for $n = 7$ and 8.

To calculate the transport coefficients, we use equation (4.16) with $c_l = \hat{k} \cdot c$ and observe that the $j(c)$ is an eigenfunction of Ω with eigenvalue ω_8. The currents in the remaining Green–Kubo relations for the viscosities in equation (4.18) are eigenfunctions too. Hence

$$\begin{aligned} D &= \frac{\langle j|j\rangle}{\langle u|u\rangle}\left(\frac{1}{\omega_8}-\frac{1}{2}\right) = \frac{1}{2c_0^2}\left(\frac{3\chi_f\chi_s}{8\chi_g\lambda_8}-\frac{1}{2}\right) \\ \nu &= \frac{\langle \psi_5|\psi_5\rangle}{\chi_g}\left(\frac{1}{\omega_5}-\frac{1}{2}\right) = \frac{\chi_f}{\chi_g}\left(\frac{\chi_f}{4\lambda_5}-\frac{1}{2}\right) \\ \nu' &= \frac{\langle \psi_6|\psi_6\rangle}{\chi_g}\left(\frac{1}{\omega_6}-\frac{1}{2}\right) = \frac{\chi_s}{4\chi_g}\left(\frac{\chi_s}{4\lambda_6}-\frac{1}{2}\right). \end{aligned} \tag{5.16}$$

The inner products $\langle \ldots | \ldots \rangle$ and susceptibilities, defined in sections 3 and 4, are linear combinations of the weights $\kappa(1) = \kappa_1$ and $\kappa(\sqrt{2}) = \kappa_2$. To calculate the eigenvalues λ_n we first construct the (symmetric) matrix $\Omega\kappa$ from the collision rules of [4]. Next, we apply the matrix $\Omega\kappa$ to the eigenvectors u_n to find the eigenvalues λ_n. The results are listed in table 2.

Table 2. Eigenvectors and eigenvalues of the operator $\Omega\kappa$, defined as $\Omega\kappa u_n = -\lambda_n u_n$. As $\{u_1, u_2, u_3, u_4\}$ are collisional invariants, their eigenvalues are equal to 0. The eigenvectors u_7 and u_8 have the same eigenvalue because they are related by a symmetry of the lattice. The shorthands $f_1 = f(1) = \rho_s/4$ and $f_2 = f(\sqrt{2}) = \rho_f/4$ have been used.

n	Eigenvector u_n	Eigenvalue λ_n
1	δ_{c1}	0
2	$\delta_{c\sqrt{2}}$	0
3	c_x	0
4	c_y	0
5	$c_x c_y$	$4f_1f_2(1-f_1)^3(1-f_2)^3 + 4f_2^2(1-f_2)^2$
6	$\frac{1}{2}(c_x^2 - c_y^2)$	$4f_1^2(1-f_1)^2$
7	$(c^2 - \frac{5}{3})c_x$	$6f_1f_2(1-f_1)^3(1-f_2)^3$
8	$(c^2 - \frac{5}{3})c_y$	

5.3. Staggered transport coefficients

As a typical example we consider the geometric staggered diffusivity (3.2) in Boltzmann approximation,

$$\widetilde{D}_\theta = \chi_f^{-1} j_f \left([(-)^{\theta\cdot c} - 1 - \Omega]^{-1} - \tfrac{1}{2}\right) \kappa j_f \tag{5.17}$$

with $\theta \cdot c = c_x + c_y$. The inverse matrix $[(-)^{\theta\cdot c} - 1 - \Omega]^{-1}$ also possesses square symmetry, so that the vector $[(-)^{\theta\cdot c} - 1 - \Omega]^{-1}\kappa j_f = A\kappa c_l + B\kappa j(c)$. The unknown coefficients A, B can be determined by multiplying both sides of the equation respectively by $c_l[(-)^{\theta\cdot c} - 1 - \Omega]^{-1}$ and $j(c)[(-)^{\theta\cdot c} - 1 - \Omega]^{-1}$. After solving for A and B, $\widetilde{D}_\theta$ in (5.17) follows as

$$\widetilde{D}_\theta = \frac{2\chi_g}{\chi_s}\left(\frac{1}{\omega_8}-\frac{1}{2}\right) = \frac{3\kappa_2}{\lambda_8} - \frac{\kappa_2}{\kappa_1} - \frac{1}{2}. \tag{5.18}$$

The staggered diffusivity (3.12) and damping coefficients (4.9) can be calculated similarly. Those involving vector currents are related to the eigenvalue ω_8, i.e.

$$D_\theta = \frac{\chi_g}{2\chi_f}\left(\frac{1}{\omega_8}-\frac{1}{2}\right)$$
$$\Lambda_{\perp o} = \frac{\chi_g}{\chi_s}\left(\frac{1}{\omega_8}-\frac{1}{2}\right) \tag{5.19}$$
$$\Lambda_{\parallel o} = \frac{\chi_s}{4\chi_g}\left(\frac{1}{\omega_8}-\frac{1}{2}\right).$$

On the other hand the coefficient Λ_e involve tensor currents, so they contain the eigenvalues ω_5 and ω_6. Calculation gives

$$\Lambda_{\perp e} = \tfrac{1}{2}\nu \qquad \Lambda_{\parallel e} = 2\nu'. \tag{5.20}$$

The subtracted currents in the Green–Kubo formulas (4.9) for the staggered transport coefficients guarantee that the inverse matrix $(\Delta(\theta,\alpha)+\Omega)^{-1}$ exists in the orthogonal complement of the null subspace. For example, if one would try to calculate $\xi_\parallel$ in equation (1.4) as derived for FHP model in the eight-bit LGCA one would find a divergent result. This is because the current $c_\parallel^2$, associated with $\xi_\parallel$, has a projection over $a_f(c) = \delta_{c\sqrt{2}}$, which is a conserved quantity in the eight-bit model. Thus $\xi_\parallel$ of equation (1.4), when calculated in the eight-bit model, would be divergent. However, in FHP models, $c_\parallel^2$ is orthogonal to all conserved quantities and the matrix $\gamma(\theta,1)$ in (5.6), when acting on $c_\parallel^2$, gives a well defined result. Similarly the current in $\Lambda_{\parallel o}$ has a subtracted part $c_s^2 c_\parallel$, proportional to the conserved staggered θ-momentum, which makes it finite. In the tensor currents of (1.4) no subtracted parts appear because the only available staggered invariant $c_\parallel$ is a vector.

The results for the transport coefficients are summarized in table 1. We further introduced the notations $f_1 \equiv f(1) = \rho_s/4$, $f_2 \equiv f(\sqrt{2}) = \rho_f/4$ and $\kappa_i = f_i(1-f_i)$ with $i = 1, 2$. The column 'current' in table 1 lists the corresponding b-vector $j(c)$ as occurring in the Green–Kubo formulas (3.9), (3.12), (3.15), (4.9), (4.15) and (4.19).

6. Discussion

We have studied the presence of spurious modes, both in eight- and nine-bit models. We found two kind of invariants: *dynamic* ones, with a high frequency modulation $(-1)^t$, and *geometric* ones without such a modulation. All of them are staggered in space according to a sublattice division, specified by the θ-vector. Among the dynamic staggered modes of the eight-bit model we have found the novel phenomena of propagating waves. Such waves can occur for a given model only if there exist for the same sublattice division two conserved staggered densities: one of scalar and one of vector character. Since the θ-sublattice division breaks the full cubic symmetry of the eight-bit model, the propagation speed for those waves is anisotropic.

We also derive Green–Kubo expressions for all diffusivities and damping constants, associated with the unphysical modes, and evaluate them in Boltzmann approximation. Finally, we suggest a systematic method for detecting staggered invariants for

a given sublattice division characterized by a θ-vector. The method is a direct consequence of the equation (A.5) of appendix A, and states that $\sum_{rc} a(c|\theta,\alpha)\, e^{\alpha t+\theta\cdot r} n(c,r,t)$ is an staggered invariant if $a(c|\theta,\alpha)$ satisfies the relation

$$(-1)^{\alpha+\theta\cdot c} a(c|\theta,\alpha) = a(c|\theta,\alpha) \tag{6.1}$$

and if $a(c|\theta,\alpha)$ is a linear combination of the standard collisional invariants. They are for the present model c, $\delta_{c\vec{1}}$, $\delta_{c\sqrt{2}}$.

Inspection of table 1 shows that there exist only three independent transport coefficients D, ν and ν' in Boltzmann approximation. All remaining transport coefficients are proportional to one of these. The coefficients of proportionality are equilibrium susceptibilities. For instance, the damping constants of the staggered waves satisfy the equalities $\Lambda_{\perp e} = \frac{1}{2}\nu$ and $\Lambda_{\|e} = 2\nu'$. A similar relation holds for the staggered diffusivity $\xi_\perp = \nu$ in the FHP models [10, 14] in Boltzmann approximation. In Lorentz gases on square lattices, where standard and staggered number densities satisfy a diffusion equation, Binder and Ernst [7] have given a general argument to show that the Green–Kubo formulas for the normal and staggered diffusion coefficients are identical for arbitrary densities, using a relationship for the conditional probability in the staggered and normal case. Similar relationships for the probabilities of slow and fast particles seem to exist here, but we have been unable to show the equality of staggered and standard transport coefficients beyond the Boltzmann approximation. Furthermore the computer simulations of the FHP model in [11] seem to suggest that the relation $\xi_\perp = \nu$ breaks down beyond Boltzmann approximation.

Finally, a comparison is made with the work of Chopard and Droz [4]. These authors define a heat conductivity λ_k through the relation $q = -\lambda_k \nabla T_k$ where q is the heat current and T_k the 'kinetic temperature', defined through the equilibrium pressure $p = \frac{1}{2}\rho T_k$, with $\rho = \rho_s + \rho_f$. As the eight-bit model is an ideal Fermi gas, its pressure $p(\rho, T)$ is a complicated function of density and *thermodynamic temperature* T which differs strongly from their kinetic temperature [22]. Their result for the heat conductivity is

$$\lambda_k = \frac{p}{T_k^2}\left(\frac{2}{\omega_8} - 1\right). \tag{6.2}$$

The authors also obtain a Dufour coefficient for single component thermal fluid model. According to irreversible thermodynamics, such transport coefficient does not exist in single component systems. If one uses the temperature T as defined in (irreversible) thermodynamics and statistical mechanics, one can show straightforwardly that the Green–Kubo expressions for the diffusion coefficient D in equation (3.15) is related to the Green–Kubo formula for the heat conductivity λ_H in the same model, (when interpreted as a single component thermal fluid) through

$$\lambda_H = \frac{c_0^2 \chi_s \chi_f}{4T^2 \chi_g} D. \tag{6.3}$$

Our result for the heat conductivity in Boltzmann approximation follows then from equation (5.16) to have a form similar to equation (6.2), with p replaced by $\kappa_1\kappa_2/\chi_g$.

This difference as well as the non-vanishing of the Dufour coefficient in [4], is caused by their use of a temperature concept which is conflict with the thermodynamics and irreversible thermodynamics [22].

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Appendix

The purpose of the present appendix is to prove the relation $\Delta(\boldsymbol{\theta},\alpha)a(\boldsymbol{c}|\boldsymbol{\theta},\alpha)=0$ for any spurious staggered invariant (either geometric $\alpha=0$ or dynamic $\alpha=1$). Let us consider a staggered conserved quantity, defined as:

$$A(t)=\sum_{\boldsymbol{r}\boldsymbol{c}} a(\boldsymbol{c}|\boldsymbol{\theta},\alpha)(-)^{\alpha t+\boldsymbol{\theta}\cdot\boldsymbol{r}} n(\boldsymbol{c},\boldsymbol{r},t) \tag{A.1}$$

where $a(\boldsymbol{c}|\boldsymbol{\theta},\alpha)$ is a linear combination of collisional invariants, satisfying

$$\sum_{\boldsymbol{c}} a(\boldsymbol{c}|\boldsymbol{\theta},\alpha)I(\boldsymbol{c}|n)=0. \tag{A.2}$$

By combining (A.2) with the evolution equation (5.1) we obtain:

$$\sum_{\boldsymbol{c}} a(\boldsymbol{c}|\boldsymbol{\theta},\alpha)(-)^{\alpha t+\boldsymbol{\theta}\cdot\boldsymbol{r}}[n(\boldsymbol{c},\boldsymbol{r}+\boldsymbol{c},t+1)-n(\boldsymbol{c},\boldsymbol{r},t)]=0. \tag{A.3}$$

Summing this equation over all sites $\boldsymbol{r}$ and using the relation $A(t+1)=A(t)$, we obtain the following expression

$$\sum_{\boldsymbol{r}\boldsymbol{c}} a(\boldsymbol{c})(-)^{\alpha t+\boldsymbol{\theta}\cdot\boldsymbol{r}} n(\boldsymbol{c},\boldsymbol{r},t)\left[(-1)^{\alpha+\boldsymbol{\theta}\cdot\boldsymbol{c}}-1\right]=0. \tag{A.4}$$

It must hold for any configurations of particles $\{n(\boldsymbol{c},\boldsymbol{r},t)\}$. Hence

$$(-)^{\alpha+\boldsymbol{\theta}\cdot\boldsymbol{c}} a(\boldsymbol{c}|\boldsymbol{\theta},\alpha)=a(\boldsymbol{c}|\boldsymbol{\theta},\alpha). \tag{A.5}$$

This equation has been discussed in section 6 as a method for searching staggered invariants.

References

[1] Frisch U, Hasslacher B and Pomeau Y 1986 *Phys. Rev. Lett.* **56** 1505
[2] 1990 *Lattice Gas Methods for Partial Differential Equations* ed G D Doolen (Reading, MA: Addison-Wesley)
[3] Kadanoff L P, McNamara G and Zanetti G 1989 *Phys. Rev.* A **40** 4527
[4] Chopard B and Droz M 1988 *Phys. Lett.* **126A** 476
[5] d'Humières D, Lallemand P and Frisch U 1986 *Europhys. Lett.* **2** 291

[6] Chen S, Lee M, Zhao K H and Doolen G D 1989 *Physica* D **37** 42
[7] *Binder* P M and Ernst M H 1990 *Physica* A **164** 91
[8] Ernst M H 1991 *Liquids, Freezing and the Glass Transition* ed D Levesque, J P Hansen and J Zinn-Justin, Les Houches, Session LI, 1989 (New York: Elsevier)
[9] Qian Y H 1991 *PhD dissertation* Universitè Pierre et Marie Curie
[10] d'Humières D, Qian Y H and Lallemand P 1989 *Discrete Kinetic Theory, Lattice Gas Dynamics and Foundations of Hydrodynamics* ed R Monaco (Singapore: World Scientific)
[11] Zanetti G 1989 *Phys. Rev.* A **40** 1539
[12] Naitoh T, Ernst M H and Dufty J W 1990 *Phys. Rev.* A **42** 7187
[13] Hardy J, Pomeau Y and de Pazzis O 1973 *J. Math. Phys.* **14** 1746
Hardy J, de Pazzis O and Pomeau Y 1976 *Phys. Rev.* A **13** 1949
[14] Frisch U, d'Humières D, Hasslacher B, Lallemand P, Pomeau Y and Rivet J P 1987 *Complex Systems* **1** 649
[15] Ernst M H and van Velzen G A 1989 *J. Stat. Phys.* **57** 455
[16] Ernst M H and Dufty J W 1990 *J. Stat. Phys* **58** 57
[17] Brito R, Ernst M H and Kirkpatrick T R 1991 *J. Stat. Phys.* **62** 283
[18] Ernst M H 1990 *Fundamental Problems in Statistical Mechanics* vol VII ed H van Beijeren (Amsterdam: North-Holland) p 321
[19] Wolfram S 1986 *J. Stat. Phys.* **45** 471
[20] Ernst M H and Dorfman J R 1975 *J. Stat. Phys.* **12** 311
[21] Das S P and Ernst M H to be published
[22] Ernst M H 1991 *Discrete Models of Fluid Dynamics* ed A S Alves (Singapore: World Scientific)