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Comment on "Abnormal Diffusion in Wind-tree Lattice Gases"

B.Th. Bouwens
M.H. Ernst
Institute for Theoretical Physics, State University,
3508 TA Utrecht, The Netherlands

P.M. Binder
Center for Nonlinear Studies, Los Alamos National Laboratory,
Los Alamos, NM 87545, USA

Abstract. The Boltzmann value of the diffusion coefficient in Gates's lattice wind-tree model reported in reference [1] is corrected. The new expression is in agreement with low-density simulations.

The low-density value of the diffusion coefficient calculated in reference [1] for a model of Gates [2] is incorrect. Here we obtain the correct expression, which agrees well in the relevant low-density regime with the molecular dynamics measurement of reference [1] and with the new simulation data reported in table 1.

The model under consideration is a lattice version of the Ehrenfest wind-tree model, in which trees are *left-turning* scatterers placed randomly at a fraction c of the sites of a square lattice [2].

Let $p_i(n, t)$ represent the probability of finding the wind particle at time t at site $n = \{n_x, n_y\}$ with arrival ("precollisional") velocity e_i, $i = 1, 2, 3, 4$

c	D (Boltzmann)	D $(t = 128)$	D $(t = 512)$
0.1	2.25	2.24	2.22
0.2	1.00	1.00	0.94
0.3	0.58	0.58	0.55
0.4	0.38	0.35	0.32
0.5	0.25	0.21	0.18

Table 1: Scatterer concentration, D^0_{xx} from equation (4) and diffusion coefficient (slope of the mean-squared displacement versus time) measured at 128 and 512 time steps.

(mod 4), equal to one of the nearest-neighbor lattice vectors. A configuration of scatterers is denoted by the set of quenched random variables $\{c_n\}$, where c_n takes the values 0 or 1 if site n is empty or occupied by a tree, respectively.

The Liouville equation for the deterministic lattice Lorentz gas, introduced in reference [1], is

$$p_i(n + e_i, t + 1) = (1 - c_n)p_i(n, t) + c_n p_{i-1}(n, t) \tag{1.1}$$

In the Boltzmann approximation all collisions in which the moving particle returns to a previously visited scatterer are neglected. In this approximation the average over the configurations of scatterers $\{c_n\}$ can be directly performed by replacing $\langle c_n \rangle$ by its average value c. This yields the model's Boltzmann equation. It reads, in the notation of reference [3],

$$p_i(n + e_i, t + 1) = [(1 + cT)p(n, t)]_i \tag{1.2}$$

where T_{ij} is a 4×4 collision matrix, formally written as $T = b - 1$, with $bp_i = p_{i-1}$. We note that, contrary to the statement in reference [1] the giral scattering rules do not possess the full symmetry of the square lattice. The diffusion tensor $D_{\alpha\beta}$, where α, β denote cartesian components (x, y), is given by the long-time behavior of $\frac{1}{2}\Delta_t\langle r_\alpha(t) r_\beta(t)\rangle$, where $\Delta_t a(t) = a(t+1) - a(t)$ is a forward time difference. It is therefore symmetric in α and β (Onsager symmetry), and given by the Green-Kubo formula,

$$D_{\alpha\beta} = \frac{1}{2}\sum_{\tau=0}^{\infty} [\varphi_{\alpha\beta}(\tau) + \varphi_{\beta\alpha}(\tau) - \varphi_{\alpha\beta}(0)] \tag{1.3}$$

where $\varphi_{\alpha\beta} = \langle v_\alpha(t) v_\beta(t)\rangle$ is the velocity correlation function. According to reference [3] it is given in the Boltzmann approximation by the symmetric part of

$$\frac{1}{4}\sum_i e_{i\alpha}(-cT)^{-1}_{ij} e_{j\beta} - \frac{1}{4}\delta_{\alpha\beta} \tag{1.4}$$

The term involving $\frac{1}{2}\varphi_{\alpha\beta}(0) = \frac{1}{4}\delta_{\alpha\beta}$, is the "propagation diffusion" resulting from the discrete structure of space and time [4]. As it is of relative order c, it was neglected in the low density limit of reference [3]. To evaluate equation (1.4) we calculate the relevant eigenvectors and eigenvalues of T_{ij}, defined through $cTv = -\lambda v$. The eigenvectors are $v_j^{\pm} = e_{jx} \pm ie_{jy}$, with corresponding eigenvalues $\lambda_{\pm} = c(1 \pm i)$. Inserting these results in equation (1.4) yields for the diffusion tensor in Gates's model

$$D^0_{xx} = D^0_{yy} = (4c)^{-1}(1 - c) \tag{1.5}$$

In reference [1] only D^0_{xx} has been considered for which the incorrect value $(4c)^{-1}(2 - c)$ was reported. Equation (1.5) resolves the apparent discrepancy between the values of the diffusion coefficient at *low densities*, measured by computer simulations, and those calculated from the Boltzmann equation.

This is clearly shown in table 1, where some new simulation data for $D(t) = \frac{1}{4}\Delta_t\langle r^2\rangle$ are shown at intermediate times and densities.

This agreement is to be expected, as the physical arguments for a breakdown of the Boltzmann equation in reference [5] do not apply to Gates's model. However, as soon as a nonvanishing fraction of the scatterers consists of reflectors the Boltzmann value is expected to be completely incorrect in the limit of small densities. A more sophisticated kinetic theory is required to correctly describe the diffusion coefficient.

Acknowledgments

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