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1992 J. Phys. A: Math. Gen. 25 L949

(http://iopscience.iop.org/0305-4470/25/15/009)

J. Phys. A: Math. Gen. 25 (1992) L949–L954. Printed in the UK

LETTER TO THE EDITOR

A fluctuation formula for the non-Galilean factor in lattice gas automata

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Received 12 March 1992

Abstract. A lattice gas automaton lacks Galilei invariance, and equilibria of systems moving with a finite speed $|\vec{u}|$ are not simply related by a Galilei transformation to the equilibrium distribution in the rest frame. In the hydrodynamic description of low speed equilibria in lattice gas automata a factor $G(\rho)$ appears in the nonlinear convective term, $\vec{\nabla} \cdot G(\rho)\rho\vec{u}\vec{u}$, of the Navier–Stokes equation, that differs from unity due to lack of Galilei invariance. For this non-Galilean factor an expression in terms of fluctuating quantities is derived, in a grand ensemble where the total momentum is fluctuating around a zero average. The formula is valid as long as there exists a unique equilibrium state. Consequently, the results can also be used for a direct simulation of $G(\rho)$ in lattice gas models where the explicit form of the equilibrium distribution is not known, such as in models that violated semi-detailed balance.

The purpose of this letter is (i) to derive for a cellular automaton fluid a fluctuation formula for the non-Galilean factor $G(\rho)$, in an equilibrium state where the total momentum fluctuates around a *vanishing* average (basic equilibrium), and (ii) to point out that this fluctuation formula can be used to measure the non-Galilean factor by means of computer simulations in lattice gas automata (LGA) after they have relaxed to a state of equilibrium.

Why is the non-Galilean factor of interest? It has been shown [1] that the macroscopic equation of motion for the LGA yields the Navier–Stokes equation for an incompressible fluid, provided the lattice gas time t is rescaled to $t/G(\rho)$, and its kinematic viscosity ν to $\nu G(\rho)$. In applications of lattice gas techniques to nonlinear flow problems, knowledge of $G(\rho)$ is indispensible. In the standard method of determining $G(\rho)$ one needs to measure effects, quadratic in the flow fields, in the limit of vanishing fluid flow. Furthermore, the theoretical predictions of $G(\rho)$, based on the Boltzmann equation, are very poor for models that violate detailed balance [2].

The basic assumption is that after a sufficient number of time steps the LGA reaches a unique equilibrium state, described by a phase space density $\rho(s)$, where s denotes the microstate or configuration of the entire LGA. However, we do not impose the so-called condition of semi-detailed balance (SDB) [1], that ensures that the equilibrium state is fully factorized over the nodes $\vec{r}$ of the lattice and over all b different velocity directions $\vec{c}_0, \vec{c}_1, \ldots, \vec{c}_{b-1}$.

The state of a node is denoted by $s(\vec{r}) = \{s_0(\vec{r}), s_1(\vec{r}), \ldots, s_{b-1}(\vec{r})\}$, where $s_i(\vec{r}) = 0, 1$ is the occupation number of channel $(\vec{r}, i)$ and $s = \{s(\vec{r}_1), s(\vec{r}_2), \ldots, s(\vec{r}_V)\}$ denotes the state of the entire system of V nodes. A

0305-4470/92/150949+06$04.50

time evolution step of the LGA consists of a collision step followed by free propagation of all particles towards neighbouring nodes, in the direction of the particle velocities $\vec{c}_i$. During the collision step *local* collision rules are applied to each single node state $s(\vec{r})$ independently. Only collisions that conserve the local particle number $\rho(\vec{r}) = \sum_i s_i(\vec{r})$, momentum $\vec{g}(\vec{r}) = \sum_i \vec{c}_i s_i(\vec{r})$ and possibly energy $e(\vec{r}) = \sum_i \frac{1}{2}\vec{c}_i^2 s_i(\vec{r})$ are allowed. This implies that the total particle number $N(s) = \sum_{\vec{r},i} s_i(\vec{r})$, the total momentum $\vec{P}(s) = \sum_{\vec{r},i} \vec{c}_i s_i(\vec{r})$ and possibly the total energy $E(s) = \sum_{\vec{r},i} \frac{1}{2}\vec{c}_i^2 s_i(\vec{r})$ are conserved quantities.

If the system is isolated the equilibrium ensemble is described by the phase space density (not normalized),

$$\begin{aligned}\rho_0(s|\mathcal{A}) &\sim \mathcal{D}(s)\,\delta(N(s),\mathcal{N})\,\delta(\vec{P}(s),\vec{\mathcal{P}})\,\delta(E(s),\mathcal{E}) \\ &\sim \mathcal{D}(s)\,\delta(\mathbf{A}(s),\mathcal{A}) \qquad (1)\end{aligned}$$

where $\delta(a,b)$ is a Kronecker delta and $\mathcal{A} = (\mathcal{N},\vec{\mathcal{P}},\mathcal{E},\ldots)$ a set of constants. The set of dynamic variables $\mathbf{A}(s) = \{N(s),\vec{P}(s),E(s),\ldots\}$ represents the complete set of global invariants of a *thermal* LGA where the total number of particles $N(s)$, the total momentum $\vec{P}(s)$, as well as the total energy $E(s)$ are conserved. In an *athermal* LGA without energy conservation, the constraint $\delta(E(s),\mathcal{E})$ is simply dropped. If there exist spurious invariants [3], they should also be included in the set $\mathbf{A}(s)$. If the LGA satisfies the SDB condition, the degeneracy factor equals $\mathcal{D}(s) = 1$. Then $\rho_0(s) = \rho_0(\mathbf{A}(s))$ has a universal form, that only depends on the microstate through the global invariants. If the SDB condition is violated, then $\mathcal{D}(s) \neq 1$, and the occupations of different velocity channels on the same or on different nodes may be correlated [4, 5]. The explicit form of the degeneracy factor $\mathcal{D}(s)$ is in general not known.

Instead of describing the LGA as an isolated system by a microcanonical ensemble with all extensive variables $\mathbf{A}(s) = (N(s),\vec{P}(s),E(s),\ldots)$ kept fixed, we will describe it as an open system in contact with reservoirs of particles, momentum and energy, i.e.

$$\begin{aligned}\rho_0(s|\mathbf{b}) &\sim \mathcal{D}(s)\exp[b\cdot\mathbf{A}(s)] \\ &\sim \mathcal{D}(s)\exp[\alpha N(s) + \vec{\gamma}\cdot\vec{P}(s) - \beta E(s)] \qquad (2)\end{aligned}$$

where $\mathbf{b} = \{\alpha,\vec{\gamma},-\beta\}$ are the conjugate parameters. In this ensemble the extensive quantities fluctuate, and their average values $\langle N\rangle$, $\langle\vec{P}\rangle$ and $\langle E\rangle$ are determined by the parameters b. The parameter value $\vec{\gamma} \neq 0$ represents a finite speed equilibrium in uniform translation with velocity $\vec{u} = \langle\vec{P}\rangle/\langle N\rangle$, and $\vec{\gamma} = 0$ represents a *basic* equilibrium ($\vec{u} = 0$), in which the average momentum vanishes, $\langle\vec{P}\rangle = 0$.

We now consider the non-Galilean factors. The normalized distribution function for the finite speed equilibrium will be written as

$$\mathcal{P}_0(s|\vec{\gamma}) = \mathcal{P}_0(s|\vec{0})\cdot\frac{\exp(\vec{\gamma}\cdot\vec{P})}{\langle\exp(\vec{\gamma}\cdot\vec{P})\rangle_0} \qquad (3)$$

where $\vec{\gamma} = 0$ denotes the basic equilibrium. Expanding (3) for small values of the thermodynamic parameter $\vec{\gamma}$ we find

$$\rho_0(s|\vec{\gamma}) = \rho_0(s|\vec{0})\{1 + \gamma\cdot\vec{P} + \tfrac{1}{2}\vec{\gamma}\vec{\gamma} : (\vec{P}\vec{P} - \langle\vec{P}\vec{P}\rangle_0) + \mathcal{O}(\gamma^3)\}. \qquad (4)$$

The average flow velocity $\vec{u}$ is related to $\vec{\gamma}$ by

$$\langle N\rangle\vec{u} = \langle\vec{P}\rangle = \gamma\cdot\langle\vec{P}\vec{P}\rangle_0 + \mathcal{O}(\gamma^3) = \tfrac{1}{d}\vec{\gamma}\langle P^2\rangle_0 + \mathcal{O}(\gamma^3) \tag{5}$$

where d is the dimensionality. We have used the fact that for lattice gas models with the proper symmetries, all third rank tensors vanish identically and all second rank tensors are diagonal [1]. The *pressure tensor* in a low speed equilibrium can be obtained by averaging the microscopic momentum flux

$$\overleftrightarrow{T} = \sum_{\vec{r},i}\vec{c}_i\vec{c}_i s_i(\vec{r}) = \overleftrightarrow{Q} + T\,\overleftrightarrow{1} \qquad \overleftrightarrow{Q} = \sum_{\vec{r},i}(\vec{c}_i\vec{c}_i - \tfrac{1}{d}c_i^2\,\overleftrightarrow{1})s_i(\vec{r}) \tag{6}$$

where $\overleftrightarrow{Q}$ is the traceless part of $\overleftrightarrow{T}$ and $T \equiv T_{\alpha\alpha}/d$ (Greek indices will be used to denote Cartesian components of vectors and tensors and summation is performed for repeated indices). From (4) it follows that

$$\begin{aligned}\langle T_{\alpha\beta}\rangle &= \langle T_{\alpha\beta}\rangle_0 + \tfrac{1}{2}\gamma_\mu\gamma_\nu\langle P_\mu P_\nu\delta T_{\alpha\beta}\rangle_0 + \mathcal{O}(\gamma^3)\\ &= \{p_0V + \tfrac{1}{2d}\gamma^2\langle P^2\delta T\rangle_0\}\delta_{\alpha\beta} + \tfrac{1}{2}\gamma_\mu\gamma_\nu\langle P_\mu P_\nu\delta Q_{\alpha\beta}\rangle_0 + \mathcal{O}(\gamma^3)\end{aligned} \tag{7}$$

where $\delta A = A - \langle A\rangle_0$ and we have used the identity $\langle A\delta B\rangle_0 = \langle B\delta A\rangle_0$. The kinetic pressure, $p = \langle T\rangle/V$, is a function of the thermodynamic state variables. To proceed we have to distinguish between *thermal* models, with state variables $\rho = \langle N\rangle/V$, $e = \langle E\rangle/V$ and $\vec{u} = \langle\vec{P}\rangle/V$, so that $p = p(\rho, e, u)$ is the equation of state, and *athermal* models where ρ and $\vec{u}$ are the only state variables so that $p = p(\rho, u)$. In basic equilibrium, where $\vec{u} = 0$, we have $p_0 = p_0(\rho_0, e_0)$ for thermal models, and $p_0 = p_0(\rho_0)$ for athermal models.

Consider first thermal models. The pressure $p_0(\rho_0, e_0)$ in (7) is a function of the average particle density ρ_0 and energy density e_0, calculated in basic equilibrium. They differ by amounts of $\mathcal{O}(\gamma^2)$ from the actual equilibrium values, i.e.

$$\begin{aligned}V\Delta\rho &\equiv \langle N\rangle - \langle N\rangle_0 = \tfrac{1}{2d}\gamma^2\langle P^2\delta N\rangle_0 + \mathcal{O}(\gamma^3)\\ V\Delta e &\equiv \langle E\rangle - \langle E\rangle_0 = \tfrac{1}{2d}\gamma^2\langle P^2\delta E\rangle_0 + \mathcal{O}(\gamma^3)\,.\end{aligned} \tag{8}$$

Therefore

$$p_0(\rho_0, e_0) = p_0(\rho, e) - \left(\frac{\partial p_0}{\partial\rho}\right)_e\Delta\rho - \left(\frac{\partial p_0}{\partial e}\right)_\rho\Delta e\,. \tag{9}$$

Combining (7), (8) and (9) then yields

$$\langle T_{\alpha\beta}\rangle = \{p_0(\rho, e)V + \tfrac{1}{2d}\gamma^2\langle P^2\delta\hat{T}\rangle_0\}\delta_{\alpha\beta} + \tfrac{1}{2}\gamma_\mu\gamma_\nu\langle P_\mu P_\nu\delta Q_{\alpha\beta}\rangle_0 + \mathcal{O}(\gamma^3)\,. \tag{10}$$

Here $\delta\hat{T}$ is a so-called *subtracted* (non-thermodynamic) fluctuation, defined as

$$\delta\hat{T} = \delta T - \left(\frac{\partial p_0}{\partial\rho}\right)_e\delta N - \left(\frac{\partial p_0}{\partial e}\right)_\rho\delta E\,. \tag{11}$$

It is *orthogonal* to the fluctuations in the thermodynamic variables δN and δE, in the sense that $\langle\delta\hat{T}\delta N\rangle_0 = \langle\delta\hat{T}\delta E\rangle_0 = 0$.

Next consider athermal models. Then Δe and δE in the above equations should be set equal to zero, and consequently the subtracted fluctuation for athermal models becomes

$$\delta\hat{T} = \delta T - \frac{\mathrm{d}p_0}{\mathrm{d}\rho}\delta N = \delta T - \frac{\langle \delta T \delta N\rangle_0}{\langle \delta N \delta N\rangle_0}\delta N \tag{12}$$

which is again orthogonal to the thermodynamic fluctuation δN. The projected fluctuations (11) and (12) can easily be generalized to thermal and athermal multicomponent mixtures by replacing $\delta\rho$ and δN by $\delta\rho_l$ and δN_l and summing over the component label l.

We now concentrate on the last term of (10). The tensor $\langle P_\mu P_\nu \delta Q_{\alpha\beta}\rangle_0$ is assumed to be traceless and isotropic, and therefore necessarily has the form [1]

$$\langle P_\mu P_\nu \delta Q_{\alpha\beta}\rangle_0 = F\{\delta_{\mu\alpha}\delta_{\nu\beta} + \delta_{\mu\beta}\delta_{\nu\alpha} - \tfrac{2}{d}\delta_{\mu\nu}\delta_{\alpha\beta}\}\,. \tag{13}$$

By contracting indices we obtain

$$F = \frac{1}{(d-1)(d+2)}\langle P_\alpha P_\beta \delta Q_{\alpha\beta}\rangle_0\,. \tag{14}$$

The non-Galilean factors $G(\rho)$ and $G_1(\rho)$ are defined by†

$$\langle \overleftrightarrow{T}\rangle/V = p(u)\,\overleftrightarrow{1} + G(\rho)\rho\vec{u}\vec{u} \qquad p(u) = p_0 - \tfrac{1}{d}G_1(\rho)\rho u^2\,. \tag{15}$$

Combining (10) and (13)–(15), and using (5) to replace $\vec{\gamma}$ by $\vec{u}$, we arrive at the following expressions for $G(\rho)$ and $G_1(\rho)$

$$\begin{aligned} G(\rho) &= \frac{d^2\rho V}{(d-1)(d+2)}\frac{\langle P_\alpha P_\beta \delta Q_{\alpha\beta}\rangle_0}{\langle P^2\rangle_0^2} \\ G_1(\rho) &= G(\rho) - \tfrac{1}{2}d^2\rho V\frac{\langle P^2\delta\hat{T}\rangle_0}{\langle P^2\rangle_0^2}\,. \end{aligned} \tag{16}$$

All averages are to be taken in *basic equilibrium* ($\langle\vec{P}\rangle_0 = 0$). It is essential in (16) to consider an open system, where the total momentum fluctuates around its (zero) average. The equilibrium fluctuation formulae for the non-Galilean factors are the new result of this letter.

Some general comments on the properties of these results should be made. In thermal models, where all energy is purely kinetic, $e_0 = (d/2)p_0$, and $\delta\hat{T}$ vanishes identically, $\delta\hat{T} = \delta T - \frac{2}{d}\delta E = 0$. Consequently $G_1(\rho) = G(\rho)$. In models where particles have internal energy $\delta\hat{T}$ is non-vanishing and the general expression (11) has to be used. In athermal models with a single speed ($|\vec{c}_i| = c$ for all i), the pressure $p_0 = (c^2/d)\rho_0$. Again $\delta\hat{T}$ vanishes identically and $G_1(\rho) = G(\rho)$.

It has been assumed in (13) that the fourth rank tensor is isotropic. This is only true for a very limited set of lattices, such as the triangular or face-centered hypercubic lattice [1]. For different lattices (e.g. square or cubic) the fourth rank tensor (13) contains three independent scalars $G(\rho)$, $G_1(\rho)$ and $G_2(\rho)$, that can be calculated in a similar fashion.

† Of course, in thermal models the non-Galilean factors also depend on the energy density e.

Many lattice gas models contain additional spurious conserved quantities, such as the staggered total momentum. These invariants can be straightforwardly included in the set **A** of equations (1) and (2). For instance, in models with a conserved staggered momentum A_θ, the staggered flow field $w_\theta = \langle A_\theta \rangle / \langle N \rangle$ plays a role very similar to $\vec{u}$ and one has to add extra terms, quadratic in w_θ, to the right hand side of (15) and (16), which again involves factors $G(\rho)$ [3, 7].

The main importance of the previously derived fluctuation formulae is their validity for models that violate semi-detailed balance [4, 5], as we shall discuss later on. Of course, the results do also apply to all standard models [1] that obey detailed or semi-detailed balance, and consequently possess a universal equilibrium distribution of the form (2) with $\mathcal{D}(s) = 1$ (see [5]). In a universal equilibrium the distribution function completely factorizes over different nodes and velocity channels, so that

$$\begin{aligned} \langle \delta s_i(\vec{r}) \delta s_j(\vec{r}') \rangle_0 &= \kappa^{(2)} \delta_{ij} \delta(\vec{r}, \vec{r}') \\ \langle \delta s_i(\vec{r}) \delta s_j(\vec{r}') \delta s_k(\vec{r}'') \rangle_0 &= \kappa^{(3)} \delta_{ij} \delta_{jk} \delta(\vec{r}, \vec{r}') \delta(\vec{r}', \vec{r}'') \end{aligned} \tag{17}$$

where the average occupation number, $f_i^0 = \langle s_i(\vec{r}) \rangle_0 = [1 + \exp(-\alpha + \frac{1}{2}\beta c_i^2)]^{-1}$, is the Fermi distribution in basic equilibrium, and

$$\kappa_i^{(2)} = f_i^0(1 - f_i^0) \qquad \kappa_i^{(3)} = f_i^0(1 - f_i^0)(1 - 2f_i^0) \,. \tag{18}$$

In athermal models f_i^0, $\kappa_i^{(2)}$ and $\kappa_i^{(3)}$ are independent of the velocity label i and $f = f_i^0 = \rho/b$ is the reduced density. With the help of (17) we obtain

$$\langle P_\alpha P_\beta \delta Q_{\alpha\beta} \rangle_0 = V \left(\frac{d-1}{d} \right) \sum_i c_i^4 \kappa_i^{(3)} \qquad \langle P^2 \rangle_0 = V \sum_i c_i^2 \kappa_i^{(2)} \tag{19}$$

and combination with (16) gives

$$G(\rho) = \begin{cases} \left(\dfrac{\rho d}{d+2} \right) \dfrac{\sum_i c_i^4 \kappa_i^{(3)}}{\{\sum_i c_i^2 \kappa_i^{(2)}\}^2} & \text{(thermal)} \\ \left(\dfrac{bd}{d+2} \right) \left(\dfrac{1-2f}{1-f} \right) \dfrac{\sum_i c_i^4}{\{\sum_i c_i^2\}^2} & \text{(athermal).} \end{cases} \tag{20}$$

The result for the athermal models follows from that for the thermal models.

Next consider the non-Galilean factor $G_1(\rho)$ that enters in the kinetic pressure $p(u)$ of a finite speed equilibrium (see equation (15)). For all thermal models with purely kinetic energy and all single speed models it has already been argued that $\delta \hat{T} = 0$ and $G_1(\rho) = G(\rho)$. As an illustration we calculate $G_1(\rho)$ for athermal multispeed models. Here

$$\frac{\mathrm{d}p_0}{\mathrm{d}\rho} = \frac{\sum_i c_i^2 \kappa_i^{(2)}}{d \sum_i \kappa_i^{(2)}} = \frac{1}{bd} \sum_i c_i^2 \equiv c_0^2 \tag{21}$$

where c_0 is the speed of sound. We then arrive at

$$G_1(\rho) = G(\rho) - \left(\frac{1-2f}{1-f} \right) \frac{\sum_i c_i^2 (c_i^2 - d c_0^2)}{2bd c_0^4} \,. \tag{22}$$

These explicit expressions (20) and (22) cover all results for non-Galilean factors, calculated in the literature so far (see for example [6]).

In conclusion we note that in the derivation of the equilibrium fluctuation formulae (16) for the non-Galilean factors, only the existence of a unique equilibrium state has been assumed, but no knowledge about the explicit form of the equilibrium distributions (1) and (2) is required (except for the relationship between closed and open systems). Consequently, the present fluctuation formulae apply also to LGAs that violate semi-detailed balance, where the ensemble density has the non-universal form (1) or (2) with a non-trivial degeneracy factor $\mathcal{D}(s) \neq 1$.

From a computer simulation point of view there is the advantage that now a method is available for measuring the non-Galilean factor *in basic equilibrium*. However, the present method requires that an ensemble be used where the total momentum *fluctuates* around a (zero) average. As $\vec{P}$ is fixed in a single run, one should average over many different realizations. Furthermore, one should wait a sufficient number of time steps for each run, so that the system can reach equilibrium. Another possiblity is to measure the fluctuations in only a small part of system, during a single run. This small part acts as an open system in contact with a reservoir of momentum. Other methods have always been based on measurements on a system out of equilibrium e.g. using the definition of $G(\rho)$

$$G(\rho) = \lim_{\vec{u}\to 0} \rho V \frac{\langle T_{xy} \rangle}{\langle P_x \rangle \langle P_y \rangle}$$

where the stress tensor and the momentum are measured in a low speed equilibrium state.

One of us (MHE) would like to thank J W Dufty, U Frisch, M Hénon, A Noullez and J P Rivet for stimulating discussions, and l'Observatoire de Nice, where this research was initiated, for its hospitality in the spring of 1991. HJB is financially supported by the Stichting voor Fundamenteel Onderzoek der Materie (FOM), which is sponsored by de Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO). RB is sponsored by the DGICYT (Spain) grant PB88-0140, FOM and Universidad Complutense through the program 'Bolsas 92'.

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