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J. Phys. A: Math. Gen. 35 (2002) L579–L584

PII: S0305-4470(02)40172-2

LETTER TO THE EDITOR

Fluctuations in the lattice gas for Burgers' equation

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Received 2 August 2002 Published 1 October 2002 Online at stacks.iop.org/JPhysA/35/L579

Abstract

The Langevin equation for the biased random hopping of particles onto unoccupied sites of a lattice is obtained from the master equation for finite systems by invoking a limit theorem due to Kurtz. For a weakly asymmetric process with diffusive scaling, the continuum limit of this equation yields a deterministic equation that is equivalent to Burgers' equation. The stochastic equation for the leading lattice corrections is derived and the approach to the continuum limit is illustrated with simulations.

PACS numbers: 02.50.-r, 05.40.-a, 47.40.Nm

Driven lattice gases are used to model physical phenomena in a variety of settings [1-5]. The dynamics of such lattice gases are determined by transition rules for site occupation numbers that are expressed in terms of the occupancies of neighbouring sites at the preceding time step. This provides the basis for a multiscale approach to nonequilibrium systems in that microscopic fluctuations are incorporated within stochastic transition rules of a master equation, while a continuum equation of motion, derived from this master equation, describes the macroscopic evolution of the coarse-grained system. One of the central issues in such studies is the nature and strength of the fluctuations as the system is coarse-grained.

In this letter, a general procedure is described for deriving exact equations of motion for driven lattice gases from their master equations. We use this method to obtain the Langevin equation for the asymmetric exclusion process, i.e. the biased random hopping of particles onto unoccupied sites of a lattice. The continuum limit of this Langevin equation is a deterministic equation that is equivalent to Burgers' equation, while the leading lattice corrections account for the discrepancies between solutions to Burgers' equation and simulations on finite lattices. Although the connection between the asymmetric exclusion process and Burgers' equation is well known [6–11], our approach provides an exact analytic expression for the fluctuations in the lattice and coarse-grained systems as well as a framework for calculating the stochastic corrections to the continuum limit.

Burgers' equation,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2} \tag{1}$$

is the simplest equation that incorporates the competing effects of a convective nonlinearity and ordinary linear diffusion [12, 13]. This equation has been used to study the development of

0305-4470/02/410579+06\$30.00 © 2002 IOP Publishing Ltd Printed in the UK L579

turbulence and the propagation of disturbances, including shock waves [14]. Stochastic forms of Burgers' equation have been proposed for randomly stirred fluids [15], surface growth [16], traffic flow [17, 18], population dynamics [19] and cardiac dynamics [20].

We consider the asymmetric exclusion process on a one-dimensional lattice [6–11] whose sites *i* have occupation numbers n_i that indicate whether the site is occupied $(n_i = 1)$ or unoccupied $(n_i = 0)$. Every configuration **N** of this lattice is specified completely by an array of all the n_i : **N** = { $n_1, n_2, ...$ }. The probability $P(\mathbf{N}, \tau)$ of finding configuration **N** at time τ is a solution of the master equation [21],

$$\frac{\partial P}{\partial \tau} = \sum_{\mathbf{r}} \left[W(\mathbf{N} - \mathbf{r}; \mathbf{r}) P(\mathbf{N} - \mathbf{r}, \tau) - W(\mathbf{N}; \mathbf{r}) P(\mathbf{N}, \tau) \right]$$
(2)

where $W(\mathbf{N}; \mathbf{r})$ is the transition rate from \mathbf{N} to $\mathbf{N} + \mathbf{r}$, and $\mathbf{r} = \{r_1, r_2, \ldots\}$ is the array of all site jump lengths r_i .

The 'particles' on our lattice hop to a nearest neighbour site with probabilities per unit time p_+ to the right and $p_- = 1 - p_+$ to the left, but the move is allowed only if the target site is unoccupied. Thus, the total transition rate is the sum of transition rates W_+ to the right and W_- to the left,

$$W_{\pm}(\mathbf{N};\mathbf{r}) = p_{\pm} \sum_{i} \left[n_{i}(1 - n_{i\pm 1})\delta(r_{i}, -1)\delta(r_{i\pm 1}, 1) \prod_{j\neq i, i\pm 1} \delta(r_{j}, 0) \right]$$
(3)

where $\delta(i, j)$ is the Kronecker delta and the summation extends over all lattice sites.

The equation of motion for this lattice gas is obtained by first performing a Kramers– Moyal expansion [21–23] of the master equation. This requires expanding the first term on the right-hand side of (2), which relies on two criteria [21]. The first is that $W(\mathbf{N}; \mathbf{r})$ is a sharply peaked function of \mathbf{r} in that there is a $\delta > 0$ such that $W(\mathbf{N}; \mathbf{r}) \approx 0$ for $|\mathbf{r}| > \delta$. This 'small jump' condition is satisfied by our rules because the difference in successive configurations is at most unity on two nearest neighbour sites. The second condition is that $W(\mathbf{N}; \mathbf{r})$ is a slowing-varying function of \mathbf{N} , i.e. $W(\mathbf{N} + \Delta \mathbf{N}; \mathbf{r}) \approx W(\mathbf{N}; \mathbf{r})$ for $|\Delta \mathbf{N}| < \delta$. Since $n_i = 0$ or $n_i = 1$, changing an occupation number in (3) by one unit may change the transition rate of processes involving that site discontinuously, in violation of this condition. To alleviate this problem, we replace the unit jumps in (3) with rescaled jumps Ω^{-1} , where Ω is a 'largeness' parameter that controls the magnitude of the intrinsic fluctuations. We also transform the time according to $\tau \rightarrow \tau / \Omega$ to preserve the original transition rate. The transformed master equation is

$$\frac{\partial P}{\partial \tau} = \int [\widetilde{W}(\mathbf{N} - \mathbf{r}; \mathbf{r}) P(\mathbf{N} - \mathbf{r}, \tau) - \widetilde{W}(\mathbf{N}; \mathbf{r}) P(\mathbf{N}, \tau)] \, \mathrm{d}\mathbf{r}$$
(4)

with the left and right transition rates \widetilde{W}_{\pm} given by

$$\widetilde{W}_{\pm}(\mathbf{N};\mathbf{r}) = p_{\pm}\Omega\sum_{i}\left[n_{i}(1-n_{i\pm1})\delta\left(r_{i}+\frac{1}{\Omega}\right)\delta\left(r_{i\pm1}-\frac{1}{\Omega}\right)\prod_{j\neq i,i\pm1}\delta(r_{j})\right]$$
(5)

in which $\delta(x)$ is the Dirac δ -function.

The central quantities in the expansion of the master equation are the moments

$$K_i^{(1)}(\mathbf{N}) = \int r_i \widetilde{W}(\mathbf{N}; \mathbf{r}) \, \mathrm{d}\mathbf{r} \sim O(1) \tag{6}$$

$$K_{ij}^{(2)}(\mathbf{N}) = \int r_i r_j \widetilde{W}(\mathbf{N}; \mathbf{r}) \,\mathrm{d}\mathbf{r} \sim O(\Omega^{-1}) \tag{7}$$

Table 1. The moments $K_i^{(1)}$ and $K_{ij}^{(2)}$ defined in (10) and (11) for each configuration $\{n_{i-1}, n_i, n_{i+1}\}$ of a site *i* and its nearest neighbour sites $i \pm 1$.

$\{n_{i-1}, n_i, n_{i+1}\}$	$K_i^{(1)}$	$K_{ij}^{(2)}$
{0, 0, 0}	0	0
$\{1, 0, 0\}$	p_+	$p_+(\delta_{ij} - \delta_{i-1,j})$
$\{0, 1, 0\}$	-1	$p(\delta_{ij} - \delta_{i-1,j}) + p_+(\delta_{ij} - \delta_{i+1,j})$
$\{0, 0, 1\}$	p_{-}	$p_{-}(\delta_{ij} - \delta_{i+1,j})$
$\{0, 1, 1\}$	$-p_{-}$	$p_{-}(\delta_{ij} - \delta_{i-1,j})$
$\{1, 0, 1\}$	1	$p_+(\delta_{ij} - \delta_{i-1,j}) + p(\delta_{ij} - \delta_{i-1,j})$
$\{1, 1, 0\}$	$-p_{+}$	$p_+(\delta_{ij} - \delta_{i+1,j})$
$\{1, 1, 1\}$	0	0

and, in general, $K^{(n)} \sim O(\Omega^{1-n})$. With these orderings in Ω , a limit theorem due to Kurtz [23–25] states that, as $\Omega \to \infty$, the solution of the master equation (2) is approximated, with an error of order $\ln \Omega / \Omega$, by that of the Langevin equation [23],

$$\frac{\mathrm{d}n_i}{\mathrm{d}\tau} = K_i^{(1)}(\mathbf{N}) + \eta_i \tag{8}$$

with Gaussian noises η_i that have zero mean, $\langle \eta_i(\tau) \rangle = 0$, and covariances

$$\langle \eta_i(\tau)\eta_j(\tau')\rangle = K_{ij}^{(2)}(\mathbf{N})\delta(\tau - \tau').$$
⁽⁹⁾

For the transition rates in (3), these moments can be written as

$$K_i^{(1)}(\mathbf{N}) = \frac{1}{2}\Delta^2 n_i + (p_+ - p_-)\left(n_i - \frac{1}{2}\right)\left(\Delta^- n_i + \Delta^+ n_i\right)$$
(10)

and

$$K_{ij}^{(2)}(\mathbf{N}) = \left(n_i - \frac{1}{2}\right) \Delta^2(n_i \delta_{ij}) - \left(n_i - \frac{1}{2}\right) \delta_{ij} \Delta^2 n_i - \frac{1}{2} n_i \Delta^2 \delta_{ij} + \frac{1}{2} (p_+ - p_-) [(\Delta^+ n_i) (\Delta^+ \delta_{ij}) - (\Delta^- n_i) (\Delta^- \delta_{ij})]$$
(11)

where $\Delta^{-}n_{i} = n_{i} - n_{i-1}$, $\Delta^{+}n_{i} = n_{i+1} - n_{i}$, $\Delta^{2}n_{i} = n_{i-1} - 2n_{i} + n_{i+1}$, and these operators act only on the first index of δ_{ij} . The first three terms on the right-hand side of (11) account for exclusion, while the last term accounts for hopping bias.

The moments in (10) and (11) for each local configuration of a site *i* and its nearest neighbours $i \pm 1$ are compiled in table 1. The hopping bias and the exclusion are both evident in the variation of these moments with the local configuration. The coupling between nearest neighbour sites in the second moment enforces particle conservation in that a change of the occupation on a site results in compensating changes on nearest neighbouring sites, insofar as exclusion allows. One of the key points to be discussed below is how the different terms in (11) transform under coarse-graining.

The continuum equation of motion corresponding to (8) and (9) is obtained by first introducing coarse-grained space and time variables through the diffusive scaling transformation, $x = \epsilon i$ and $t = \epsilon^2 \tau$, where $\epsilon > 0$ parametrizes the extent of the coarse-graining. The corresponding transformation of the occupation numbers is $n_i(\tau) = \varphi(\epsilon i, \epsilon^2 \tau)$, where φ is an analytic function in both arguments. With these transformations, the leading-order terms in $K^{(1)}$ are

$$K^{(1)}(\varphi) = \frac{\epsilon^2}{2} \frac{\partial^2 \varphi}{\partial x^2} + \frac{\epsilon^4}{4!} \frac{\partial^4 \varphi}{\partial x^4} + \dots + 2\epsilon (p_+ - p_-) \left(\varphi - \frac{1}{2}\right) \left(\frac{\partial \varphi}{\partial x} + \frac{1}{3!} \frac{\partial^3 \varphi}{\partial x^3} + \dots\right).$$
(12)

By requiring that $p_- - p_+ = \epsilon$, in which case $\epsilon \to 0$ also corresponds to the weakly asymmetric limit, we obtain

$$K^{(1)}(\varphi) = \frac{\epsilon^2}{2} \frac{\partial^2 \varphi}{\partial x^2} - 2\epsilon^2 \left(\varphi - \frac{1}{2}\right) \frac{\partial \varphi}{\partial x} + O(\epsilon^4).$$
(13)

For $K^{(2)}$, the coarse-graining transformations, together with the identifications

$$\delta_{ij} = \epsilon \delta(x - x') \qquad \delta(\tau - \tau') = \epsilon^2 \delta(t - t') \tag{14}$$

yield

$$K^{(2)}(\varphi)\delta(\tau - \tau') = \epsilon^5 \frac{\partial}{\partial x} \left\{ \varphi(\varphi - 1) \left[\frac{\mathrm{d}}{\mathrm{d}x} \delta(x - x') \right] \right\} \delta(t - t') + O(\epsilon^7)$$
(15)

which, according to (9), imply a coarse-grained noise $\eta_i(\tau) = \epsilon^{5/2}\eta(x, t)$. The terms of order ϵ^5 are derived from the first three terms on the right-hand side of (11) and are therefore associated only with exclusion. The remaining term, contained in the ϵ^7 corrections, accounts for hopping bias. Thus, as $\epsilon \to 0$, the importance of hopping bias on the fluctuations diminishes more rapidly than that of exclusion. By substituting these transformations into (8) and taking the limit $\epsilon \to 0$, we obtain the deterministic equation

$$\frac{\partial\varphi}{\partial t} = \frac{1}{2} \frac{\partial^2 \varphi}{\partial x^2} - 2\left(\varphi - \frac{1}{2}\right) \frac{\partial\varphi}{\partial x}.$$
(16)

The transformation

$$\varphi(x,t) = \frac{1}{2} + \frac{1}{4}u\left(x,\frac{1}{2}t\right)$$
(17)

yields Burgers' equation (1) for u.

The comparison of solutions of the master equation (2), as exemplified by lattice simulations, with a standard solution of (16) [26] (cf (17)),

$$\varphi(x,t) = \frac{1}{2} - \frac{\sinh x}{2(\cosh x + e^{-t/2})}$$
(18)

is shown in figure 1. This solution is considered over the spatial interval $-80 \le x \le 80$ and compared to stochastic lattice gas simulations with 100,250 and 1000 sites at t = -60, -40, 0. The simulations are initialized by averaging over individual realizations with site occupation probabilities determined by (18) at t = -60. Since, for this solution, $u \to 0$ as $x \to \infty$ and $u \to 1$ as $x \to -\infty$, we impose a source of particles at the left boundary (x = -80) and a sink at the right boundary (x = 80). Each simulation was averaged over 8000 independent realizations.

As time increases from t = -60, the plateau near the origin of (18) disappears and a 'shock' front is formed. The simulations show the same qualitative behaviour, but the details of the profile are faithfully reproduced only by the larger system sizes, i.e. those corresponding to smaller ϵ . For 100 sites, the sharpness of the features in the Burgers solution is smeared out and there is an appreciable broadening of the shock front at t = 0. For 1000 sites, the simulations show only a slight deviation at the shock front at t = 0; simulations with a somewhat larger number of sites are essentially indistinguishable from the Burgers solution. Thus, the continuum limit of the biased random walk of particles with exclusion does indeed approach the solution of Burgers' equation, in agreement with the passage from (10) and (11) to (16).

The differences between the simulations and solution (18) can be explained by the lattice corrections to (16). In the spirit of the central limit theorem, we write

$$n_i(\tau) = \varphi(\epsilon i, \epsilon^2 \tau) + \epsilon^{1/2} \xi(\epsilon i, \epsilon^2 \tau)$$
(19)



Figure 1. Comparison of solution (18) of equation (16) (solid line) with simulations of the asymmetric exclusion process (full symbols) for lattices of sizes L = 100, 250, 1000, corresponding to $\epsilon = 1.6, 0.64, 0.16$, respectively, at times t = -60, -40, 0. In each panel, the abscissa indicates the range of the spatial variable $(-80 \le x \le 80)$ and the ordinate the range of the solution $(0 \le \varphi \le 1)$.

substitute into (10) and (11), and collect terms proportional to $\epsilon^{5/2}$ to obtain the equation of motion for the lattice correction ξ ,

$$\frac{\partial\xi}{\partial t} = \frac{1}{2} \frac{\partial^2 \xi}{\partial x^2} - 2 \frac{\partial}{\partial x} (\varphi \xi) + \frac{\partial \xi}{\partial x} + \eta$$
(20)

where the noise has zero mean and covariance

$$\langle \eta(x,t)\eta(x',t')\rangle = \frac{\partial}{\partial x} \left\{ \varphi(\varphi-1) \left[\frac{\mathrm{d}}{\mathrm{d}x} \delta(x-x') \right] \right\} \delta(t-t').$$
(21)

As discussed above, this noise accounts only for the exclusion rule, the hopping bias being a higher order effect. The structure of (10) and (11) means that the differential equation for the ξ is linear with coefficients determined by φ . In other words, the fluctuations 'follow' the deterministic solution.

A complete characterization of $\xi(x, t)$ would require the solution of (20) and (21). We will focus instead on some general features, beginning with the average $\langle \xi(x, t) \rangle$. Since the η have zero mean and φ is a deterministic quantity, the equation for $\langle \xi \rangle$ is

$$\frac{\partial \langle \xi \rangle}{\partial t} = \frac{1}{2} \frac{\partial^2 \langle \xi \rangle}{\partial x^2} - 2 \frac{\partial}{\partial x} (\varphi \langle \xi \rangle) + \frac{\partial \langle \xi \rangle}{\partial x}.$$
(22)

The initial condition on the total solution is determined by φ , so (19) indicates that $\langle \xi(x,0) \rangle = 0$. Moreover, since the boundary conditions at $x = \pm 80$ are also subsumed by the deterministic part of the solution, we must have that $\langle \xi(-80,t) \rangle = \langle \xi(80,t) \rangle = 0$. Thus, the solution to (22) vanishes identically: $\langle \xi(x,t) \rangle = 0$.

Returning to (20), we first observe that, as $x \to \pm \infty$, the noise covariance in (21) vanishes, so $\lim_{x\to\pm\infty} \xi(x,t) = 0$, as follows from the solution of (22). This is precisely what one would expect from simulations, since, as $x \to -\infty$, all sites are occupied ($\varphi \to 1$), while, as $x \to \infty$, all sites are empty ($\varphi \to 0$). In both cases, the transition rates in (3) vanish. Alternatively, according to (21), in regions where φ deviates significantly from these asymptotic values, the noise asserts its strongest influence, as is indeed observed in figure 1.

To summarize, we have obtained an exact equation of motion for the biased random walk with exclusion on finite lattices. The corresponding continuum equation, obtained from a coarse-graining transformation with diffusive scaling in the weakly asymmetric limit, is Burgers' equation. The leading lattice corrections describe the fluctuations in the simulations of this lattice gas. The considerations leading to these equations of motion apply to a large class of driven lattice systems, even those with non-analytic transition rules, such as growth models [27–29] and sandpile models [30]. These applications are being explored further for several models.

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