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TITLE DIFFUSION IN LATTICE FLUIDS

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DIFFUSION IN LATTICE FLUIDS

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ABSTRACT

Diffusion is the transport of mass caused by molecular motion. In this article we review recent studies of the motion of one tagged particle in (a) a static, disordered medium, and (b) a bath of moving particles, both in two-dimensional lattices. We find in the first study that diffusion only exists if the particle-scatterer collision rules are non-deterministic. In the second study we find that the two-dimensional diffusion coefficient exists, apparently without a logarithmic divergence. We also find that several tagged-particle collision rules are consistent with the moving particle rules, leading to the non-uniqueness of the diffusion coefficient. These results are relevant to the study of diffusion in lattice gas automata.

1. Introduction

Recent developments [1-4] show cellular automaton models to be a promising alternative, rather than a replacement, to numerical solutions of partial differential equations.

In particular, there has been a lot of work in the area of fluid mechanics [3,4]. Several two and three-dimensional models have provided simulations that agree extremely well with experiments. Even though these microscopic models involve Newtonian particles which collide elastically, the correspondence of their macroscopic behavior to the Navier-Stokes equation is surprising. In the present article we deviate from most other studies in several respects:

(1) We study specifically the phenomenon of diffusion.

(2) We study gases at rest rather than high Reynolds number flows.

(3) We are more concerned with quantitative and qualitative changes in behavior resulting from the modelling, rather than with agreement between models and reality.

(4) The studies here usually involve the calculation of macroscopic properties (diffusion coefficients and autocorrelation functions) from ensemble averages of microscopic measurements. Typically, this involves Einstein's diffusion equation [6] or Green-Kubo formulas.

This article will proceed as follows: in section 2 we review the microscopic origin of diffusion; in section 3 we present the models for the lattice Lorentz gas, along with some analytical results. In section 4 we extend the Lorentz models to include moving scatterers, i.e., other particles. Section 5 compares the results of the previous two sections to computer simulations. Finally section 6 contains a summary and conclusions. Much of the work reported here has been the result of collaborations with M.H.Ernst, G.A. van Velzen, D.d'Humières and L.Poujol.

2. One-particle diffusion in two dimensions

The diffusion equation,

$$\partial_t n = D\nabla^2 n \tag{1}$$

is the archetype of parabolic differential equations; it describes a ubiquitous phenomenon in nature. In his 1905 paper on suspended particles, Einstein [5] related the diffusion coefficient of Brownian particles to their average displacement by

$$< x^2 >= 2Dt \tag{2}$$

When one tries to replace the random walker by a Newtonian particle with a random potential, two possibilities arise:

(1) for a point particle moving among fixed scatterers, the diffusion coefficient exists, except for overlapping square scatterers. In the latter case, retracing events lead to a vanishing diffusion coefficient[6].

(2) for a particle in a two-dimensional fluid, transport properties in two dimensions (viscosity and diffusion coefficients) diverge logarithmically with the characteristic length of the fluid. This is caused by long-time tails in the velocity autocorrelation function. As discussed by Pomeau and Résibois[7], the theories leading to these results are somewhat unsatisfactory. The problematic long-time tail can be traced back to mass and momentum conservation [8]. The reason that the diffusion coefficient exists in case (1) above is that momentum is not conserved, leading to a correlation function that decays as $t^{-(d+1)/2}$ rather than $t^{-d/2}$.

In the next two sections we will construct lattice analogues of the two cases presented above.

3. Lattice Lorentz gases

Consider a two-dimensional square lattice; we define directions i=0,1,2,3. We associate with them nearest neighbor lattice vectors ρ_i. Fixed scatterers are placed randomly at the nodes with probability c. The system of many noninteracting particles is described by the probability density in Γ-space, $p_i(n,t;\{c_n\})$, which is the probability of finding a particle moving in direction i at site n in a given configuration of scatterers $\{c_n\}$. We associate with each site n a random variable with value $c_n = 0$ with probability 1-c, $c_n = 1$ otherwise. The distribution function of moving particles can be obtained by

$$f_i(n,t) = < p_i(n,t) > \tag{3}$$

where the brackets indicate an average over configurations of scatterers. Collisions between moving particles and scatterers occur only at integer values of time. At such values the velocities are not well-defined. We choose to define $f_i(n,t)$ as the distribution function just after time t. I will now describe two of the models and give their respective Liouville equations.

Model I: If a scatterer is present, the particle velocity ρ_i becomes either ρ_{i+1} or ρ_{i-1} (modulo 4), each with probability 1/2.

The Liouville equation is

$$p_i(n,t+1) = (1-c_n)p_i(n-\rho_i,t) + \frac{1}{2}c_n[p_i(n-\rho_{i+1},t) + p_i(n-\rho_{i-1},t)] \tag{4}$$

Model II: This model has deterministic collision rules. The velocity ρ_i changes to ρ_{i-1} or ρ_{i+1} if the time step is odd or even, respectively. This leads to the Liouville equation

$$p_i(n,t+1) = (1-c_n)p_i(n-\rho_i,t) + c_n p_{i+\pi(t)}(n-\rho_i,t) \tag{5}$$

where $\pi(t) = (-1)^t$.

By recasting the Liouville equation in terms of a collision and a streaming operator [9], one can solve it for the first model by performing a Fourier-Laplace transform of the probability for a displacement[10]. One obtains for this model the following diffusion coefficient:

$$D = \frac{1}{2c} - \frac{1}{4} \tag{6}$$

For model II in a hexagonal lattice, the diffusion coefficient is given by the same expression as equation (6), without the factor 2 in the first term. For model II, there are two complications: (1) the collision operator is time-dependent, and (2) there is no equilibrium distribution. We have found that including the possibility of reflection modifies the above result directly, not as a higher-order correction.

A final observation is that the particle-and-scatterer models described in this section seem to approximate better the Lorentz model with convex scatterers, while the earlier models of Gates[11] are closer to the Ehrenfest wind-tree model which has square scatterers.

4. Tagged fluids

The results of the previous section can be easily extended to predict the self-diffusion coefficient of the well-known square lattice fluid of Hardy, de Pazzis and Pomeau[7] (HPP).

Figure 1 shows the possible tagged-untagged particle collisions consistent with the HPP model. As discussed by Binder and d'Humières[13], any combination of two or four-particle collisions from this set has the consequence that the tagged particle is representative of any fluid particle; this is why we can speak of self diffusion. From this observation it follows that the diffusion coefficient is not unique in lattice models.

We will consider two models: model III consists of collision 2A plus the HPP rules for untagged particles, while in model IV we consider all collisions.

It turns out that the Boltzmann level solution for the Lorentz gas can be used to derive expressions for the HPP self-diffusion coefficient. It can be seen from figure 1 that certain configurations of bath particles act as "scatterers" to the tagged particle. Inserting the probabilities of such events in terms of the concentration of bath particles, one obtains

$$D_{III} = \frac{1}{2c}(1 + \frac{3}{2}c - c^2 + ...) \tag{7}$$

and

$$D_{IV} = \frac{1}{6c}(1 - \frac{1}{2}c + \frac{2}{3}c^2 + ...) \tag{8}$$

As in the previous section, these results should only hold for low enough densities.

5. Simulations

In this section we review numerical simulations of the diffusion coefficient for several of the models presented above.

Table 1 shows averages over 200 configurations for times up to 20 mean-free paths. The model studied is the hexagonal-lattice version of model I. These results appeared originally in figure 7 of reference 14. The densities studied are lower than 1/64, and the agreement between theory and experiment is excellent.

Table 2 shows averages over 5000 configurations and 5000 time steps. These results appeared originally in figure 2 of reference 15. Although the results for model II should not be expected to agree with equation (6), the general agreement between this equation and simulations for models I and II is quite good.

Finally, table 3 shows averages over 2000 configurations and 4096 time steps for models III and IV. These results were originally reported in reference 13. The results in tables 1 and 2 come from simulations in an infinite field, while those in table 3 come from a periodically repeated 256x512 field.

The agreement between theory and simulations is excellent, except for model IV at high densities where a superdiffusive zig-zag phenomenon, caused by alternating deflections, comes into play.

Density.	Equation 6.	Simulations(I).	Simulations (II)
0.05	9.75	8.2 ± 1.6	9.0 ± 1.8
0.10	4.75	3.3 ± 0.7	6.0 ± 1.2
0.20	2.25	1.5 ± 0.3	4.5 ± 0.9

Table 1: Density of scatterers, equation 6, and simulations for models I and II.

Density.	Equation 6, modified.	Simulations (II)
2^{-10}	1024.	$1096. \pm 100.$
2^{-8}	256.	$190. \pm 25.$
2^{-6}	64.	$60. \pm 6.$
2^{-4}	16.	$15.0 \pm 2.$

Table 2: Density of scatterers, equation 6 modified for hexagonal lattice and simulations for model II.

Density.	Equation 7.	Simulations (III).	Equation 8.	.Simulations (IV)
0.0625	8.8	8.8 ± 0.7	2.55	2.25 ± 0.3
0.125	4.95	5.1 ± 0.4	1.25	1.4 ± 0.2
0.250	3.3	3.5 ± 0.3	0.61	0.69 ± 0.1
0.500	3.8	4.2 ± 0.4	0.32	0.73 ± 0.1

Table 3: Density of particles, equation 7, simulations for model III, equation 8 and simulations for model IV.

The diffusion coefficient values for model II are only valid for short times. As stated in section 3, for any configuration of scatterers the phase space decomposes into independent orbits. The particle recurs with probability one, which leads to abnormal diffusion through the mechanism of orbiting events which is discussed in reference 6. In the wind-tree model it is a different type of event that leads to abnormal diffusion. The fact that deterministic Lorentz models behave diffusively only for times smaller than that of a typical orbit seems to be exclusive to lattice models. A typical distribution of orbit lengths is given in reference 14, and a mean-square displacement versus time plot is given in reference 15.

Reference 15 also contains preliminary reports of measurements of the velocity autocorrelation function, $C(t) =< v(0)v(t) >$. For the Lorentz model we find $C(t) \sim t^{\alpha}$. The values of α are -1.5 ± 0.3 for model I and -1.0 ± 0.2 for model II. Preliminary simulations for the tagged-particle models show exponential decay of this function.

Finally, the diffusive behavior in the tagged-particle systems seems to persist for times longer than what it takes the particle to traverse the system.

Also, we find no logarithmic divergence of the diffusion coefficient. The latter results come from simulations in a 32x32 field.

6. Summary and conclusions

In this paper I have reviewed several lattice gas models for diffusion. coefficients of these models. Comparison of simulations to higher-order analytical expressions for one of these models[16] will be available in the near future. The simulations for particle-scatterer models show that diffusion exists for probabilistic collision rules: for deterministic rules, closed orbits equivalent to the infinite limit of orbiting events cause abnormal diffusion. Alternating left-right deflections can also cause zig-zag events which for short enough times increase the diffusion coefficient.

For tagged-untagged particle models, the most striking result is that a number of collision rules are consistent with the undifferentiated particle collision rules, leading to the non-uniqueness of the self-diffusion coefficient. The results in the previous section point to the existence of diffusion in a two-dimensional fluid. The origin of this phenomenon is unknown; a possibility is mode coupling with the ill-defined viscous mode in the HPP system. Perhaps recent simulations in a hexagonal lattice tagged-particle system will help in clearing this issue[17].

I hope that the models and results reviewed here will provide the basis for rigorous studies in the high-density behavior of lattice gas models.

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Figure 1

Tagged-untagged collisions that can be derived from the HPP model.