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Staggered Diffusivities in Lattice Gas Cellular Automata

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The majority of LGCAs has spurious conservation laws, the so-called staggered invariants, first discovered by Kadanoff, McNamara, and Zanetti. Consequently there are additional hydrodynamic modes of diffusive type, which modify mode coupling theories and the nonlinear fluid dynamic equations. The diffusivities of these staggered modes are evaluated in the mean field approximation for LGCAs on triangular lattices, starting from the Green–Kubo formulas for the staggered diffusivities.

KEY WORDS: Staggered invariants; lattice gas cellular automata; CA-fluids; staggered diffusivities; Green–Kubo relations.

1. INTRODUCTION

The majority of cellular automata fluids (CA)[1–8] possesses, apart from the usual conservations laws for particle number N, total momentum $\mathbf{P}$, and possibly total energy H, additional conserved quantities, the *staggered invariants*, H_θ. They are caused by the extremely simplified dynamics of LGCAs, mainly due to the discreteness of both space and time and due to the local conservation rules. In CA-fluids out of equilibrium, these spurious invariants give rise to slowly decaying staggered densities $h_\theta(\mathbf{r}, t)$. At the linear level this leads to new modes or elementary excitations, a phenomenon analogous to fermion doubling in lattice gauge theories.[9]

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Consequently, the set of nonlinear fluid dynamic equations for these CA-fluids has to be extended with additional equations that couple in a nonlinear fashion to the standard Navier–Stokes equations. Also, additional nonlinear coupling terms of $\mathcal{O}(h_\theta^2)$ appear in the Euler part of the Navier–Stokes-equations.[1,2,10]

Therefore, the existence of these slow modes will affect the time evolution of the macroscopic flow field and that of other hydrodynamic densities in CA-fluids. The extra appearance of $\mathcal{O}(h_\theta^2)$ terms in the Euler equations will also modify the mode coupling theory.[1,6,10] The long-time tails in current–current correlation functions will in general have additional long-time contributions from pairs of staggered modes.[1,6,10–12]

At the level of linear excitations the staggered modes do not couple to the standard fluid modes. They are purely diffusive and their Fourier transform satisfies

$$\partial_t h_\theta(\mathbf{q}, t) = -q^2 \Lambda_\theta(\hat{q})\, h_\theta(\mathbf{q}, t) \tag{1.1}$$

The staggered diffusivity $\Lambda_\theta(\hat{q})$ depends on the direction $\hat{q}$ of the wave vector $\mathbf{q}$, and can be expressed as a Green–Kubo relation.[2,6] With respect to the standard transport coefficients, Rivet[13] was the first author to study the Green–Kubo relations for the shear viscosity in CA-fluids.

To study the effects of the spurious modes on nonlinear hydrodynamic equations and mode coupling theories, knowledge of the staggered diffusivities is indispensable. The goal of the present paper is to present a simple method to evaluate explicitly the Green–Kubo formulas for staggered diffusivities. Up till now it was only possible to evaluate the Green–Kubo relations for the standard transport coefficients, such as viscosities and diffusion coefficients.[14] In Boltzmann approximation, the standard transport coefficients are expressed as matrix elements of the inverse collision operator Ω. It will be shown that the staggered diffusivities involve matrix elements of the inverse of $(\Delta + \Omega)$, where the operator Δ is related to discrete translation over a lattice distance. We also note that identical results can be obtained[12] starting directly from the Boltzmann equation without using the Green–Kubo formalism.[6]

The CA-fluid models of interest here have only staggered momentum densities as additional slow modes. Examples are the six- or seven-bit FHP models[15] on the triangular lattice, the quasi-three-dimensional 24-bit FCHC model,[3,16] and the thermal eight- or nine-bit models on a square lattice and their three-dimensional extensions with energy conserving collisions.[3–5] In a Lorentz gas on a square lattice[8] or in the four-bit CA-fluid on the square lattice there exist also staggered number density modes,[7] which will not be considered here.

This paper is organized as follows: in Section 2 the staggered

invariants are presented together with the Green–Kubo formula for the staggered diffusivity, which describes the relaxation of the corresponding conserved density. In Section 3 the kinetic propagator is constructed in the mean field or Boltzmann approximation. In Section 4 this propagator is diagonalized and the usual transport coefficients are obtained. In the last section the staggered diffusion coefficients are evaluated explicitly.

2. STAGGERED DIFFUSIVITIES

The microscopic definition of the staggered momentum density is given in terms of occupation numbers:

$$h_\theta(\mathbf{r}, t) = \sum_i (-)^{t+\boldsymbol{\theta}\cdot\mathbf{r}} c_{i\theta} n_i(\mathbf{r}, t) \tag{2.1}$$

where $n_i(\mathbf{r}, t)$ is the occupation number of the ith link $\mathbf{c}_i$ at lattice site $\mathbf{r}$ and $c_{i\theta} = \hat{\theta} \cdot \mathbf{c}_i$ is its θ component. A b-bit model contains a set of b different velocity states $\mathbf{c}_i$ per site, which includes in general the nearest neighbor lattice vectors (FHP models), or, in the square lattice models,[4] even next nearest neighbor lattice vectors and possibly a rest particle, $\mathbf{c}_i = 0$. The vectors $\boldsymbol{\theta}$ labeling the staggered modes are reciprocal lattice vectors, implying that $\boldsymbol{\theta} \cdot \mathbf{r}$ is an integer. In the FHP models there exist *three* independent staggered momentum densities, corresponding to $\boldsymbol{\theta} = (0, 2/\sqrt{3})$, $\boldsymbol{\theta}' = (-1, -1/\sqrt{3})$, $\boldsymbol{\theta}'' = (1, -1/\sqrt{3})$. In the eight- or nine-bit square lattice models there are *two* independent staggered momentum densities with $\boldsymbol{\theta} = (0, 1)$ and $\boldsymbol{\theta}' = (1, 0)$.

The macroscopic averages of (2.1) over some nonequilibrium state and the long-wavelength components of the microscopic density (2.1) decay for large times according to the diffusion equation (1.1). The staggered diffusivity is given by[6]

$$\begin{aligned} \Lambda_\theta(\hat{q}) &= \Lambda_\theta^k(\hat{q}) + \Lambda_\theta^p(\hat{q}) \\ &= \lim_{s \to 0} \lim_{q \to 0} \chi_\theta^{-1} \sum_{i,j} c_{iq} c_{i\theta} [\tilde{\Gamma}(\mathbf{q} + \pi\boldsymbol{\theta}, s + \pi i) - \tfrac{1}{2}]_{ij} c_{jq} c_{j\theta} \end{aligned} \tag{2.2}$$

(provided the limits exist). The term $\Lambda_\theta^k(\mathbf{q})$ containing Γ is referred to as the kinetic part; the term $\Lambda_\theta^p(\hat{q})$ obtained by setting $\Gamma = 0$ is referred to as the *propagating part* of the transport coefficient. Here $c_q = \hat{q} \cdot \mathbf{c}$ and $c_\theta = \hat{\theta} \cdot \mathbf{c}$ are the components of $\mathbf{c}$ parallel to the unit vectors $\hat{q}$ and $\hat{\theta}$, respectively. Furthermore, Γ is the Fourier–Laplace transform of the kinetic propagator or equilibrium time correlation function

$$\tilde{\Gamma}_{ij}(\mathbf{q}, s) = \sum_{t=0}^{\infty} e^{-st} \sum_{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \langle \delta n_i(\mathbf{r}, t)\, \delta n_j(\mathbf{0}, 0) \rangle$$

$$= \frac{1}{M} \langle \tilde{n}_i(\mathbf{q}, s)\, n_j^*(\mathbf{q}, 0) \rangle \equiv \langle \tilde{n}_i(\mathbf{q}, s) \mid n_j(\mathbf{q}, 0) \rangle \tag{2.3}$$

The average $\langle \cdots \rangle$ is taken over an equilibrium ensemble and M is the number of sites in the lattice. The symbol $n_i(\mathbf{q}, t)$ denotes the Fourier transform of the fluctuation in the occupation number $\delta n_i(\mathbf{r}, t) = n_i(\mathbf{r}, t) - \langle n_i \rangle$ and $\tilde{n}_i(\mathbf{q}, s)$ is its discrete Laplace transform. The Fourier–Laplace transform of (2.1) reads in this notation $\tilde{h}_\theta(\mathbf{q}, s) = \sum_j c_{j\theta} \tilde{n}_j(\mathbf{q} + \pi\boldsymbol{\theta}, s + \pi i)$. Finally, the equilibrium susceptibility or equal-time correlation function is

$$\chi_\theta = \langle h_\theta(\mathbf{q}) \mid h_\theta(\mathbf{q}) \rangle = \sum_i c_{i\theta}^2 \kappa_i \equiv \chi \tag{2.4}$$

where the fluctuation formula $\langle n_i(\mathbf{q}) \mid n_j(\mathbf{q}) \rangle = \langle (\delta n_i)^2 \rangle\, \delta_{ij} \equiv \kappa_i \delta_{ij}$ has been used. The diffusivity $\Lambda_\theta(\hat{q}) = \hat{q}_\alpha \hat{q}_\beta \xi_{\alpha\beta}(\boldsymbol{\theta})$ depends on the second-rank tensor field $\xi_{\alpha\beta}(\boldsymbol{\theta}) = \xi_1(\delta_{\alpha\beta} - \hat{\theta}_\alpha \hat{\theta}_\beta) + \xi_2 \hat{\theta}_\alpha \hat{\theta}_\beta$. For all lattices with inversion symmetry this tensor contains two scalar diffusion coefficients ξ_1 and ξ_2, so that $\Lambda_\theta(\hat{q}) = \xi_1 + (\xi_2 - \xi_1)(\hat{q} \cdot \hat{\theta})^2$. They are given by

$$\begin{aligned} \xi_1 &= \lim_{s \to 0} \lim_{q \to 0} \chi^{-1} \sum_{i,j} c_{i\perp} c_{i\theta} [\tilde{\Gamma}(\mathbf{q} + \pi\boldsymbol{\theta}, s + \pi i) - \tfrac{1}{2}]_{ij}\, c_{j\perp} c_{j\theta} \\ \xi_2 &= \lim_{s \to 0} \lim_{q \to 0} \chi^{-1} \sum_{i,j} c_{j\theta}^2 [\tilde{\Gamma}(\mathbf{q} + \pi\boldsymbol{\theta}, s + \pi i) - \tfrac{1}{2}]_{ij}\, c_{j\theta}^2 \end{aligned} \tag{2.5}$$

provided the limits in (2.2) exist. Furthermore, $c_\perp = \hat{\theta}_\perp \cdot \mathbf{c}$ with $\hat{\theta}_\perp$ a unit vector perpendicular to $\boldsymbol{\theta}$. These coefficients can be split into two parts, the kinetic part ξ^k and the propagation part ξ^p, defined as

$$\begin{aligned} \xi_1^p &= \xi_1 - \xi_1^k = -\tfrac{1}{2} \sum_i c_{i\perp}^2 c_{i\theta}^2 \\ \xi_2^p &= \xi_2 - \xi_2^k = -\tfrac{1}{2} \sum_i c_{i\theta}^4 \end{aligned} \tag{2.6}$$

From here on we restrict the presentation to *athermal models* where energy and number conservation are equivalent (single-speed models) or where energy is not conserved at all. In both cases $\langle n_i \rangle \equiv f = \rho/b$ is the reduced density ($0 \leqslant f \leqslant 1$) and ρ the average occupation per site. Furthermore,

$$\begin{aligned} \kappa &= \langle (\delta n_i)^2 \rangle = f(1 - f) \\ \chi &= \kappa \sum_i c_{i\theta}^2 = \kappa \sum_i c_{ix}^2 \equiv \kappa b c_0^2 \end{aligned} \tag{2.7}$$

for a b-bit d-dimensional model with sound velocity c_0.

To display clearly the difference between the staggered diffusivities (2.2) and the standard transport coefficients, we also quote the Green–Kubo relation for the standard transport coefficients,

$$L = \lim_{s \to 0} \lim_{q \to 0} \chi^{-1} \sum_{i,j} w(\mathbf{c}_i)[\tilde{\Gamma}(\mathbf{q}, s) - \tfrac{1}{2}]_{ij} w(\mathbf{c}_j) \tag{2.8}$$

With the choices $w(\mathbf{c}) = c_x c_y$ and $w(\mathbf{c}) = d^{-1}c^2 - c_0^2$ we obtain, respectively, the shear ($L = \eta/\rho$) and bulk viscosity ($L = \zeta/\rho$).

It should be noted that the formulas for ξ_1 and ξ_2 as quoted in Eq. (5.13) of ref. 6 are not entirely correct, but that for $\Lambda_\theta(\hat{q})$ is correct. Also, Zanetti's formula[2] for $\Lambda_\theta(\hat{q})$ contains a misprint.[17] The "projected" current $\tilde{J}_j^i$ in his Eq. (16) should be replaced by the current J_j^i as given in (2.2).

3. KINETIC EQUATION

The time evolution of CA-fluids consists of a collision step over the time interval (t^-, t^+) with $t^\pm = t \pm \varepsilon$ $(\varepsilon \downarrow 0)$ and a propagation step over the interval $(t^+, t^- + 1)$. The *collision* step can be represented by

$$n_i(\mathbf{r}, t^+) - n_i(\mathbf{r}, t^-) = I_i(n(t^-)) \tag{3.1}$$

and the *propagation* step by

$$n_i(\mathbf{r}, t^+) = n_i(\mathbf{r} + \mathbf{c}_i, t^- + 1) \equiv S n_i(\mathbf{r}, t^- + 1) \tag{3.2}$$

where S is the free streaming operator.

The collision term is nonlinear in the occupation numbers, i.e., in a b-bit model, $I_i(n)$ contains at most b δn's, each referring to a different velocity channel. Its explicit form has been discussed extensively in the literature[15,16] for different sets of collision rules, lattices, and dimensionalities. The collision rules may be deterministic or stochastic; they conserve particle number and momentum, but not necessarily energy. From now on all occupation numbers $n_i(\mathbf{r}, t) = n_i(\mathbf{r}, t^+)$ refer to *postcollision states* and the combined evolution equations (3.1) and (3.2) can be expressed as

$$n_i(\mathbf{r}, t + 1) = n_i(\mathbf{r} - \mathbf{c}_i, t) + I_i(S^{-1} n(t)) \tag{3.3}$$

By iterating this equation t times, one obtains the formally exact series for $n_i(\mathbf{r}, t)$ expressed as a polynomial of degree b^t in the occupation numbers $n_k(\mathbf{r}', 0)$. This series can be substituted in (2.3) to obtain the exact time evolution of the kinetic propagator $\tilde{\Gamma}(\mathbf{q}, s)$.

Here we only consider the approximation of uncorrelated collisions, also referred to as the mean field or Boltzmann approximation. It implies that one *neglects* the occurrence of recollisions of particles that did collide before. Therefore any term of degree m ($1 \leqslant m \leqslant b^t$) in this approximate series contains m occupation numbers referring to m *different* one-particle states $\{\mathbf{r}', \mathbf{c}_{i'}\}$. In the same approximation the kinetic propagator (2.3) can be calculated straightforwardly by multiplying the approximate series for $\delta n_i(\mathbf{r}, t)$ by $\delta n_j(\mathbf{0}, 0)$ and averaging over an equilibrium ensemble. Using the property $\langle n_l(\mathbf{r}', 0)\, \delta n_j(\mathbf{0}, 0)\rangle = \kappa \delta_{lj} \delta_{r'0}$, one can factorize the average of a product of n's into a sum of products, i.e.,

$$\left\langle \delta n_j(\mathbf{0}) \prod_{l=1}^{m} n_l(\mathbf{r}_l) \right\rangle = \kappa f^{m-1} \sum_{l=1}^{m} \delta_{lj} \delta_{\mathbf{r}_l \mathbf{0}} \tag{3.4}$$

where $f = \langle n_i \rangle$ and one can resum the series as a tth power of a single-time-step evolution. This mean field approximation is implemented most simply in Eq. (3.3) by making the replacement $n_i = f + \delta n_i$. The collision term becomes

$$I_i(n) = I_i(f) + \sum_k \Omega_{ik} \delta n_k + \sum_{k,l} \Omega_{ikl} \delta n_k \delta n_l + \cdots \tag{3.5}$$

and one *neglects* all nonlinear terms in δn_i. On account of the relation $I_i(f) = 0$, the time evolution for uncorrelated collisions becomes

$$\delta n_i(\mathbf{r}, t+1) = \delta n_i(\mathbf{r} - \mathbf{c}_i, t) + \sum_j \Omega_{ij} \delta n_j(\mathbf{r} - \mathbf{c}_j, t) \tag{3.6}$$

After Fourier–Laplace transformation [see (2.3)], we obtain the solution

$$\tilde{n}_i(\mathbf{q}, s) = \sum_k [\exp(s + i\mathbf{q} \cdot \mathbf{c}_i)] \left(\frac{1}{\exp(s + i\mathbf{q} \cdot \mathbf{c}) - 1 - \Omega} \right)_{ik} n_k(\mathbf{q}, 0) \tag{3.7}$$

where $(A(c))_{ij} = A(c_i)\, \delta_{ij}$ is a diagonal matrix. Substitution of (3.7) into (2.3) and use of the relation $\langle n_i(\mathbf{q}, 0) \mid n_j(\mathbf{q}, 0)\rangle = \kappa \delta_{ij}$ yields for the kinetic propagator in the *mean field approximation*,

$$\tilde{T}_{ij}(\mathbf{q}, s) = [\kappa \exp(s + i\mathbf{q} \cdot \mathbf{c}_i)] \left(\frac{1}{\exp(s + i\mathbf{q} \cdot \mathbf{c}) - 1 - \Omega} \right)_{ij} \tag{3.8}$$

In the same approximation the staggered diffusivities become

$$\begin{aligned} \xi_1 &= -\frac{\kappa}{\chi} \sum_{i,j} c_{i\perp} c_{i\theta} \left(\frac{1}{\Delta + \Omega} + \frac{1}{2} \right)_{ij} c_{j\perp} c_{j\theta} \\ \xi_2 &= -\frac{\kappa}{\chi} \sum_{i,j} c_{i\theta}^2 \left(\frac{1}{\Delta + \Omega} + \frac{1}{2} \right)_{ij} c_{j\theta}^2 \end{aligned} \tag{3.9}$$

where $\Delta_{ij} = \Delta_i \delta_{ij} = [1 - \exp(i\pi + i\pi\boldsymbol{\theta} \cdot \mathbf{c}_i)]\, \delta_{ij}$ is a diagonal matrix. We further used the relation

$$c_{i\theta} \exp(i\pi\boldsymbol{\theta} \cdot \mathbf{c}_i) = \hat{\theta} \cdot \mathbf{c}_i (-)^{\boldsymbol{\theta} \cdot \mathbf{c}_i} = -c_{i\theta}$$

because the definition of the reciprocal lattice vectors $\boldsymbol{\theta}$ guarantees that $\boldsymbol{\theta} \cdot \mathbf{c}_i$ equals ± 1 or 0 for all i. Consequently, $\Delta_i = 1 + (-)^{\boldsymbol{\theta} \cdot \mathbf{c}_i}$ is either $+2$ or 0. In a similar fashion one finds for the standard transport coefficients

$$L = -\frac{\kappa}{\chi} \sum_{ij} w(\mathbf{c}_i) \left(\frac{1}{\Omega} + \frac{1}{2} \right)_{ij} w(\mathbf{c}_j) \tag{3.10}$$

Schmitz and Dufty[18] have shown that the matrix of transport coefficients is nonnegative definite. This implies that the eigenvalues λ_α of Ω, defined as

$$\Omega u_\alpha = -\lambda_\alpha u_\alpha \tag{3.11}$$

satisfy the inequalities $0 \leqslant \lambda_\alpha \leqslant 2$.

4. DIAGONALIZATION OF Ω FOR THE FHP MODELS

In this section we construct a basis of eigenvectors for Ω in the six-bit and seven-bit FHP models, defined on the triangular lattice by orthogonalizing the tensor products $c_\alpha c_\beta c_\gamma \cdots$ ($\alpha, \beta, \gamma, \ldots = x, y$). No restrictions are required on the collision rules except that they support the conservation laws of number and momentum and that they are invariant under the group of symmetry transformations of the triangular lattice, being rotations over $\pi/3$ and reflections in the x and y axes.

Let us start with the seven-bit model. We label the velocities as $\mathbf{c}_0 = (0, 0)$, $\mathbf{c}_i = (\cos \frac{1}{3}\pi(i-1),\ \sin \frac{1}{3}\pi(i-1))$, $i = 1, 2, \ldots, 6$. The eigenvectors associated with the conservation laws (where $\lambda_\alpha = 0$) are

$$\begin{aligned} u_1 &= 1 = (1, 1, 1, 1, 1, 1, 1) \\ u_2 &= c_x = \tfrac{1}{2}(0, 2, 1, -1, -2, -1, 1) \\ u_3 &= c_y = \tfrac{1}{2}\sqrt{3}\,(0, 0, 1, 1, 0, -1, -1) \end{aligned} \tag{4.1}$$

We complete the basis with the following vectors:

$$\begin{aligned} u_4 &= c_x c_y = \tfrac{1}{4}\sqrt{3}\,(0, 0, 1, -1, 0, 1, -1) \\ u_5 &= c_x^2 - c_y^2 = \tfrac{1}{2}(0, 2, -1, -1, 2, -1, -1) \\ u_6 &= (4c_x^2 - 3)\, c_x = (0, 1, -1, 1, -1, 1, -1) \\ u_7 &= \tfrac{1}{2}c^2 - c_0^2 = \tfrac{1}{14}(-6, 1, 1, 1, 1, 1, 1) \end{aligned} \tag{4.2}$$

where the sound velocity c_0 for the seven-bit FHP models is given by $c_0^2 = \frac{3}{7}$ on account of Eq. (2.7). These vectors form a complete orthogonal basis of the seven-dimensional space.

The next step is to prove that these vectors are eigenvectors of Ω. To do this, we construct Table I, showing how the vectors $u_4,\ldots, u_7$ change under rotations and reflections, operations that leave Ω invariant (the double arrow indicates invariant subspaces under the action of the symmetry transformation). Notice that these symmetry transformations are simply permutations of the second through seventh component of the 7-vectors in (4.1)–(4.2). Consider first the reflections in that table. The signs show that $\{u_4\}$, $\{u_6\}$, $\{u_5, u_7\}$ are invariant subspaces under the action of Ω. The rotations over $\pi/3$ decompose the $\{u_5, u_7\}$ subspace into two one-dimensional invariant subspaces because u_7 has a well-defined parity, but u_5 does not. Then, the seven-dimensional space has been decomposed into seven one-dimensional invariant subspaces of Ω. As a consequence, Ω is diagonal in this basis.

From Table I more information can be obtained using the invariance of Ω under a rotation over $\pi/3$. A rotation over $\pi/3$ applied to u_4 gives a linear combination of u_4 and u_5 and vice versa. Using that both u_4 and u_5 are eigenvectors, it is easily proved that $\lambda_4 = \lambda_5$.

For the six-bit model the proof proceeds in a similar fashion. Here one has a six-dimensional basis obtained from (4.1) and (4.2) by dropping the *first* component. The vector u_7 vanishes identically because $2c_i^2 = c_0^2 = 1$ for all i. Table I remains valid. By analyzing the reflections, it follows that $\{u_4\}$, $\{u_5\}$, $\{u_6\}$ are invariant subspaces. The eigenvalues for the FHP-I, II, and III models are listed in Table II.

The use of this eigenvector basis greatly simplifies all calculations.

Table I. Symmetries of the Linearized Collision Operator Ω and the Transformation of $u_4,\ldots, u_7$ under these Operations[a]

	u_4		u_5	u_6	u_7
Reflection Y $(x \to -x)$	−		+	−	+
Reflection X $(y \to -y)$	−		+	+	+
Rotation $\pi/3$		$\Leftrightarrow$		−	+
Rotation $2\pi/3$		$\Leftrightarrow$		+	+
Rotation π	+		+	−	+

[a] The double arrow means that u_4 is written as a linear combination of u_4 and u_5 and vice versa under rotations of $\pi/3$ and $2\pi/3$. For six-bit models the table remains valid except for the last column (see text).

Table II. Eigenvalues of the Linearized Collision Operator for the FHP Models[a]

	u_1, u_2, u_3	u_4, u_5	u_6	u_7
FHP-I	0	$3f(1-f)^3$	$6f^2(1-f)^2$	—
FHP-I′	0	$3\kappa(1+2\kappa)$	$6\kappa^2$	—
FHP-II	0	$f(1-f)^3(7-4f)$	$3f(1-f)^2(3f^2-4f+3)$	$7f(1-f)^4$
FHP-III	0	$\kappa(7-8\kappa)$	$3\kappa(3-4\kappa)$	$7\kappa(1-2\kappa)$

[a] The FHP-I′ model is a self-dual model constructed with the collision rules (200), (300), (320), and (400) of Table 1 of ref. 15. κ is defined as $f(1-f)$.

For example, the shear viscosity in (3.10) for all FHP models is simply

$$\frac{\eta}{\rho} = \nu = \frac{1}{3} u_4 \left(-\frac{1}{\Omega} - \frac{1}{2} \right) u_4 = \frac{1}{4} \frac{1}{\lambda_4} - \frac{1}{8} \tag{4.3}$$

where $\chi/\kappa = \sum_i c_{ix}^2 = 3$. Similarly, we obtain from (2.8) and (3.10) that the bulk viscosity vanishes for the FHP-I model and is given by

$$\frac{\zeta}{\rho} = \frac{1}{3} u_7 \left(-\frac{1}{\Omega} - \frac{1}{2} \right) u_7 = \frac{1}{14} \frac{1}{\lambda_7} - \frac{1}{28} \tag{4.4}$$

in FHP-II and III models.

5. MEAN FIELD VALUES OF STAGGERED DIFFUSIVITIES

To evaluate the staggered diffusion coefficients ξ_1 and ξ_2, we investigate the symmetry properties of the matrix $\Delta + \Omega = (-)^{1+\boldsymbol{\theta}\cdot\mathbf{c}} + 1 + \Omega$ appearing in (3.9). By symmetry, ξ_1 and ξ_2 are the same for $\boldsymbol{\theta}$, $\boldsymbol{\theta}'$, and $\boldsymbol{\theta}''$. It is convenient to choose a special coordinate system in which $c_{i\theta} = c_{iy}$ and $c_{i\perp} = c_{ix}$. Then Δ is invariant under reflection in the y axis ($x \to -x$) because $\boldsymbol{\theta}\cdot\mathbf{c} = c_y$ does not change its sign, but also under reflections in the x axis because $\boldsymbol{\theta}\cdot\mathbf{c}$ changes its sign, but $(-)^{\boldsymbol{\theta}\cdot\mathbf{c}}$ does not. The matrix Δ is no longer invariant under $\pi/3$ rotations. The analog of Table I is Table III. It shows how the vectors $u_1, \ldots, u_7$ change under transformations which leave $\Omega + \Delta$ invariant. Then, the invariant subspaces are $\{u_3\}$, $\{u_4\}$, $\{u_2, u_6\}$, $\{u_1, u_5\}$ for the FHP-I model and $\{u_3\}$, $\{u_4\}$, $\{u_2, u_6\}$, $\{u_1, u_5, u_7\}$ for the FHP-II and III models. Moreover, the vectors u_3 and u_4 are eigenvectors

$$(\Omega + \Delta) u_3 = \Omega u_3 = 0 \tag{5.1}$$

$$(\Omega + \Delta) u_4 = \Omega u_4 = -\lambda_4 u_4 \tag{5.2}$$

Table III. The Same as in Table I for the $(\Omega + \Delta)$ Operator[a]

	u_1	u_2	u_3	u_4	u_5	u_6	u_7
Reflection $Y(x \to -x)$	+	−	+	−	+	−	+
Reflection $X(y \to -y)$	+	+	−	−	+	+	+

[a] Now all the vectors are displayed because u_1, u_2, and u_3 are no longer eigenvectors of $(\Omega + \Delta)$.

where the explicit form of the diagonal matrix $\Delta_{ij} = \Delta_i \delta_{ij}$ with $\Delta_i = (2, 2, 0, 0, 2, 0, 0)$ for the seven-bit models. In the six-bit models, the first component of Δ_i above is simply dropped.

Equation (5.2) shows that the current $u_4 = c_x c_y$ is a simultaneous eigenfunction of $(\Omega + \Delta)$ and Ω with the same eigenvalue. Consequently, the shear viscosity η/ρ in (4.3) and the staggered diffusion coefficient ξ_1 are equal for all FHP models, and given by

$$\xi_1 = \frac{\eta}{\rho} = \frac{1}{3} u_4 \left(\frac{1}{\lambda_4} - \frac{1}{2} \right) u_4 = \frac{1}{4} \frac{1}{\lambda_4} - \frac{1}{8} \tag{5.3}$$

The calculation of ξ_2 in (3.9) is somewhat more involved because $c_{i\theta}^2 = c_{iy}^2$ is not an eigenfunction of $(\Omega + \Delta)$. From the symmetry properties of the different subspaces we deduce for the six-bit models that $(\Omega + \Delta)^{-1} c_y^2$ lies in the $\{u_1, u_5\}$ subspace

$$(\Omega + \Delta)^{-1} c_y^2 = a_1 u_1 + a_5 u_5 \tag{5.4}$$

We multiply this equation with $u_1(\Omega + \Delta)$ and $u_5(\Omega + \Delta)$, respectively, and calculate the matrix elements $\Delta_{11} = \Delta_{15} = \Delta_{55} = 4$, where $\Delta_{\alpha\beta} = u_\alpha \Delta u_\beta$ are the matrix elements of Δ in the representation (4.1) and (4.2). Then we obtain two coupled linear equations with solution $a_5 = 3/2\lambda_5 = 3/4 - a_1$. The staggered diffusivity ξ_2 in the six-bit models follows then from (3.9), (5.3), and (4.2), with the result

$$\xi_2 = \frac{9}{4} \left(\frac{1}{\lambda_5} - \frac{1}{2} \right) \tag{5.5}$$

where λ_5 for FHP-I and its self-dual extension FHP-I′ are given in Table II.

In the seven-bit models we deduce similarly

$$(\Omega + \Delta)^{-1} c_y^2 = b_1 u_1 + b_5 u_5 + b_7 u_7 \tag{5.6}$$

The three coupled linear equations are solved for b_1, b_5, b_7 and Eq. (5.6) is inserted into (3.9). This yields for the staggered diffusivity in the seven-bit models

$$\xi_2 = \frac{63}{8} \frac{(2-\lambda_5)(2-\lambda_7)}{14\lambda_5 + 4\lambda_7 - 9\lambda_5\lambda_7} \tag{5.7}$$

with λ_5 and λ_7 given in Table II for the FHP-II and FHP-III model. For the special case of the FHP-III model these results agree with those of Zanetti.

A comment should be made about the first Enskog approximation to the staggered and standard transport coefficients in (3.9) and (3.10). It comes down to assuming that the current $w(c)$ in (3.10) and the currents $c_x c_y$ and c_y^2 in (3.9) are approximate eigenvectors of Ω and $(\Omega + \Delta)$, respectively. In the models discussed here $w(c)$ and $c_x c_y$ are exact eigenvectors of, respectively, Ω and $\Omega + \Delta$. So the first Enskog approximation gives here the exact result for η, ζ, and ξ_1.

For most intermolecular potentials the first Enskog approximation is an excellent approximation (correct within a few percent) to calculate

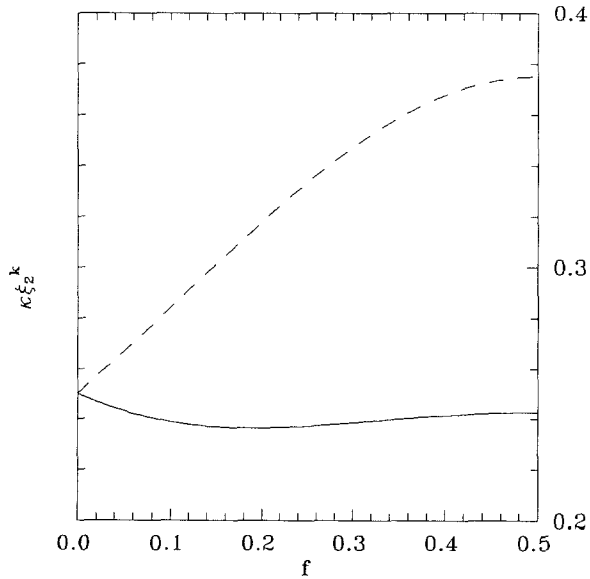

Fig. 1. The kinetic part ξ_2^k of the staggered diffusivity defined in Eq. (2.6) versus reduced density in the self-dual FHP-III model. The solid line corresponds to the exact Boltzmann value and the dashed line to the first Enskog approximation. Both curves coincide in the low-density limit ($f \to 0$).

viscosities, heat conductivity, and diffusion coefficients.[19] To test this approximation on the staggered diffusivity ξ_2 in (3.9), we assume that $(\Omega + A)^{-1} c_y^2 \simeq A c_y^2$ with $A^{-1} = c_y^2(\Omega + A) c_y^2 / c_y^2 c_y^2$. Proceeding then in the same manner as in (5.4) and (5.6), we obtain the first Enskog approximation to ξ_2^k in the FHP-III model, i.e.,

$$\xi_2^{\mathrm{CE}} - \xi_2^p = [4\kappa(1 - \tfrac{4}{3}\kappa)]^{-1} \tag{5.8}$$

The left-hand side of (5.8) is plotted in Fig. 1 versus the reduced density f and compared with the exact Boltzmann value (5.7). As $f \to 0$, the quantity $[\xi_2^k]_{\mathrm{CE}}$ approaches ξ_2^k, as can be seen analytically from (5.7). However, at higher densities the first Enskog approximation to ξ_2^k is a very poor approximation. It is typically 50–80% larger than the exact value (5.7).

In summary, we have presented in this paper a simple method to compute both the standard and the staggered diffusion coefficients directly from the Green–Kubo relations. The method exploits the symmetries of the collision rules and, consequently, of the underlying lattice. It can be extended to the FCHC and the temperature-dependent nine-bit model with minor changes. The results for these models will be presented elsewhere.

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