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Self-diffusion in CA fluids

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Abstract. Tagged particle properties, such as the diffusion coefficient and velocity autocorrelation function, are calculated in the mean-field approximation for all standard lattice gas cellular automata defined on (hyper)cubic, square and triangular lattices and on a line. Tagged particle dynamics is introduced through maximally random or minimally random collision rules. For a completely filled lattice the former reduces to a random walk, the latter to ballistic motion.

1. Introduction

The fluid transport coefficients, such as shear and bulk viscosity, of lattice gas cellular automata (LGCA) for all basic models have been calculated in the mean-field or Boltzmann approximation by Hénon [1], d'Humières and Lallemand [2], and by Dubrulle *et al* [3]. Analytic results for the diffusion coefficient D and the closely related velocity autocorrelation function (VACF) of a tagged or coloured particle in the same set of basic models are scarce [4–7], and vary with the chosen collision rules between tagged and fluid particles, even within a given model. This can be seen from [4], where the first few terms in the density expansion of the diffusion coefficient are calculated analytically for two choices of tagged particle collision rules in the square lattice 4-bit HPP model, introduced by Hardy, Pomeau and de Pazzis [8]. The bit number b (here $b = 4$) denotes the number of allowed velocity channels per node.

Frenkel and co-workers have calculated the self-diffusion coefficient D for the two-dimensional 7-bit FHP-III model [6] (a version of the triangular lattice gas introduced by Frisch, Hasslacher and Pomeau [2]) and for the quasi-three-dimensional 24-bit face-centred hypercubic (FCHC) model [7]. Here D was given in terms of a polynomial of degree $(b-1)$. The counting involved in obtaining its coefficients was essentially done by computer. In their formulation of tagged particle dynamics, to which we refer as *maximally random collision rules*, they used the fact that in LGCA a particle loses its identity in any interacting ('active') or non-interacting collision. This property is also imposed on tagged particle dynamics, where one defines stochastic collision rules such that the tagged particle has an equal probability of being in any possible outgoing velocity channel, in interacting as well as non-interacting collisions. For a completely filled lattice the tagged particle becomes a simple random walk on a regular lattice.

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There are a great variety of possible choices for tagged particle dynamics, all satisfying the essential requirement that a colour-blind observer sees the same collision rules as in a CA fluid without tags. Apart from the maximally random collision rules we shall also introduce *minimally random collision rules*, which can be considered as a stochastic extension of the tagged particle dynamics of [4]. Here the tagged particle continues its straight-line motion in non-interacting collisions and is only scattered with equal probability in any outgoing velocity channel in an interacting collision (with momentum exchange between particles). For a completely filled lattice the motion of the tagged particle becomes ballistic.

In this paper we derive analytic results starting from the expression for the self-diffusion coefficient in a LGCA [9,10]

$$D = \sum_{t=0}^{\infty} \frac{1}{d}\langle \boldsymbol{v}(0)\cdot\boldsymbol{v}(t)\rangle - \frac{1}{2d}\langle v^2(0)\rangle \tag{1}$$

where d is the number of dimensions and $\langle\cdots\rangle$ is an average over an equilibrium ensemble. If correlations between subsequent collisions are neglected (Boltzmann or mean-field approximation), then according to [7] the above expression reduces to

$$\begin{aligned} \varphi(t) &\equiv \frac{1}{d}\langle \boldsymbol{v}(0)\cdot\boldsymbol{v}(t)\rangle = \varphi(0)(1-\lambda)^t \\ D &= \varphi(0)\left(\frac{1}{\lambda}-\frac{1}{2}\right) \end{aligned} \tag{2}$$

where the 'eigenvalue' λ is defined through $\varphi(1) = \varphi(0)(1-\lambda)$ and is related to the mean free time between collisions, $t_0 = -[\ln(1-\lambda)]^{-1}$. The single-eigenvalue *ansatz* or 'single relaxation time approximation' (2) is not always exact, as we shall see later. It does hold for single-speed models with at most one additional type of rest particle. In this case, it can be shown by symmetry arguments [8] that any vector $\boldsymbol{v}(t)$, invariant under the isometries that leave $\boldsymbol{v}(0)$ invariant, is proportional to it, i.e. $\boldsymbol{v}(t) \sim \boldsymbol{v}(0)$, which implies (2) as we shall see later. However, it is difficult to assess *a priori* the limits of validity of this approximation. Later on we shall in fact see classes of multiple-speed models, where equations (2) hold or break down depending on the choice of tagged particle collision rules.

For tagged particle dynamics with the maximally random collision rules we calculate λ directly from the VACF after one time step and find the following very general result:

$$1-\lambda = \frac{(1-f)}{(b-1)f}[1-(1-f)^{b-1}] \tag{3}$$

where $f = \rho/b$ is the reduced density per node ($0 < f < 1$) and b the bit number. This result holds in any single-component athermal LGCA fluid for any dimension ($d = 1, 2, \ldots$) for any set of *fluid* collision rules, consistent with particle and momentum conservation and consistent with the symmetry of the underlying lattice. For instance, models having moving or rest particles with different masses have to be excluded, as well as mixtures and temperature-dependent LGCA.

As we are studying the VACF in equilibrium, the existence of an equilibrium state has been assumed implicitly, and consequently the probability distribution factorizes

into probability distributions per channel. This implies at least the assumption of a semi-detailed balance. LGCA violating the semi-detailed balance approach a steady state, different from thermal equilibrium, in which the probability distribution no longer factorizes. There is no reason to expect that Einstein's formula for the self-diffusion (1) and other Green–Kubo relations for transport coefficients have any meaning in this steady state.

This result, quoted in (3), will be derived in section 2. In section 3 we apply the minimally random tagged particle collision rules to the commonly used models. As it turns out, even there (2) is still correct. In section 4 we present a 5-bit model with minimally random collision rules where (2) is not applicable, and we have to construct the Lorentz–Boltzmann equation. There v turns out to be a linear combination of two eigenfunctions, requiring adequate changes in the mean-field results for diffusion coefficient and VACF.

2. Maximally random collision rules

The calculation of the VACF involves two steps. In step (i) we consider a p-tuple collision, where the tagged particle has initial velocity c_0. Let $\{c\}$ and $\{c^*\}$ be respectively the sets of p incoming and outgoing velocities. Then, the expected velocity of the tagged particle after one time step due to this collision is $(1/p)\sum'_{c^*} c^* = (1/p)\sum'_{c} c$. This is a consequence of momentum conservation. The summations extend either over the outgoing or over the incoming set of velocities. Let $\overline{v}_p(1|c_0)$ denote the expected velocity, summed over all possible sets of p-tuple collisions. In total we have for the expected velocity of the tagged particle after one time step, given its initial velocity c_0

$$\overline{v}(1|c_0) = \sum_{p=1}^{b} \overline{v}_p(1|c_0) f^{p-1}(1-f)^{b-p} \tag{4}$$

where $f^{p-1}(1-f)^{b-p}$ is the probability to have exactly $(p-1)$ fluid particles at the node.

In fact, for the calculation of $\overline{v}(1|c_0)$ we may just as well sum over all incoming velocities, and the distinction between interacting and non-interacting collisions is irrelevant. Consequently $\overline{v}(1|c_0)$ and the eigenvalue λ do not depend on the collision rules for the fluid particles.

In step (ii) we calculate $\overline{v}_p(1|c_0)$ where obviously $\overline{v}_1(1|c_0) = c_0$. If only one *fluid* particle is present in channel c of the node under consideration, the expected velocity is $\frac{1}{2}(c + c_0)$. Adding the contributions of all binary collisions requires a summation over *all* velocity channels except c_0, i.e.

$$\overline{v}_2(1|c_0) = \tfrac{1}{2}\sum_{c \neq c_0}(c_0 + c) = \tfrac{1}{2}(b-1)c_0 - \tfrac{1}{2}c_0 \tag{5}$$

where the relation $\sum_c c = 0$ has been used. More generally for a p-tuple collision one can choose a set of $(p-1)$ channels $[p-1] = \{c_1, c_2, \ldots, c_{p-1}\}$ out of the set $[b-1]$, which does not contain c_0. This can be done in $\binom{b-1}{p-1}$ possible ways. The

combinatorial factor $\binom{b}{p}$ vanishes for $p > b$. So

$$\begin{aligned}\overline{v}_p(1|c_0) &= \frac{1}{p}\sum_{[p-1]\subset[b-1]}\left(c_0 + \sum_{c\in[p-1]} c\right)\\ &= \frac{1}{p}\left[\binom{b-1}{p-1} - \binom{b-2}{p-2}\right]c_0\\ &= \frac{1}{b-1}\binom{b-1}{p}c_0 .\end{aligned} \tag{6}$$

The double sum on the first line reduces to $\binom{b-2}{p-2}\sum_{c\neq c_0} c_0$ where $\binom{b-2}{p-2}$ is the number of times a specific c appears in the total sum. Finally, inserting (6) into (4), with the help of Newton's binomial formula, yields

$$\begin{aligned}\overline{v}(1|c_0) &= \frac{1}{b-1}\sum_{p=1}^{b-1}\binom{b-1}{p} f^{p-1}(1-f)^{b-p}c_0\\ &= \frac{(1-f)}{(b-1)f}[1-(1-f)^{b-1}]c_0\\ &\equiv (1-\lambda)c_0\end{aligned} \tag{7}$$

with the eigenvalue λ given by (3). The VACF $\varphi(1)$ itself is obtained after averaging over c_0

$$\begin{aligned}\varphi(1) &= \frac{1}{db}\sum_{c_0} c_0\cdot\overline{v}(1|c_0) = \varphi(0)(1-\lambda)\\ \varphi(0) &= \frac{1}{db}\sum_{c} c^2 \equiv c_s^2\end{aligned} \tag{8}$$

where c_s is in fact the speed of sound in athermal lattice gases.

The result for $\overline{v}(1|c_0)$ and $\varphi(1)$ above are *exact* for all densities. The probabilistic reasoning leading to these results is exact as long as colliding particles are *uncorrelated*, i.e. do not recollide with particles they have met before (*ring collisions*). The *mean-field or Boltzmann approximation* neglects all correlated collision sequences by assuming that (7) is valid for any two consecutive time steps, i.e.

$$\overline{v}(t+1|v(t)) = (1-\lambda)\overline{v}(t) = (1-\lambda)^{t+1}c_0. \tag{9}$$

From here the mean-field results in (2) follow immediately.

3. Minimally random collision rules

Using these collision rules the tag remains on the incoming velocity unless an interacting p-tuple collision occurs, where the outcome equals c_0 plus an expected excess

velocity $((1/p)\sum_c c - c_0)$. Let $\overline{w}_p(1|c_0)$ be the expected excess velocity summed over all *interacting* p-tuple collisions, then

$$\overline{v}(1|c_0) = c_0 + \sum_{p=2}^{b} \overline{w}_p(1|c_0) f^{p-1}(1-f)^{b-p}. \tag{10}$$

Now the possible sets of interacting p-tuple collisions depend very strongly on the model. For the square-lattice HPP model there is only one binary collision with vanishing expected velocity. So $\overline{w}_2(1|c_0) = -c_0$ and

$$\lambda_{\mathrm{HPP}} = f(1-f)^2 \tag{11}$$

in agreement with Binder's results [4]. In the 6-bit FHP-I model [2] only binary and triple collisions occur, yielding similarly

$$\lambda_I = f(1-f)^3. \tag{12}$$

In the collision saturated version of the 6-bit FHP-I′ model, defined in table 1 of [2], additional triple and quadruple collisions occur, yielding

$$\lambda_{\mathrm{I}'} = \tfrac{1}{3} f(1-f)^2(3 + 13f - 10f^2). \tag{13}$$

Using the collision table (table 2) of [2] we find for the FHP-II

$$\lambda_{\mathrm{II}} = f(1-f)^3(3 - 4f + 2f^2) \tag{14}$$

and for the FHP-III

$$\lambda_{\mathrm{III}} = f(1-f)^5\{3 + 9x + \tfrac{49}{4}x^2 + \tfrac{53}{5}x^3\} \tag{15}$$

with $x = f/(1-f)$. For the different versions of the FCHC model [3,7] not all collision rules are available in the literature. We have not attempted to give any explicit expression for λ. However, in general $\overline{w}_p(1|c_0) = Ac_0$ and the constant A and $\overline{v}(1|c_0)$ can be calculated most conveniently by some algebraic manipulation program.

4. Lorentz–Boltzmann equation

In cases where $\overline{v}(1|c)$ is not a multiple of c equation (2) is not valid. In order to evaluate the Green–Kubo formula (1) one needs to construct the lattice Lorentz–Boltzmann equation. It describes the time evolution of the coloured (tagged) particle distribution $g(c, r, t)$ in a sea of uncoloured particles, that is in equilibrium except for its colour distribution, i.e.

$$g(c, r + c, t) - g(c, r, t) = I(c \mid g) \equiv -\Omega_{cc'} g(c', r, t). \tag{16}$$

The collision term $I(c \mid g)$ of the CA fluid is linear in $g(c, r, t)$ and depends furthermore on the equilibrium distribution $f = \rho/b$ of the fluid particles. For a b-bit model the collision operator $\Omega_{cc'}$ is a $b \times b$ matrix and $g(c, r, t)$ a b-vector with components labelled by c.

Following the method of [11,12] and using a matrix notation, one shows that in the mean-field approximation

$$D = \frac{1}{db} c_x \left(\frac{1}{\Omega} - \frac{1}{2} \right) c_x . \tag{17}$$

In the same approximation one finds for the VACF that

$$\varphi(t) = (db)^{-1} c_x (1 - \Omega)^t c_x . \tag{18}$$

If each Cartesian component $c_\alpha (\alpha = x, y, \ldots d)$ is a b-dimensional eigenvector of Ω, then (17) and (18) reduce to (2). In fact all basic models fall in this category, as has been shown in the two previous sections.

To illustrate the use of the more general (17) we consider a one-dimensional CA fluid, that has been extensively discussed in the literature [13,14]. It consists of V points on a line with periodic boundary conditions. At each lattice point there are five velocity channels $c_k = k$ $(k = 2, 1, 0, -1, -2)$, each of which can be occupied by at most one particle. Interacting collisions between fluid particles occur only if at most two particles are present at the same node. They are described by the (non-self-dual) collision rules

$$\begin{aligned} c_1 + c_{-1} &\Longleftrightarrow c_2 + c_{-2} \\ c_0 + c_{-1} &\Longleftrightarrow c_1 + c_{-2} \\ c_0 + c_1 &\Longleftrightarrow c_2 + c_{-1} . \end{aligned} \tag{19}$$

For the tagged particle dynamics we use the minimally random collision rules†. The expected excess velocity of these binary collisions is then

$$\begin{aligned} \overline{w}_2(1 \mid c_1) &= \tfrac{1}{2}[c_1 + c_{-2} + c_0 + c_1 + c_{-2} + c_1] - 3c_1 = -3c_1 \\ \overline{w}_2(1 \mid c_2) &= [c_2 + c_{-2} + c_2 + c_{-1}] - 2c_2 = -\tfrac{7}{4} c_2 \end{aligned} \tag{20}$$

and $\overline{v}(1|c) \neq (1 - \lambda)c$. To calculate the diffusion coefficient in (17) we need the Lorentz–Boltzmann equation (16) and construct the 5×5 collision matrix using minimally random collision rules in (19). The result is

$$\begin{aligned} I(c_2 \mid g) &= \tfrac{1}{2} f(1 - f)^3 \{-4g_2 + 2g_1 + g_0 + g_{-1}\} \equiv -\Omega_{2j} g_j \\ I(c_1 \mid g) &= \tfrac{1}{2} f(1 - f)^3 \{2g_2 - 6g_1 + g_0 + 2g_{-1} + g_{-2}\} \equiv -\Omega_{1j} g_j \\ I(c_0 \mid g) &= \tfrac{1}{2} f(1 - f)^3 \{g_2 + g_1 - 4g_0 + g_{-1} + g_{-2}\} \equiv -\Omega_{0j} g_j \end{aligned} \tag{21}$$

where $g_j = g(c_j)$ is a component of a 5-vector. The matrix elements for Ω_{ij} with $i = -1, -2$ can be obtained by interchanging $1 \longleftrightarrow -1$ and $2 \longleftrightarrow -2$.

To evaluate the diffusion coefficient one has to calculate $c\Omega^{-1}c$ in (17), where Ω is defined in (21). We observe that $\Omega^{-1}c$ is an odd function of c and hence a linear combination‡ of c and c^3, or equivalently $\Omega^{-1}c = A\psi_1 + B\psi_2$ where $\psi_1 = c = (2, 1, 0, -1, -2)$ and $\psi_2 = \frac{1}{6}(5c^3 - 17c) = (1, -2, 0, 2, -1)$ are orthogonal. After

† The case of maximally random collision rules for this model is already covered by the second section.

‡ A complete basis for this 5-dimensional space is formed by the five 5-vectors $\{1, c, c^2, c^3, c^4\}$.

determining A and B in terms of $\Omega(mn) = \psi_m \Omega \psi_n$ we find for the diffusion coefficient in (17)

$$D = 2A - 1 = \frac{20}{\Omega(11) - \Omega^2(12)/\Omega(22)} - 1 . \tag{22}$$

For the non-self-dual collision rules of (19) one obtains for the coefficients

$$\Omega(mn) = \tfrac{1}{2} f(1-f)^3 \Lambda^{(2)}_{mn} . \tag{23}$$

They have the numerical values

$$\Lambda^{(2)}_{11} = 40 \qquad \Lambda^{(2)}_{12} = \Lambda^{(2)}_{21} = -10 \qquad \Lambda^{(2)}_{22} = 80 \tag{24}$$

and lead to the following values of the diffusion coefficient:

$$D = \frac{32}{31 f(1-f)^3} - 1 . \tag{25}$$

To calculate the VACF in (18) one needs to determine the odd eigenfunctions of Ω and corresponding eigenvalues $\lambda_{1,2} = \frac{1}{2}(6 \pm \sqrt{5}) f(1-f)^3$, yielding a sum of two exponentials

$$\varphi(t) = a(1-\lambda_1)^t + b(1-\lambda_2)^t \tag{26}$$

and the coefficients $\{a, b\}$ can be easily calculated, if so desired.

The collision rules in (19) can also be extended to self-dual rules (particle–hole symmetry), by allowing a spectator particle. For this model one obtains in a similar fashion

$$\Omega(mn) = \tfrac{1}{2} f(1-f)^3 \Lambda^{(2)}_{mn} + \tfrac{1}{3} f^2 (1-f)^2 \Lambda^{(3)}_{mn} \tag{27}$$

with $\Lambda^{(2)}$ as in (24) and

$$\Lambda^{(3)}_{11} = 110 \qquad \Lambda^{(3)}_{12} = 10 \qquad \Lambda^{(3)}_{22} = 120 . \tag{28}$$

The resulting diffusion coefficient for the self-dual version of this model becomes then

$$D = \frac{228}{f(1-f)^2[279 + 270f - 25f^2]} - 1 . \tag{29}$$

The method of this section for calculating the diffusion coefficient of a tagged particle can be applied to any athermal or thermal LGCA [15,16]. From the collision rules one constructs first the Lorentz–Boltzmann operator Ω, as in (21) and subsequently $\Omega^{-1}c$. With minor modifications the method can be adapted to thermal lattice gases [17], where energy is non-trivially conserved.

5. Conclusion

The work of Hénon [1], and d'Humières *et al* [2] on transport coeficients in LGCA has been extended to include tagged particle properties in all basic LGCA models considered in the literature. We have explicitly calculated the diffusion coefficient and the VACF in the mean-field or Boltzmann approximation, that takes only uncorrelated collisions into account. Our conclusions are given in a number of comments.

(1) *Tagged particle dynamics* is specified for two extreme choices: the maximally random collision rules (MaxRCR) and minimally random collision rules (MinRCR). For the completely filled lattice ($f = 1$) the former case reduces to a standard random walk on a regular lattice; the latter to ballistic motion. With MaxRCR at $f = 1$ the eigenvalue in (2) is $\lambda = 1$, the diffusion coefficient $D = \frac{1}{2}\varphi(0)$ and the VACF $\varphi(t) = 0$ for $t \geq 1$. With MinRCR, the eigenvalue $\lambda \longrightarrow 0$, the mean free time between collisions $t_0 = -[\ln(1-\lambda)]^{-1}$ diverges, and so does the diffusion coefficient, whereas the VACF $\varphi(t) \longrightarrow 1$ for $t \geq 1$.

(2) In the *mean-field approximation* with MaxRCR the diffusion coefficient and VACF are determined through (2) and (3), and are completely *independent of the interactions of the fluid particles*. The results remain valid when all interacting collisions are replaced by non-interacting ones. This is caused by the combined effect of (i) momentum conservation and (ii) MaxRCR, which treats interacting and non-interacting collisions on equal footing. However, dependence on fluid collision rules does occur if either condition is not satisfied. For instance, the use of MaxRCR in the tagged particle correlation functions such as $\langle u(0)u(t)\rangle$ with $u = v_x^2 - v_y^2$ (here momentum conservation cannot be used to calculate the expected $u(t)$-value after one time step) leads to results depending on the detailed collision rules of the CA fluid, and so does the use of MinRCR in the VACF.

(3) In the context of long time tail studies in the FHP-III and FCHC models the mean-field results for the eigenvalue λ, diffusion coefficient and VACF in (2) have also been calculated using MaxRCR. For the 7-bit FHP-III model the eigenvalue is found to be [6]

$$\lambda = 7\sum_{m=0}^{5}\frac{1}{m+2}\binom{5}{m}f^{m+1}(1-f)^{5-m}. \tag{30}$$

Analysis shows that this formula is just a special case of (3) for $b = 7$. For the 24-bit FCHC model the result is given as [7]

$$1-\lambda = \sum_{p=1}^{b} A_p f^{p-1}(1-f)^{24-p} \tag{31}$$

where the numerical values of the coefficients A_p are tabulated. Analysis shows that these coefficients are in fact $A_p = (b-1)^{-1}\binom{b-1}{p}$ with $b = 24$. This result is in in agreement with (3) apart from a tiny error in [7] (the listed value $A_{23} = 0$ should be $A_{23} = \frac{1}{23}$), which has no observable effect on the diffusion coefficient.

(4) Consider a *non-interacting lattice gas* with a uniform position and velocity distribution, consistent with the symmetry of the underlying lattice. The system is contained in a box of size $L_1 \times L_2 \times \cdots \times L_d$ with periodic boundary conditions. A tag hops from particle to particle according to MaxRCR. Then, the VACF of the tag,

$\varphi(t) = \varphi(0)(1-\lambda)^t$ with λ in (3) is exact for all t smaller than the minimum of $\{L_1, L_2, \ldots, L_d\}$.

(5) The VACF of a LGCA in the mean-field approximation is only a *single exponential* $\varphi(t) = \varphi(0)(1-\lambda)^t$ in cases where the expected velocity after one time step $\overline{v}(1 \mid \boldsymbol{c})$ equals $(1-\lambda)\boldsymbol{c}$ with a λ-value independent of the incoming velocity, i.e. where $\boldsymbol{c}$ is an eigenvector of the Lorentz–Boltzmann collision operator Ω for the tagged particle. In general the VACF is a sum of exponentials $\sum_i a_i(1-\lambda_i)^t$ where λ_i are eigenvalues of Ω (see equations (26) and (18)).

(6) The *first Enskog approximation* for the calculation of transport coefficients [18] assumes an approximate solution of the Boltzmann equation, $\Omega \boldsymbol{F}(\boldsymbol{c}) = \boldsymbol{c}$, (it is an integral equation in the case of continuous velocities) of the form of an approximate eigenfunction $\boldsymbol{F}(\boldsymbol{c}) = A\boldsymbol{c}$. This is equivalent to the ansatz $\varphi(t) = \varphi(0)[\varphi(1)/\varphi(0)]^t = \varphi(0)[1-\lambda]^t$ for the VACF. The transport coefficient obtained in this manner (and denoted by $[D]_0$) is correct to within a few per cent for all intermolecular potentials. To see how this works out in lattice gases we consider the one-dimensional 5-bit LGCA of equations (19)–(25). Here the first Enskog approximation to D in (17) is obtained by setting $\Omega(12) = 0$ in (22), yielding

$$[D]_0 = \frac{1}{f(1-f)^3} - 1 . \tag{32}$$

It equals D in (25) to within a few per cent.

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