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Exact domain wall theory for deterministic TASEP with parallel update

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Abstract
We develop an exact domain wall theory (DWT) for the totally asymmetric exclusion process (TASEP) with parallel update and deterministic ($p = 1$) bulk motion. Remarkably, the dynamics of this system can be described by the motion of a domain wall not only on the coarse-grained level but also exactly on the microscopic scale for arbitrary system size. All properties of this TASEP, not only stationary but also time-dependent, are shown to follow from the solution of a bivariate master equation whose variables are not only the position but also the velocity of the domain wall. In the continuum limit this exactly soluble model then allows us to perform a first principle derivation of a Fokker–Planck equation for the position of the wall.

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Nature abounds with problems controlled by unidirectional one-dimensional transport. The transport may be in channels (as in porous materials or across cell membranes) or along rails (e.g. the cytoskeleton of biological cells). The analogy to road and pedestrian traffic has reinforced interest in such systems and spurred research aimed at uncovering common characteristics.

Several simple models have been proposed for the description of such phenomena. Among these the totally asymmetric simple exclusion process (TASEP) has become a major paradigm of out of equilibrium systems. In this model each site $1, 2, \ldots, L$ of a finite one-dimensional lattice (see figure 1) is either empty or singly occupied. Particles are injected onto site 1,
Figure 1. TASEP of sites 1, 2, ..., L. Red discs represent particles and arrows represent transition probabilities for the particles; this work studies the case $p = 1$. A particle carrying a ‘flag’ separates a low from a high density phase (see text).

may hop to the right if their target site is empty, and are removed from site $L$. The order in which these steps are performed (the ‘updating scheme’) completes the definition of a specific TASEP.

The random sequential update [1, 2] often used for the TASEP leads to large fluctuations in individual velocities. In real road or pedestrian traffic, particle motion is not subject to such large fluctuations. Sophisticated traffic models based on TASEP therefore rather use parallel update [3]. When applied to the TASEP, parallel update is defined as follows: the configuration at time $t + 1$ is obtained from the one at time $t$ by moving with probability $p$ each particle with an empty target site one step to its right; filling the leftmost site 1 with probability $\alpha$ if empty; and removing the particle on site $L$, if any, with probability $\beta$.

Exact results on TASEPs, in particular concerning their stationary states [4–6], are known for various updating schemes but require considerable mathematical sophistication. In order to obtain results that are beyond the scope of exact solutions, Kolomeisky et al [7] have applied the more general phenomenological approach of domain wall theory (DWT) to TASEP. Their implementation, to which we shall refer as simple DWT (SDWT), successfully predicts dynamical TASEP quantities when the update is random sequential [8–10] at least in a part of the phase diagram [11–13] (when $\alpha$ and $\beta$ reach some critical values the maximal current allowed by the bulk dynamics is reached in certain spatial domains and DWT fails). SDWT can be easily adapted to variants with modified kinetics [14–17] and geometries [18–21], or be used as a basis for more general discussions [22]. For other updates, however, observed discrepancies with exact [19, 23] or numerical [24, 25] results call for an adapted DWT such as proposed in [23, 26] for sublattice parallel update.

The purpose of this communication is to build a complete and exact (and not only phenomenological) DWT for the TASEP with parallel update and $p = 1$. The detailed study of this model was initiated by Tilstra and Ernst [27] before the advent of DWT. Although exact expressions have been obtained for the stationary state [6, 28] no exact dynamical solution has been exhibited up to now. Here we show that there exists a pair of domain wall variables (to be called the ‘flag position’ and the ‘flag velocity’) that satisfies an exact master equation. We then derive a DWT from first principles, which appears to contain a diffusion constant $D$ different from the one in SDWT.

1. Simple domain wall theory for the TASEP

We shall first summarize the SDWT approach. DWT approximates the system by two spatially uniform domains separated by a domain wall. On the right of the wall, the queue of particles that have been blocked at the exit constitutes a jammed phase, while on the left a free flow
domain is sustained by the entrance boundary. The domain wall, assumed to be of negligible width, is located at a position \( i \) that fluctuates with time. Let \( \rho_\pm \) be the average particle densities of the right and left domain, respectively, and \( j_\pm \) the corresponding currents, all supposed known. The first postulate of SDWT, as applied by [7] and tested by [29], is that the probability \( P_i(t) \) to find the domain wall on \( i \) at time \( t \) satisfies the master equation

\[
\frac{dP_i(t)}{dt} = D_+ P_{i-1}(t) + D_- P_{i+1}(t) - (D_+ + D_-)P_i(t)
\]

with reflecting boundary conditions at \( i = 1 \) and \( i = L \). If this equation is true at all, it should be possible to express the a priori unknown coefficients \( D_\pm \) in terms of the basic model parameters. Mass conservation constrains the value of the drift \( \delta = D_+ - D_- = \frac{j_+}{\rho_+} - \frac{j_-}{\rho_-} \). However, as rightly pointed out by Kolomeisky et al [7], an extra hypothesis concerning the current fluctuations is needed to determine the stochastic part of the motion represented by \( D \equiv (D_+ + D_-)/2 \), which in the continuum limit becomes the diffusion constant of a Fokker–Planck equation. Given that for TASEP \( j_\pm = 0 \) implies \( D_\pm = 0 \), in SDWT the values of \( \frac{j_\pm}{\rho_\pm} \) are then interpreted as arrival rates at the wall location of particles (holes) from the free flow (jammed) domain. The further assumption that these latter processes are independent leads to \( D_\pm = j_\pm / (\rho_+ - \rho_-) \), so that \( D = \frac{1}{2} \frac{j_+ + j_-}{\rho_+ - \rho_-} \). For the random sequential update, the SDWT expressions for \( D_\pm \) are supported by the fact that, for large systems, they reproduce correctly the exactly known \([4, 5]\) stationary density profile when there is no maximal current domain. Besides, in the case of random sequential update many TASEP properties, both dynamical and stationary, are reproduced accurately by SDWT [7, 29]. However, as mentioned, SDWT is not appropriate for updates with low fluctuations, and we shall now derive a complete DWT in the case of the deterministic parallel update. In contrast to SDWT, this derivation is exact and thus no postulates are needed.

2. The flag: definition and dynamics

The \( p = 1 \) TASEP with parallel update has completely deterministic bulk dynamics allowing a maximal current equal to 1; only the entrance and exit processes are stochastic. Then the maximal current phase is reduced to the point \( \alpha = \beta = 1 \) and the DWT is expected to work everywhere else in the phase diagram. Two domains may coexist in this model, a free flow domain on the left and a jammed domain on the right. In the free flow domain particles enter randomly at the left and advance at unit velocity; two successive particles are separated by at least one hole. The site occupation probabilities \( \rho_i(t) \) then satisfy simple recursion relations in space: if \( i \) is occupied, \( i - 1 \) is empty; and if \( i \) is empty, \( i - 1 \) is occupied with probability \( \alpha \). This can be simply written

\[
\rho_{i-1}(t) = \alpha(1 - \rho_i(t)) \tag{2}
\]

The jammed domain has a symmetrical structure obtained by exchanging particles and holes, \( \alpha \) and \( \beta \), and right and left. The domains have [30]

\[
j_- = \rho_- = \frac{\alpha}{1 + \alpha}, \quad j_+ = \beta \rho_+ = \frac{\beta}{1 + \beta} \tag{3}
\]

For \( \alpha < \beta \) the free flow domain invades the bulk and the system is said to be in the free flow phase, while, symmetrically, for \( \alpha > \beta \) the jammed domain invades the bulk and the system is in the jammed phase. The critical line is \( \alpha = \beta \).

We introduce a marker that will turn out to play the role of a domain wall. We say that the leftmost particle ever to have been blocked carries a flag similar to the shock marker introduced in [31]. If no particle in the system has ever been blocked, the flag occupies by convention a virtual site \( L + 1 \). A typical configuration is depicted in figure 1. A consequence of choosing
deterministic bulk dynamics is that a particle can get blocked only if its predecessor has been blocked, so that by induction all particles to the right of the flag have also undergone blocking. Since no particle to the left of the flag has ever been blocked, the flag motion traces out the boundary between two qualitatively different domains, namely the free flow domain, whose particles have never been blocked, and the jammed domain, whose particles have already been blocked at least once.

The flag definition given in this paper, which is with respect to the particles, breaks the particle–hole symmetry. A similar flag could be defined with respect to the holes and a symmetric description would consider the joint distribution of two flag variables. However, we will show that it is possible to write closed equations involving only one flag.

With random sequential update shock profiles have traditionally been studied by introducing second-class particles \([32]\). A second-class particle (noted 2) may exchange its position with an ordinary particle (1) located on its left \((12 \rightarrow 21)\) or with a hole (0) located on its right \((20 \rightarrow 02)\). As a result, a second-class particle remains loosely coupled to the shock position. With parallel update the rule of motion of such a particle is not unique: one must choose what the motion of the second-class particle will be in the configuration 120. In the limit case where in this configuration the second-class particle always hops to the right (to the left), its dynamics becomes equivalent to the dynamics of the flag of the particles (of the holes) in the bulk. We will see that our definition of the flag provides a consistent set of boundary conditions for the second-class particle.

We are now interested in the time evolution of the probability distribution \(P_i(t)\) of the flag position. At each time step the flag may execute hops \(i \rightarrow i, i \pm 1\) according to the rules below. When the flag carrying particle blocks the forward move of a particle to its left, the flag is transferred to this latter particle, that is, hops one lattice distance to the left. In the other cases the flag remains attached to its carrier particle which may either hop forward or stay on the same site. It can be seen that the random motion of the flag has a memory of one time step.

Indeed, let us define \(P^a_i(t)\) for \(a = 0, \pm 1\) as the probability that at time \(t\) the flag is on site \(i\) and has arrived there by a move of \(0, \pm 1\) lattice units in the preceding time step, respectively (for lighter notation we shall omit the 1 in the superscript). Hence \(a\) may be interpreted as the flag velocity between \(i - 1\) and \(i\).

Conditional on the flag having arrived at site \(i\) with velocity \(a\) we know the following. Site \(i\) is occupied by a particle for sure and \(i + 1\) is occupied with probability \(1 - \beta\). For \(a = +1\), site \(i - 1\) is empty and for \(a = 0\) or \(a = -1\), it is occupied with probability \(\alpha\). This knowledge determines the probabilities for what will happen at the next time step. We set \(P^a_i(t) = 0\) and \(P^0_i(t) \equiv 0\). We have to find first the equations for the three values of \(a\) separately and then notice that, quite remarkably, the cases \(a = 0\) and \(a = -1\) can be taken together by introducing

\[
P^{-1}_i(t) = P^{-0}_i(t) + P^{0}_i(t)\]

for \(1 \leq i \leq L + 1\). The equations for \(P^{-0}\) and \(P^{+}\) then read

\[
P_{i}^{-0}(t + 1) = \alpha P_{i+1}^{-0}(t) + (1 - \alpha) \beta P_{i-1}^{-0}(t) + (1 - \beta) P_{i}^{+}(t),
\]

\[
P_{i}^{+}(t + 1) = (1 - \alpha) \beta P_{i-1}^{-0}(t) + \beta P_{i}^{+}(t),
\]

for \(2 \leq i \leq L - 1\) and \(3 \leq i \leq L\), respectively. Near the left boundary we have the two special equations

\[
P_{1}^{-0}(t + 1) = \alpha P_{2}^{-0}(t) + (1 - \beta) P_{1}^{-0}(t),
\]

\[
P_{1}^{+}(t + 1) = \beta P_{1}^{-0}(t).
\]

The right boundary requires more attention. If the flag has just arrived on site \(L + 1\) (i.e. has \(a = 1\)), then site \(L\) is occupied with probability \(r_0 = 0\). But if the flag stays on \(L + 1\) (has \(a = 0\)), this probability evolves with each time step. Let \(r_{i}\) be the occupation probability of
site $L$ after the flag has stayed on $L + 1$ for $u$ time steps. The $r_u$ can be calculated from an elementary recursion in $u$. Indeed, let $p^0_u$ and $p^L_u$ be the probability that the flag has stayed on $L + 1$ for $u$ time steps and that site $L$ is occupied or empty, respectively. When the flag is on $L + 1$ the free flow domain takes over the whole system so that we have

$$p^0_{u+1} = \alpha p^L_u,$$

$$p^L_{u+1} = \beta p^0_u + (1 - \alpha)p^L_u$$

with the initial condition $p^0_0 = 1 - p^L_0 = \alpha$. After the recurrence (6) is solved, $r_u$ may be calculated using $r_u = p^0_u / (p^0_u + p^L_u)$.

In order to accommodate this memory effect at the right boundary into a Markovian description, we write $P^{−0}_{L+1, u}(t) = \sum_{u=1}^{\infty} P^{−0}_{L+1, u}(t)$ in which $P^{−0}_{L+1, u}(t)$ takes into account the time $u$ the flag has spent on site $L + 1$ since its latest arrival there. The special evolution equations near the right boundary then read

$$P^{−0}_{L, t + 1} = \sum_{u=1}^{\infty} (1 - \beta)r_u P^{−0}_{L+1, u}(t) + (1 - \alpha)(1 - \beta)P^{−0}_{L}(t) + (1 - \beta)P^{+}_{L}(t),$$

$$P^{−0}_{L+1, t + 1} = P^{+}_{L+1, t}.$$  

$$P^{−0}_{L+1, u}(t + 1) = (1 - (1 - \beta)r_u)P^{−0}_{L+1, u-1}(t), \quad u \geq 2.$$  

The closed system of equations (4)–(7), valid for all $L \geq 2$ constitutes the master equation of our ‘flag theory’. The total probability $\sum_{L=1}^{L+1} \sum_{u=0, \pm} P^{\pm}_{t}(t)$ can of course be checked to be conserved.

The stationary state solution of equations (4)–(7) reads

$$P^{+, \text{stat}}_{1} = 0$$

$$P^{−0, \text{stat}}_{i} = \beta^{-1} P^{+, \text{stat}}_{i+1} = \frac{1}{Z} \left( \frac{\beta}{\alpha} \right)^{i-1}, \quad 1 \leq i \leq L$$

$$P^{−0, \text{stat}}_{L+1} = \frac{1 + \alpha \beta}{Z} \left( \frac{\beta}{\alpha} \right)^{L}$$

$$P^{−0, \text{stat}}_{L+1, u} = \frac{\prod_{j=1}^{u} (1 - (1 - \beta)r_j)}{\sum_{u'=1}^{\infty} \prod_{j=1}^{u'-1} (1 - (1 - \beta)r_j)} P^{−0, \text{stat}}_{L+1, u-1},$$

where $Z$ is the normalization constant ensuring that $\sum_{i=1}^{L+1} \sum_{u=0, \pm} P^{\pm, \text{stat}}_{i} = 1$. It shows that the probability $P^{\pm, \text{stat}}_{i}$ is concentrated near the left (the right) boundary when $\alpha > \beta$ (when $\alpha < \beta$), within a penetration depth $\xi = |\log(\beta/\alpha)|^{-1}$, in agreement with the findings of [27]. The stationary probability distribution $P^{\pm, \text{stat}}_{i}$ is plotted in figure 2. In contrast to the wall in SDWT theory, here the flag has a microscopic definition, and thus $P^{\pm, \text{stat}}_{i}$ can be directly measured in Monte Carlo simulations. The agreement with our exact theory is excellent as expected.

### 3. Density profile

Now we wish to calculate the density profile. Let $\rho^{\pm}_{i,j}$ (with $1 \leq i, j \leq L$) be the expected particle density on site $j$ conditionally on the flag being at $i$ with velocity $a$. In SDWT theory this profile would be assumed to be a step function. However here one can compute exactly the corrections to the step profile. We anticipate that this ‘flag-dependent profile’ (FDP) depends only on the difference $j - i \equiv k$. The $\rho^{\pm}_{i,k}$ follow from the appropriate recursion relation in space (the ones for the free flow and the jammed phase for $k < 0$ and $k > 0$, respectively); the knowledge of the flag velocity $a$ at site $i$ provides the starting values. For example the $k < 0$ part of $\rho^{0}_{k,0}$ may be calculated by noting that the site to the left of the flag is a site of the free
Figure 2. Stationary probability distribution of the position of the flag \( P_{\text{stat}} \) for \( \alpha = 0.5 \) and varying \( \beta \) in a system of size \( L = 40 \). Lines are the analytical predictions from equations (4)–(7) and empty circles are the result of Monte Carlo simulations. The distribution is exponential apart from particular values on the two extremal sites. For \( \beta < \alpha \) the wall is most likely located near the entrance and the jammed domain invades the bulk while for \( \beta > \alpha \) the situation is reversed. In the critical case \( \alpha = \beta \) the probability distribution is flat.

Figure 3. Flag dependent density profile \( \rho_{-0} \) for \( \alpha = 0.60 \) and \( \beta = 0.75 \). The flag is located at \( k = 0 \). For \( k \to \pm \infty \) the density tends to the bulk values \( \rho_{\pm} \) as \( \sim (-\alpha)^{|k|} \) on the left and as \( \sim (-\beta)^{k} \) on the right. Dotted lines are guides to the eye.

flow domain with a particle on its right, which gives \( \rho_{-1} = \alpha \). The recurrence relation (2) then yields

\[
\rho_{k} = \frac{1 - (-\alpha)^{|k|}}{1 + \alpha}, \quad k < 0.
\] (9)

The value of \( \rho_{k \geq 0} \) may be calculated analogously to give the whole function shown in figure 3. For \( i = L + 1 \) the special \( u \)-dependent FDPs \( \rho_{-0}^{a_{i,u}} \) may be calculated similarly.

The time-independent profiles \( \rho^{a_{j}} \) are attached to the frame of reference of the moving flag. The time-dependent density \( \rho_{j}(t) \) at site \( j \) is the average of \( \rho_{j-1}^{a_{j-1}} \) with respect to the distributions \( P_{i}^{a}(t) \)

\[
\rho_{j}(t) = \sum_{i=1}^{L} \sum_{a=-0,+} \rho_{j-1}^{a_{j-1}} P_{i}^{a}(t) + \rho_{j-(L+1)}^{a_{j-(L+1)}} P_{L+1}^{a}(t) + \sum_{u=1}^{\infty} \rho_{j-(L+1),a}^{a_{j-(L+1),a}} P_{L+1,0}^{a}(t).
\] (10)
Figure 4. (a) Stationary density profile for $L = 5$, $\alpha = 0.2$ and $\beta = 0.8$. Open blue diamonds: SDWT. Black crosses and open red squares: Monte Carlo simulation and the flag theory of this work (equation (11)), respectively. Lines are guides to the eye.

(b) Stationary density profile in the scaling limit for $\beta = 0.5$ and $\epsilon = 1$. Blue dotted line: SDWT. It is distinctly different from the red dashed line, obtained from equation (17) and representing the flag theory of this work. Continuous lines: Monte Carlo simulations for different lengths $L$ converging to the flag theory prediction.

Figure 4(a) shows that our Monte Carlo results for the stationary state, even for a small system, $L = 5$, are in excellent agreement with the flag theory, as expected of an exact theory. In the stationary case we recover the already known result of equation (7) in [6] by combining equations (8), (10) and the expressions of the $\rho^a_k$, $\rho_{stat}^j = (1 - \beta)\alpha L + 1 - \alpha (1 - \alpha)\beta L + 1 - (1 - \alpha)(1 - \beta)\alpha L + 1 - \beta(\beta L - 1)$. (11)

4. Scaling limit

We now scale the lattice coordinate as $x = i/L$ and consider the limit $L \to \infty$, adopting the notation $P^0(t) \equiv L^{-1}P^a(x, t)$. For $\alpha, \beta < 1$ the FDPs then become step functions as in SDWT. We will show that, in the large $L$ limit, it is possible to extract from (4)–(7) an equation for the position distribution of the flag $P = P^0 - P^+ + P^-$ alone. We introduce the shorthand notation $Q \equiv (1 - \beta)P^+ - \beta(1 - \alpha)P^-$, $\Delta_1 A(t) \equiv A(t + 1) - A(t)$ for any quantity $A$, and $\delta \equiv \frac{\beta - \alpha}{1 - \alpha \beta}$. We also define

$$D_1 \equiv \frac{\alpha + \beta - 2\alpha \beta}{2(1 - \alpha \beta)}.$$ (12)

When Taylor expanding all quantities in equations (4) around $x = i/L$ we find

$$\Delta_1 P = -\frac{\delta}{L} \frac{dP}{dx} + D_1 \frac{d^2 P}{dx^2} - \frac{(1 + \beta)\alpha}{L} \frac{dQ}{dx} - \frac{(1 - \beta)\alpha}{2L^2} \frac{d^2 Q}{dx^2} + O(L^{-3}).$$ (13a)

$$\Delta_1 Q = -(1 - \alpha \beta)Q - \frac{\beta(1 - \alpha^2)}{L(1 - \alpha \beta)} \frac{dP}{dx} + \frac{\alpha \beta(\beta - \alpha)}{L(1 - \alpha \beta)} \frac{dQ}{dx} + O(L^{-2}).$$ (13b)

We may solve equation (13b) for $Q$ in terms of $P$. The term $-(1 - \alpha \beta)Q$ in this equation causes $Q$ to decay to values $\sim L^{-2}$ on a time scale $\sim L^0$ (which was the reason for defining $Q$ as we did) and hence, on time scales $\gg L^0$,

$$Q = -\frac{\beta(1 - \beta)(1 - \alpha^2)}{L(1 - \alpha \beta)} \frac{dP}{dx} + O(L^{-2}).$$ (14)
Substituting equation (14) in equation (13a) gives
\[ \Delta_t \mathcal{P} = -\frac{\delta \mathcal{P}}{\mathcal{Q}} + \frac{D}{L} \frac{\partial^2 \mathcal{P}}{\partial x^2} + O(L^{-3}), \]
(15)
in which the diffusion constant is given by \( D \equiv D_1 + D_2 \) where \( D_1 \) is given by (12) and \( D_2 \) stems from \( \mathcal{Q} \),
\[ D_2 \equiv \frac{\alpha \beta (1 - \alpha^2)(1 - \beta^2)}{(1 - \alpha \beta)^3}. \]
(16)
Note that the constant \( D \) given above differs from the one found by Belitsky et al [31], which actually applies to a particular type of shock. Our exact expression (12),(16) for \( D \) disagrees with that of SDWT and also with equation (56) from [23], conjectured on the basis of an exact calculation.

Whereas equation (15) is valid for arbitrary \( \alpha, \beta \), it is of interest near the phase transition line \( \alpha = \beta \) to investigate the scaling limit \( L \to \infty \) with \( \beta - \alpha = c/L \) and the constant \( c \) fixed. Repeating the calculation with \( \tau \equiv t L^{-2} \) we find that in this limit \( D = (1 - \beta^2)^{-1} \) while SDWT would have given \( D = \beta(1 - \beta)^{-1} \). \( \mathcal{P} \) satisfies the Fokker–Planck equation
\[ \partial_\tau \mathcal{P} = (1 - \beta^2)^{-1} (-c \partial_x \mathcal{P} + \beta \partial_x^2 \mathcal{P}). \]
(17)
The boundary conditions associated with equation (17) may be derived from equations (5) and (7) by a calculation similar to that of [33] (section 5). On the time scale \( \tau \) the memory effect at \( i = L + 1 \) collapses and we obtain at both ends of the interval standard zero current boundary conditions. Figure 4(b) shows that the profile obtained by Monte Carlo simulation of a size \( L \) system indeed converges in the scaling limit toward the stationary distribution of equation (17).

This work arose from the need to extend the DWT beyond random sequential update. Here, in the context of the \( \rho = 1 \) TASEP with parallel update, we developed a full DWT which, in contrast to the SDWT, is exact even at the microscopic scale and for systems of any finite size. Indeed, the dynamics of this model can be reduced to a Markov process more complicated than that of SDWT and involving the position and speed of a ‘flag’. In the continuum limit a Fokker–Planck equation results, but with a diffusion constant different from that of SDWT and in agreement with Monte Carlo simulations. The diffusion constant that we have obtained can now be used to predict various dynamical properties of the system.

In contrast with many exact solutions available in the literature, ours is valid not only in the stationary state but also for nonstationary time evolutions. The exact calculation of this work rests on the deterministic character of the dynamics, and could probably be extended to other deterministic updates such as frozen shuffle update [24]. The main merit of our result is however to exist as a landmark in the field of exact solutions that may guide the development of approximate domain wall theories.

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**References**

