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Thermal Cellular Automata Fluids

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The concepts of local temperature and local thermal equilibrium are introduced in the context of lattice gas cellular automata (LGGAs) whose dynamics conserves energy. Green–Kubo expressions for thermal transport coefficients, in particular for the heat conductivity, are derived in a form, equivalent to those for continuous fluids. All thermal transport coefficients are evaluated in Boltzmann approximation as thermal averages of matrix elements of the inverse Boltzmann collision operator, fully analogous to the results for continuous systems, and fully model-independent. The collision operator is expressed in terms of transition probabilities between in- and out-states. Staggered diffusivities arising from spuriously conserved quantities in LGCAs are also calculated. Examples of models with either cubic or hexagonal symmetries are discussed, where particles may or may not have internal energies.

KEY WORDS: Thermal lattice gas; cellular automata; temperature definition; Green–Kubo formula; heat conductivity; diffusion coefficient; speed of sound.

1. INTRODUCTION

Lattice gas cellular automata (LGCAs) form interesting statistical mechanical models$^{(1,2)}$ with extremely simplified dyanmics. They consist of many interacting particles moving on a regular space lattice with a small set of different speeds. These models are being used for simulating nonequilibrium fluid flow on a computer. In the earlier versions of LGCAs$^{(1)}$ all particles had the same speed apart from rest particles. Energy was either not conserved or just corresponded to number conservation. Therefore *temperature* did not exist for such systems. Later, multiple-

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speed models were introduced in order to have systems with microscopic energy conservation, temperature, temperature gradients, and heat conductivity.(3–11) The LGGA has the same conserved densities as the continuous fluid, i.e., mass, momentum, and energy density.

The goals of this paper are: (i) To introduce in the context of lattice gases the concepts of local temperature T and local thermal equilibrium, consistent with thermodynamics and statistical mechanics. (ii) To derive in a systematic, model-independent fashion Green–Kubo formulas for thermal transport coefficients in accordance with irreversible thermodynamics,(12) in particular for the heat conductivity of such LGCAs, following the method of ref. 13 for athermal LGCA's. (iii) To evalulate the transport coefficients in Boltzmann approximation as thermal averages of matrix elements of the inverse collision operator, fully analogous to the results for continuous fluids and fully model-independent,(14) (iv) To illustrate the results for lattice gases with cubic or hexagonal symmetry and for particles with or without internal energy. For one of the models we present some explicit results.

Although there exist scattered results(3–11) for specific models, none of the above issues has been systematically addressed in the lattice gas context. We also like to emphasize the importance of defining temperature in accordance with thermodynamics and statistical mechanics, and of defining thermodynamic driving forces and corresponding transport coefficients in accordance with irreversible thermodynamics.(12) Frequently nonstandard definitions of temperature(6,7) and thermal transport coefficients(3,8) are used in the lattice gas literature.

The equilibrium statistical mechanics of thermal LGCAs, when formulated in terms of occupation numbers for the different sites and velocity channels, is essentially that of an ideal Fermi gas (see Section 2); there are no statistical correlations between occupation numbers of different channels or different sites. The study of LGCAs out of equilibrium is very similar to that of continuous fluids. The concept of local temperature(2) in a nonequilibrium LGCA is introduced through the concept of *local equilibrium*, and not by setting the kinetic energy or pressure proportional to T.(3,6) In any ideal Fermi gas the kinetic energy is a nontrivial function of density and temperature. In lattice gases it is even bounded from above because of the finite number of one-particle states per site. The equations of motion for the conserved densities constitute the usual set of hydrodynamic equations. In the present paper we consider linear transport. Thus, the dissipative fluxes in the hydrodynamic equations are proportional to the gradients of the thermodynamic fields and can be expressed in the form of the linear constitutive relations of irreversible thermodynamics.(12)

Owing to the discrete nature of space and time, an LGCA is usually plagued by additional conserved quantities$^{(15)}$ as compared to continuous fluid. They give rise to slowly varying local densities, and hence the usual set of hydrodynamic equations has to be extended by additional equations of motion for the spuriously conserved quantities which involve extra transport coefficients for the LGCA.

In Section 3 we present the lattice gas generalization of the Green–Kubo formulas when compared with the heat conductivity and other thermal transport coefficients, which are supposedly valid for any d-dimensional space lattice with an arbitrary number of different velocity states, and collision rules conserving energy, particle number, and linear momentum. The energy ε_i assigned to a particle may be purely kinetic, or partly kinetic and partly internal. The heat conductivity, being a second-rank tensor, is isotropic on lattices with cubic or hexagonal symmetry. The appearance of the energy as a new conserved variable in thermal LGCAs also induces drastic changes in the explicit form of the currents in the Green–Kubo formulas when compared to athermal models.

The Green–Kubo formulas are given in terms of time correlation functions, measured in equilibrium states described by the canonical or grand canonical Gibbs distribution. We want to emphasize that these formulas should not be applied without further justification to systems with collision rules or transition rates that do not satisfy (semi)-detailed balance$^{(1)}$ with respect to the Gibbs distribution. In such systems the structure of the local and global equilibrium state is an open problem.

Section 4 is devoted to extending kinetic theory methods to lattice gases, starting with the Boltzmann approximation. Subsequently one may implement the ring approximation as recently developed for two- and three-dimensional athermal LGCAs.$^{(16-18)}$ The Boltzmann approximation, as presented here, generalizes Hènon's formula$^{(19)}$ for the viscosity in athermal LGCAs to arbitrary transport coefficients for LGCAs with temperature. It is independent of any specific model and lattice symmetry.

The third part of the paper (Section 4) gives three different examples of thermal lattice gases with different lattice symmetries and with or without internal energies and shows some numerical results. We end with a discussion in Section 5.

2. THERMODYNAMICS OF THERMAL LATTICE GASES

2.1. Microdynamics

Lattice gas cellular automata consist of a collection of N particles with a finite number of b different velocities, which can be at the sites of a regular d-dimensional lattice with V sites and periodic boundary conditions. Its state is specified by the set of occupation numbers $n(\mathbf{c}, \mathbf{r}, t)$, where $n(\mathbf{c}, \mathbf{r}, t) = 1$ if the single-particle state $(\mathbf{c}, \mathbf{r})$ is occupied and 0 otherwise. The collision rules are deterministic or stochastic and obey the usual conservation laws of number $N = \sum_{rc} n(\mathbf{c}, \mathbf{r}, t)$, momentum $\mathbf{P} = \sum_{rc} \mathbf{c} n(\mathbf{c}, \mathbf{r}, t)$, and energy $H = \sum_{rc} \varepsilon(c)\, n(\mathbf{c}, \mathbf{r}, t)$. Here $\varepsilon(c) = \frac{1}{2}c^2 + \varepsilon_0(c)$ is the energy of a particle in state $\mathbf{c}$, which may include an internal energy $\varepsilon_0(c)$, depending on the model considered. Possible spurious conservation laws, which are artifacts of the discrete structure of space and time, must also be included$^{(13)}$ (see Section 3.3).

The time evolution of the LGCA can be expressed by the microdynamic equation

$$n(\mathbf{c}, \mathbf{r} + \mathbf{c}, t + 1) = n(\mathbf{c}, \mathbf{r}, t) + I_c(n(t)) \tag{2.1}$$

where $I_c(n(t))$ denotes the collision terms in velocity channel $\mathbf{c}$. It depends in a nonlinear fashion on the occupation numbers $n(\mathbf{c}, \mathbf{r}, t)$ at site $\mathbf{r}$ with $\mathbf{c} = \{\mathbf{c}_0, \mathbf{c}_1, \mathbf{c}_2, ..., \mathbf{c}_{b-1}\}$, the bit number b being the number of velocity states per site. The conservation laws imply the relation

$$\sum_c a(\mathbf{c})\, I_c(n(t)) = 0 \tag{2.2}$$

where $a(\mathbf{c}) = \{1, \mathbf{c}, \varepsilon(c), ...\}$ are the collisional invariants. It ensures the existence of local conservation laws with the locally conserved *microscopic* densities, denoted by a caret,

$$\hat{a}(\mathbf{r}, t) = \sum_c a(\mathbf{c})\, n(\mathbf{c}, \mathbf{r}, t) \tag{2.3}$$

For the three collisional invariants listed above, $\hat{a}$ consists of the set $\{\hat{\rho}, \hat{\mathbf{g}}, \hat{e}\}$, where $\hat{\rho}$ is the mass density, $\hat{\mathbf{g}}$ is the momentum density, and $\hat{e}$ is the total energy density. These correspond, respectively, to the conserved quantities $\{N, \mathbf{P}, H\}$, where N is the total number of particles, $\mathbf{P}$ is the total momentum, and H is the total energy of the system.

2.2. Equilibrium Properties

In thermal equilibrium, the state of a lattice gas is conveniently described by a grand ensemble with a phase space density proportional to $\exp(\mathbf{b} \cdot \mathbf{A})$, where $\mathbf{A} = \{N, H, \mathbf{P}, \mathbf{A}_s\}$ includes all spurious invariants $\mathbf{A}_s$ and all physical ones, and $\mathbf{b} = \{\alpha, -\beta, \gamma, \mathbf{b}_s\}$ denotes all conjugate thermodynamic variables. By setting $\gamma = 0$ and $\mathbf{b}_s = 0$, one ensures that

$\langle \mathbf{P} \rangle = 0$ and $\langle \mathbf{A}_s \rangle = 0$, and the ensemble reduces to the grand canonical ensemble with a phase space density proportional to $\sim \exp(\alpha N - \beta H)$.

In equilibrium, the LGCA is very similar to an ideal Fermi gas. The distribution function or the average occupation of a single-particle state with velocity $\mathbf{c}$ at site $\mathbf{r}$ is given by

$$f^0(c) = \langle n(\mathbf{c}, \mathbf{r}) \rangle = \{1 + \exp[-\alpha + \beta \varepsilon(c)]\}^{-1} \tag{2.4}$$

where $\beta = 1/k_B T$ is the inverse temperature and α/β the chemical potential. The density $\rho = \sum_c f^0(c)$ is restricted to $0 < \rho < b$, where b is the bit number. The equilibrium correlations of the fluctuations $\delta n(\mathbf{c}, \mathbf{r})$ are entirely determined by Fermi statistics and there are no spatial correlations in a lattice gas, i.e.,

$$\begin{aligned} \langle \delta n(\mathbf{c}, \mathbf{r})\, \delta n(\mathbf{c}', \mathbf{r}') \rangle &= \kappa(c)\, \delta_{cc'} \delta_{rr'} \\ \kappa(c) &= f^0(c)[1 - f^0(c)] \end{aligned} \tag{2.5}$$

From these results there follow immediately the equilibrium properties of the thermal lattice gases, such as pressure p and entropy per particle s, i.e.,

$$\begin{aligned} p &= (1/d) \sum_c c^2 f^0(c) \\ \rho s &= \sum_c \{ f^0(c) \ln[f^0(c)] + [1 - f^0(c)] \ln[1 - f^0(c)] \} \end{aligned} \tag{2.6}$$

and the speed of sound $c_0^2 = (\partial p / \partial \rho)_s$.

2.3. The Local Equilibrium Distribution

The *nonequilibrium state* of a continuous fluid or LGCA can be described at the macroscopic level by the *average* local densities of number, energy, and momentum, $a(\mathbf{r}, t) = \langle \hat{a}(\mathbf{r}, t) \rangle_{\mathrm{ne}}$, where the average is taken over a nonequilibrium ensemble. These quantities are slowly varying in space and time. A state of *local equilibrium* is described by the local equilibrium distribution,

$$\langle n(\mathbf{c}, \mathbf{r}) \rangle_l = f_l(\mathbf{c}, \mathbf{r}) = \{1 + \exp[-b(\mathbf{r}) \cdot a(\mathbf{c})]\}^{-1} \tag{2.7}$$

The set of thermodynamic fields $b(\mathbf{r}, t) = \{\alpha(\mathbf{r}, t), -\beta(\mathbf{r}, t), \gamma(\mathbf{r}, t), \mathbf{b}_s(\mathbf{r}, t)\}$ are conjugate to the *average* or *macroscopic* densities $a(\mathbf{r}, t) = \{\rho(\mathbf{r}, t), e(\mathbf{r}, t), \mathbf{g}(\mathbf{r}, t) = \rho(\mathbf{r}, t)\, \mathbf{u}(\mathbf{r}, t), \mathbf{a}_s(\mathbf{r}, t)\}$. They are defined through the relations $a(\mathbf{r}, t) = \langle \hat{a}(\mathbf{r}, t) \rangle_l$, where the label l denotes an average calculated with the local equilibrium distribution.

The hydrodynamic equations for the macroscopic local densities $a(\mathbf{r}, t)$ are obtained[2] by averaging the microscopic local conversation laws (2.1) and by making leading-order expansions in the gradients of the thermodynamic fields around equilibrium. The local conservation laws for $a(\mathbf{r}, t)$ contain the local currents $\langle J_a(\mathbf{r}, t)\rangle_{\text{ne}}$, consisting of a nondissipative Euler part, $\langle J_a(\mathbf{r}, t)\rangle_l$, and a dissipative Navier–Stokes part, $\Delta J_a(\mathbf{r}, t)$. The latter part defines the linear transport coefficients $L_{aa'}$ through the constitutive relations[12]

$$\Delta J_a(\mathbf{r}, t) = -\sum_{a'} L_{aa'} \nabla b_{a'}(\mathbf{r}, t) \tag{2.8}$$

where $\{\nabla b_a\}$ is the set of thermodynamic driving forces. The Green–Kubo formulas for $L_{aa'}$ are discussed in the next section. These average equations are valid for long times and long distances and can be written in the form of the fluid dynamic equations.

3. THERMAL TRANSPORT COEFFICIENTS

3.1. Green–Kubo Relations

The presentation in this section strongly emphasizes that transport coefficients of thermal LGCAs are fully described by the well-known Green–Kubo formulas for continuous fluids[20,21] with a few minor adaptations for the discreteness of space and time. The transport coefficient $L_{aa'}$ for any d-dimensional thermal LGCA with point particles (single-site collisions) is given by the following Green–Kubo relation,[13]

$$L_{aa'} = \lim_{s\to 0} V^{-1} \sum_{t=0}^{\infty}{}^{*} e^{-st} \langle \hat{J}_a(t)\hat{J}_{a'}\rangle \tag{3.1}$$

where V is the total number of sites in the system whenever the linear transport coefficients exist. Two minor modifications of the Green–Kubo formulas for continuous fluids are: the appearance of an asterisk and of a discrete time sum instead of an integral. The asterisk on the summation indicates that the term with $t = 0$ has a weight 1/2. This same term, multiplied by (-1), is referred to in the lattice gas literature[1] as the *propagation part of the transport coefficient.*

Green–Kubo relations always contain *subtracted* current $\hat{\mathbf{J}} = \{\hat{J}_a\}$ which read in b-vector and $b \times b$-matrix notation

$$\begin{aligned}\hat{\mathbf{J}} &= \mathbf{J} - \delta\mathbf{A} \cdot \langle \delta\mathbf{A}\,\delta\mathbf{A}\rangle^{-1} \cdot \langle \delta\mathbf{A}\mathbf{J}\rangle \\ &= \sum_{r,c} \hat{\mathbf{j}}(\mathbf{c})\,\delta n(\mathbf{c}, \mathbf{r}, t)\end{aligned} \tag{3.2}$$

The explicit form of the single-particle current $\hat{\jmath}(c)$ will be specified when discussing specific transport coefficients. The unsubtracted current is

$$\mathbf{J} = \sum_{r,c} c_x \mathbf{a}(\mathbf{c})\, \delta n(\mathbf{c}, \mathbf{r}, t) \tag{3.3}$$

Here $\delta n(\mathbf{c}, \mathbf{r}, t) = n(\mathbf{c}, \mathbf{r}, t) - \langle n \rangle$ is the fluctuation of the occupation number around total equilibrium. The set of fluctuations of global invariants, $\delta \mathbf{A}$, includes not only N, H, $\mathbf{P}$ in thermal models, but *all* spurious invariants (spurious collisional invariants, staggered invariants, geometric or checkerboard invariants,...) of the model under consideration. Equation (3.2) implies the orthogonality relation $\langle \hat{\mathbf{J}}\, \delta \mathbf{A} \rangle = 0.$(13) The transport matrix $L_{aa'}$ of Green–Kubo formulas for CA fluids is a *nonnegative-definite* matrix, implying that $L_{aa} \geqslant 0$ for all a.(22) It also includes the spurious transport coefficients, connected with the spurious slow modes.

Next, we discuss the specific transport coefficients that appear in the fluid dynamic equations. The *heat conductivity* λ is defined as the coefficient of proportionality between the dissipative heat current and the temperature gradient, i.e., $\mathbf{q}^D = -\lambda\, \nabla T \equiv L_{TT} \nabla \beta$, with $L_{TT} = k_B T^2 \lambda$. In all thermal d-dimensional LGCAs with point particles the conductivity is given by L_{TT} in (3.1) with a subtracted heat current $\hat{J}_T$ calculated from (3.2). It satisfies the orthogonality relation $\langle \hat{J}_T \mathbf{P} \rangle = 0$. The single-particle current $\hat{\jmath}_T(\mathbf{c})$ introduced on the second line of (3.2) is

$$\hat{\jmath}_T(\mathbf{c}) = c_x(\varepsilon(c) - h) \tag{3.4}$$

The function h is the usual enthalpy per particle,(20,21)

$$\begin{aligned} h &= \frac{\langle J_{Tx} P_x \rangle}{\langle P_x^2 \rangle} = \frac{\sum_c c^2 \varepsilon(c)\, \kappa(c)}{\sum_c c^2 \kappa(c)} \\ &= \frac{\langle \delta p\, \delta H \rangle}{\langle \delta p\, \delta N \rangle} = \left(\frac{\partial \alpha}{\partial \beta}\right)_p = \left(\frac{\partial e}{\partial \rho}\right)_s \end{aligned} \tag{3.5}$$

where $\delta p = (dV)^{-1} \sum_{rc} c^2 \delta n(\mathbf{c}, \mathbf{r})$ and $\delta H = \sum_{rc} \varepsilon(c)\, \delta n(\mathbf{c}, \mathbf{r})$ are, respectively, the microscopic pressure and energy fluctuations. We also have used a number of thermodynamic identities that will be needed later. These formulas apply equally well to the continuous fluid, except the one with the discrete velocity summations.

Similarly, the fourth-rank viscosity tensor for the thermal LGCA relates the dissipative part of the stress tensor to the gradient of the flow field $\mathbf{u}$ through

$$\sigma^D_{\alpha\beta} = -\rho \nu_{\alpha\beta\gamma\delta} \nabla_\gamma u_\delta \tag{3.6}$$

where $\alpha\beta\gamma\delta = \{x, y, z, \dots\}$ label Cartesian components. Here $\mathbf{u}$ is related to the thermodynamic field $\boldsymbol{\gamma}$ by $\rho\mathbf{u} = \chi_g \boldsymbol{\gamma}$, and the susceptibility χ_g is given by $\chi_g = V^{-1}\langle P_x^2 \rangle = (1/d) \sum_c c^2 \kappa(c)$. The Green–Kubo relation for the viscosity tensor becomes then$^{(2)}$

$$\nu_{\alpha\beta\gamma\delta} = (V\chi_g)^{-1} \sum_{t=0}^{\infty}{}^{*}\, e^{-st} \langle \hat{J}_{\alpha\beta}(t) \hat{J}_{\gamma\delta} \rangle \tag{3.7}$$

with the subtracted current $\hat{J}_{\alpha\beta}$ defined through

$$\begin{aligned} \hat{J}_{\alpha\beta} &= J_{\alpha\beta} - \delta_{\alpha\beta} \left(\frac{\partial p}{\partial e}\right)_{\rho} \delta H - \delta_{\alpha\beta} \left(\frac{\partial p}{\partial \rho}\right)_{e} \delta N \\ \hat{j}_{\alpha\beta} &= c_\alpha c_\beta - \delta_{\alpha\beta} \left(\frac{\partial p}{\partial e}\right)_{\rho} \varepsilon(c) - \delta_{\alpha\beta} \left(\frac{\partial p}{\partial \rho}\right)_{e} \end{aligned} \tag{3.8}$$

The second line defines the one-particle current $\hat{j}$ as in (3.2). The subtracted current on the first line is the same as for the continuous fluid,$^{(20,21)}$ but very different from that of an athermal LGCA, where energy is not a conserved variable. For comparison we quote the current for the *athermal* (AT) models,

$$\begin{aligned} \hat{J}^{\mathrm{AT}}_{\alpha\beta} &= J_{\alpha\beta} - \delta_{\alpha\beta} \left(\frac{dp}{d\rho}\right) \delta N \\ \hat{j}^{\mathrm{AT}}_{\alpha\beta} &= c_\alpha c_\beta - \delta_{\alpha\beta} \left(\frac{dp}{d\rho}\right) \end{aligned} \tag{3.9}$$

where $(dp/d\rho) = c_0^2$ determines the sound velocity in athermal models.

So far we have not used the symmetry of the underlying lattice. First we consider a lattice with cubic symmetry. Then the viscosity tensor involves in general three independent viscosities,

$$\nu_{\alpha\beta\gamma\delta} = \nu\{\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma} - 2\delta^{(4)}_{\alpha\beta\gamma\delta}\} + 2\vartheta\left\{\delta^{(4)}_{\alpha\beta\gamma\delta} - \frac{1}{d}\delta_{\alpha\beta}\delta_{\gamma\delta}\right\} + \zeta\delta_{\alpha\beta}\delta_{\gamma\delta} \tag{3.10}$$

The cubic invariant tensor $\delta^{(4)}_{\alpha\beta\gamma\delta}$ is equal to 1 if all indices $\alpha, \beta, \gamma, \delta$ are equal, and is zero otherwise. The Green–Kubo formulas for the *shear viscosity* $\nu = \nu_{xyxy}$ and *cubic viscosity* $\vartheta = \nu_{xxxx}$ can be obtained from (3.7) and (3.8). They are given by diagonal elements of the transport matrix. The explicit expressions for the corresponding single-particle currents are, respectively,

$$\begin{aligned} \hat{j}_{xy}(\mathbf{c}) &= c_x c_y \\ \hat{j}_{xx}(\mathbf{c}) &= \tfrac{1}{2}(c_x^2 - c_y^2) \end{aligned} \tag{3.11}$$

The viscosity ϑ is, for instance, of physical significance in the absorption coefficients of elastic waves in the hard-sphere solid, which orders into a hexagonally closed-packed lattice at sufficiently high density.$^{(23)}$

The bulk viscosity $\zeta = (1/d^2)\nu_{\alpha\alpha\beta\beta}$ is obtained by contraction of (3.10). The first and second terms on the right-hand side are traceless tensors. Combination of (3.6) and (3.10) shows that the trace of the stress tensor, $\sigma^D_{\gamma\gamma} = -\zeta \nabla \cdot \mathbf{u}$, only involves the bulk viscosity ζ. This is also the standard definition of bulk viscosity in continuous fluids. Its Green–Kubo expression is given by (3.7) with a subtracted current $\hat{J}_{\alpha\alpha}$, which is the trace of (3.8).

If the underlying lattice is triangular, as in the two-dimensional FHP model, or face-centered hypercubic, as in the quasi-three-dimensional FCHC model,$^{(1)}$ then fourth-rank tensors such as (3.10) are isotropic and $\nu = \vartheta$. If one wants to study properties of isotropic fluid flow by means of lattice gases, one can approximately recover isotropy in the nonlinear Navier–Stokes equations by using the FHP or FCHC models, or by finetuning the available free parameters in cubic models so as satisfy the isotropy condition $\nu = \vartheta$.

3.2. Boltzmann Approximation

The Green–Kubo relations considered in the previous subsection are exact, provided the transport coefficients exist. They require the solution of the complete N-body dynamics (2.1). In the Boltzmann approximation the dynamics is only treated approximately, in the sense that ring collisions and other correlated collisions between particles are neglected. Very recently a more sophisticated ring kinetic theory, which is well known in the context of continuous fluids,$^{(24,25)}$ has also been developed for LGCAs. Here we restrict ourselves to the Boltzmann approximation. Then the nonequilibrium average $\langle I_c(n(t))\rangle_{\text{ne}}$ of (2.1) is replaced by $I_c(f)$, where $f(\mathbf{c}, \mathbf{r}, t) = \langle n(\mathbf{c}, \mathbf{r}, t)\rangle_{\text{ne}}$. Thus the average of the product of occupation numbers is factorized into a product of averages. This means that the collisions of the particles are treated as being completely uncorrelated. By taking the average of (2.1), one obtains

$$f(\mathbf{c}, \mathbf{r} + \mathbf{c}, t + 1) = f(\mathbf{c}, \mathbf{r}, t) + I_c(f) \tag{3.12}$$

In the evaluation of the Green–Kubo formulas only the linearized kinetic equation is needed.$^{(26)}$ Thus, we expand $I_c(f)$ in deviations from total equilibrium to obtain

$$I_c(f) = I_c(f^0) - \Omega_{cc'}\delta f_{c'} - \Omega_{cc'c''}\,\delta f_{c'}\,\delta f_{c''} + \cdots \tag{3.13}$$

where $I_c(f^0)=0$, and δf_c is short for $\delta f(\mathbf{c}, \mathbf{r}, t) = f(\mathbf{c}, \mathbf{r}, t) - f^0(c)$. Here $\Omega_{cc'}$ is the linearized Boltzmann collision operator. Closely following the analysis for the athermal models, as given in refs. 16 and 26, we find that the Green–Kubo formula reduces to

$$L_{aa} = \sum_{c',c} \hat{j}_a(\mathbf{c}') \left[\frac{1}{\Omega} - \frac{1}{2}\right]_{c'c} \kappa(c)\, \hat{j}_a(\mathbf{c}) \tag{3.14}$$

This provides the *Boltzmann approximation* to any transport coefficient in thermal lattice gas models, and even includes all athermal models as a special case for $\beta = 0$. It has the same general structure and validity as the Chapman–Enskog results(14) for continuous gases. The explicit forms of the currents have been specified in the previous subsection. Below we will specify the collision operator in terms of the transition probabilities between in-states and out-states for any detailed balance model. We note the appearance of the thermal weight $\kappa(c)$ of (2.5), which is absent in athermal models. In a continuous gas $\kappa(c)$ is replaced by a Maxwellian $\sim \exp(-\frac{1}{2}\beta c^2)$ and velocity summations are replaced by integrations.

From the collision rules for the specific model under consideration we can construct $I_c(f)$ and obtain $\Omega_{cc'}$ explicitly. For the detailed balance models of interest here the collisions at a single node can be specified by a symmetric transition probability $A(s \to s') = A(s' \to s)$ from an in-state, specified by a set of occupation numbers $s = \{s_i(r)\}$, to an out-state $s' = \{s_i'(r)\}$. The label i refers to the velocity state $\mathbf{c}_i$ with $(i = 0, 1,..., b-1)$. For detailed definitions of the symbols we refer to ref. 1. We express the collision operator $\Omega_{ij} \equiv \Omega_{c_i c_j}$ explicitly in terms of $A(s \to s')$ following Section 8.2 of ref. 1, with the result

$$\Omega_{ij}\kappa(c_j) = \sum_{s',s} (s_i - s_i')\, A(s \to s')\, p_0(s) s_j \tag{3.15}$$

This formula should be compared with the linear Boltzmann collision operator in Eq. (8.23) of ref. 1 for athermal models. In the present case $p_0(s)$ is the completely factorized probability distribution of occupation numbers at a single node $\mathbf{r}$ in true *thermal* equilibrium, given by

$$\begin{aligned} p_0(s) &= \prod_{j=0}^{b-1} \{[f^0(c_j)]^{s_j}[1-f^0(c_j)]^{1-s_j}\} \\ &= \frac{\exp[\alpha\hat{\rho}(r\,|\,s) - \beta\hat{e}(r\,|\,s)]}{\sum_{\{n\}} \exp[\alpha\hat{\rho}(r\,|\,n) - \beta\hat{e}(r\,|\,n)]} \end{aligned} \tag{3.16}$$

where $\hat{\rho}(r\,|\,s) = \sum_j s_j(r)$ and $\hat{e}(r\,|\,s) = \sum_j \varepsilon(c_j)\, s_j(r)$ are, respectively, the total number of particles and total energy at node $\mathbf{r}$. The distribution function depends on temperature β and chemical potential α, or equivalently on density ρ. We further observe that the product matrix $(\Omega\kappa)_{ij} = \Omega_{ij}\kappa(c_j)$ is symmetric on account of detailed balance, and can be cast into a similar form as Eq. (8.23) of ref. 1 for athermal models. Note, however, that the matrix Ω_{ij} is not symmetric.

The evaluation of (3.14) either requires the solution $B_a(c)$ of the linear system of equations $\Omega B_a = \kappa\hat{j}_\alpha$ (which is the analog of the Chapman–Enskog integral equation for continuous gases$^{(14)}$) or a decomposition of $\kappa\hat{j}_a$ into eigenvectors of Ω. Which method to use is a matter of convenience and depends somewhat on the model under consideration (see Section 4). We illustrate here the decomposition into eigenvectors. The transport coefficients can be calculated in terms of right eigenfunctions and eigenvalues of the $b \times b$ collision matrix Ω, i.e.,

$$\Omega\kappa\psi_n = \omega_n \kappa\psi_n \tag{3.17}$$

They are orthogonal with respect to a weighted *thermal* inner product

$$\langle \psi_n | \psi_m \rangle = \sum_c \kappa(c)\, \psi_n(c)\, \psi_m(c) \tag{3.18}$$

where $\kappa(c)$ is a weight factor defined in (2.5). The transport coefficient can then be expressed as

$$L_{aa} = \sum_n \frac{|\langle \hat{j}_a | \psi_n \rangle|^2}{\langle \psi_n | \psi_n \rangle} \left\{ \frac{1}{\omega_n} - \frac{1}{2} \right\} \tag{3.19}$$

with eigenvalues satisfying the inequalities, $0 \leqslant \omega_n < 2$.

The simplest case is realized whenever the current $\kappa\hat{j}_a$ itself is an eigenvector of Ω. This occurs in the majority of athermal lattice gases with a small (depending on the number of space dimensions) number of speeds, such as in the 4-bits HPP model$^{(1)}$ and in the 4-bits model of ref. 27, in 6- and 7-bits models on a triangular lattice,$^{(1)}$ and in the 24-bits FCHC model.$^{(1)}$ The same holds for the 8- and 9-bits thermal models$^{(3,4,6)}$ on a square lattice.

In that case only the term with $n = a$ contributes and (3.19) can be written as

$$L_{aa} = \frac{\langle \hat{j}_a | \hat{j}_a \rangle^2}{\langle \hat{j}_a | \, \Omega_j \, | \hat{j}_a \rangle} - \frac{1}{2} \langle \hat{j}_a | \hat{j}_a \rangle \tag{3.20}$$

Using (3.17), we have expressed the eigenvalue ω_a in terms of a *thermal* matrix element of the collision operator, i.e.,

$$\langle \hat{j}_a | \, \Omega \, | \hat{j}_a \rangle = \sum_{cc'} \hat{j}_a(c')\, \Omega_{c'c}\, \kappa(c)\, \hat{j}_a(c) \tag{3.21}$$

where the product matrix $\Omega\kappa$ has been defined in (3.15). The present formula (3.20) includes as special cases the viscosity formulas (3.39) of ref. 19 and formula (8.25) of ref. 1 for the isotropic athermal lattice models in these papers.

In general, however, (3.20) is not correct as more eigenvalues are involved, as in (3.19). In ref. 2 this was shown, for instance, for a 5-bits one-dimensional model. It is also the case in b-bits triangular lattice gases with $b \geqslant 12$ (see Section 4).

The formula (3.20) may, however, be used as a first estimate of the Boltzmann value of the transport coefficients. In fact, in the case of continuous gases it represents the well-known *first Enskog approximation* to the solution of the Chapman–Enskog integral equation, $\Omega B_a = \kappa \hat{j}_a$, obtained by expanding $B_a(c)$ in terms of Sonine polynomials.(14) It is an approximation to the Boltzmann value of transport coefficients that is usually correct within a few percent.

3.3. Staggered Diffusivities

Model-independent expressions for transport coefficients related to spurious conservation laws do not exist, because these invariants depend crucially on the number of different speeds involved and, less sensitively, on the underlying lattice and collision rules. The most frequently occurring spurious invariant is the total staggered momentum, discovered by Kadanoff *et al.*(15) It occurs not only in the athermal 6- and 7-bits models on the triangular lattice, but also in many thermal models on square or cubic lattices, such as the 8- and 9-bits thermal models on the square lattice.(28)

We therefore treat the diffusivity related to the slowly decaying staggered momentum mode as a prototypical example. Each staggered invariant is characterized by a reciprocal lattice vector $\boldsymbol{\varepsilon}$,(15,28) and denoted by

$$H_\varepsilon = \sum_{r} h_\varepsilon(\mathbf{r}, t) = \sum_{r,c} (-)^{t + \boldsymbol{\varepsilon} \cdot \mathbf{r}} (\boldsymbol{\varepsilon} \cdot \mathbf{c})\, n(\mathbf{c}, \mathbf{r}, t) \tag{3.22}$$

There may be a set of such $\boldsymbol{\varepsilon}$-vectors. They give rise to new slow, staggered densities h_ε. At the level of linear deviations from equilibrium, the equations of motion for these staggered densities do not couple to the usual set of hydrodynamic variables and satisfy a simple diffusion equation,

$$\partial_t h_\varepsilon(\mathbf{k}, t) = -k^2 \xi(\hat{k})\, h_\varepsilon(\mathbf{k}, t) \tag{3.23}$$

where $\xi(\hat{k})$ is the staggered diffusivity and $\hat{k}$ is the unit vector parallel to $\mathbf{k}$. The staggered diffusivity can also be expressed[15,28] in terms of Green–Kubo relations (3.1) with the corresponding current defined as

$$\hat{J}_{\varepsilon}(t)=\sum_{r,c}(-)^{t+\boldsymbol{\varepsilon}\cdot\mathbf{r}}(\hat{k}\cdot\mathbf{c})(\boldsymbol{\varepsilon}\cdot\mathbf{c})\,\delta n(\mathbf{c},\mathbf{r},t) \tag{3.24}$$

The $\hat{k}$-dependent diffusivity can be split into two diffusion constants,

$$\xi_{\varepsilon}(\hat{k})=(\hat{k}\cdot\boldsymbol{\varepsilon})^2\xi_{\|}+(\hat{k}\cdot\boldsymbol{\varepsilon}_{\perp})^2\xi_{\perp} \tag{3.25}$$

where $\boldsymbol{\varepsilon}_{\perp}$ is the unit vector perpendicular to $\boldsymbol{\varepsilon}$. The parallel and perpendicular diffusivities can be evaluated in Boltzmann approximation. We write out the result obtained for the perpendicular diffusivity,

$$\xi_{\perp}=\frac{1}{\chi_g}\sum_{c,c'}\hat{j}_{\perp}(\mathbf{c})\left[\frac{1}{\Omega-\Delta}-\frac{1}{2}\right]_{cc'}\kappa(c')\,\hat{j}_{\perp}(\mathbf{c}') \tag{3.26}$$

where the susceptibility χ_g is defined above (3.8). The matrix $\Delta_{cc'}$ is diagonal and is given by $\Delta_{cc'}=\Delta(c)\delta_{cc'}=[1+(-)^{\boldsymbol{\varepsilon}\cdot\mathbf{c}}]\,\delta_{cc'}$. The expression for $\xi_{\|}$ is obtained by replacing $\hat{j}_{\perp}$ by $\hat{j}_{\|}$, and the currents are given by

$$\hat{j}_{\perp}=(\boldsymbol{\varepsilon}_{\perp}\cdot\mathbf{c})(\boldsymbol{\varepsilon}\cdot\mathbf{c}) \qquad \text{and} \qquad \hat{j}_{\|}=(\boldsymbol{\varepsilon}\cdot\mathbf{c})^2 \tag{3.27}$$

The above expressions represent the Boltzmann approximation to the staggered diffusivity. They are only applicable to models that do have staggered momentum invariants. The calculation of (3.25) requires again the solution $B(c)$ of a system of linear equations, $(\Omega-\Delta)B=\kappa\hat{j}$. This equation does not resemble the Chapman–Enskog integral equations, because of the appearance of the Δ operator.

4. THREE THERMAL LGCAs

4.1. Nine-Bits Square Lattice Gas

In a strictly formal sense one may interpret an athermal binary mixture LGCA with slow (*cold*) and fast (*hot*) particles as a thermal one-component model,[8] although there is no exchange of energy between hot and cold particles. The Green–Kubo expressions for binary diffusion coefficient and heat conductivity are then simply proportional.[9]

Here we take the point of view that a lattice gas during thermalization should allow a redistribution of particles over the different energy states. In order to allow energy exchange between hot and cold particles, multispeed models are required with at least three different speeds. The three models to be considered below all satisfy this minimal requirement. We first consider different versions of the 9-bits model on the square lattice.(4,6,7)

The state of the system is given by the set of occupation numbers $n(\mathbf{c}, \mathbf{r}, t)$, where $n(\mathbf{c}, \mathbf{r}, t)$ is equal to 1 if the velocity channel $\mathbf{c}$ at site $\mathbf{r}$ is occupied and vanishes otherwise. The collisions, referred to as *a, b, c, d*-collisions, are shown in Fig. 1. They conserve particle number, momentum, and kinetic energy. The particles have no internal energy. There are in total nine possible velocity states. There is one rest particle with speed $|c| = 0$, four slow particles with speed $|c| = 1$, and four fast particles with speed $|c| = \sqrt{2}$.

The currents in the Green–Kubo formulas for particles without internal energy simplify, as pressure p and energy density $e = (d/2)\,p$ are essentially the same. The microscopic expression (3.4) for the heat current contains the enthalpy per particle h, which reduces to

$$h = \frac{1}{2}\, d \left(\frac{\partial p}{\partial \rho}\right)_s = \frac{1}{2}\, d c_0^2 = \frac{\sum_c c^4 \kappa(c)}{2 \sum c^2 \kappa(c)} \tag{4.1}$$

as follows from (3.5). Similarly, the subtracted current for the viscosity reduces to

$$\begin{aligned} \hat{J}_{\alpha\beta} &= J_{\alpha\beta} - \delta_{\alpha\beta}(2/d)\,\delta H \\ \hat{j}_{\alpha\beta} &= c_\alpha c_\beta - \delta_{\alpha\beta} c^2/d \end{aligned} \tag{4.2}$$

Consequently, the bulk viscosity, $\zeta = (1/d^2)\, \nu_{\alpha\alpha\beta\beta}$, *vanishes identically*. This is because the trace of (4.2), $\hat{J}_{\alpha\alpha} \equiv 0$, or alternatively, the unsubtracted current, $J_{\alpha\alpha} = (2/d) H$, it itself a conserved quantity. The vanishing of the bulk viscosity in *thermal* lattice gases is a general result for models with

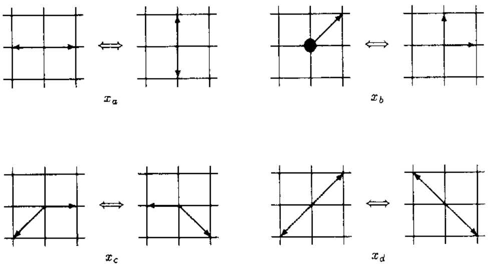

Fig. 1. The collision rules for the *thermal* LGCA. The black circle in collision (b) represents a rest particle. Scattering from in-states into out-states occurs with probability x_p ($p = a, b, c, d$).

particles that possess only kinetic energy. In *athermal* LGCAs the bulk viscosity only vanishes in single-speed models. The 9-bits model has two staggered momentum invariants, given by (3.22) with two independent choices for ε, namely (1, 0) and (0, 1).

Further evaluation requires specification of the collision rules. One may impose the collision rules (A) where the collisions in Fig. 1 only occur in the absence of all other particles. An alternative set of rules (B) is: binary collisions between like particles, i.e., (a)-collisions and (d)-collisions, occur irrespective of the presence of unlike particles. Some extra parameters x_p ($p = a, b, c, d$) might be introduced into the model by imposing that the in-state of a p-collision scatters with probability x_p into the out-state (see Fig. 1). With probability $1 - x_p$, in-states and out-states are equal. There exist many more alternatives for constructing collision rules that conserve number, energy, and linear momentum, involving 2-, 3-,..., up to 7-tuple collisions. The models can be made self-dual, yielding interesting extensions into the temperature–density plane of the symmetry between low and high densities that exists in the self-dual athermal LGCAs.

The transition probabilities $A(s \to s')$ for the different alternatives can be read off from Fig. 1 and the Ω-matrix can be constructed with the help of Eq. (3.14).

The analytic expressions for the transport coefficients (3.15) are found as functions of the chemical potential α and the inverse temperature β,

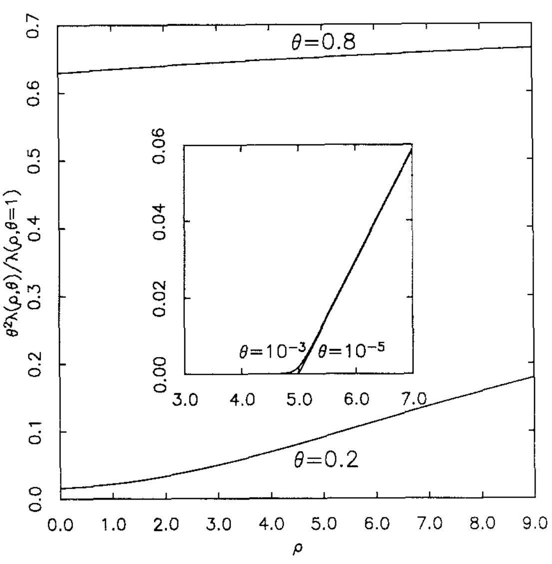

Fig. 2. Isotherms for the heat conductivity $\theta^2\lambda(\rho, \theta)$, normalized with respect to its value at $\theta = 1$, versus the density ρ in the 9-bits model.

because Ω in (3.15) and $\kappa(c)$ in (2.5) depend on these parameters. To obtain the transport coefficients as functions of density ρ and reduced temperature $\theta \equiv \exp(-\frac{1}{2}\beta)$, one has to solve α as a function of ρ and θ from $\rho(\alpha, \beta) = \sum_c f^0(c)$, and insert the result into (3.14). In the numerical calculations we set the probabilities for different collisions $x_a = x_b = x_c = x_d = 1$ and use the collision rule A, described above.

In Fig. 2 we show how the heat conductivity $\theta^2 \lambda(\rho, \theta)$ varies with density. It is normalized with respect to its value at $\theta = 1$ in order to remove effects coming from the obvious density dependence of the collision frequencies, the ν's. The figure indicates that, for moderate to high temperatures, $\lambda(\rho, 1)$ contains the dominant density dependence, leaving the normalized function almost structureless. However, for vanishingly small values of θ, i.e., at very low temperature, there appear discontinuities in the ρ dependence of the thermal conductivity, which are visible around the density $\rho = 5$ and can be analyzed in detail from the analytic expressions. In Fig. 3 we show the isochores for the heat conductivity as a further illustration. The further analytic evaluation and a graphical presentation of the Boltzmann results for all transport coefficients in the 9-bits model will be published elsewhere.(29)

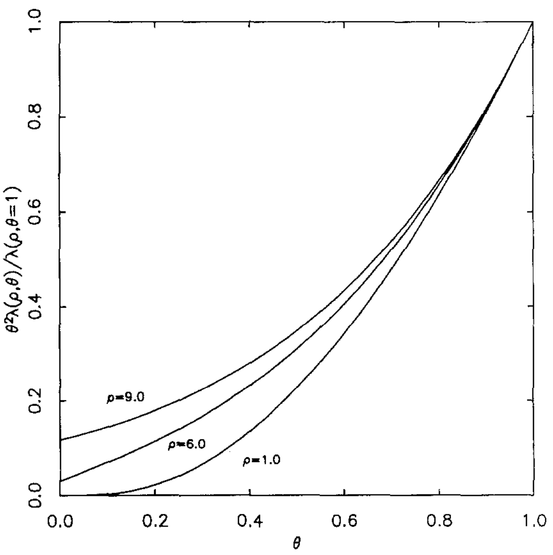

Fig. 3. Isochores for the heat conductivity $\theta^2 \lambda(\rho, \theta)$, normalized with respect to its value at $\theta = 1$, versus temperature θ in the 9-bits model.

4.2. Nineteen-Bits Triangular Lattice Gas

This model, recently introduced by Grosfils *et al.*,(30) is a thermal model with nontrivial energy conservation and with isotropic fourth-rank tensors. There are no staggered momentum invariants. The particles live on a triangular lattice, there is one rest particle, and 3×6 particles with speed $c = 1$, $c = \sqrt{3}$, and $c = 2$, respectively. Their energy is *purely kinetic*. Therefore the results (4.1) and (4.2) apply. The bulk viscosity vanishes for all densities and temperatures. As the viscosity tensor (3.7) is isotropic, the shear viscosity ν and the cubic viscosity ϑ are equal. We further note that the *shear viscosity* in the present model cannot be expressed in a form similar to Eq. (3.20) or to Eq. (8.25) of ref. 1. The reason is that the current $\hat{J}_{\alpha\beta}$ or equivalently $Q_{\alpha\beta} = c_\alpha c_\beta - \delta\alpha\beta c^2/d$ is not an eigenfunction of the Boltzmann collision operator Ω, but has components in *three* different eigenspaces. This can be seen by extending the symmetry considerations of ref. 26. For detailed calculations of the transport coefficients we refer to ref. 31.

4.3. Thirteen-Bits Triangular LGCA with Internal Energy

This model(32) with isotropic fourth-rank tensors serves to illustrate the effects of internal energy on heat conductivity and bulk viscosity. The result is again analogous to the continuous case, where the bulk viscosity is nonvanishing for a dilute gas with internal degrees of freedom, but vanishing without. There is one rest particle, six slow particles with $c = 1$, and six fast ones with $c = \sqrt{3}$. There are no staggered invariants.

The total energy per particle, $\varepsilon(c) = \frac{1}{2}c^2 + \varepsilon_0(c)$, consists of kinetic energy, $\frac{1}{2}c^2$, and internal energy, $\varepsilon_0(c)$. The latter is only nonvanishing for fast particles, where the internal energy is $\varepsilon_0(\sqrt{3}) = -\frac{1}{2}$ and the total energy is $\varepsilon(\sqrt{3}) = 1$. In the present model the energy density and pressure are different, and the corresponding currents (3.4) and (3.8) do not simplify any further. The bulk viscosity, which is nonvanishing in this model, and the shear viscosity cannot be expressed in the form (3.20), because the current $\hat{J}_{\alpha\beta}$ has components in *two* different eigenspaces of Ω.

5. DISCUSSION

This paper presents a systematic extension of the theory of *athermal* lattice gases to *thermal* ones, both for equilibrium statistical mechanics, as well as for the evaluation of transport coefficients in the Boltzmann approximation. The formulation of transport coefficients is model-independent, and is applicable whenever the transport coefficients exist. The resulting explicit expressions for thermal transport coefficients in terms of collision integrals are the direct counterparts of the corresponding collision integrals in the Chapman–Enskog theory.(14)

The close parallels with continuous systems as well as consistency with concepts from statistical mechanics and irreversible thermodynamics have been emphasized throughout this work.

By setting $\beta = 0$ in the present formulas (infinite temperature), and using the collision rules or transition probabilities $A(s \rightarrow s')$ of the athermal models, one recovers the explicit expressions for the transport coefficients, as derive in refs. 1 and 19. The thermal conductivity is of particular interest, because it does not occur in any of the standard athermal lattice gases. However, the bulk viscosity is also strongly affected by energy conservation. It vanishes identically in all *thermal* LGCAs, where particles only possess kinetic energy. In *athermal* lattice gases the bulk viscosity is in general nonvanishing (except for single-speed models). However, if the particles in a *thermal* lattice gas also possess internal energy, then the bulk viscosity is nonvanishing. The last property has a direct analog in the bulk viscosity of continuous gases without and with internal degrees of freedom.

Before closing, we recall that the Navier–Stokes equations and their corresponding linear transport coefficients do not exist in two-dimensional systems, as a consequence of the long-time tails. Navier–Stokes equations with finite transport coefficients can only be an approximation in some intermediate time regime, which may be extremely long in most relevant lattice gases.(33)

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