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Microscopic-Shock Profiles: Exact Solution of a Non-equilibrium System.

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Abstract. – The full microscopic structure of macroscopic shocks is obtained exactly in the one-dimensional totally asymmetric simple exclusion process from the complete solution of the uniform stationary non-equilibrium state of a system containing two types of particles—«first» and «second» class. The width of the shock as seen from a second-class particle diverges as the inverse square of its strength when the latter goes to zero. In that limit the steady state exhibits long-range correlations and weakly bound states of second-class particles.

Introduction. – There is much interest, physical and mathematical, in the behaviour of model systems of particles on a lattice evolving microscopically under conservative stochastic dynamical rules and described macroscopically by a continuous density field satisfying equations of hydrodynamic type [1, 2]. Of particular interest are models for which the macroscopic equations produce shocks. In such cases it is clear that the hydrodynamic equations do not tell the full story; in fact, because of the discontinuities in the density and consequent infinities in the derivatives which enter the equations, shocks correspond to non-unique weak solutions of these equations, and, to find the physical solution, the equations have to be supplemented by additional conditions or be treated as the limit of equations with non-zero viscosity. The microscopic level has of course no room for such extra conditions and its study is therefore essential for a complete understanding of the behaviour of shocks [3].

Unfortunately, even molecular-dynamics simulations of shocks in real particle systems can only be carried out very partially with the currently available supercomputers [3], so model systems such as the one-dimensional asymmetric simple exclusion process are important. In this model, particles on the lattice jump independently at random times with rate 1 to adjacent sites, choosing the site to their right with probability p, and to their left with

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probability $1-p$, provided the target site is unoccupied [1,4]. The density profile of this system on macroscopic spatial and temporal scales x and t is described for $p \neq 1/2$ in the appropriate hydrodynamic scaling limit by the inviscid Burgers' equation [1,2]

$$\frac{\partial u(x,t)}{\partial t} + (2p-1)\frac{\partial}{\partial x}[u(1-u)] = 0. \tag{1}$$

This means that there exists a limiting scaling for which the actual random microscopic density exactly tracks the solution of the Burgers' equation.

This equation can produce shocks; for example, there is a solution of (1) such that $u(x,t) = u_+$ for $x > x_0(t)$ and $u(x,t) = u_-$ for $x < x_0(t)$, where $u_+ > u_-$ (when $p > 1/2$) and the shock position $x_0(t)$ moves with the constant velocity $(2p-1)(1-u_+-u_-)$. We now ask about the corresponding microscopic behaviour: can one see an abrupt change at that scale or is the jump in densities spread out over very large microscopic distances?

To analyse the shock microscopically one must first locate it—that is, define precisely its position—on the microscopic level. This may be done by introducing a special *second-class particle* [5] into the system, which evolves by a modified dynamical rule: it behaves like a regular (first-class) particle when jumping to an empty site but must give way to any regular particle that tries to jump on it (by exchanging places with the latter). For $p > 1/2$ this dynamics makes the velocity of the second-class particle decrease with density and then gives it a drift towards regions of positive density gradient. This keeps the second-class particle near the shock and its position may then conveniently be taken as the definition of the (microscopic) shock location. With this definition it has been established that shocks are sharp even on the microscopic level [6,7]; specifically, that the microscopic (ensemble-averaged) particle density at site j, as viewed from the second-class particle, has a time-invariant distribution which approaches the densities $\rho_\pm = u_\pm$ at $\pm\infty$. In practice, this means that one can see the discontinuity on the scale of a few intermolecular distances, something consistent with computer simulations on real particle systems and with experiments [3]. Computer studies of this shock profile are described in [8], see also [9].

In this note we present the exact microscopic structure of such a shock for the case $p = 1$. We obtain our results by first finding the exact translation-invariant stationary state of a related model system, introduced in [7], which considers a system with uniform densities ρ_1 and ρ_2 of first- and second-class particles (f.c.p. and s.c.p.). It is in fact easy to show that when this uniform system is viewed from some chosen s.c.p., all s.c.p.'s to the right of the chosen one behave as f.c.p.'s, while all s.c.p.'s to the left of it behave as unoccupied sites or holes. Whit this identification the chosen s.c.p. in the uniform system sees exactly the same microscopic shock profile as a single s.c.p. in a system containing only f.c.p.'s in which the density approaches $\rho_+ = \rho_1 + \rho_2$ at $+\infty$ and $\rho_- = \rho_1$ at $-\infty$ [7].

This two-species model is of independent interest as an example of a driven diffusive system [10]. Such systems have particle-conserving transition rates which do not satisfy detailed balance with respect to the stationary state and are expected to exhibit long-range spatial correlations in two or more dimensions [10-12]. Our one-dimensional model also exhibits such behaviour when the density of the second-class particles goes to zero.

For ρ_2 non-zero, the exponential decay of correlations in the uniform system gives an exponential approach to the asymptotic densities for the one-component shock, with a characteristic length ξ which diverges as $(\rho_+ - \rho_-)^{-2}$ when $(\rho_+ - \rho_-) = \rho_2 \to 0$. In the limit $\rho_2 \to 0$ there still exists a microscopic «shock» consisting of an excess density of particles in front of any given s.c.p. and of holes at the back of it, which decays to zero as $|j|^{-1/2}$; by contrast, the mean-field result found in [8] is $|j|^{-1}$. In this limit there are also long-range correlations between the second-class particles: a pair of s.c.p.'s in a system with a uniform non-zero density of f.c.p.'s will form a bound state with the probability of separation r between them decaying as $r^{-3/2}$.

Exact solution. – The exact stationary state of our two-species totally asymmetric simple exclusion process is based on earlier work [13] (see also [14]) for a one-component finite system with open boundaries; the solution can be extended to the partially asymmetric case [15]. We work first on a ring of N sites containing N_1 f.c.p.'s, N_2 s.c.p.'s and $N_0 \equiv \equiv N - N_1 - N_2$ holes. A configuration is specified by an N-tuple $(\tau_1, \tau_2, \ldots, \tau_N)$, where $\tau_i = 0$ if site i is empty, $\tau_i = 1$ if there is an f.c.p. at site i, and $\tau_i = 2$ if there is an s.c.p. at site i. During a time interval dt each adjacent pair of sites in the system of the type 10, 12 or 20 has probability dt of being exchanged. It is easy to see that any configuration can evolve into any other, so that the system is ergodic and there is a unique stationary probability measure. This measure which assigns a weight $w(\tau)$ to each configuration $\tau = (\tau_1, \tau_2, \ldots, \tau_N)$ is determined by the stationary form of the master equation. It satisfies the following balance condition:

$$\sum_{\{i \mid \tau_i \tau_{i+1} = 10,\ 12,\ \text{or}\ 20\}} w(\tau) = \sum_{\{i \mid \tau_i \tau_{i+1} = 01,\ 21,\ \text{or}\ 02\}} w(\tau^{i,\, i+1}), \tag{2}$$

where τ^{ij} denotes the configuration obtained from $\tau = (\tau_1, \ldots, \tau_N)$ by interchanging τ_i and τ_j.

If either N_0, N_1 or N_2 equals zero, then the system reduces to the one-component asymmetric simple exclusion process whose stationary measure is well known: all configurations are equally likely. In the general case the stationary measure will be constructed with the aid of matrices or operators D and E which satisfy [13]

$$DE = D + E \tag{3}$$

and the matrix $A = DE - ED$ which, from (3), satisfies the relations

$$DA = AE = A. \tag{4}$$

Explicit forms of these matrices are given below. We will show that the probability $w(\tau)$ in the stationary state for fixed N_1, N_2 is given [15], up to an overall normalizing factor, by

$$w(\tau_1, \ldots, \tau_N) = \operatorname{tr}[X_1 \ldots X_N], \tag{5}$$

where $X_i = E$ if $\tau_i = 0$, $X_i = D$ if $\tau_i = 1$, and $X_i = A$ if $\tau_i = 2$.

To verify that (5) provides the weights of a stationary measure, we substitute this formula on both sides of (2); it is then convenient to write $X_1 \ldots X_N$, possibly after a cyclic permutation which will not affect the trace, in terms of blocks of consecutive identical matrices: $X_1 \ldots X_N = Y_1^{k_1} \ldots Y_m^{k_m}$, where each Y_j is D, A, or E, and $Y_j \neq Y_{j+1}$, $Y_m \neq Y_1$. Now, in the term on the left-hand side of (2) indexed by i we use the algebraic relations (3) and (4) to replace the product $X_i X_{i+1}$ by a sum of two operators or a single operator—that is, DE is replaced by $D + E$, while DA and AE are replaced by A. The net effect of these replacements is that each D-block (respectively, E-block) gives rise to a term in which the rightmost (respectively, leftmost) factor in the block has disappeared; notice that in the case of a DE boundary we get a term for each block. Thus we find

$$\sum_{\{i \mid \tau_i \tau_{i+1} = 10,\ 12,\ \text{or}\ 20\}} \operatorname{tr}[X_1 \ldots X_i X_{i+1} \ldots X_N] = \sum_{\{j \mid Y_j = D,\, E\}} \operatorname{tr}[Y_1^{k_1} \ldots Y_j^{k_j - 1} \ldots Y_m^{k_m}]. \tag{6}$$

If we make the same replacements for the product $X_{i+1} X_i$ in each term on the right-hand side of (2), then the net effect is that the D-blocks lose their leftmost and the E-blocks their rightmost factors. Therefore, each side of (6) gives rise to the same terms and thus (5) satisfies (2).

To obtain the matrices D, E and A, write $D = I + d$ and $E = I + e$, where I is the identity matrix. Then (3) gives $de = I$. If D and E were finite, they would have to commute, giving $A = 0$. Therefore, to obtain a non-trivial solution we must take infinite matrices: an explicit solution [13] is that d is the right and e the left shift on semi-infinite vectors:

$$D_{ij} = \delta_{i,j} + \delta_{i,j-1}, \qquad E_{ij} = \delta_{i,j} + \delta_{i,j+1} \quad \text{and} \quad A_{ij} = \delta_{i,1}\delta_{j,1}, \qquad i, j \geq 1. \tag{7}$$

A is then the projector on the first component, $A = |1\rangle\langle 1|$ with $|1\rangle = [1, 0, 0, ...]$, and has trace 1.

An important consequence of this matrix formulation and of the fact that the matrix A is a one-dimensional projector is the absence of correlations between regions separated by second-class particles. In particular, in the infinite-volume limit, there is a factorization about any site i occupied by a second-class particle,

$$\langle f(\tau)\, g(\tau) \,|\, \tau_i = 2\rangle = \langle f(\tau) \,|\, \tau_i = 2\rangle \langle g(\tau) \,|\, \tau_i = 2\rangle, \tag{8}$$

whenever f (respectively, g) depends only on the configuration to the left (respectively, right) of i.

Shock structure and other properties. – Once the weight of each configuration in the steady state is known, one can in principle calculate all the correlation functions for arbitrary N_1, N_2 and N, and then consider various infinite-volume limits $N \to \infty$. In practice, this limit is actually taken in a «grand canonical» ensemble after introducing fugacitylike parameters which are later converted back to densities. We consider several situations: a finite density of both first-class and second-class particles ($N_1/N \to \rho_1$, $N_2/N \to \rho_2$), a single second-class particle with a non-zero density of first-class particles ($N_1/N \to \rho$, $N_2 = 1$), and two second-class particles with a non-zero density of first-class particles ($N_1/N \to \rho$, $N_2 = 2$). All these cases can be treated using similar techniques. Here we will summarize our results in the first two cases, leaving the detailed derivation for a future longer version of the present work [15], and will sketch the calculation in the third and easiest case, that of two second-class particles.

We first consider the case of finite densities of both types of particles, in which for each choice of ρ_1 and ρ_2 the infinite-volume limit yields a translation-invariant measure which is stationary for the two-species asymmetric-exclusion dynamics. One interesting feature of the measure that emerges from explicit computation [15] is that, conditioned on the presence of an s.c.p. at some site i, the distribution of f.c.p.'s to the *right* of i and of holes to the *left* of i are just product measures with densities ρ_1 and $1 - \rho_1 - \rho_2$, respectively.

To obtain the shock profile from this measure in the one-component system with asymptotic densities $\rho_+ = \rho_1 + \rho_2$ and $\rho_- = \rho_1$, we pick any s.c.p. in the two-component system and let its instantaneous position specify the origin of the lattice. We then define δ_j as the probability that the site j is occupied by an f.c.p. for $j < 0$ and that it is occupied by either an f.c.p. or s.c.p. for $j > 0$. δ_i gives the shock profile in the one-component totally asymmetric simple exclusion process, seen in the randomly moving frame of a single s.c.p. This follows from the observation made earlier that each s.c.p. in the two-component system behaves as if all the s.c.p.'s at its left were holes and all s.c.p.'s at its right were f.c.p.'s. An explicit computation gives [15]

$$\delta_{-1} = \rho_+ \rho_- , \qquad \delta_1 = \rho_+ + \rho_- - \rho_+ \rho_- , \tag{9}$$

and for all $j \geq 2$

$$\delta_{-j} - \delta_{-1} = \delta_1 - \delta_j = \sum_{n=1}^{j-1}\sum_{p=0}^{n-1}\binom{n}{p}\binom{n-1}{p}\frac{(\rho_+\rho_-)^{n-p}[(1-\rho_+)(1-\rho_-)]^{p+1}}{p+1}. \tag{10}$$

Notice that these shocks have the symmetry property $\delta_j + \delta_{-j} = \rho_+ + \rho_-$. It is also easy to check from (9) and (10) that δ_j converges exponentially: $|\delta_j - \rho_\pm| \sim \exp[-|j|/\xi]$ as $j \to \pm\infty$ when $\rho_+ > \rho_-$, where the characteristic length ξ measures the microscopic width of the shock as seen from the s.c.p. This length ξ diverges as $(\rho_+ - \rho_-)^{-2}$ when $\rho_+ \to \rho_-$.

We can obtain the limiting shock shape when $\rho_- = \rho_+$ directly from (10) or we can equivalently consider the case of a single s.c.p. in a system of f.c.p.'s at a uniform non-zero density ρ. Physically, one expects that the s.c.p. will be attracted by fluctuations with a positive-density gradient of f.c.p.'s, so that the average density d_j of f.c.p.'s at position j (in the frame where the s.c.p. is at the origin) will have a non-trivial profile. We have calculated this profile exactly [15] from the steady state (5) and found in the limit of an infinite system size ($N \to \infty$ with $N_1/N \to \rho$ and $N_2 = 1$) that $d_1 = 2\rho - \rho^2$, $d_{-1} = \rho^2$, and for all $j \geq 2$

$$d_{-j} - d_{-1} = d_1 - d_j = \sum_{n=1}^{j-1}\sum_{p=0}^{n-1}\binom{n}{p}\binom{n-1}{p}\frac{(1-\rho)^{2n-2p}\rho^{2p+2}}{p+1}. \tag{11}$$

From this exact expression, which is equivalent to that obtained from (10) for δ_j when $\rho_2 \searrow 0$ and $\rho_1 = \rho$, one can show that for large j the profile is a power law: $|d_j - \rho| \sim |j|^{-1/2}$. The exponent 1/2 disagrees with the exponent 1 obtained from a mean-field argument [8].

The last case we consider is the case of a pair of s.c.p.'s in an infinite system of f.c.p.'s at a non-zero density ρ. In that case, we find that the probability $P_\infty(r)$ that two s.c.p.'s are a distance r apart (in an infinite system) is given by

$$P_\infty(r) = \sum_{p=0}^{r-1}\binom{r}{p}\binom{r-1}{p}\frac{\rho^{2n-2p-1}(1-\rho)^{2p+1}}{p+1}. \tag{12}$$

This shows that the two second-class particles form a bound state of a rather unusual kind, since $P_\infty(r) \sim r^{-3/2}$ and the average distance is infinite. (We can say that this is an *algebraic* bound state in contrast with the normally encountered exponentially decaying bound states.)

The derivation of (12) is rather easy when one uses the grand canonical ensemble. If we introduce a parameter x which plays the role of a fugacity for the f.c.p., so that the weight of any configuration with N_1 first-class particles is multiplied by x^{N_1}, then the probability (in the grand canonical ensemble) of finding the two second-class particles a distance r apart, on a ring of N sites (for simplicity we choose here N to be odd and r to be the shorter distance between the two particles on the ring) is

$$P_N(r) = \langle 1|C^{r-1}|1\rangle\langle 1|C^{N-r-1}|1\rangle\Big[\sum_{s=1}^{(N-1)/2}\langle 1|C^{s-1}|1\rangle\langle 1|C^{N-s-1}|1\rangle\Big]^{-1}, \tag{13}$$

where the matrix C is defined by

$$C = xD + E, \tag{14}$$

i.e. $C_{ij} = \delta_{i,j+1} + (1+x)\delta_{i,j} + x\delta_{i,j-1}$ for $i \geq 1$ and $j \geq 1$. Expression (13) arises because when one sums over all the occupations of the $N-2$ sites one is adding at each site a matrix D with weight x and a matrix E with weight 1, giving at each site a matrix C. The limit $N \to \infty$ then follows easily: from the explicit expression of the matrix C, whose elements can be interpreted in terms of random walks, one can show that for any n [15]

$$\langle 1|C^n|1\rangle = \sum_{p=0}^{n} \binom{n+1}{p}\binom{n}{p}\frac{x^p}{p+1}, \tag{15}$$

which gives for large n

$$\langle 1|C^n|1\rangle \sim (\sqrt{x}+1)^{2n}/n^{3/2}. \tag{16}$$

From this asymptotic behaviour it follows that the density ρ is related in the large-N limit to the fugacity x by $\rho = \sqrt{x}/(\sqrt{x}+1)$; then replacing x by $\rho^2/(1-\rho)^2$ in (13) and (15) one obtains in the large-N limit (12).

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