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Microscopic models of macroscopic shocks

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We present some rigorous and computer-simulation results for a simple microscopic model, the asymmetric simple exclusion process, as it relates to the structure of shocks.

13.1 Introduction

In this chapter our concern is the underlying microscopic structure of hydrodynamic fields, such as the density, velocity and temperature of a fluid, that are evolving according to some deterministic autonomous equations, e.g., the Euler or Navier-Stokes equations. When the macroscopic fields described by these generally nonlinear equations are smooth we can assume that on the microscopic level the system is essentially in local thermodynamic equilibrium [1]. What is less clear, however, and is of particular interest, both theoretical and practical, is the case where the evolution is not smooth—as in the occurrence of shocks. Looked at from the point of view of the hydrodynamical equations these correspond to mathematical singularities—at least at the compressible Euler level—possibly smoothed out a bit by the viscosity, at the Navier-Stokes level. But what about the microscopic structure of these shocks? Is there really a discontinuity, or at least a dramatic change in the density, at the microscopic scale or does it look smooth at that scale?

It is clear that this question cannot be answered by the macroscopic equations. Also, both the traditional methods of deriving these equations from the microscopic dynamics, which use (uncontrolled) Chapmann-Enskog type expansions [2], and the more recent mathematical methods, which use ergodic properties of the microscopic dynamics and the large separation between microscopic and macroscopic space-time scales, appear at first glance

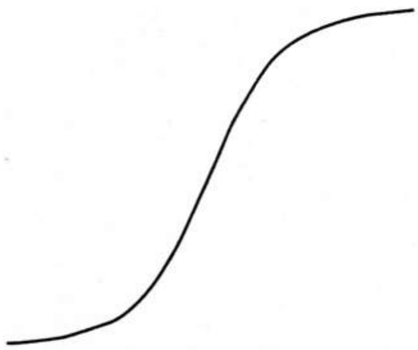

Fig. 13.1. Smooth initial data for Burgers' equation.

to require that the hydrodynamic fields vary smoothly on the macroscopic scale [1,3,4]. In fact until recently all rigorous derivations of hydrodynamical equations were restricted to macroscopic times when their solutions are smooth. This is in particular the case for the derivation of the inviscid Burgers' equation [5],

$$\frac{\partial u(x,t)}{\partial t} + c\frac{\partial}{\partial x}\{u(x,t)\,[1-u(x,t)]\} = 0, \tag{13.1}$$

from various microscopic model systems. Burgers' equation can produce shocks: smooth initial data of the form shown in Fig. 13.1 quickly evolve into a discontinuous profile. After a long time the macroscopic profile takes the form sketched in Fig. 13.2. The validity of the derivations of (13.1) stops, however, just at the development of the discontinuity. It is therefore quite remarkable that recently F. Rezakhanlou was able to extend previous results and prove the validity of (13.1) in describing the time evolution of a microscopic model system *even after the formation of a shock* [6].

13.2 Microscopic model

The microscopic model that Rezakhanlou considered is the so-called asymmetric simple exclusion process or ASEP (some generalizations are possible). In this model the microscopic system consists of particles on some lattice (typically Z^d) in which there is hard-core exclusion preventing more than one particle from occupying a given lattice site at any one time. The configuration of the system is specified by $\eta = \{\eta_i : i \in Z^d, \eta_i = 0, 1\}$. The time evolution proceeds by allowing every particle independently to attempt to jump to one of its neighboring sites at a rate τ^{-1}. Once it decides to jump it chooses a direction $\mathbf{e}_\alpha \in \{\pm\mathbf{e}_1, \pm\mathbf{e}_2, \ldots, \pm\mathbf{e}_d\}$ with probability $p_{\mathbf{e}_\alpha}$ (the

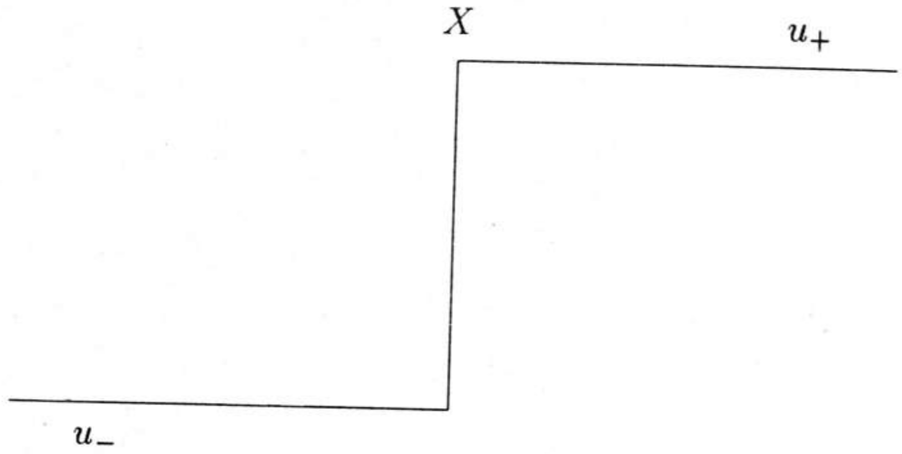

Fig. 13.2. For large times, the shock is located at a position X and moves with velocity $v = c(1 - u_+ - u_-)$.

$\mathbf{e}_\alpha$ form a basis for the lattice). The jump is actually performed only if the target site is empty—otherwise the particle does not go anywhere. The dynamics is symmetric if $p_{\mathbf{e}_\alpha} = p_{-\mathbf{e}_\alpha}$ for all α; otherwise it is asymmetric.

In all cases the only stationary translation-invariant states are product measures ν_ρ, $\rho \in [0, 1]$, where ρ is the average density at any given site: $\langle \eta_i \rangle_{\nu_\rho} = \rho$, $\langle \eta_i \eta_j \rangle_{\nu_\rho} = \rho^2$ $(i \neq j)$, $\langle \eta_i \eta_j \eta_k \rangle_{\nu_\rho} = \rho^3$ $(i, j, k$ distinct), etc. These states can be thought of as the equilibrium state of a lattice gas with on-site hard-core interaction. Note, however, that the dynamics obeys detailed balance with respect to these stationary states only for the symmetric case. (There is also, in the asymmetric case, a stationary non-translation-invariant state in which the density approaches unity along the direction of the asymmetry, e.g., along the $\mathbf{e}_1$-direction if $p_{\mathbf{e}_1} > p_{-\mathbf{e}_1}$ and $p_{\mathbf{e}_\alpha} = p_{-\mathbf{e}_\alpha}$ for $\alpha > 1$. The dynamics satisfies detailed balance with respect to such 'blocked' states, which can be thought of as equilibrium states in the presence of a constant external 'electric' field [7]. These states, however, will not be relevant in our further consideration.)

To study the microscopic structure of our model system, whose macroscopic evolution is described by (13.1), we start the system in a nonuniform state that converges under rescaling to a piecewise-smooth density $u_0(x)$. For simplicity we will state results only for the one-dimensional (1D) case, but most of the results carry over to higher dimensions. A simple initial state corresponds to having each site occupied independently with probability $\langle\eta_i\rangle_0 = u_0(\epsilon i)$, where $u_0(x)$ takes values in $[0,1]$. The parameter ϵ measures the ratio of the microscopic to macroscopic length scales. For a typical system, deterministic, autonomous, macroscopic evolution is achieved in the limit $\epsilon \to 0$. More precisely, let us count the number of particles in a macroscopic region of length Δ, containing Δ/ϵ sites, located at a point x at a macroscopic time t, corresponding to microscopic time t/ϵ ('Euler scaling') and divide by the number of sites, to obtain

$$N^\epsilon(x,t,\Delta) = \frac{\epsilon}{\Delta} \sum_{i=[x/\epsilon]}^{[(x+\Delta)/\epsilon]} \eta_i(t\epsilon^{-1}). \tag{13.2}$$

A theorem then says that as $\epsilon \to 0$ the random variable $N^\epsilon(x,t,\Delta)$ converges almost surely, i.e., for almost every microscopic configuration, to a deterministic quantity

$$N^\epsilon(x,t,\Delta) \to \frac{1}{\Delta}\int_x^{x+\Delta} u(x,t)\,dx, \tag{13.3}$$

where $u(x,t)$ satisfies (13.1) with initial condition $u(x,0) = u_0(x)$. For simplicity we consider $\tau = 1$, which gives $c = 2p-1$.

13.2.1 Shock tracking

Given the existence of singularities in the hydrodynamic equation we return to our original question: what about the microscopic structure of these shocks? Actually, we first must answer a more basic question: how does one locate the shock? If $u_- = 0$ this is an easy question; the first particle determines the shock position. No such simple tool will work if $u_- > 0$; however, there is a device that has been used with great success: the *second-class particle* [8].

The second-class particle is a special particle added to the system whose position is updated via a modified dynamical rule: basically the second-class particle behaves like a particle when attempting to jump to other sites, but it behaves like a hole when other particles (now called first-class particles) attempt to jump to its site. A second-class particle in the region of density ρ will have a mean velocity equal to $(2p-1)(1-2\rho)$. This gives the second-class particle a drift towards the location of any shock, and in 1D its position may be used as the microscopic definition of the shock position. (In more than 1D one can still use second-class particles to track the shock, but one cannot necessarily define the position in this way.)

13.3 Detailed shock structure

Using the second-class particle to define the shock position, it has been shown that the shock front in the 1D ASEP remains sharp even on the microscopic level [8-12]. When $p = 1$ there is additional information about the structure of the microscopic system at the location of the shock, i.e., about the 'shape' of the shock as seen from the point of view of the second-class particle. This amounts to determining the time-invariant distribution of first-class particles relative to the second-class particle's location. It is done by first examining what happens when we add many second-class particles to the ASEP, and then studying the nonequilibrium stationary states of this two-species system. One recovers the original shock profile [13,14] via a trick of [11]. For the case $p = 1$, total asymmetry, this correspondence is particularly easy to describe: in a system with a density ρ_1 of first-class particles and ρ_2 of second-class particles, if we take the point of view of a specific second-class particle then all second-class particles in front of it behave as first-class particles, while all second-class particles behind it behave like holes. Thus this particular particle sees the same microscopic shock profile as a single second-class particle in a system containing density $u_- = \rho_1$ on the left and $u_+ = \rho_1 + \rho_2$ on the right.

The ordinary ASEP has a trivial stationary state in a closed or infinite system, but exhibits interesting behavior when combined with nontrivial boundary conditions. This model was solved exactly in [15,16], by embodying the ASEP dynamics into an algebra. An extension of this algebra serves to solve the two-species model (on a ring or in infinite volume); these results are presented in [13,14,17-19]. The primary fact needed to derive all the other results is that the probability that a given configuration occurs in the stationary distribution $P(\eta_1, \eta_2, \ldots, \eta_N)$ is proportional to $\mathrm{Tr}[X_1 X_2 \cdots X_N]$ where $X_i = \mathcal{O}_k$ if $\eta_i = k$ (k takes values 0, 1, 2) and the operators $\mathcal{O}_k$ satisfy the algebra

$$\mathcal{O}_2 = [\mathcal{O}_1, \mathcal{O}_0], \qquad \mathcal{O}_1\mathcal{O}_0 = \mathcal{O}_1 + \mathcal{O}_0. \tag{13.4}$$

A specific representation of the operators $\mathcal{O}_k$ is then used to determine various properties of the two-species stationary state. A convenient representation is $(\mathcal{O}_0)_{ij} = \delta_{i,j} + \delta_{i-1,j}$, $(\mathcal{O}_1)_{ij} = \delta_{i,j} + \delta_{i,j-1}$, $(\mathcal{O}_2)_{ij} = \delta_{i,1}\delta_{j,1}$, where $i, j \in \{1, 2, 3, \ldots\}$. If one now considers a grand-canonical ensemble in which the particles and holes have fugacities z_0, z_1, and z_2, then the partition function and other expectations can be expressed in terms of the traces of powers of $G = z_0\mathcal{O}_0 + z_1\mathcal{O}_1 + z_2\mathcal{O}_2$. This allows many results to be formulated in terms of known results for random walks since G is the (unnormalized) transition matrix for a biased random walk restricted to the nonnegative half-line.

The solution illustrates several novel features of the stationary state, such as the properties that two second-class particles will form a state where the particles are bound together yet the expectation of their distance is infinite and that certain correlations between particles are unexpectedly zero—neither property was predicted prior to the development of the exact solution. It also describes the full microscopic structure of a shock. Defining the density about the position of the second-class particle as $\delta_i = \langle \eta_{X+i} \rangle$, where X is the position of the second-class particle, one has

$$\delta_i = \begin{cases} u_+ + u_-(1-u_+) - g_i, & i > 0, \\ u_- u_+ + g_{-i}, & i < 0, \end{cases} \tag{13.5}$$

where

$$g_i = \sum_{n=1}^{i-1} \sum_{m=0}^{n-1} \frac{1}{m+1} \binom{n}{m} \binom{n-1}{m} (u_- u_+)^{m+1} [(1-u_-)(1-u_+)]^{n-m}. \tag{13.6}$$

This shows in particular that there is an exponential approach to the product measure with density u_+ or u_- as we move away from the second-class particle. The correlation length diverges as $(u_+ - u_-)^{-2}$ when $u_+ \to u_-$.

An interesting feature of the exact solution is that the shock profile is *not* monotonic. The profile for $u_- = 1/4$, $u_+ = 3/4$ is plotted in Fig. 13.3.

It is not at all clear whether this structure is the 'true' nature of the shock or whether it is an artifact resulting from determining the shock position via the use of the second-class particle. This is an important question—of course one is interested in the shock's own inherent structure, but it appears that the only reliable tool for studying the shock has so much structure of its own that the shock itself may become obscured. In particular, when the asymptotic densities on either side of the shock are the same, and we would expect there not to be any shock at all, the second-class particle still produces a nontrivial density profile.

To overcome this problem one can attempt to separate the portion of the probability measure resulting from the motion of the second-class particle from that due to the inherent shock structure. This is not easy, however—although the macroscopic definition of a shock is clear, there is no one simple and consistent way to define the exact location of a shock on the microscopic scale. A multitude of definitions exists, and the microscopic structure may depend on the definition that is chosen.

One can attempt to eliminate the second-class particle altogether. The second-class particle has significant theoretical advantages, but other types

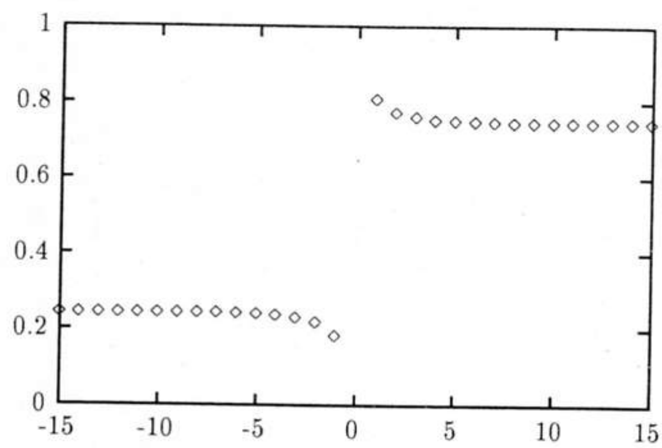

Fig. 13.3. The profile for $u_- = 1/4$, $u_+ = 3/4$.

of shock 'tracers' may more accurately (or more intuitively) identify the instantaneous shock location. If the tracer particle need only follow the shock, rather than also obey the ASEP dynamics as the second-class particle does, it may possibly avoid the artifacts seen in the shock as defined by the second-class particle. One can then study the shock structure using these other measurements, both theoretically and numerically, and see how it compares with results determined through the use of second-class particles. One possibility is the use of the instantaneous ASEP configuration as a background potential field for a random walker, which will have a distribution centered around the shock position. All such indicators examined so far produce a nonmonotone profile—which seems intrinsic to using a probe sensitive to local variations in the environment for determining the instantaneous position of a global change superimposed on many local fluctuations.

One can also study particle models other than the ASEP and examine their shock structure. After all, one is not so much interested in the detailed behavior of the ASEP as the structure of shocks in particle systems in general. If the behavior in the ASEP turns out to be generic then it is a very useful model; if it is very different from that in other models then it is simply an obscure special case that has an exact solution. One possible avenue of study is the Boghosian-Levermore model [20], which has the same hydrodynamic behavior [20,21] and shock position fluctuations [21,22] as the

ASEP but where preliminary numerical studies indicate that a variant of the second-class particle behaves more intuitively than in the ASEP.

13.3.1 Shock fluctuations

Although the front remains sharp, its position fluctuates around the deterministic macroscopic velocity. How big are these fluctuations? One obtains different results depending on the method of measurement. If we compute expectations over both initial conditions and dynamics, the standard deviation of the shock position grows as $t^{1/2}$, standard diffusive behavior [1]. On the other hand it is known that if one computes instead the variance just over the dynamics, i.e., fixes the initial conditions, the growth in time is $o(t^{1/2})$ [12], *subdiffusive*. Numerical studies and heuristic analysis indicate that the correct growth is $t^{1/3}$ in this case [21-23].

These questions have been investigated also in more general systems. For example one can consider systems with interactions between the particles in which the rates of exchange between the contents of sites i and j in a configuration η, $c(i,j;\eta)$, leading to a new configuration $\eta^{i,j}$ has the form

$$c(i,j;\eta) = c^{(0)}(i,j;\eta)e^{-\beta E(i-j)(\eta_i-\eta_j)}, \tag{13.7}$$

where $c^{(0)}(i,j;\eta)$ satisfies detailed balance for an equilibrium Gibbs distribution with some Hamiltonian $H_0(\eta)$, i.e.,

$$c^{(0)}(i,j;\eta)/c^{(0)}(i,j;\eta^{ij}) = e^{-\beta[H_0(\eta^{i,j})-H_0(\eta)]}. \tag{13.8}$$

For a review of the behavior of these driven diffusive systems see [24]. Then the translation-invariant stationary distributions are generally not product measures, but can still be classified by their density ρ, i.e., there are, at least at high temperatures, measures μ_ρ such that $\langle\eta_i\rangle_{\mu_\rho} = \rho$, $\langle\eta_i\eta_j\rangle - \rho^2 \to 0$ as $|i-j| \to \infty$.

Burgers' equation (13.1) needs to be generalized to fit driven diffusive systems. Based on the assumption (which can be proven in many cases) that on the appropriate spatial and temporal scale the probability distribution is locally that of a stationary state with local density $u(x,t)$, we can evaluate the current $J(u(x,t))$ entering the conservation law,

$$\frac{\partial u(x,t)}{\partial t} + \frac{\partial}{\partial x}J(u(x,t)) = 0. \tag{13.9}$$

In the ASEP we have

$$\begin{aligned} J(u) &= [p\langle\eta_i(1-\eta_{i+1})\rangle_{\nu_u} - (1-p)\langle\eta_{i+1}(1-\eta_i)\rangle_{\nu_u}]/\tau \\ &= (2p-1)u(1-u)/\tau, \end{aligned} \tag{13.10}$$

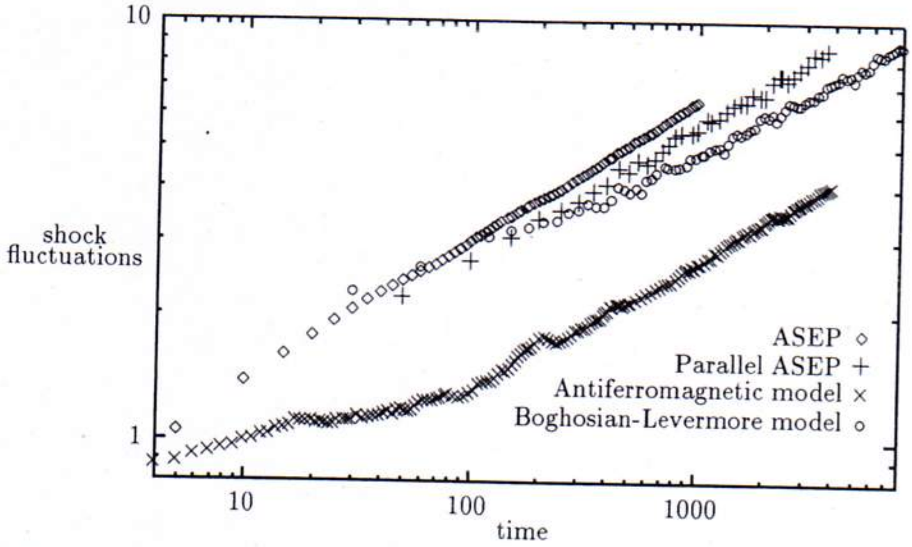

Fig. 13.4. Numerical evaluation of shock fluctuation exponents for ASEP and other models.

which gives equation (13.1) with $c = (2p-1)/\tau$.

One expects that the scaling of the fluctuations in these models should be universal, for example the exponents should not depend on the details of the model but only on gross features such as the dimension, symmetry properties, etc. An extensive series of computer simulations of the motion of shock fronts in a variety of 1D stochastic lattice models with parallel and serial dynamics, infinite and finite temperatures, and ferromagnetic and antiferromagnetic particle interactions, was conducted [22], and this was found to be the case: all the models have the same shock fluctuation exponents, as illustrated by the slopes in Fig. 13.4. This strengthens the rationale for using the exceptionally uncomplicated ASEP in the first place.

In addition, it was shown [22,25] that this exponent could be changed if the dynamics were tuned to a special critical point: when one considers the current $J(\rho)$ as a function of the density ρ in a uniform system, if the system is at a point where $\partial^2 J/\partial\rho^2 = 0$ then the fluctuations will be reduced from the universal value of $O(t^{1/3})$. In the ordinary ASEP we have $J = (2p-1)\rho(1-\rho)$ and $\partial^2 J/\partial\rho^2 = 2 - 4p \neq 0$, and there is no critical point. However, a variant with non-nearest-neighbor jumps allowed has a current $J = \rho(1-\rho)[1/2 + \rho^3 + (1-\rho)^3]$ and therefore at $\rho = 1/2$ one has

$\partial^2 J/\partial\rho^2 = \partial^3 J/\partial\rho^3 = 0$, where one finds that the standard deviation of the shock position grows as $t^{1/4}$ [22,25].

13.4 Models with blockages

A variation of the ASEP can produce shocks that do not move: one introduces a 'blockage' on one bond (or hypercolumn of bonds in more than 1D); the transition rates are reduced for particles jumping between one particular pair of nearest-neighbor sites [26]. Particles pile up behind the blockage and the density is reduced in front of it; if one uses periodic boundary conditions the transition from low to high density will result in a stable shock localized at a position that depends on the blockage and the average density. Now initial conditions are irrelevant and one would expect the previous scaling of the growth of fluctuations in time to be converted into a spatial scaling.

Actually, however, there are two components to the shock fluctuations—the aforementioned 'dynamical randomness' producing the $L^{1/3}$ behavior, and a 'blockage randomness', since the timing of jumps across the blockage is random. The variance of the shock position due to the blockage randomness is proportional to the expected net number of excitations in the system and thus provides no contribution when the system is half-filled, i.e., when the number of particles is the same as the number of holes; and indeed a half-filled system of size L has shock fluctuations of order $L^{1/3}$, which confirms the behavior observed earlier. In general the blockage randomness produces fluctuations that scale as $L^{1/2}$. The validity of this picture can be seen by changing the dynamics to reduce artificially the noise resulting from the blockage jumps while keeping the rest of the system (relatively) unchanged. This new system has fluctuations that scale as $L^{1/3}$ for *all* densities, further reinforcing the belief in the exponent 1/3.

Of course the model with a blockage provides two subjects worthy of study: the region around the blockage as well as the region around the shock. The motivation for this model came from studying the shock, but the blockage has proved to be very interesting as well, and is perhaps of more general interest, serving as a model for long-range correlations and phase transitions in nonequilibrium systems: it exhibits the sensitivity to changes in parameters that are typical of driven diffusive systems; a local change in the transition rates (i.e., the jump rate across the blockage) has a global effect [27] in that the system segregates into high- and low-density phases.

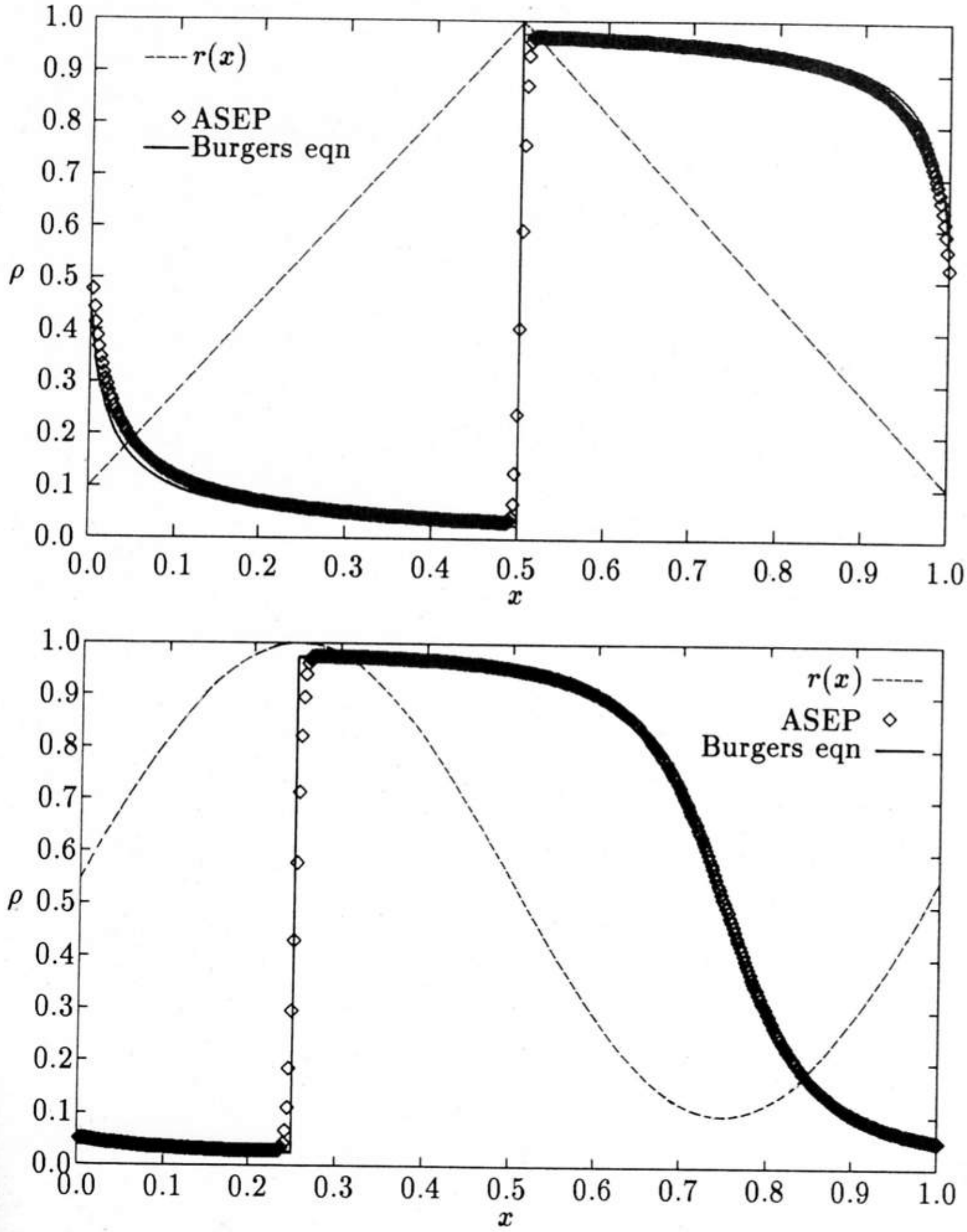

Fig. 13.5. Two examples of rate functions: stationary solutions of (13.12) with average value 1/2, and the stationary density of the ASEP with 500 sites and the same rate function.

We know quite a bit about this model [28]. Consider the case $p = 1$. Exact finite volume results serve to bound the allowed values for the current in the infinite system. This proves the existence of a gap in the allowed density corresponding to a nonequilibrium phase transition in the infinite system: specifically, only states with $|\rho - 1/2| \geq \delta(r)$ are permitted, where r is the blockage transmission rate, $\delta(\cdot)$ is a nonincreasing function with $\delta(1) = 0$, and there exists r^*, $0 < r^* < 1$, such that $\delta(r^*) > 0$. Numerical results indicate that $\delta(r) > 0$ for all $r < 1$. Note that the ASEP can be used to model traffic flow [29]. The result that $\delta(r) > 0$ for all $r < 1$ indicates that an arbitrarily small highway disruption can produce a traffic jam in situations in which the flow would be maximal without the obstruction.

One also knows the exact coefficients of a series expansion for the current as a function of the blockage rate:

$$\begin{aligned} J(r) = r - \frac{3}{2}r^2 + \frac{19}{2^4}r^3 - \frac{5\times59\times73}{2^{10}\times3^3}r^4 + \frac{13\times33613\times177883}{2^{26}\times3^7}r^5 \\ -0.3278724755(1)r^6 + O(r^7). \end{aligned} \tag{13.11}$$

The series expansion, derived from exact solutions of small finite systems (obtained using MAPLE V), is known to be asymptotic for all sufficiently large systems. Padé approximants based on this series, which make specific assumptions about the nature of the singularity at maximal transmission, match the numerical data for the 'infinite' system to one part in 10^4.

13.4.1 Extended defects

A blockage is a localized defect in an otherwise translation-invariant system. One can also consider extended defects. One model for this is an exclusion process where the rates vary over the system. In keeping with a hydrodynamic picture, we consider a smooth rate function r on the unit circle, i.e., the jump rate at site i is $r(i/L)$. Then the hydrodynamic equation governing this process is expected to be

$$\frac{\partial u(x,t)}{\partial t} + \frac{\partial}{\partial x}\{r(x)u(x,t)\,[1 - u(x,t)]\} = 0\,. \tag{13.12}$$

The key feature in determining the behavior of (13.12) is the minimum of the function r. Consider stationary viscosity solutions $u(x)$ of (13.12) (obtained by considering the limit of adding a vanishingly small viscosity term). Let $u_\pm(x) = [1 \pm \sqrt{1 - r_{\min}/r(x)}\,]/2$, assuming that $r_{\min}$ is the unique minimum of r located at $x_{\min}$. Then we have three types of solutions: if $\int u(x)\,dx \geq \int u_+(x)\,dx$ the solution is of the form $u(x) = [1 + \sqrt{1 - R/r(x)}\,]/2$ with

$R \le r_{\min}$; if $\int u(x)\,dx \le \int u_-(x)\,dx$ the solution is of the form $u(x) = [1-\sqrt{1-R/r(x)}\,]/2$ with $R \le r_{\min}$; otherwise the solution is discontinuous, with $u(x) = u_+(x)$ to the left of $x_{\min}$ and $u(x) = u_-(x)$ to the right of $x_{\min}$. This results in a solution continuous at $x_{\min}$ and discontinuous at some arbitrary other point.

Does this have anything to do with the particle system? In Fig. 13.5 we see two examples of rate functions: stationary solutions of (13.12) with average value 1/2, and the stationary density of the ASEP with 500 sites and the same rate function. Thus we see that shocks are not caused by discontinuities in the jump rates, but can occur and remain stable even when the rates vary smoothly.

If r has multiple minima, the picture is much less clear; certainly numerous weak stationary solutions of (13.12) exist but it is not clear if they have anything to do with the particle system and whether they exist as the limit of vanishing viscosity.

We would like to thank Francis Alexander and Eugene Speer for helpful discussions. Our work was supported in part by AFOSR Grant 4-26435. See also the added note [30].

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[30] *Note added in proofs.* B. Derrida, J. L. Lebowitz and E. Speer have recently obtained results about the structure of the shock for the case when the asymmetry is not total, $\frac{1}{2} < p < 1$. They find in particular that for any asymptotic densities ρ_+ and ρ_-, there exists a p^* such that for $p \le p^*$ the local density profile, as seen from the second class particle, is monotone. For $\rho_+ = 1$, $\rho_- = 0$, $p^* = 1$. O. Costin, J. L. Lebowitz and E. Speer have found additional evidence (but no proof) that the behavior of the current $J(r)$ is, in the case of a single blockage, as described in Sec. 13.4.