Physica A 177 (1991) 366–372
North-Holland

Two-tag correlation functions in one-dimensional lattice gases

S.N. Majumdar and Mustansir Barma
Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay 400005, India

Correlations between two labelled particles are studied in a one-dimensional lattice gas with nearest neighbour hopping. Fluctuations in the distance between the first particle (at time t) and the other (at time 0) are studied analytically and by Monte Carlo, with unbiased and biased hopping. In the latter case, the tag–tag correlation shows a nonmonotonic dependence on t. A stochastic harmonic theory, based on an exact mapping to an interface model, suggests a scaling form for the correlation as a function of t and the difference between the labels. Monte Carlo data are consistent with scaling. In the unbiased case, the scaling function given by the harmonic theory seems to be exact.

1. Introduction

The general problem of interactions between random walkers is of interest from several points of view [1]. A simple but important instance is hard core exclusion in a lattice gas – particles hop between nearest neighbour sites of a lattice, subject to the constraint that no site is more than singly occupied. Of particular interest in this system is the study of tracer diffusion, in which the dynamics of a single tagged particle is followed.

A number of results pertaining to the tagged process are known in one dimension [2–5]. Let there be N_S sites of which $N_P = \rho N_S$ are occupied by particles. A randomly chosen particle attempts to hop, rightward with probability p ($\geqslant \frac{1}{2}$), and leftward with probability q, with $p+q=1$; the hard core constraint is ensured by allowing the hop to complete only if the sought site is unoccupied. N_P attempted hops constitute one time step. In steady state, the drift velocity v_P of any particular tagged particle is known [5] to be $(p-q)(1-\rho)$ and the mean squared displacement of a tagged particle around its mean position grows asymptotically as Dt, with $D=(p-q)(1-\rho)$. But if the bias is zero, the variance grows anomalously slowly [2], as $At^{1/2}$, with $A=(2/\pi)^{1/2}(1-\rho)/\rho$.

In physical terms, this slow growth can be understood as a cage effect arising from hard core exclusion, as in one dimension a particle is always hemmed in by its neighbours. More surprising is the fact that the anomalously slow growth of fluctuations seems to disappear the moment the bias is nonzero. The resolution of this puzzle involves an exact mapping [6] between the tagged particle problem and a model of

0378-4371/91/$03.50

one-dimensional interface dynamics. The mapping also suggests the definition of a "sliding tag" process in which one of the tags is a function of t. The mapping to the interface model and the sliding tag process are discussed in section 2. The sliding tag process clearly shows how anomalous fluctuations (growing as $t^{1/3}$) arise in the biased case.

In order to have a signature of anomalous time dependence in the tagged particle problem, it is essential, in general, to consider correlations involving two particles with distinct labels. Accordingly, in section 3, we study, both analytically and by Monte Carlo simulation, the fluctuations in the separation between a labelled particle at time t and another labelled particle at time 0. In the unbiased case, we find that fluctuations increase monotonically in time. By contrast, in the biased case, two-tag fluctuations decrease, reach a minimum value and then increase. One can understand these effects by analyzing a harmonic, stochastic model of the equivalent interface. The theory suggests that scaling forms should hold, and Monte Carlo results are found to conform with this. In the unbiased case, the scaling function can be found analytically, using a harmonic theory; in the biased case, the harmonic theory provides a qualitative understanding of the phenomena, but does not correctly predict the scaling variable.

2. Mapping to interface model

In this section we describe an exact mapping between the tagged particle problem and an interface model [6]. The mapping suggests the definition of the sliding tag process, which helps in the understanding of universality classes in this problem.

Label particles sequentially $n=1, 2, ..., N_P$, and let $y(n)$ denote the location of the nth particle. The interface model is defined by interpreting n as a horizontal coordinate, and $y(n)$ as the interface height at n. Each allowed configuration of particles maps into an interface configuration, and vice versa. The heights satisfy $y(n+1) \geqslant y(n)+1$, and the interface as a whole has mean slope $1/\rho$. In each time step, the local height tends to increase or (decrease) by 1 with probability p (or q), and actually changes if and only if $y(n+1)-y(n)>1$ remains valid for all n.

The bias has a strong effect on interface dynamics. When bias is absent ($p=q=\frac{1}{2}$) the interface fluctuates around its mean position but does not move bodily. When the bias is nonzero, the interface moves with the particle drift velocity v_P, and the dynamics describes a growing interface. Local height fluctuations in the interface model translate directly into tagged particle correlations. In this respect, our model differs from earlier equivalences [7,8] between the particle and interface problems.

Analysis of a continuum model by Kardar, Parisi and Zhang [9] (KPZ) has led to an improved understanding of interface dynamics in one dimension. The equation of motion of the interface is

$$\frac{\partial y}{\partial t}=\frac{1}{2}\frac{\partial^2 y}{\partial n^2}+a_1\frac{\partial y}{\partial n}+a_2\left(\frac{\partial y}{\partial n}\right)^2+\eta(n,t)\,, \tag{1}$$

where the coefficients a_1 and a_2 are nonzero only if the interface is growing with a net velocity, and $\eta(n, t)$ represents Gaussian, uncorrelated noise. This continuum model seems to represent quite well, in a general way, the physics of several discrete $(1+1)$-dimensional interfacial models, and it is interesting to see what the KPZ results predict for the tagged particle problem.

In the unbiased case, we have a nongrowing but fluctuating interface, corresponding to $a_1=a_2=0$ in eq. (1). The rms fluctuations of the local height in the resulting interfacial model (considered by Edwards and Wilkinson [10], and earlier, in a different context, by Hammersley [11]) are proportional to $t^{1/4}$. This is precisely the answer for the tagged particle problem in this case.

With nonzero bias in the tagged particle problem, we have a growing interface, for which both a_1 and a_2 are nonzero in eq. (1). In this case, rms fluctuations of height at fixed n grow as $t^{1/2}$, which accords with the known, normal diffusive growth of fluctuations in the tagged particle problem.

The more interesting and important point is that the a_1 term can be eliminated by the Galilean shift $n'=n+a_1t$, $t'=t$. The KPZ analysis then shows that the rms fluctuations grow anomalously slowly, as $t^{1/3}$, in the shifted frame of reference. There are interesting implications for the tagged particle problem. The Galilean shift corresponds to a shift in tag space, and so leads to the consideration of the sliding tag correlation function

$$\sigma_b^2(t)=\langle[y(n_t,t)-y(n_0,0)-(1-b)v_{\rm P}t]^2\rangle\,. \tag{2}$$

Here b is a parameter which characterizes the Galilean shift, in terms of which the shifted tag n_t is $n_0-b\rho v_{\rm P}t$. The last term in eq. (2) is the shift in position caused by going into a moving frame with velocity $v_{\rm F}=(1-b)v_{\rm P}$. Only for $b=b_{\rm c}\equiv a_1/\rho v_{\rm P}$ can one completely eliminate the a_1 term in eq. (1) by Galilean shift, and only for this critical value do the height fluctuations $\sigma^2_{b_{\rm c}}(t)$ vary as $t^{2/3}$; for $b\neq b_{\rm c}$, $\sigma_b^2(t)$ varies as t. From particle–hole symmetry, it follows [6] that $(1-\rho)b_{\rm c}(\rho)+\rho b_{\rm c}(1-\rho)=1$. For the half-filled case $\rho=\frac{1}{2}$, this condition leads to $b_{\rm c}(\frac{1}{2})=1$. For other values of ρ, a numerical study reveals $b_{\rm c}(\rho)=\rho/(1-\rho)$. The corresponding velocity of the critical inertial frame is $v_{\rm c}(\rho)=(1-b_{\rm c})v_{\rm P}=(1-2\rho)(p-q)$, which coincides with $\partial(\rho v_{\rm P})/\partial\rho$, the average drift speed of density fluctuations [12,13].

In summary, for most values of the sliding tag parameter b, mean squared fluctuations grow linearly in t. But for the critical value $b_{\rm c}$ (which corresponds to the elimination of the a_1 term in eq. (1)) the variance grows as $t^{2/3}$.

3. Two-tag correlation functions

In this section, we show that there is a signature of anomalous behaviour in correlations involving two particles with fixed tags n_0 and $n_0 - \Delta n$. Define a correlation function which monitors fluctuations in the distance between n_0 at time 0 and $n_0 - \Delta n$ at time t,

$$\sigma_2^2(\Delta n, t) \equiv \langle [y(n_0 - \Delta n, t) - y(n_0, 0) + \Delta n/\rho - v_P t]^2 \rangle . \tag{3}$$

In the steady state, the expectation value of the quantity within parentheses is zero. Fig. 1 shows Monte Carlo results for the variation of σ_2^2 with t, and brings out a strong difference between the unbiased (fig. 1a) and biased (fig. 1b) cases. While σ_2^2 increases monotonically with t in the absence of bias, it is strongly nonmonotonic when bias is nonzero. In both cases, results depend on the separation Δn of the two tags. In the unbiased case, the large time behaviour follows $\sigma_2^2 \sim t^{1/2}$. In the biased case, the lower envelope of the curves describes the critical locus σ_{2c}^2 of the sliding tag process and varies as $t^{2/3}$.

We now attempt an analytical description of this behaviour, based on the equivalent interface model of section 2. As we shall see below, a harmonic stochastic treatment of interface dynamics explains quantitatively the behaviour of σ_2^2 in the un-

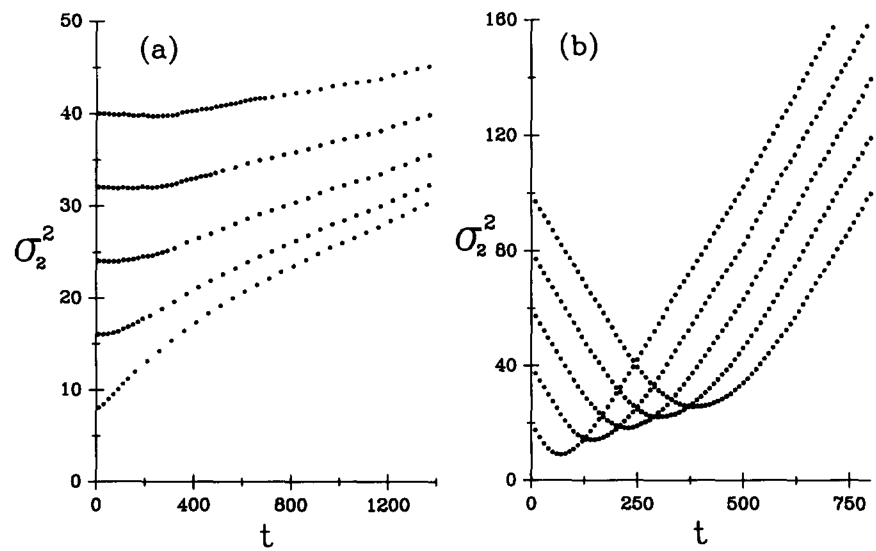

Fig. 1. Monte Carlo data for a system with $N_S = 90\,000$, $N_P = 45\,000$. (a) Unbiased case, $p = 0.5$. Each point is an average over 10 runs. Different sets (moving upwards) correspond to tag separations $\Delta n = 4$, 8, 12, 16, 20. (b) Biased case, $p = 0.75$. Each point is obtained from a single run. Different sets (moving upwards) correspond to tag separations $\Delta n = 10$, 20, 30, 40, 50. The lower envelope of the curves varies as $t^{1/3}$.

biased case, and provides a qualitative understanding of the trends in the biased case. In the harmonic theory, the height $y(n, t)$ depends linearly on the heights at neighbouring n's, and is modulated by noise,

$$y(n,t)=Qy(n-1,t-1)+Py(n+1,t-1)+\eta(n,t)\ , \tag{4}$$

where the couplings P and Q satisfy $P+Q=1$. The difference $P-Q$ is a measure of the bias. Periodic boundary conditions are used, so $y(0,t)$ stands for $y(N_P,t)-N_S$ and $y(N_P+1,t)$ for $y(1,t)+N_S$. The noise $\eta(n,t)$ satisfies $\langle\eta(n,t)\rangle=0$, and $\langle\eta(n,t)\,\eta(n',t')\rangle=w^2\delta_{n,n'}\delta_{t,t'}$. The initial condition is taken to be $y(n,0)=n/p$. The mean value $\langle y(n,t)\rangle$ is given by $y(n,0)+(P-Q)t/p$, and the deviation $h(n,t)=y(n,t)-\langle y(n,t)\rangle$ is found by Fourier transform to be

$$h(n,t)=\frac{1}{2\pi N_P}\sum_k \mathrm{e}^{-ikn}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta\,\mathrm{e}^{-i\theta t}\,\tilde{\eta}(k,\theta)}{1-(Q\,\mathrm{e}^{ik}+P\,\mathrm{e}^{-ik})\,\mathrm{e}^{i\theta}}\,, \tag{5}$$

where $\tilde{\eta}(k,\theta)=\sum_{n=1}^{N_P}\sum_{t=1}^{\infty}\eta(n,t)\,\mathrm{e}^{i(nk+t\theta)}$. The correlation function of interest becomes

$$\sigma_2^2(\Delta n,t)=\lim_{t_0\to\infty}\langle[h(n_0-\Delta n,t+t_0)-h(n_0,t_0)]^2\rangle\ , \tag{6}$$

the limit $t_0\to\infty$ being taken to ensure steady state. The result, in the thermodynamic limit, is

$$\sigma_2^2=\frac{w^2}{PQ}\sum_{r=0}^{t}\binom{t}{r}P^rQ^{t-r}\,|\tfrac{1}{2}(t-\Delta n)-r|\ . \tag{7}$$

At large times t, the variable $z=(r-Pt)/\sqrt{PQt}$ is distributed normally, and we find

$$\sigma_2^2=w^2\left(\frac{t}{2\pi PQ}\right)^{1/2}\int \mathrm{d}z\left|z+\frac{t(p-\frac{1}{2})-\frac{1}{2}\Delta n}{\sqrt{PQt}}\right|\mathrm{e}^{-z^2/2}\ . \tag{8}$$

In the unbiased case ($P=Q=\frac{1}{2}$) the large-time result can be written in the scaling form

$$\sigma_2^2(\Delta n,t)=w^2\,\Delta n\,Y_u(t/(\Delta n)^2) \tag{9}$$

with the scaling function given by

$$Y_u(z)=2[\mathrm{erf}(1/\sqrt{2z})+\sqrt{2z/\pi}\,\mathrm{e}^{-1/2z}]\ . \tag{10}$$

$Y_u(z)$ approaches a constant as $z\to 0$ and varies as $z^{1/2}$ as $z\to\infty$. As suggested by eq. (9), we rescaled the Monte Carlo data and plotted $\sigma_2^2/\Delta n$ versus $z=t/(\Delta n)^2$ for several values of Δn, and found data collapse. Representative results are shown in fig. 2a (only two values of Δn are shown for clarity). The analytical scaling function Y_u of eq. (10) is also plotted for comparison. In general, there would be a uniform time-rescaling factor to account for the difference of time steps in the Monte Carlo and

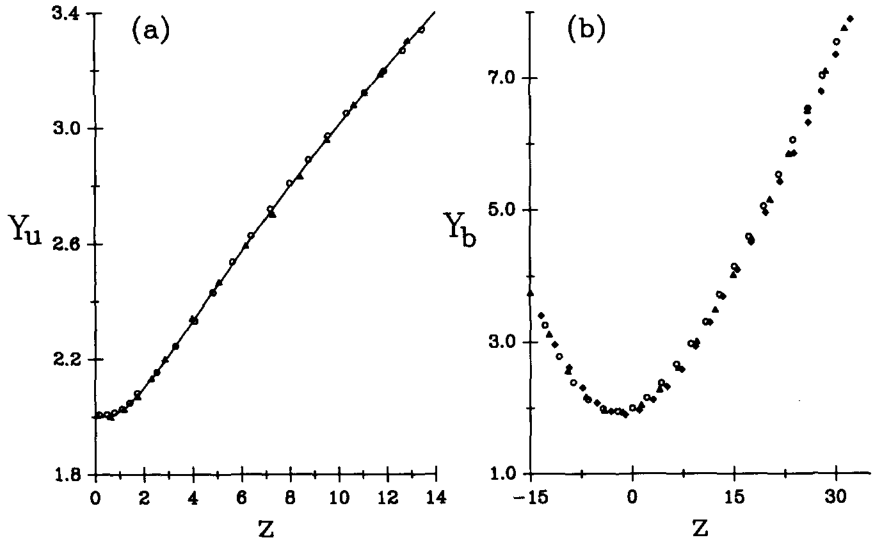

Fig. 2. Scaling functions. (a) Unbiased case: $Y_u = \sigma_2^2/\Delta n$ obtained from Monte Carlo data of fig. 1a for $\Delta n = 8$ (open circles) and $\Delta n = 12$ (triangles) plotted against $z = t/(\Delta n)^2$. The continuous curve is a plot of $Y_u(z/2)$ defined in eq. (10). (b) Biased case: $Y_b = \sigma_2^2/(\Delta n)^{2/3}$, obtained from Monte Carlo data of fig. 1b for $\Delta n = 10$ (open circles), $\Delta n = 20$ (triangles) and $\Delta n = 30$ (diamonds), plotted against $z = [t - t^*(\Delta n)]/(\Delta n)^{2/3}$ with $t^*(\Delta n) = \Delta n/\rho^2(p-q) = 8\Delta n$.

stochastic harmonic model; in this case, the factor is 2, and the continuous curve is a plot of $Y_u(z/2)$. The agreement with the Monte Carlo data is very good, and we conjecture that Y_u is the exact scaling function for the two-tag process.

In the biased case ($P \neq Q$), the difference $P - Q$ is a measure of the bias, but there is no unique way to determine P and Q in terms of p, q and ρ. The continuum limit of eq. (4) lacks the nonlinear term of eq. (1), known to be important for a complete description of the dynamics of a growing interface. Nevertheless, harmonic theory provides a reasonably good qualitative description. For instance, analysis of eq. (8) yields a nonmonotonic dependence of σ_2^2 on t, with a minimum at $t = t^*$ and a scaling form in the vicinity of the minimum,

$$\sigma_2^2(\Delta n, t) \approx (\Delta n)^{\phi} Y_b(z) , \qquad z = \frac{t - t^*(\Delta n)}{(\Delta n)^{\phi}} . \tag{11}$$

Here t^* is proportional to Δn for sufficiently large Δn, implying a variation $\sigma_2^2 \sim (t^*)^{\phi}$ for the envelope of the curves in fig. 1b. The harmonic theory incorrectly predicts $\phi = 1/2$. Matching to the known result for the envelope [6] yields $\phi = 2/3$. Monte Carlo data, rescaled in accordance with eq. (11), are plotted in fig. 2b. Results are consistent with scaling.

4. Conclusion

Two-tag correlations clearly show the signature of anomalous behaviour in both non-driven (unbiased) and driven (biased) one-dimensional lattice gases, in contrast to single-tag correlations, which show only diffusive spreads in driven systems. Two-tag correlations grow monotonically in the unbiased case, and non-monotonically in the biased case. Scaling descriptions are valid for both. In the unbiased case, it is conjectured that the stochastic harmonic theory gives the exact form (eq. (10)) of the scaling function.

Acknowledgements

We thank V. Krishnamurthy for helping us with the figures. MB would like to take this opportunity to acknowledge many stimulating interactions with Michael E. Fisher, both at a professional and personal level.

References

[1] M.E. Fisher, J. Stat. Phys. 34 (1984) 667.
[2] T.M. Ligget, Interacting Particle Systems (Springer, New York, 1983), and references therein.
[3] P.M. Richards, Phys. Rev. B 16 (1977) 1393.
[4] S. Alexander and P. Pincus, Phys. Rev. B 18 (1978) 2011.
[5] A. DeMasi and P.A. Ferrari, J. Stat. Phys. 38 (1985) 603.
[6] S.N. Majumdar and M. Barma, Phys. Rev. B, to appear.
[7] M. Plischke, Z. Racz and D. Liu, Phys. Rev. B 35 (1987) 3485.
[8] D. Dhar, Phase Transitions 9 (1987) 51.
[9] M. Kardar, G. Parisi and Y.C. Zhang, Phys. Rev. Lett. 56 (1986) 889.
[10] S.F. Edwards and D.R. Wilkinson, Proc. R. Soc. London A 381 (1982) 17.
[11] J.M. Hammersley, Proc. Fifth Berkeley Symp. Math. Stat. Probab. 3 (1967) 89.
[12] H. van Beijeren, R. Kutner and H. Spohn, Phys. Rev. Lett. 54 (1985) 2026.
[13] H. van Beijeren, J. Stat. Phys., to appear.