Facilitated Asymmetric Exclusion

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We introduce a class of facilitated asymmetric exclusion processes in which particles are pushed by neighbors from behind. For the simplest version in which a particle can hop to its vacant right neighbor only if its left neighbor is occupied, we determine the steady-state current and the distribution of cluster sizes on a ring. We show that an initial density downstep develops into a rarefaction wave that can have a jump discontinuity at the leading edge, while an upstep results in a shock wave. This unexpected rarefaction wave discontinuity occurs generally for facilitated exclusion processes.

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In the asymmetric exclusion process (ASEP), sites of a lattice are occupied by single particles, each of which can hop at a fixed rate to a neighboring vacant site on the right [1–5]. This versatile model describes many systems, including traffic [6–9], ionic conductors [10], and RNA transcription [11,12]. Despite its simplicity, the properties of the ASEP are rich and deep. For example, a density that increases with x leads to a propagating shock wave, similar to a traffic jam that propagates along a congested road. Conversely, when the initial density drops quickly as a function of x, a rarefaction wave arises in which the drop gradually smooths out, as occurs in stopped traffic after a stoplight turns green. Macroscopic aspects of these phenomena can be understood from hydrodynamic theories [13,14], while the fluctuations about these macrostates continue to be actively investigated [15–19].

In this work, we investigate facilitated asymmetric exclusion. We primarily focus on occupancy facilitation in which a particle can hop to its vacant right neighbor only if its left neighbor is also occupied (Fig. 1). This model was proposed by Basu and Mohanty [20] in the context of nonequilibrium absorbing state phase transitions. We also investigate distance facilitation in which the rate at which a particle hops to a vacant right site is a decreasing function of the distance between a particle and its closest left neighbor.

The notion of facilitated exclusion is part of a general class of ASEP models in which the hopping rate of a particle depends on more than just the occupancy of the neighboring site [6–8,20,21]. For example, in glassy dynamics the particle mobility decreases as the local density increases [22]. Conversely, the presence of nearby particles may increase hopping rates; for example, in molecular motor models a moving particle can exert a hydrodynamic force that pushes other particles along [23]. Moreover, a subset of phase space in occupancy facilitated exclusion can be mapped onto the ASEP of extended objects [11,12,21,24–26], a model that was formulated to mimic the traffic of ribosomes along RNA.

In occupancy facilitation, a mean-field hypothesis for the current is $J = \rho^2(1-\rho)$; the expression accounts for the presence of two particles and one vacancy and represents a natural generalization of the current $J = \rho(1-\rho)$ in the ASEP. As we show below, the current in facilitated exclusion actually has a very different density dependence. We also develop a hydrodynamic description for an initial density step and predict that a rarefaction wave develops a discontinuity at the leading edge. Finally, we provide a general criterion to understand this unexpected phenomenon in the framework of distance facilitation.

Finite ring.—We first determine the density dependence of the current on a finite ring in occupancy facilitation. The key to understanding the steady-state spatial distribution of particles is the notion of islands. An island is a string of occupied sites that are delimited at both ends by vacant sites (Fig. 1). Each hopping event transforms a triplet $\bullet\bullet\circ$ into $\bullet\circ\bullet$. Depending on the occupancy of the next site, the number of islands either increases, $\bullet\bullet\circ\circ \to \bullet\circ\bullet\circ$, or remains the same, $\bullet\bullet\circ\bullet \to \bullet\circ\bullet\bullet$, but cannot decrease. Thus the system eventually reaches a state where the number of islands is maximal.

For $\rho \le \frac{1}{2}$, the constraint that the number of islands can never decrease ensures that the system eventually reaches a static state that consists of immobile single-particle islands. The approach to the final state has a rich time dependence [27], particularly in the marginal case $\rho = \frac{1}{2}$, where the number of active particles asymptotically decays as $t^{-1/2}$ (see also Refs. [28–30]).

In the $\rho > \frac{1}{2}$ steady state, the requirement that the number of islands is maximal ensures that adjacent vacancies must be separated by at least one particle. Furthermore,

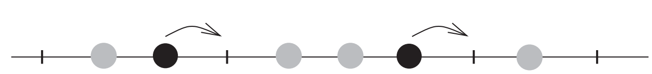

FIG. 1. Illustration of occupancy facilitated asymmetric exclusion. Particles that are eligible to hop to the right are dark, while immobile particles are shaded. This configuration contains islands of lengths 2, 3, and 1 (left to right).

configurations that contain the maximal number of islands are equiprobable. Indeed, let $P(C)$ be the steady-state probability of being in a maximal-island configuration C. Then the stationarity condition is

$$P(C)\sum_{C'}R(C\to C') = \sum_{C'}P(C')R(C'\to C), \tag{1}$$

where $R(C\to C')$ is the evolution rate from configuration C to C'. Since $R=1$ if an evolution step is allowed and 0 otherwise, we need to count the number of ways into and out of a configuration to solve Eq. (1).

The evolution out of a configuration is triggered by triplets of the form $\bullet\bullet\circ$ at the right edge of any island of length ≥ 2. The system can evolve into the configuration C from another maximal-island configuration by the process $\bullet\bullet\circ\bullet\to\bullet\circ\bullet\bullet$. This evolution can only happen at the left edge of an island of length ≥ 2. Hence there is an equal number of terms on both sides of Eq. (1). If $P(C)$ are equal for all configurations, Eq. (1) is clearly satisfied. Thus, all maximum-island configurations are equiprobable in the steady state.

The probability of a maximum-island configuration therefore equals $\mathcal{C}^{-1}$, where $\mathcal{C}$ is the total number of such configurations with N particles and V vacancies on a ring of $L=N+V$ sites. To determine $\mathcal{C}$, consider an arbitrary site that we label by i. If this site is occupied, there are N possible locations between the N particles to put the V vacancies (Fig. 2). If site i is unoccupied, there are $N-1$ possible places to put the remaining $V-1$ vacancies. In both cases, we cannot put more than one vacancy between consecutive particles or else the number of islands would not be maximal. The number of such configurations is therefore given by

$$\mathcal{C} = \binom{N}{V} + \binom{N-1}{V-1}. \tag{2}$$

To obtain the steady-state current, consider the flow across a link between arbitrary adjacent sites i and $i+1$. For a particle to move across this link, the consecutive sites $i-1$ and i must be occupied, while site $i+1$ must be vacant. We now enumerate the number of maximum-island configurations that are consistent with the presence of this triplet by noting that there are $N-2$ places between the remaining particles to place the $V-1$ remaining vacancies so that no two vacancies are adjacent. Thus the number of allowed configurations consistent with the presence of this triplet is $\binom{N-2}{V-1}$. The current across link $(i, i+1)$ is therefore (see Fig. 3)

$$J = \frac{\binom{N-2}{V-1}}{\mathcal{C}} \to \frac{(1-\rho)(2\rho-1)}{\rho}, \tag{3}$$

with $\rho=\frac{N}{L}$ held constant in the limit N, $L\to\infty$. (This result can be mapped into an equivalent expression for the current in the ASEP of extended objects [11,12,21,24–26]; we return to this correspondence below.) The current is zero at $\rho=\frac{1}{2}$, since the system eventually reaches the static state of alternating particles and vacancies. The current is also zero at $\rho=1$, where no evolution is possible. The maximal current arises when $\rho^*=\frac{1}{\sqrt{2}}$, where $J(\rho^*)\equiv J_{\max}=3-2\sqrt{2}\approx 0.1716$.

We can also determine I_n, the density of islands of length n. Using the same enumeration that gave the number of allowed configurations, there are $V-2$ remaining vacancies that can be distributed among the $N-n-1$ places between the rest of the particles so that there are no consecutive vacant sites. There are $\binom{N-n-1}{V-2}$ such configurations. Since each configuration has equal weight, the density of islands of length n is

$$I_n = \frac{\binom{N-n-1}{V-2}}{\binom{N}{V}+\binom{N-1}{V-1}} \to \frac{(1-\rho)^2}{\rho}\left(\frac{2\rho-1}{\rho}\right)^{n-1}, \tag{4}$$

where the latter equality applies for $n \ll L$; both Eqs. (3) and (4) were also derived in Refs. [20,21] by independent methods. The island length distribution decays as λ^n, with $\lambda=(2\rho-1)/\rho$, rather than $\lambda=\rho$ which occurs for a random particle distribution. Since $(2\rho-1)/\rho<\rho$, long islands are suppressed compared to a random distribution; this feature is a consequence of the constraint that the number of islands is maximal. From these island probabilities we recover the particle density from $\rho=\sum nI_n$, while the current J can alternatively be expressed as the probability to have an island that contains at least two particles, $J=\sum_{n\geq 2}I_n$.

Density step.—Let us now study the evolution of a density step on the infinite line by occupancy facilitation. Initially, the density to the left of the origin is ρ_-, while the density to the right is ρ_+. For a downstep, where $\rho_->\rho_+$, the density profile within a hydrodynamic description evolves by the continuity equation $\frac{\partial\rho}{\partial t}+\frac{\partial J}{\partial x}=0$, which we may solve by the method of characteristics [13]. The solution is a function of a scaled variable, $z\equiv x/t$, so $\rho(x,t)=f(z)$. Using the steady-state current expression (3) for the flux, we find that the scaled profile is composed of distinct segments in which the density is either constant or given by $f=(2+z)^{-1/2}$. Thus the density profile is

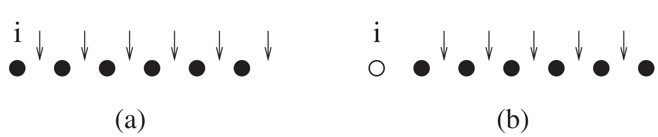

FIG. 2. Illustration of the number of places that V vacancies can be placed among N particles (filled circles) with site i (a) occupied or (b) vacant.

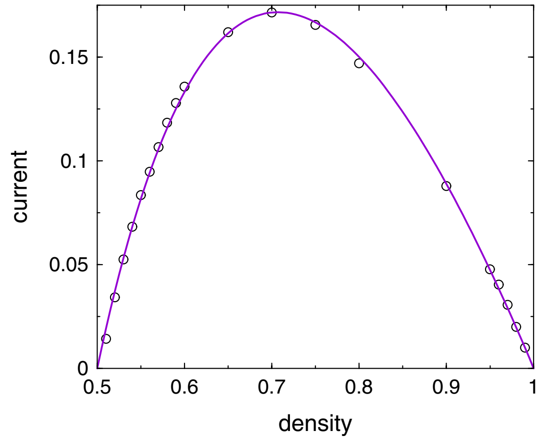

FIG. 3 (color online). Current versus density for occupancy facilitation. The smooth curve is the prediction (3), while the circles are simulation data from 10^4 realizations on a ring of 10^5 sites.

$$f = \begin{cases} \rho_- & z < z_- \\ (2+z)^{-1/2} & z_- < z < z_+ \\ \rho_+ & z > z_+. \end{cases} \tag{5}$$

The position of the left interface z_- is determined from continuity: $(2+z_-)^{-1/2} = \rho_-$. When $\rho_- > \rho^* = \frac{1}{\sqrt{2}}$, we have $z_- < 0$. In this situation, the density at the origin $\rho(0)$ is universal and it coincides with the density ρ^* that maximizes the current in Eq. (3). Therefore, the number of particles that penetrates into the region $x > 0$ is $N(t) = J[\rho(0)]t = J_{\max}t$.

To determine the location of the right interface z_+, we apply the constraint that the initial mass within $[z_-, z_+]$ must equal the mass in this region at some later time plus the net influx into this region. In scaled units, this conservation statement is

$$-\rho_- z_- + \rho_+ z_+ = \int_{z_-}^{z_+} \frac{dz}{\sqrt{2+z}} + J_- - J_+, \tag{6}$$

with $J_\pm = J(\rho_\pm)$.

Different density profiles arise depending on whether $\rho_+ < \frac{1}{2}$ or $\rho_+ > \frac{1}{2}$. In the former case the right interface is located at $z_+ = [2 - 3\rho_+ - 2\sqrt{(1-\rho_+)(1-2\rho_+)}]/\rho_+^2$. As z passes through z_+ the density jumps from the value $(2+z_+)^{-1/2}$ to ρ_+. For example, when $(\rho_-, \rho_+) = (1, 0)$, $z_+ = \frac{1}{4}$ and the magnitude of the density drop is $\frac{2}{3}$ (Fig. 4). The discontinuity at the front of a rarefaction wave arises because the leading particle cannot move unless "pushed" by neighboring particles from behind. Consequently, the density at the leading edge must be nonzero.

For $\rho_+ \geq \frac{1}{2}$, this jump discontinuity disappears, and the density profile is everywhere continuous. Continuity at $z = z_+$ now gives $\rho_+ = (2+z_+)^{-1/2}$, which manifestly solves Eq. (6). For this class of rarefaction waves, the density is sufficiently large ahead of the wave that the leading edge can get pulled ahead, and there is no need for a pileup of particles from behind to push the wave front forward.

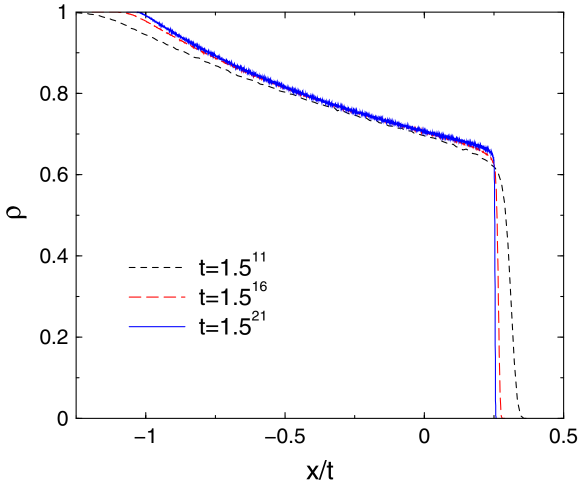

FIG. 4 (color online). Scaled density profile of facilitated exclusion starting from the step initial condition $\rho_- = 1$ and $\rho_+ = 0$. The simulation data are based on 10^5 realizations for three representative times and are visibly indistinguishable from the prediction of Eq. (5) when $t = 1.5^{21}$.

To study shock waves, we suppose that $\frac{1}{2} < \rho_- < \rho_+$ and consider a large region that includes the interface. The particle influx to this region is J_-, while the outflux is J_+. The net flux must equal the change in mass $c(\rho_- - \rho_+)$ inside this region, where c is the shock wave speed. Hence $c = (J_- - J_+)/(\rho_- - \rho_+)$. Using the expression (3) for the current, the shock wave speed is

$$c = (\rho_- \rho_+)^{-1} - 2. \tag{7}$$

The shock propagates to the right if $\rho_- < (2\rho_+)^{-1}$ and to the left otherwise.

Our results can be extended to a more stringent occupancy facilitation in which r consecutive sites to the left of a particle must be occupied for a particle to hop to a vacant right neighbor [20,27]. (For example, for $r = 3$ the rightmost particle in $\circ \bullet \bullet \bullet \circ$ cannot move, while the update $\bullet \bullet \bullet \bullet \circ \to \bullet \bullet \bullet \circ \bullet$ is possible.) A steady state with a nonvanishing current and a maximal number of islands, each of length $\geq r$, arises when $\rho > \frac{r}{1+r}$. All such configurations are again equiprobable.

We now discuss the connection between occupancy facilitation and the ASEP of extended objects [11,12,21,24–26]. In the maximal-island steady-state regime with density $\rho \geq \frac{1}{2}$, we may equivalently view a particle followed by a vacancy as an extended object of length $k = 2$ which hops to the left. Since vacancies cannot be adjacent in the steady state, these extended objects obey exclusion and perform a simple ASEP (Fig. 5). This connection continues to hold with the more stringent r-tuple occupancy facilitation. In the region of phase space where

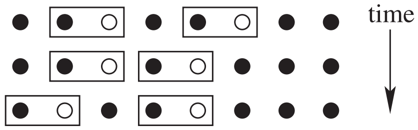

FIG. 5. Equivalence between occupancy facilitated exclusion for the case $r = 1$ and the ASEP of dimers (rectangles) that hop to the left.

$\rho \geq \frac{r}{r+1}$, the steady-state behavior of the system maps to the ASEP of extended objects with length $k = 1 + r$.

Finally, we treat distance facilitation. Finding the current even for the simple example in which the hopping rate equals ℓ^{-1}, where ℓ is the distance to the nearest left particle, is challenging. The hydrodynamic behavior, however, is robust, and the rarefaction wave discontinuity always arises [27]. We can demonstrate the universality of this phenomenon from basic features of the current-density relation. We know that $J(0) = J(1) = 0$, and we expect that $J(\rho)$ has a single maximum at some density ρ^*. Applying the scaling ansatz for the continuity equation shows that either ρ is constant or $\frac{dJ}{d\rho} = z$. The rarefaction wave therefore has the form

$$\rho(z) = \begin{cases} \rho_- & z < z_- \\ I(z) & z_- < z < z_+ \\ \rho_+ & z > z_+, \end{cases}$$

where $I(z)$ is the inverse function of $z = \frac{dJ}{d\rho}$. Differentiating this relation with respect to z in the region $z_- < z < z_+$ gives $J_{\rho\rho}\rho_z = 1$. If $J_{\rho\rho}$ is everywhere negative (as in the standard ASEP), then ρ_z must also be negative. Thus the density $\rho(z)$ continuously decreases until it reaches ρ_+. However, if $J_{\rho\rho}$ is positive at some low density, then ρ_z would become positive. Thus the smallest possible density $\rho_{\min}$ in a rarefaction wave occurs at the point where $J_{\rho\rho}$ vanishes. If $\rho_{\min} > \rho_+$, there must be a jump discontinuity at the leading edge.

Thus an inflection point in the current-density relation signals a rarefaction wave discontinuity. Such an inflection point must exist for any facilitation mechanism, since $J_{\rho\rho}(\rho^*) < 0$ at the maximum ρ^* and $J_{\rho\rho} > 0$ for small ρ. One example of such a current-density relation is $J \sim \rho^{\alpha+1}$ as $\rho \to 0$ that arises for distance facilitation with hopping rate $\ell^{-\alpha}$.

In summary, facilitated asymmetric exclusion has features that are dramatically different from simple asymmetric exclusion. The most prominent is the jump discontinuity at the leading edge of rarefaction waves. This phenomenon arises in a broad class of cooperative transport models with facilitated dynamics.

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