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Relaxation spectrum of the asymmetric exclusion process with open boundaries

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Abstract. We calculate numerically the exact relaxation spectrum of the totally asymmetric simple exclusion process (TASEP) with open boundary conditions on lattices up to 16 sites. In the low- and high-density phases and along the nonequilibrium first-order phase transition between these phases, but sufficiently far away from the second-order phase transition into the maximal-current phase, the low-lying spectrum (corresponding to the longest relaxation times) agrees well with the spectrum of a biased random walker confined to a finite lattice of the same size. The hopping rates of this random walk are given by the hopping rates of a shock (a domain wall separating stationary low- and high-density regions), which are calculated in the framework of a recently developed non-equilibrium version of Zel'dovich's theory of the kinetics of first-order transitions. We conclude that the description of the domain wall motion in the TASEP in terms of this theory of boundary-induced phase transitions is meaningful for very small systems of the order of ten lattice sites.

1. Introduction: domain wall dynamics in driven diffusive systems

In the context of equilibrium phase coexistence or when studying the dynamical origin underlying critical non-equilibrium phenomena such as coarsening processes the question arises to which extent large-scale notions such as domain size or interface width really play a role in very small systems. This becomes important, for example, if one tries to relate a mesoscopic description of a many-body system in terms of lattice gas models [1–3] to real systems where the size of particles is not necessarily much smaller than the entire region within which they interact. More pointedly—and particularly so in low dimensional systems—the question is when fluctuations in the mesoscopic variables become so large compared to system size that a description in terms of coarse-grained degrees of freedom (intermediate between the mesoscopic variables and system size) loses its meaning? This is the issue we wish to address in a specific nonequilibrium context, namely, the dynamics of a domain wall (a coarse-grained notion) in a one-dimensional lattice gas model kept far from equilibrium by choosing open boundary conditions which support a finite steady-state current. Driven diffusive systems of this kind have become relevant in the study of ion channels [4, 5], biopolymers [6–8], traffic flow [9] and other complex systems of essentially one-dimensional topology [10].

The prototypical example studied here is the totally asymmetric simple exclusion process (TASEP), a lattice gas model for which an exact solution of the steady state properties has been found [11–13]. In this model each lattice site can be occupied by at most one particle. Particles attempt to move to the right with unit rate after an exponentially distributed random waiting time with unit mean. If the neighbouring site is empty, the attempt succeeds, otherwise

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it is rejected. At site 1 particles are injected with rate α and at site L particles are removed with rate β. The bulk stationary states (characterized by a spatially constant bulk density ρ) are uncorrelated. Hence there is a stationary particle current of strength

$$j = \rho(1-\rho) \tag{1}$$

which has a maximum $j^* = 1/4$ at $\rho^* = 1/2$. Considering the bulk density as order parameter, the nonequilibrium phase diagram of the model has a first-order phase transition between a low-density phase with bulk density $\rho = \alpha < 1/2$ and a high-density phase with bulk density $\rho = 1-\beta > 1/2$ along the curve $\alpha = \beta < 1/2$. Second-order transitions take place from both phases to a maximal current phase with bulk density $\rho = 1/2$ defined by the region $\alpha > 1/2, \beta > 1/2$.

Which bulk steady state the system selects, i.e. the stationary bulk density as a function of the boundary densities $\rho^- = \alpha$, $\rho^+ = 1-\beta$, can be understood in terms of the interplay of density fluctuations and the motion of a shock [14,15]. This shock, marking a rapid increase of the local density, may be seen as a domain wall separating a *stationary* (not equilibrium!) region of low density ρ^- to another stationary region of high density ρ^+. We have shown (assuming the system size to be large) that the (non-equilibrium) first-order transition at $\alpha = \beta$ can be explained in a way similar to the Zel'dovich theory of the kinetics of (equilibrium) first-order transitions [16]. The domain wall motion is understood as diffusion of the 'size of the high-density segment'. The 'elementary processes' that change the length of the filled region consist of hopping of the domain wall to the right and left at rates $D^{\pm}$ respectively. Postulating continuous-time random walk dynamics we conjectured the individual rates to take the values [14]

$$D^{\pm} = j^{\pm}/(\rho^+ - \rho^-) \tag{2}$$

with incoming and outgoing currents $j^{\pm} = j(\rho^{\pm})$ given by (1). The mean velocity of the domain wall

$$v_s = D^+ - D^- = \frac{j^+ - j^-}{\rho^+ - \rho^-} \tag{3}$$

is determined by mass conservation. Since in general $j^+ \neq j^-$ the domain wall performs a biased random walk (figure 1), leaving the bulk of the system in a region of high density ρ^+ if the domain wall velocity is negative and in a region of low density ρ^- if v_s is positive. A first-order transition takes place for $j^+ = j^-$. In this case the domain wall performs an unbiased random walk, leaving the bulk of the system in a state of coexistence of the low- and high-density segments.

In this theory, which describes the approach to stationarity (i.e. the late-time behaviour of the model), the domain wall is imagined to be a soliton-like collective mode of the many-body system which essentially behaves like a single particle and remains stable at all times. This picture is not restricted to the TASEP for which the properties of the shock are well understood [17–20], but is believed to be generic for driven one-component systems as long as there is a stable domain wall [15]. In view of the coarse-grained nature of this approximation it should be recognized that the assignment of the domain wall position to a lattice site (which is implicit in the random walk picture) leaves much room for arbitrariness; it is analogous to the problem of defining the location of the interface between coexisting phases in an equilibrium system [21]. Yet the theory explains the correct location of the phase transition lines in many driven diffusive systems [3], and also reproduces the exactly known shock diffusion coefficient [22] of the TASEP defined on an infinite lattice

$$D = \frac{1}{2}(D^+ + D^-) = \frac{1}{2}\frac{j^+ + j^-}{\rho^+ - \rho^-} \tag{4}$$

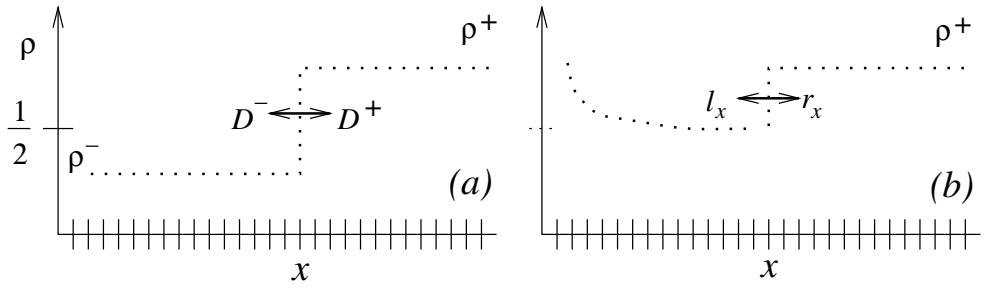

Figure 1. (*a*) Schematic presentation of a (0|1) domain wall at position x, connecting a homogeneous stationary phase of low density $\rho^- < 1/2$ with a stationary phase of high density $\rho^+ > 1/2$. The domain wall hops one lattice unit to the right with rate D^+ and to the left with rate D^-. In figure (*b*) the $(m|1)$-domain wall connects the inhomogeneous maximal-current phase with bulk density $\rho = 1/2$ with a high-density phase of density $\rho^+ > 1/2$. Here the hopping rates l_x, r_x are space dependent, approaching the bulk values $D^{\pm}$ far away from the boundary. The reference profile $\rho(x)$ at the edge of the maximal-current phase AT the point $(\alpha, 1/2)$, independent of β. The asymptotic densities at the boundaries of a finite system are imagined to be fixed at all times.

and the exact localization length [12, 13] of the boundary density profile in the TASEP with open boundaries.

On the other hand, some simple implications of this dynamic non-equilibrium domain wall theory have not yet been tested. If the late-time behaviour of a very large system can really be viewed as being dominated by the domain wall motion and if this domain wall behaves like a single-particle mode, then one expects the longest relaxation times in the *many-body* relaxation spectrum of the TASEP with open boundaries to be given by those of a *single* random walker with hopping rates (2). Once this is established the question arises of just how large the system has to be for this non-rigorous description to be reasonably accurate.

With this in mind we study here the approach of the TASEP to its stationary nonequilibrium state in terms of the intrinsic relaxation times of the stochastic many-body process. First we derive the random walk dynamics of a domain wall that one expects from the theoretical scenario (section 2). The comparison of the theoretically predicted relaxation times with those found numerically is presented in section 3. These results are evaluated with emphasis on the degree of accuracy of the theory in small systems in section 4. Some concluding remarks are presented in section 5. Without loss of generality we consider throughout this paper the regime $\beta < 1/2$. The relaxation times in that part of the domain $\alpha < 1/2$ which is not discussed here follow from particle–hole symmetry.

2. Random walk of a domain wall

The position of the domain wall is viewed as a lattice site x^* located between two stationary regions of average densities $\rho^{\pm}$. We stress that we do not provide a definition of what this lattice site should be in a given configuration of the lattice gas, defined by discrete occupation numbers $n_x(t) = 0, 1$. For the ASEP such a site could be defined by the position of a second-class particle [17] which is driven into a region of maximal density gradient, but in the general case there is no analogous construction and hence we do not make use of it. We only assume that such a position could be defined and explore the consequences of this assumption for the relaxation spectrum of the full process.

Ignoring any possible internal structure of the 'interface', i.e. the intrinsic order parameter profile, we consider the whole region $x \geqslant x^*$ to the right of the domain wall position to belong

to the ρ^+-segment and the whole of the region to the left ($x < x^*$) to belong to the ρ^--segment (figure 1). The domain wall position in a system of L sites then can take $L+1$ values. Position $x = 1$ corresponds to the system being completely in the high-density phase, while $x = L+1$ corresponds to a pure low-density phase. We remark that due to a quantum algebra symmetry of the process this highly idealized picture of the domain wall structure is exact for a special relation between ρ^+ and ρ^- [20,23], but not in general [19] and not in the cases studied below.

We start with a discussion of the domain wall dynamics in the bulk of a very large system. First we consider the case $\rho^- = \alpha < 1/2$, $\rho^+ = 1-\beta > 1/2$, corresponding to a (0|1) domain wall in a notation similar to that of [14].

According to [14] the domain wall performs a lattice random walk with the bulk rates (2), but reflecting boundary conditions since the domain wall can never leave the system because of the fixed boundary densities. At the boundary sites $x = 1$ and $x = L+1$ one therefore expects a left-hopping rate $l_1 = 0$ at site 1 and a right-hopping rate $r_{L+1} = 0$ at site $L+1$. In the simplest approximation one assumes bulk dynamics for the remaining two boundary rates: one takes $r_1 = D^+$ as the right-hopping rate at site 1 and $l_{L+1} = D^-$ as the left-hopping rate at site $L+1$. At all other sites close to the boundary the hopping rates are assumed to equal the bulk rates. The probability distribution $P(x)$ for the position of the domain wall then satisfies the master equation

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}P(x,t) &= D^-P(x+1,t) + D^+P(x-1,t) - (D^+ + D^-)P(x,t) \\
\frac{\mathrm{d}}{\mathrm{d}t}P(1,t) &= D^-P(2,t) - D^+P(1,t) \\
\frac{\mathrm{d}}{\mathrm{d}t}P(L+1,t) &= D^+P(L,t) - D^-P(L+1,t).
\end{aligned} \tag{5}$$

Here $2 \leqslant x \leqslant L$. The stationary distribution satisfies detailed balance and has the form

$$P^*(x) \propto u^{2x} \tag{6}$$

with

$$u^2 = D^+/D^-. \tag{7}$$

Thus the stationary probability of finding the domain wall decays exponentially from the boundary towards which it is biased.

To obtain the relaxational behaviour we reformulate the reflection property by extending the range of validity of the bulk equation to all integers and at the same time imposing the boundary conditions $D^+P(0,t) = D^-P(1,t)$ and $D^+P(L+1,t) = D^-P(L+2,t)$ for all times t. This ensures that both the bulk equation and the boundary equations are satisfied at all times. The master equation can now be solved with a plane wave ansatz of the form

$$P_x(t) = \sum_p A_p(0)\mathrm{e}^{-\epsilon t}(\mathrm{e}^{\mathrm{i}px} + B_p u^{2x}\mathrm{e}^{-\mathrm{i}px}). \tag{8}$$

This gives the reciprocal relaxation times $\epsilon_p = D^+(1-\mathrm{e}^{-\mathrm{i}p}) + D^-(1-\mathrm{e}^{\mathrm{i}p})$ as a function of the 'momentum' p. Satisfying the boundary conditions fixes $B_p = -(1-u^{-2}\mathrm{e}^{\mathrm{i}p})/(1-\mathrm{e}^{-\mathrm{i}p})$ and requires

$$\mathrm{e}^{2\mathrm{i}p(L+1)} = u^{2L+2}. \tag{9}$$

The solution of this equation yields quantized complex values $p_n = \pi n/(L+1) - \mathrm{i}\ln u$, with $n = 1, \ldots, L$. Thus the spectrum (9) is real and one finds the relaxation times

$$\tau_n = \left[D^+ + D^- - 2\sqrt{D^+D^-}\cos\left(\pi n/(L+1)\right)\right]^{-1}. \tag{10}$$

These relaxation times depend on both $\alpha = \rho^-$ and $\beta = 1 - \rho^+$ through the relation (2). In the thermodynamic limit one obtains the longest relaxation time

$$\tau = \left[D^+ + D^- - 2\sqrt{D^+ D^-} \right]^{-1}. \tag{11}$$

This quantity is finite for a biased random walk with $D^+ \neq D^-$ (finite-size corrections are of order $1/L^2$), but diverges proportionally to L^2 for the symmetric case $D^+ = D^-$.

For $\alpha > 1/2$ the theory predicts a $(m, 1)$-domain wall [14] which is composed of a segment corresponding to the high-density phase with $\rho^+ = 1 - \beta > 1/2$ on the right and the maximal current phase (m) on the left with bulk density $\rho = 1/2$ for *all* α. The m-segment does not have constant density close to the boundary, as was assumed in the discussion of the domain wall dynamics above. Instead, the density profile decays rather slowly proportional to $1/\sqrt{x}$ from the true left-boundary value α to its bulk value $1/2$. In the framework of the domain wall picture the bulk density of the left (maximal current) segment plays the role of ρ^- which is now understood as an *effective* left-domain-wall density. Hence $\rho^- = 1/2 \neq \alpha$ for all $\alpha > 1/2$ and one expects for a large system relaxation times (10) which do *not* depend on α. However, due to the slow algebraic decay of the density profile one can also expect the relaxational behaviour to be dominated by the bulk dynamics only in rather large systems of the order of thousands of sites.

3. Relaxation spectrum of the TASEP

The relaxation times of the TASEP can be calculated by diagonalizing the time evolution operator H of the process for finite systems. By construction, the lowest eigenvalue of H is zero (with the associated eigenvector being the stationary distribution) while the real parts of the higher eigenvalues are the reciprocals of the relaxation times. Hence the low-lying excitations correspond to the longest-living modes. The generator H of the ASEP is closely related to a non-Hermitian 'quantum' Hamiltonian of an anisotropic ferromagnetic spin-$\frac{1}{2}$ Heisenberg chain [24]. Following standard procedures described in detail in [3] we use the spin-$\frac{1}{2}$ Pauli matrices $\sigma_k^{x,y,z}$ acting on site k of the chain and define the particle annihilation/creation operators $s_k^{\pm} = (\sigma_k^x \pm \mathrm{i}\sigma_k^y)/2$ and the projectors $n_k = (1 - \sigma_k^z)/2$ on particles and $v_k = 1 - n_k$ on vacancies respectively. For the TASEP with open boundaries one then has

$$H = \sum_{k=1}^{L-1} (n_k v_{k+1} - s_k^+ s_{k+1}^-) + n_1 - s_1^+ + v_L - s_L^-. \tag{12}$$

Notice that due to the lack of detailed balance (corresponding to the intrinsic nonequilibrium nature of the process) the excitation spectrum may have complex eigenvalues which appear in complex conjugate pairs.

For a periodic system exact finite-size analysis of the Bethe ansatz equations for the spectrum of H yields longest relaxation times increasing with system size as L^z with the dynamical exponent $z = 3/2$ [24, 25]. This analysis, however, does not provide information about the domain wall motion since the existence of a stable domain wall requires non-periodic boundary conditions with different boundary densities kept fixed at all times. This is realized in the open system outside the maximal current phase $\alpha, \beta > 1/2$, inside which a domain wall is not stable [3] and longest relaxation times with the same finite-size scaling properties as in the periodic system are expected. This is in agreement with numerical finite-size estimates [26].

Like the periodic system, the open quantum spin chain (12) is also an integrable model [27, 28]. However, due to the lack of particle number conservation no analogue of the Bethe ansatz equations has been found yet. For this reason we are not able to calculate the

exact asymptotic behaviour of the low-lying part of the spectrum. However, it is possible to calculate the eigenvalues of small systems up to approximately 20 lattice sites by numerical diagonalization of H. These eigenvalues allow us to assess the validity of the domain wall theory in small systems.

Since the generator H is an asymmetric matrix the numerical diagonalization is more difficult than in the standard case of symmetric or Hermitian matrices. Nevertheless there are methods available which allow us to perform a numerically exact calculation of the eigenvalues. The results presented below have been obtained applying two methods. For system sizes up to $L = 10$ we used a complete diagonalization routine from the standard package LAPACK. For larger systems we applied an iterative Arnoldi algorithm [29]† to calculate the low-lying part of the spectrum.

A chain of L sites has 2^L eigenvalues and hence $2^L - 1$ excited states. On the other hand, the domain wall theory predicts only a subset of L eigenvalues corresponding to excited states. In order to compare the theoretical prediction with the spectrum of the TASEP it is necessary to identify those eigenvalues of the TASEP which correspond to the postulated domain wall modes. To this end we note that for α, β much smaller than $1/L$ the domain wall picture becomes exact [30]. Moreover, at such small values of α and β the full random walk spectrum (which has eigenvalues of the order of $\alpha + \beta$) is below the remaining excitation spectrum of the TASEP, which from perturbation theory can be seen to have eigenvalues of the order of unity and larger. Using this property we plot the low-lying part of the spectrum of the TASEP as a function of α and β and identify as the domain wall eigenvalues for finite α, β those which become the known domain-wall eigenvalues at very small α, β.

In figure 2 we show the low-lying spectrum for several system sizes. We plot real parts of the eigenvalues along two curves $\alpha = \beta$ and $\beta = \alpha/2$ in the region $\alpha < 1/2$, corresponding to a (0|1) domain wall. One observes many level crossings, which is not surprising because of the integrability of the system. Also shown are the eigenvalues of a random walker given by (10). For sufficiently small α they coincide with the lowest-lying eigenvalues of the TASEP. The agreement is very good up to $\alpha \approx 1/L$ along the line $\alpha = \beta$ and for significantly larger values of α (up to $\alpha \approx 2/L$) along the line $\beta = \alpha/2$. This is quite remarkable and encouraging with regard to the robustness of the random walk model as good agreement could be expected from perturbation theory only for both α, β significantly less than $1/L$.

Before discussing further how these random walk eigenvalues relate to the TASEP spectrum, we note some other spectral properties which we found intriguing, but for which we have no explanation.

(1) As α increases some real eigenvalues merge to form a pair of complex conjugate eigenvalues of which only the real part is shown. A similar phenomenon was observed as a function of field strength in the Rubinstein–Duke model [7], which is a two-species driven lattice gas describing the motion of an entangled polymer chain under the influence of an external electrical field as, for example, in gel electrophoresis. We do not have an explanation for this phenomenon except to say that complex eigenvalues are related to the presence of currents (corresponding to absence of detailed balance). It is not clear, however, why these special complex pairs appear only for sufficiently high α. Other complex conjugate pairs appear as soon as $\alpha > 0$.

(2) In all system sizes considered, alternating eigenvalues of the random walk branch merge with another real eigenvalue (not belonging to the random walk branch) to form a complex conjugate pair at some value of α. Up to this value of α the agreement of the TASEP

† A sophisticated package ARPACK, which implements the Arnoldi method, can be found in [29] in the directory pub/people/software/ARPACK.

eigenvalue with the corresponding random walk eigenvalue is good; for larger α it quickly deteriorates.

(3) For $\alpha = \beta$ the total number $\Sigma_L(\alpha)$ of real eigenvalues seems to follow some interesting pattern. For fixed α the difference $\Delta = \Sigma_L - \Sigma_{L-1}$ appears to approach a constant value for even values of L as L increases. This difference decreases with increasing α: $\Delta(0.05) = 6$ for $L \geqslant 6$; $\Delta(0.1) = \Delta(0.15) = 2$ for $L \geqslant 2$; $\Delta(\alpha) = 0$ for $\alpha \geqslant 0.2$ and $L \geqslant 6$. At $\alpha = 1/2$ one has $\Delta = 0$ for all L and $\Sigma_{2L} = 2^L$ (see table 1).

4. Finite-size effects and late-time behaviour

We have remarked earlier that the simple domain wall picture in which one assumes the existence of a lattice point separating a region of constant density ρ^- to the left from a region of constant density ρ^+ to the right is literally applicable for a special relation between ρ^+ and ρ^-. On this manifold, which is of interest only for partially asymmetric particle hopping, part of the spectrum of the exclusion process is indeed *exactly* given by the spectrum of a single random walker for any system size [23]. On the other hand, the results of [19] suggest for generic values of densities an extended intrinsic structure of the domain wall. The associated length scale (see below) is not related to the bulk correlation length—as is found in theories for equilibrium systems such as van der Waals theory [31]—but is finite and non-zero in lattice units. This in turn implies that one cannot expect to find the exact random walk spectrum in a system of finite size. However, the random walk picture of the domain wall is still expected to be valid for large enough systems, such that any hypothetical intrinsic width of the domain wall that one might define is small compared to system size.

It is also clear from the expression (2) for the hopping rates that the random walk model cannot possibly be valid in finite systems for domain walls with very small density difference $\Delta\rho = \rho^+ - \rho^-$. For the TASEP these rates diverge as one approaches $\alpha = 1/2$ along the first-order transition line $\alpha = \beta$ since $\rho^+ - \rho^- \to 0$ as $\alpha = \rho^- \to 1/2$. This would mean that the domain wall position would fluctuate over distances much larger than system size in an infinitesimal time step, thus rendering the notion of a domain wall moving within the system meaningless.

We also recall that the domain wall theory describes the behaviour at very late times of the evolution of the system. At earlier times relaxational modes within the domains are likely to interfere with the motion of the domain wall as a single physical entity. Hence one expects only the low-lying spectrum of the TASEP to coincide with the spectrum of a random walker, not the full spectrum as one—surprisingly—has for the special relation between ρ^+ and ρ^- referred to above.

What the domain wall theory therefore predicts for a small system—if applicable at all—is the presence of a set of long relaxation times which are approximately given by those of a random walker in a system of the same size for *all* parameter values, but with significant (and eventually divergent) errors as one approaches the point $\alpha = \beta = 1/2$. In particular, the longest relaxation time, corresponding to the lowest excitation in the spectrum, is expected to give the best match of all domain wall relaxation modes with those of a single random walker. This picture is consistent with the numerical observations shown in figure 2. One expects the agreement to improve for larger systems, which is also seen in the figures. The values of α at which the deviation between a given random walk eigenvalue and the corresponding eigenvalue of the TASEP exceeds some fixed value (say, 5%) increases slowly with increasing length L.

One may also compare the reciprocal of the longest random walk relaxation time in

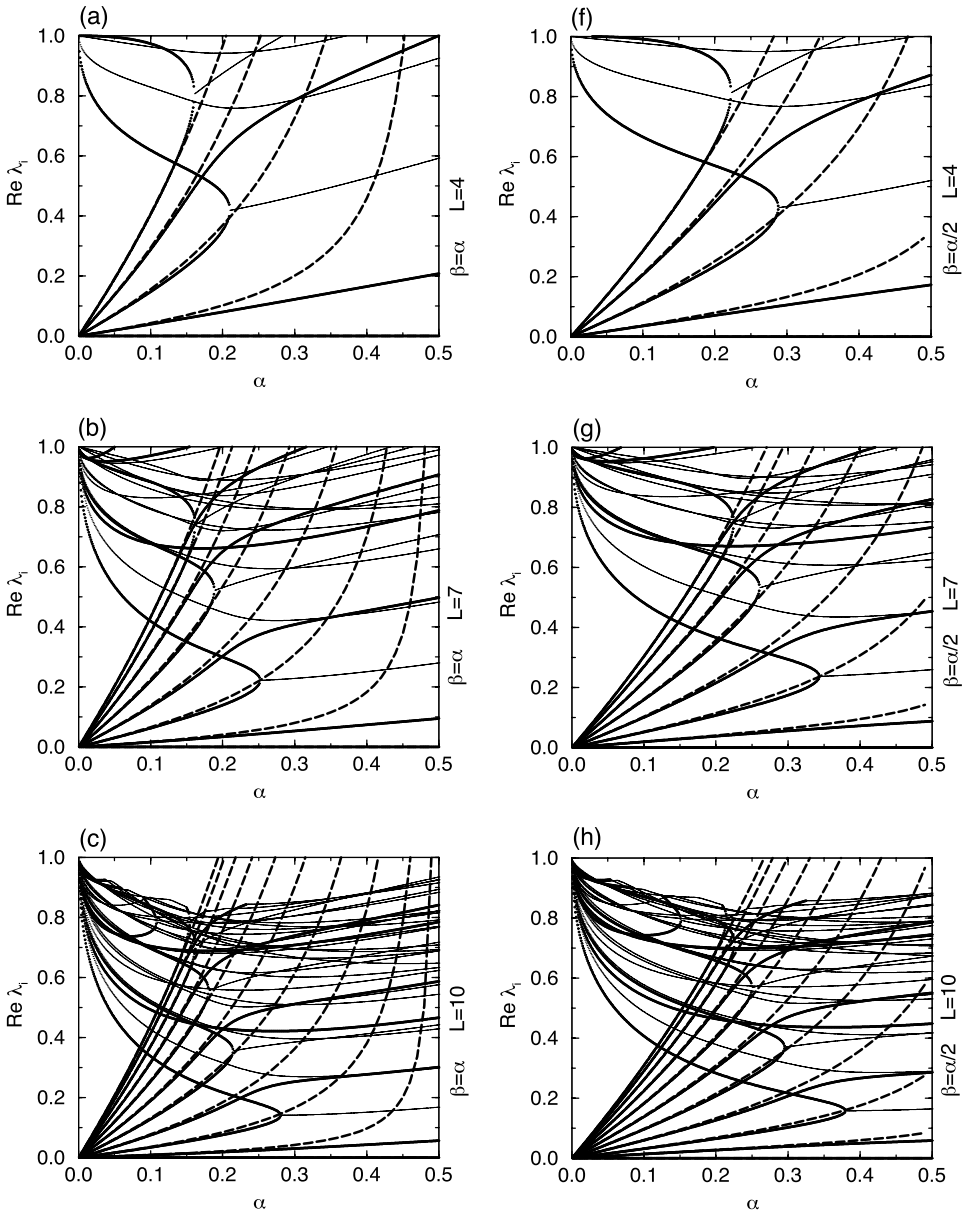

Figure 2. Real parts of the eigenvalues λ_i of the TASEP generator H in equation (12) along the two lines $\beta = \alpha$ (left) and $\beta = \alpha/2$ (right), for $L = 4, 7, 10, 13, 16$ as given in the figures. Thick solid curves represent real eigenvalues and thin solid curves are real parts of complex conjugate pairs. The random-walker spectrum according to equation (10) is shown by dashed curves. For $L = 4, 7$ all eigenvalues which have real parts up to unity are plotted, for $L = 10, 13$ we show the 60 lowest eigenvalues and for $L = 16$ only the 20 lowest ones.

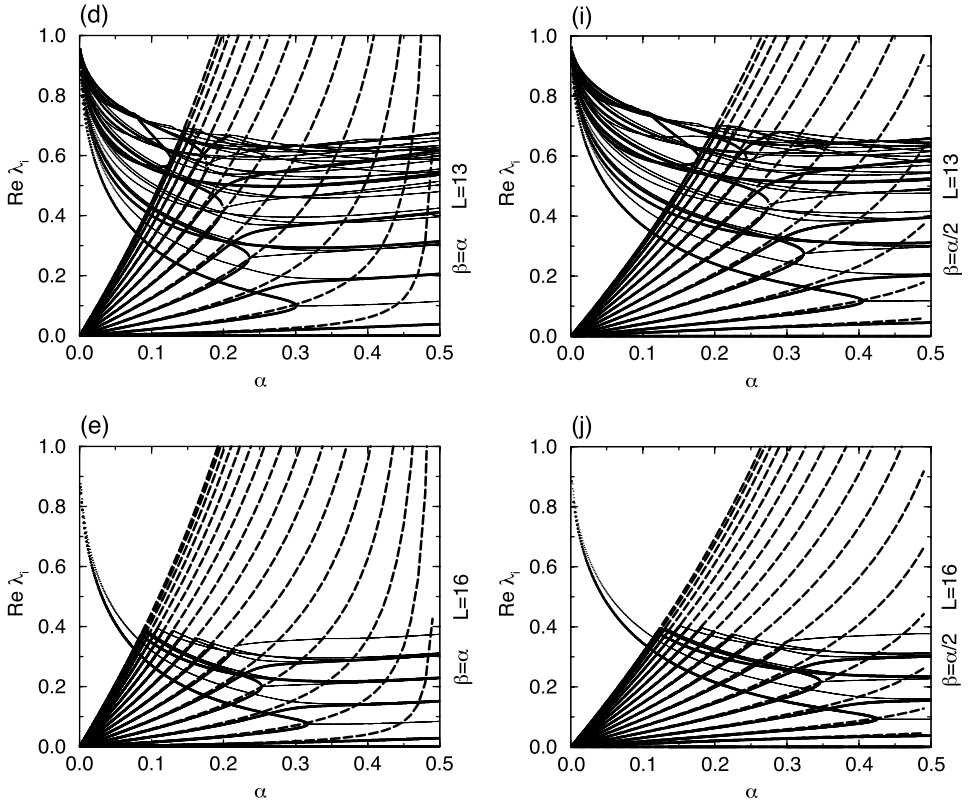

Figure 2. (Continued)

Table 1. Number of real eigenvalues in the full spectrum of the TASEP along the first-order transition line $\alpha = \beta$ for different system sizes.

$\alpha = \beta$	$L = 1$	2	3	4	5	6	7	8	9	10
0.05	2	4	6	10	14	20	28	34	50	56
0.10	2	4	6	8	12	14	22	24	42	44
0.15	2	4	6	8	12	14	22	24	40	42
0.20	2	2	4	6	10	10	18	18	36	36
...										
0.50	2	2	4	4	8	8	16	16	32	32

the thermodynamic limit (11) with finite-size extrapolants of the lowest excitation of the TASEP, calculated in [26] from the finite-size spectra using the Bulirsch–Stoer extrapolation algorithm [32]. In table (2) we show extrapolants for $\beta = 0.2$ and various values of α together with the theoretical random walk relaxation times (11). For $\alpha \leqslant 1/2$, i.e. in the regime with a $(0|1)$ domain wall, the deviation is within the 0.1% range. In the regime $\alpha > 1/2$ where the theory predicts an $(m|1)$ domain wall the deviation is approximately 20%. We recall that the domain wall theory predicts relaxation times which become independent of α for $\alpha > 1/2$. This is in agreement with the extrapolants for $\alpha \geqslant 0.6$.

We believe the much poorer agreement of the finite-size data for $\alpha > 1/2$ with the theoretical values (10) for the longest relaxation times to be partly due to finite-size effects

Table 2. Theoretical reciprocal relaxation times in the thermodynamic limit (11) and extrapolated reciprocal relaxation times from the spectrum of the TASEP for $\beta = 0.2$ and various values of α. The extrapolated data are taken from table 1 of [26].

$\tau^{-1} \times 10^2$	$\alpha = 0.1$	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
Theory	1.429	0.000	0.679	2.020	3.333	3.333	3.333	3.333	3.333	3.333
TASEP	1.428	−0.001	0.678	2.018	3.331	4.016	4.012	4.013	4.014	4.014

resulting from the inhomogeneous structure of the maximal-current segment. In order to examine whether this conjecture produces corrections which improve the agreement, we incorporate the inhomogeneous density profile into the random walk picture in the following way. Rather than postulating constant hopping rates (2) we consider space-dependent hopping rates l_x and r_x for left and right hopping respectively which are determined from the exactly known density profiles in the pure phases on the basis of the domain wall picture. The master equation for the domain wall position with right/left hopping rates r_x, l_x therefore reads

$$\frac{\mathrm{d}}{\mathrm{d}t} P(x,t) = l_{x+1} P(x+1,t) + r_{x-1} P(x-1,t) - (r_x + l_x) P(x,t) \tag{13}$$

with boundary condition $P(0,t) = P(L+2,t) = 0$ for all times, corresponding to reflecting boundaries $l_1 = r_{L+1} = 0$. As shown below, these rates approach the constant values (2) in the bulk as required by the original domain wall theory, but take into account the internal structure of the postulated domains in the vicinity of the boundary. With the rates r_x and l_x thus specified one can numerically compute the relaxation spectrum of the random walk defined by (15).

The calculation of the rates consists of four steps. (i) First we determine the stationary domain wall probability $P^*(x)$ from the exactly known stationary density profile of the TASEP within the domain wall picture. (ii) Next we reexpress the domain wall hopping rates in terms of the stationary density profile using detailed balance. (iii) We require (3) to hold everywhere except as the boundary sites as this relation is dictated by mass conservation. (iv) The remaining free parameter in the choice of rates is determined by the requirement that the exactly known diffusion coefficient (4) be recovered in the bulk of an infinite system.

Step (i). The stationary density profile $\rho(x)$ has been calculated exactly for the TASEP [12, 13]. We denote by $P^*(x)$ the stationary probability of finding the domain wall at site x. Within the domain wall picture the density profile is related to $P^*(x)$ through the relation

$$\rho(x) = \rho^-(x) + (\rho^+ - \rho^-(x)) \sum_{y=1}^{x} P^*(y) \qquad (1 \leqslant x \leqslant L). \tag{14}$$

Here $\rho^-(x)$ is a reference density profile which takes into account the postulated internal structure of the pure left domain. For a $(0|1)$ domain wall with $\alpha < 1/2$ one has $\rho^-(x) = \rho^- = \alpha$ whereas for an $(m|1)$-domain wall with $\alpha > 1/2$ the reference profile $\rho^-_{\alpha,\beta}(x) = \rho_{\alpha,1/2}$ is the exact density profile of the TASEP at the onset of the maximal phase at the point with coordinates $(\alpha, \beta = 1/2)$ (figure 1). Inverting this relation one obtains the stationary domain wall probabilities

$$\begin{aligned} P^*(1) &= \frac{\rho(1) - \rho^-(1)}{\rho^+ - \rho^-(1)} \\ P^*(x) &= \frac{\rho(x) - \rho^-(x)}{\rho^+ - \rho^-(x)} - \frac{\rho(x-1) - \rho^-(x-1)}{\rho^+ - \rho^-(x-1)} \\ P^*(L+1) &= \frac{\rho^+ - \rho(L)}{\rho^+ - \rho^-(L)}. \end{aligned} \tag{15}$$

Step (ii). Detailed balance implies for the stationary solution $P^*(x)$ the relations

$$r_{x-1}P^*(x-1) = l_x P^*(x) \tag{16}$$

for $1 \leqslant x \leqslant L+2$. This does not fully specify the hopping rates in terms of the stationary probabilities (15), but relates left- and right-hopping rates through a free function $\mu(x)$, which takes positive values. One may write

$$l_1 = 0 \tag{17}$$

$$l_x = \frac{\mu(x)}{P^*(x)} \qquad \text{for} \quad 2 \leqslant x \leqslant L+1 \tag{18}$$

$$r_x = \frac{\mu(x+1)}{P^*(x)} \qquad \text{for} \quad 1 \leqslant x \leqslant L \tag{19}$$

$$r_{L+1} = 0. \tag{20}$$

Step (iii). The stationary particle current does not depend on space because of particle number conservation (except at the boundary sites) and hence the shock velocity (3) should be constant in space as well. We implement this condition by requiring

$$r_x - l_x = v_s = D^+ - D^- \tag{21}$$

everywhere except at the boundary sites $x = 1$ and $x = L+1$. Together with (15) and (17)–(20) this yields

$$\begin{aligned} &\mu(1) = 0 \\ &\mu(x) = (D^+ - D^-)\left[\frac{\rho(x-1) - \rho^-(x-1)}{\rho^+ - \rho^-(x-1)} + \xi\right] \\ &\mu(L+2) = 0 \end{aligned} \tag{22}$$

with an arbitrary constant ξ for $2 \leqslant x \leqslant L+1$.

Step (iv). This constant is chosen to reproduce the exact bulk diffusion coefficient (4) with constant bulk hopping rates $r_x = D^+, l_x = D^-$ in the thermodynamic limit. This is equivalent to requiring $u^2 = \mu(x+1)/\mu(x)$ (cf (7), (18) and (19)) for all x and yields $\mu(x+y) = u^{2y}\mu(x)$ by iteration. In order to fix ξ we demand that this iterated relation be valid for the boundary values $x = 2$, $x + y = L+1$ of a very large system. In the thermodynamic limit the reference densities entering this expression for ξ become constant, i.e. $\rho^-(x) = \rho^- = \alpha$, and one finds

$$\xi = \frac{\rho(L) - \rho^- - (\rho(1) - \rho^-)u^{2(L-1)}}{(\rho^+ - \rho^-)(u^{2(L-1)} - 1)}. \tag{23}$$

It is straightforward to verify that with this choice of ξ one recovers in the bulk of a large system the expected relations $r_x = D^+$ and $l_x = D^-$ by using the exact expression for the density profile $\rho(x)$ [12].

Notice that as one approaches the line $\alpha = 1 - \beta$ the difference between ρ^+ and the local density at site 1 in the maximal current segment vanishes. Hence one obtains infinite hopping rates and therefore a divergent spectrum. This limits the range of validity of this phenomenological approach to the regime $\alpha < 1 - \beta$. This is analogous to the divergence of the bulk rates in the vicinity of the point $\alpha = \beta = 1/2$.

In figure 3 we show the lowest eigenvalue of the TASEP along the line $\beta = 0.25$ together with the predictions from (10) and the numerical calculation of the lowest eigenvalue of the random walk (15) for $L = 10$. Sufficiently far away from $\alpha = 1 - \beta$ the agreement of the eigenvalue of the space-dependent random walk is moderately better than that of the random

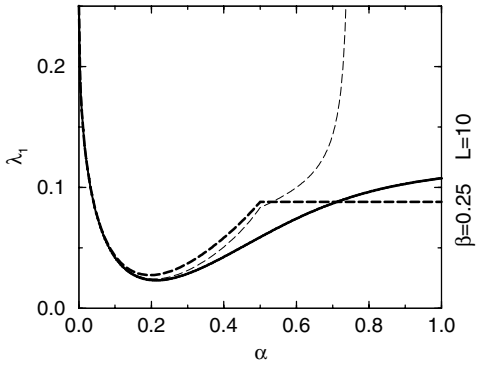

Figure 3. The lowest TASEP eigenvalue (solid curve) along the curve $\beta = 0.25$ for $L = 10$ compared to predicitions of the random-walk theory. The thick dashed curve shows the first eigenvalue according to equation (10), and the thin dashed curve is the lowest eigenvalue of the random walk in equation (15).

walk with constant rates, thus confirming the notion that the spatial structure of the density profile contributes to finite-size effects. Also the higher eigenvalues of the inhomogeneous random walk (not shown here) are closer to the corresponding eigenvalues of the TASEP than those of the homogeneous random walk. The effect is small though, and we do not wish to overemphasize its importance.

5. Conclusions

The numerical diagonalization of the stochastic generator of the TASEP with open boundary conditions yields results which are in agreement with theoretical expectation resulting from the notion that outside the maximal current phase the late-time dynamics of the TASEP are governed by the diffusive motion of a domain wall. Within the regime of a $(0|1)$ domain wall (but not close to $\alpha = \beta = 1/2$) it appears that this simple picture of a localized domain wall is applicable in good approximation in systems as small as ten lattice sites. This suggests that a domain wall indeed develops and that any internal structure of this domain wall such as an intrinsic width is much less than ten lattice units in an extended parameter range. With increasing system size this range increases. For small systems this observation is in qualitative agreement with a related result on the stationary structure of the domain wall in an infinite system which indeed suggests a very narrow region of inhomogeneity around the position of the domain wall defined by the location of a second particle [19]. However, our results are different not only in so far as we considered a finite system, but also in so far as did not specifically define the position of the domain wall on a microscopic scale and as we drew our conclusions not from stationary properties of the domain wall, but from its relaxational behaviour predicted by the domain wall theory. We also stress that our approach yields the exact longest relaxation time in the thermodynamic limit of the open system even though only the steady state is exactly known.

We believe that similar analysis can be carried out for generic lattice gas models of driven diffusive systems, thus circumventing the need for a (necessarily) ambiguous definition of the domain wall position. Thus one obtains the longest relaxation times from the current–density relation once the random walk dynamics of the domain wall have been determined. An open question to be addressed in future work is the marked decrease in accuracy of the theoretical and numerical relaxation times in the presence of the $(m|1)$ domain wall. Since the inhomogeneous structure of the m-segment is universal [33, 34] it is likely that strong finite-size corrections to the simple random walk picture are a generic feature of driven diffusive systems with an $(m|1)$ domain wall. The space dependence of the density profile may be a significant cause for the

observed discrepancies, but our results are too preliminary to be regarded as conclusive in this respect.

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References

[1] Spohn H 1991 *Large Scale Dynamics of Interacting Particles* (Berlin: Springer)
[2] Schmittmann B and Zia R K P 1995 Statistical mechanics of driven diffusive systems *Phase Transitions and Critical Phenomena* vol 17, ed C Domb and J Lebowitz (London: Academic)
[3] Schütz G M 2000 Exactly solvable models for many-body systems far from equilibrium *Phase Transitions and Critical Phenomena* vol 19, ed C Domb and J Lebowitz (London: Academic)
[4] Katz S, Lebowitz J L and Spohn H 1984 *J. Stat. Phys.* **34** 497
[5] Kukla V, Kornatowski J, Demuth D, Girnus I, Pfeifer H, Rees L, Schunk S, Unger K and Kärger J 1996 *Science* **272** 702
[6] MacDonald J T, Gibbs J H and Pipkin A C 1968 *Biopolymers* **6** 1
[7] Widom B, Viovy J L and Défontaines A D 1991 *J. Physique* I **1** 1759
[8] Schütz G M 1999 *Europhys. Lett.* **48** 623
[9] Chowdhury D, Santen L and Schadschneider A 2000 *Phys. Rep.* **329** 199
[10] Privman V (ed) 1997 *Nonequilibrium Statistical Mechanics in One Dimension* (Cambridge: Cambridge University Press)
[11] Liggett T M 1975 *Trans. Am. Math. Soc.* **179** 433
[12] Schütz G and Domany E 1993 *J. Stat. Phys.* **72** 277
[13] Derrida B, Evans M R, Hakim V and Pasquier V 1993 *J. Phys. A: Math. Gen.* **26** 1493
[14] Kolomeisky A B, Schütz G M, Kolomeisky E B and Straley J P 1998 *J. Phys. A: Math. Gen.* **31** 6911
[15] Popkov V and Schütz G M 1999 *Europhys. Lett.* **48** 257
[16] Lifshitz E M and Pitaevskii L P 1981 Physical kinetics *Course of Theoretical Physics* vol 10, ed L D Landau and E M Lifshitz (New York: Pergamon) section 99
[17] Ferrari P A, Kipnis C and Saada S 1991 *Ann. Prob.* **19** 226
[18] Ferrari P A 1993 Shocks in one-dimensional processes with drift *Probability and Phase Transition* ed G Grimmett (Cambridge: Cambridge University Press)
[19] Derrida B, Lebowitz J L and Speer E R 1997 Shock profiles in the asymmetric simple exclusion process in one dimension *J. Stat. Phys.* **89** 135–67
[20] Belitsky V and Schütz G M 2000 *Preprint*
[21] Jin A J and Fisher M E 1993 *Phys. Rev.* B **47** 7365
[22] Ferrari P A and Fontes L R G 1994 *Prob. Theor. Rel. Fields* **99** 305
[23] Krebs K 2000 *PhD Thesis*
[24] Gwa L-H and Spohn H 1992 *Phys. Rev.* A **46** 844
[25] Kim D 1995 *Phys. Rev.* E **52** 3512
[26] Bilstein U and Wehefritz B 1997 *J. Phys. A: Math. Gen.* **30** 4925
[27] Inami T and Konno H 1994 *J. Phys. A: Math. Gen.* **27** L913
[28] de Vega H-J and Gonzalez-Ruiz A 1994 *J. Phys. A: Math. Gen.* **27** 6129
[29] Webpage ftp://caam.rice.edu
[30] Derrida B, Evans M R and Mallick K 1995 *J. Stat. Phys.* **79** 833
[31] Rowlinson J S and Widom B 1982 *Molecular Theory of Capillarity* (Oxford: Oxford University Press)
[32] Henkel M and Schütz G 1988 *J. Phys. A: Math. Gen.* **21** 2617
[33] Krug J 1991 *Phys. Rev. Lett.* **67** 1882
[34] Oerding K and Janssen H K 1998 *Phys. Rev.* E **58** 1446