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Tag diffusion in driven systems, growing interfaces, and anomalous fluctuations

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Tagged diffusion in a one-dimensional hard-core lattice gas with biased nearest-neighbor hopping is mapped to a model of a growing interface. Based on the Kardar-Parisi-Zhang theory of interface dynamics, it is suggested that fluctuations, in the separation of the initial position of a tagged particle from the position at time t of a particle with tag shifted by vt at time t, grow at $t^{1/2}$ for most v, and as $t^{1/3}$ for a critical v_c. This is verified by numerical simulation, and the dependence of v_c on bias and density is found. The $t^{1/4}$ growth of fluctuations in the unbiased case is unstable with respect to both bias and $v-v_c$.

Tagged-particle diffusion in hard-core lattice gases with nearest-neighbor hopping has been of interest for several years.[1-10] In one dimension, the result is known to depend strongly on whether there is an external field, i.e, whether the hopping is biased or not. In the unbiased case, the root-mean-squared (RMS) displacement of a tagged particle grows anomalously slowly,[1-8] and varies as $t^{1/4}$ at time t; on the other hand, when the bias is nonzero, the more familiar diffusive dependence $t^{1/2}$ is found for the RMS fluctuation of a tagged particle around its mean position.[4,9,10]

It is then interesting to ask whether there is any tagged correlation function which is anomalous even with nonzero bias. In this paper we answer this question in the affirmative, by mapping the tagged-particle problem to a one-dimensional model of interface dynamics. Besides reproducing known results, our mapping leads to the identification of an important parameter, by varying which, fluctuations cross over from the diffusive $t^{1/2}$ behavior to an anomalous $t^{1/3}$ behavior. Consider a "sliding tag" process, in which we follow the fluctuations in the separation between a tagged particle (at $t=0$) and a particle (at time t) whose tag is shifted from the original one by vt. We show that for almost all values of the tag velocity v (including $v=0$, the customary tagged process) the RMS fluctuations in the presence of bias vary as $t^{1/2}$, but for a critical value v_c (which depends on bias and density) the RMS fluctuations vary anomalously, as $t^{1/3}$. We confirm these predictions, determine v_c and demonstrate various crossovers by a Monte Carlo study of the dynamics of tracer diffusion in the one-dimensional lattice gas.

Consider a one-dimensional lattice of N_S sites, of which $N_P=\rho N_S$ are occupied by particles, and assume periodic boundary conditions. In the simple exclusion process, a particle chosen at random attempts to hop with probability p to the right and probability q to the left $(p+q=1)$; the hop is completed only if the site sought is unoccupied. N_p such attempted hops constitute a single time step. This model has been studied earlier and the dynamic exponent z found to be $\frac{3}{2}$ (for $p\neq q$, $\rho=\frac{1}{2}$), by Monte Carlo methods[11] and a Bethe ansatz treatment of the relaxation matrix.[12]. Also, from a hydrodynamic description,[13] density fluctuations were found to spread anomalously rapidly $\sim t^{2/3}$.

For the tagged process in the presence of bias, the drift velocity v_P of any particular tagged particle is given by $(p-q)(1-\rho)$ and the corresponding diffusion constant D is known to be $\frac{1}{2}|p-q|(1-\rho)$.[8,9] Below, we map the tagged process to the dynamics of an interface model in which the tag appears very naturally, and thereby deduce an anomalous $\sim t^{1/3}$ behavior, not found earlier in the tagged problem.

Consider the tagged process with particles labeled $n=1,2,\dots,N_P$ sequentially at $t=0$. The ordering is preserved by the dynamics of the exclusion process. The configuration of the system is specified by the set $\{y(n)\}$ where $y(n)$ denotes the location of the nth particle. The corresponding interface model, which we call the particle height (PH) model, is obtained by interpreting the tag label n as a horizontal coordinate, and $y(n)$ as a local height. Each configuration $\{y(n)\}$ then defines a one-dimensional interface in the form of a staircase inclined to the horizontal with mean slope $1/\rho$. The interface coordinates satisfy $y(n+1)\geq y(n)+1$, and the periodic boundary conditions translate into $y(n\pm N_P)=y(n)\pm N_S$. The evolution rule is as follows: in each time step, $y(n)$ tends to increase (or decrease) by 1 with probability p (or q); it actually increases (or decreases) if and only if $y(n+1)-y(n)>1$ (or $y(n)-y(n-1)>1$). In the unbiased case ($p=q=\frac{1}{2}$), the interface does not move with a net velocity, but fluctuates around its initial position. But in the biased case ($p\neq q$), the interface moves vertically with the particle drift velocity v_P in the steady state. Our mapping differs from earlier equivalences between the particle and interface problems[11,12] in that it uses the particle tag in a direct and essential way in the translation. As a consequence, height fluctuations around the mean position of the interface translate directly into tagged particle correlations.

The mapping is useful as there has recently been significant progress in understanding universality classes in interface dynamics in one dimension. A continuum model of a growing interface was introduced and analyzed by Kardar, Parisi, and Zhang[14] (KPZ):

$$\frac{\partial y}{\partial t}=D\frac{\partial^2 y}{\partial n^2}+a_1\frac{\partial y}{\partial n}+a_2\left[\frac{\partial y}{\partial n}\right]^2+\eta(n,t) \ . \quad (1)$$

Here D is the diffusion constant, the coefficients a_1 and a_2 are nonzero if the interface has a net velocity, and $\eta(n,t)$ is a noise term which satisfies the condition $\langle \eta(n_1,t_1)\eta(n_2,t_2)\rangle=\delta(t_1-t_2)\delta(n_1-n_2)$. The KPZ model is generic in that several discrete (1+1)-dimensional interfacial models are known to exhibit the KPZ exponents.[12,11,15–18] We thus expect the PH model also to belong to the KPZ universality class.

If $a_1=a_2=0$ (nongrowing case), Eq. (1) reduces to a harmonic model with noise, solved by Hammersley[19] and by Edwards and Wilkinson[20] (HEW). The RMS fluctuations of the local height in the HEW model are proportional to $t^{1/4}$, which agrees with the answer in the tagged-particle problem in the absence of bias.

A nonzero bias implies a finite velocity v_P of the PH interface in the vertical direction. In the corresponding KPZ description, both a_1 and a_2 are nonzero for the growing interface.[14,18] With a_1 nonzero, RMS fluctuations of the height around the mean position, for fixed n, grow as $t^{1/2}$. However, the second term on the right-hand side of Eq. (1) can be eliminated by making the transformation $n'=n+a_1t$, $t'=t$ corresponding to a Galilean shift into a frame in which the drift motion of the interface is arrested. In such a frame, the growth of the interfacial width (for fixed n') is anomalously slow; the KPZ analysis leads to the conclusion that RMS fluctuations grow as $t^{1/3}$.

Let us examine the implications for the tagged-particle problem. The fact that fluctuations vary as $t^{1/2}$ for a growing interface, if n is fixed, accords with the known diffusive spread of a tagged-particle displacement around its mean in the presence of bias. A Galiliean shift in the interface problem corresponds to a shift in "tag space" in the exclusion problem, rather than in real space. We are thus led to examine correlations of the form

$$\sigma_b^2(t)=\langle\{(y(n_t,t)-y(n,0)-(1-b)v_Pt)\}^2\rangle \quad (2a)$$

with[21]

$$n_t=n-b\rho v_Pt \ . \quad (2b)$$

Here b is a parameter in terms of which the tag velocity is $\nu=b\rho v_P$. The last term on the right-hand side of Eq. (2a) guarantees that the mean value of the terms within parentheses vanishes, and represents the shift in position caused by going into a moving frame with velocity $v_F=(1-b)v_P$. Let the special tag velocity ν_c (which eliminates the bodily drift of the interface) correspond to a critical value b_c in the particle problem. It is important to know how b_c depends on bias and density. Below we derive a constraint on its density dependence, and determine it for $\rho=\frac{1}{2}$.

Although we have defined the exclusion process in terms of particle hopping, it can equally well be viewed as the backward motion of holes (sites on which there are no particles). Double occupancy of holes is forbidden, so that the relative order of tagged holes is also preserved. The average velocity of any particular hole is $v_H=-(p-q)\rho$. Consider the hole analog of the correlation function of Eq. (2b). Let the rate of change of the hole tag be $\nu'=b'(1-\rho)v_H$. The corresponding inertial frame velocity is then $v'_F=(1-b')v_H$. The value of b' (for holes) that corresponds to a certain value of b (for particles) can be found by equating the corresponding v'_F and v_F, as both refer to the velocity of the same moving frame. Moreover, the condition for criticality should be reflected simultaneously in particle and hole correlation functions, so that $b'_c(\rho)=b_c(1-\rho)$. Putting these relations together we find

$$(1-\rho)b_c(\rho)+\rho b_c(1-\rho)=1 \ . \quad (3)$$

For $\rho=\frac{1}{2}$, this condition implies $b_c(1/2)=1$ which corresponds to a critical velocity $v_c=0$. For $\rho\neq\frac{1}{2}$, Eq. (3) provides a connection between $b_c(\rho)$ in the range $\rho<\frac{1}{2}$ and the range $\rho>\frac{1}{2}$.

We performed a Monte Carlo study of the exclusion process to check the predictions based on the mapping, and to determine the dependence of b_c on bias and density. We used $N_S=90\,000$, and accessed particles in a random order in each Monte Carlo time step. Figure 1 shows the time dependence of σ for various values of b, for $\rho=\frac{1}{2}$, $p=\frac{3}{4}$. As expected from Eq. (3) the data for $b=1$ show the smallest σ. While σ^2 varies linearly with t for $b\neq1$, the variation is sublinear $\sim t^{2\theta}$ for the critical value $b_c=1$; as shown in the inset in Fig. 1 we find that for $b=b_c$, the exponent is $\theta\simeq0.32\pm0.015$, consistent with $\sigma\sim t^{1/3}$.

We did similar b scans for several values of ρ and p. We observed a crossover from $\theta=\frac{1}{2}$ (for most values of b) to $\theta=\frac{1}{3}$ (for the critical value b_c) for all $p\neq\frac{1}{2}$, and thus obtained estimates of b_c. We observed that b_c is independent of the bias $(p-q)$ and that it depends on the density

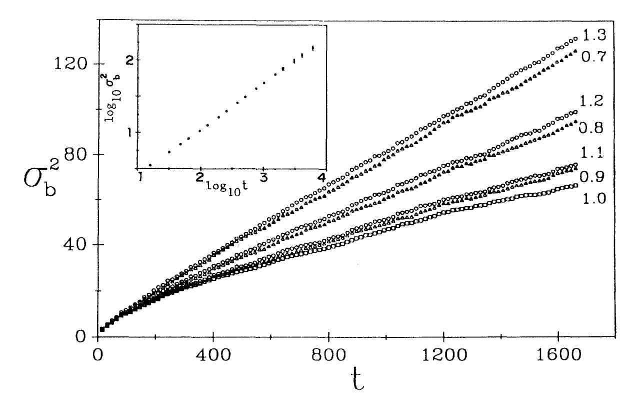

FIG. 1 The time dependence of fluctuations in the sliding-tag process for various values of b, in a Monte Carlo run with 90 000 sites, $\rho=0.5$ and $p=0.75$. The growth is linear for $b\neq1$ and sublinear for $b=b_c=1$. For $b=b_c$, the inset shows the variation on a $\log_{10}$ scale, averaged over seven longer runs. The average slope yields $2\theta\simeq0.64\pm0.03$.

ρ in a simple fashion

$$b_c(\rho)=\frac{\rho}{1-\rho} \ . \tag{4}$$

Thus the velocity of the critical inertial frame is

$$v_c(\rho)=(1-2\rho)(p-q) \ . \tag{5}$$

Our results are consistent with the simple scenario depicted in Fig. 2. There are two relevant parameters in the tagged-particle problem. The first is the bias $(p-q)$ and the second (which comes into play only when the bias is nonzero) is the deviation of b from its critical value $b_c(\rho)$ (or equivalently, the difference of the velocity of the inertial frame from that of the critical frame, v_F-v_c). The multicritical HEW fixed point, which describes fluctuations in the unbiased case, is unstable with respect to both parameters. If $b=b_c(\rho)$ is maintained, the behavior is characterized by the KPZ fixed point ($\theta=\frac{1}{3}$). On the other hand, if $b\neq b_c(\rho)$, the behavior is governed by the "diffusive" fixed point ($\theta=\frac{1}{2}$). Depending on the values of $[b-b_c(\rho)]$ and $(p-q)$, various types of crossovers are observed. In particular, if b is equal to $b_c(\rho)$ and $(p-q)$ is small, there is a regime of time over which $\sigma\sim t^{1/4}$ is observed, followed by $\sigma\sim t^{1/3}$ for larger times. Details of such crossover effects and evidence for scaling near the HEW multicritical point will be presented elsewhere.[22]

The velocity $v_c(\rho)$ in Eq. (5), which equals $\partial(\rho v_P)/\partial\rho$, arises naturally in a hydrodynamic description of the exclusion process. It was shown by van Beijeren, Kutner, and Spohn[13] that in the presence of bias in one dimension the RMS fluctuation of the center of mass grows anomalously $\sim t^{2/3}$, when viewed in a frame moving with velocity v_c. Our results show that an appropriate tagged-particle correlation function also behaves anomalously $\sim t^{1/3}$ in the same frame. By contrast, in the unbiased case, center-of-mass fluctuations are diffusive $\sim t^{1/2}$, while tracer fluctuations are anomalous $\sim t^{1/4}$.

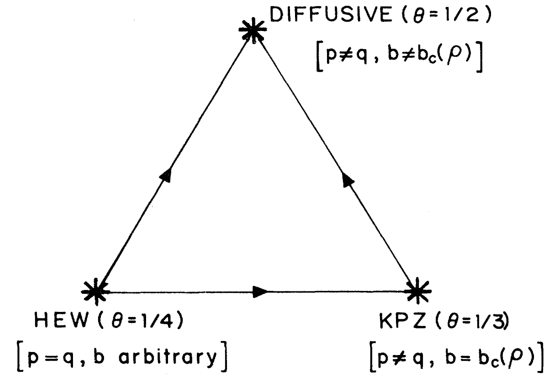

FIG. 2. The schematic depiction of relative stability of various types of behavior in tagged-particle correlations.

We note that the anomalous behavior in the sliding-tag process also affects the time dependence of correlations involving two fixed tags.[22] In higher dimensions, the equivalence between the tagged-particle problem and the PH model breaks down as the ordering of tags is not preserved. The calculation of sliding-tag correlation functions [Eq. (2)] in two[23] and higher dimensions remains an interesting open question.

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Note added in proof. After this work was submitted for publication, we learned of work by H. van Beijeren where the stochastic displacement of a mass front from its average position is shown to increase as $t^{1/3}$. We thank Prof. van Beijeren for sending us his paper before publication.

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[21]Equation (2b), which is correct in a continuum sense, must be modified for discrete n and t by replacing $b\rho v_p t$ by the integer closest to it.
[22]S. N. Majumdar and M. Barma (unpublished).
[23]In two dimensions with nonzero bias, the center of mass fluctuates anomalously $\sim t^{1/2}(\ln t)^{1/3}$ in a frame moving with velocity v_c (see Ref. 13).