Single-bottleneck approximation for driven lattice gases with disorder and open boundary conditions

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Abstract. We investigate the effects of disorder on driven lattice gases with open boundaries using the totally asymmetric simple exclusion process as a paradigmatic example. Disorder is realized by randomly distributed defect sites with reduced hopping rate. In contrast to equilibrium, even macroscopic quantities in disordered non-equilibrium systems depend sensitively on the defect sample. We study the current as a function of the entry and exit rates and the realization of disorder and find that it is, in leading order, determined by the longest stretch of consecutive defect sites (single-bottleneck approximation, SBA). Using results from extreme value statistics the SBA allows us to study ensembles with fixed defect density which gives accurate results, e.g. for the expectation value of the current. Corrections to SBA come from effective interactions of bottlenecks close to the longest one. Defects close to the boundaries can be described by effective boundary rates and lead to shifts of the phase transitions. Finally it is shown that the SBA also works for more complex models. As an example we discuss a model with internal states that has been proposed to describe transport of the kinesin KIF1A.

Keywords: driven diffusive systems (theory), phase diagrams (theory), stationary states, disordered systems (theory), defects (theory)
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1. Introduction

Driven diffusive systems play an important role in non-equilibrium statistical physics [1, 2]. Due to broken detailed balance they allow us to investigate non-equilibrium effects. In addition, they serve as models for various transport processes ranging from vehicular traffic [3, 4] to biological transport by motor proteins [5]–[7]. The paradigmatic model is the totally asymmetric simple exclusion process (TASEP) which was first introduced to describe protein polymerization in ribosomes [8]. It was solved exactly [9, 10] which allows us to study generic properties like the phase diagram and boundary-induced phase transitions [11] that also occur in more complex driven systems without resorting to approximations or simulations.

In contrast to the homogeneous case, much less is known for the TASEP with inhomogeneous hopping rates, i.e. disorder. Here in principle one has to distinguish particle-dependent and site-dependent hopping rates. The former case is simpler since it can be mapped onto an exactly solvable zero-range process [12]–[15]. Therefore, at least for periodic boundary conditions, this case is well understood. In contrast, in the latter case exact results are known only for a single defect in an otherwise deterministic system with sublattice-parallel dynamics [18]–[20]. For the general case, several numerical and (approximate) analytical investigations [21]–[24] have revealed interesting behaviour already for single defects and periodic boundary conditions. However, far less is known for finite defect densities or open boundary and, especially, a combination of both.

Apart from the fundamental theoretical interest in disorder effects in non-equilibrium systems, which are far from being well understood [25], these are also of direct relevance for applications. Typical examples are found in intracellular transport processes where

For further investigations of disordered zero-range processes, see, e.g., [16, 17] and references in the review [15].

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molecular motors often move along heterogeneous tracks like DNA or mRNA (see, e.g., [26]).

In this work we consider systems with binary disorder, i.e. with transition rates that can take two possible values that are randomly assigned to the sites. Sites with a lower transition rate are called defect sites (or slow sites due to their influence on the average velocity), while those with the higher transition rate are non-defect sites.

For periodic boundary conditions the influence of single defect sites has been clarified by Janowsky and Lebowitz [22,23]. The current through the system is limited by the transport capacity of the defect site leading to a density-independent current at intermediate densities. The corresponding steady state phase separates into a high-and low-density region separated by a shock. In contrast, at high and low densities the system is only affected locally by the presence of the defect.

The effects of finite defect density in a periodic system have been studied in detail in [27,28,24,29], mainly numerically. For binary distributions of defects, Tripathy and Barma [27,28] have classified two different regimes: (1) a homogeneous regime with a single macroscopic density and non-vanishing current and (2) a segregated-density regime, with two distinct values of density and non-vanishing current. Considering the partially ASEP where disorder was realized by inhomogeneous hopping bias, they also found a vanishing-current regime which shows two distinct densities, but with a current that vanishes asymptotically for ($L \to \infty$). They argue that phase separation can be understood by a maximum current principle: for a given mean density the system settles in a state which maximizes the stationary current. Thus the largest stretch of slow bonds acts as a current limiting segment. For the same system, Juhász et al [30] introduced an effective potential and determined trapping times in potential wells to investigate the vanishing of the current in a finite-size scaling.

In the case of open boundary conditions, not only detailed balance but also translational invariance is broken. Although in principle one expects the same phases as in the pure system, the phase boundaries and the nature of the transitions might change. For equilibrium systems the Harris criterion [31] allows us to decide whether critical behaviour is altered by weak disorder. For non-equilibrium systems no such general statements are currently available [25].

As in the periodic case, for a single defect site generically disorder-induced phase separation into macroscopic regions of different densities is observed in certain parameter regimes. The presence of defects leads to a decrease of the transport capacity and the maximum current phase is enlarged compared to the pure system [32]. These results have been generalized to systems with a single stretch of consecutive defects, called bottleneck, or two defect sites (or bottlenecks) [33–[36]. It has been shown that for such systems reliable analytical approximations exist which go beyond a simple mean field approach to take into account the relevant correlations [33,36].

For open systems with a single defect (or bottleneck) the current depends on the position of the defect [34–[36] if it is located close to a boundary. This edge effect due to the interaction between the defect and the boundary also occurs in systems with many defects and can be accounted for by effective boundary rates [36].

The focus of most previous investigations was on individual realizations of defect distributions while statistical properties of defect ensembles were not considered. Numerical investigations on ensembles have been made in [37], where the influence of
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defects on the phase transition between the low- and high-density phase of the randomly
disordered TASEP with open boundary conditions was studied. It was shown that the
position of this phase transition is sensitively sample-dependent, even for large systems.
This effect is due to defects near the boundaries which is consistent with the results in [36].
Krug [24] conjectured that the maximum current is also sample-dependent and is mainly
determined by the longest bottleneck. In [34,36] this was shown to be correct, at least
for two bottlenecks which are not too close to each other. These observations lead to the
single-bottleneck approximation (SBA) which is supported in this work by numerical and
analytical arguments.

For applications to real systems, macroscopic parameters and quantities are most
relevant. Since we have seen that macroscopic quantities can depend on microscopic
ones that can differ for different defect samples, we are mainly interested in determining
statistical properties, e.g. probability distributions and expectation values, of relevant
quantities taking an ensemble of systems rather than looking at single samples. We
therefore consider in this work a large ensemble of individual finite but large systems,
while the individual values of these quantities might vary for different samples.

The goal of this work is to understand the phase diagrams of driven lattice gases and
give quantitative approximations for the expectation values of critical parameter values
and the maximum current. Using Monte Carlo (MC) simulations, we therefore check the
validity of the SBA and the concept of effective boundary rates on individual samples
not only in the disordered TASEP, but also in a more complex model with internal
states (NOSC model without Langmuir kinetics [38,39], see the appendix), which is a
model for intracellular transport with KIF1A motor proteins5. With the help of extreme
value statistics these principles are used to derive approximations for expectation values
(section 4). After checking the accuracy of the SBA we discuss in section 5 the relevance
of various possible corrections, e.g. through edge effects or effective interactions between
the bottlenecks. Finally, in section 6 the influence of the disorder on the phase diagram
is investigated in more detail.

2. Model definition

Although our considerations are rather general, we focus here on the prototypical driven
lattice gas, the totally asymmetric simple exclusion process (TASEP). The TASEP is
defined on a lattice of \( L \) sites which can either be empty or occupied by one particle. A
particle at site \( j \) can move forward to its neighbour site \( j + 1 \) if this site is empty. The
corresponding hopping rate is denoted by \( p_j \). At the boundary sites \( j = 1 \) and \( j = L \)
particles can be inserted and removed, respectively. If site 1 is empty a particle will be
inserted there with rate \( \alpha \). On the other hand, if site \( L \) is occupied this particle will
be removed with rate \( \beta \). Here we will use a random-sequential update corresponding to
continuous-time dynamics.

In schematic form the transition rules are

\[
\begin{align*}
\text{Forward hopping in the bulk:} &\quad 10 \to 01 \quad \text{with probability } p_{j} \Delta t. \\
\text{Entry at the left boundary:} &\quad 0 \to 1 \quad \text{with probability } \alpha \Delta t. \\
\text{Exit at the right boundary:} &\quad 1 \to 0 \quad \text{with probability } \beta \Delta t.
\end{align*}
\]

5 These motor proteins belong to the kinesin family.
As the indices indicate, the hopping rates \( p_i \) are site-dependent in the disordered TASEP. Other transitions are prohibited.

We will also investigate a generalization of the TASEP where each particle can be in two different states 1, 2. This model, which is defined in the appendix, has been proposed to describe the dynamics of KIF1A motor proteins on microtubules [38, 39]. In the NOSC model the forward-rebinding rate \( \omega_f \) is a parameter controlling the average velocity of single particles for which we allow disorder.

In this paper we focus on \textit{binary disorder} for which the hopping rates on each site can take the two possible values \( p \) and \( q < p \) that are randomly distributed by the rule

\[
 p_j = \begin{cases} 
 q & \text{with prob. } \phi \\
 p & \text{with prob. } 1 - \phi.
\end{cases}
\]  

(2)

The parameter \( \phi \) is the \textit{defect density}. Sites with reduced hopping rate \( q \) will be called \textit{defect sites} or \textit{slow sites}, while those with hopping rate \( p \) are \textit{non-defect sites} or \textit{fast sites}. In the following we will set \( p = 1 \), which can always be achieved by rescaling time.

For convenience a sequence of \( l \) consecutive defect sites will be called a \textit{bottleneck of length} \( l \) in the following. A bottleneck of length \( l = 1 \) corresponds thus to an isolated slow site.

We will focus on \textit{finite but large} systems here, i.e. we neglect terms of magnitude \( \mathcal{O}(1/L) \), but keep terms \( \mathcal{O}(1/\ln L) \). This is motivated by the facts that (a) the maximum current decreases with increasing bottleneck length and (b) the length of the longest bottleneck grows logarithmically in \( L \).

3. \textbf{Single-bottleneck approximation}

Besides the macroscopic structure of the stationary state in dependence of the system parameters, i.e. the phase diagram, the main focus of our investigation will be the (stationary) maximum current \( J^* \) for fixed bulk parameters \( p \) and \( q \):

\[
 J^* = \max_{\alpha, \beta} J(\alpha, \beta).
\]  

(3)

In analogy with the terminology used in traffic engineering, we will call \( J^* \) the \textit{(transport) capacity}. Besides the macroscopic structure of the steady state, the transport capacity will serve as the main quantitative indicator for disorder effects. Furthermore the critical values \( \alpha_c \) and \( \beta_c \), where the transport capacity is reached, are of interest. In the pure TASEP one has \( J^* = J(\alpha = 1, \beta = 1) = 1/4 \) and \( \alpha_c = \beta_c = 1/2 \). Both will change in the presence of defects and, based on previous results, could even be sample-dependent.

Investigations in several works [24, 27, 36] indicate that, in the TASEP with many defects, the longest stretch of consecutive defects (\textit{bottleneck}) is the quantity that contributes most to the transport capacity. This is plausible if one assumes a local character of the bottlenecks by characterizing them by an individual transport capacity \( J_j^*(l) \) depending on the length \( l \) and (possibly) position \( j \). In the stationary state the total current is constant in space and is restricted by all bottleneck capacities, i.e. it cannot exceed the minimum of all \( J_j^*(l) \). Since the transport capacity is decreasing monotonically with bottleneck size, as was shown in [36], the minimum of \( J_j^*(l) \) corresponds to the transport capacity \( J^*(l^*) \) of the longest bottleneck which consists of \( l^* \) consecutive defects.
Table 1. Comparison of Monte Carlo (MC) and SBA results for the transport capacity $J^*$ in the disordered TASEP with different system sizes $L$ and defect densities $\phi$. The transport capacity $J^*_{MC}$ was obtained by Monte Carlo simulations for $\alpha = \beta = 0.5$ (column 6) for fixed slow hopping rate $q = 0.6$. This is compared with MC results ($J^*_{SBA}$, column 7) and the results obtained by ISA [36] ($J^*_{ISA}$, column 8) for a single-bottleneck system with one bottleneck in the bulk whose length is the same as the longest defect in the simulated disordered TASEP (column 3). Columns 4 and 5 give the distance and length of the bottleneck next to the longest one.

| $L$  | $\phi$ | $l^*$ | Distance | Length | $J^*_{MC}$ | $J^*_{SBA}$ | $J^*_{ISA}$ |
|------|--------|------|----------|--------|------------|------------|------------|
| 1000 | 0.05   | 2    | 2        | 1      | 0.2174     | 0.2294     | 0.2229     |
| 1000 | 0.1    | 3    | 12       | 1      | 0.2080     | 0.2131     | 0.2080     |
| 1000 | 0.2    | 3    | 2        | 2      | 0.1963     | 0.2131     | 0.2080     |
| 3000 | 0.1    | 3    | 4        | 1      | 0.2048     | 0.2131     | 0.2084     |
| 3000 | 0.2    | 5    | 1        | 1      | 0.1866     | 0.1925     | 0.1901     |

Smaller bottlenecks do not contribute much as long as they are not too close to the longest one [36]. This motivates the Single-Bottleneck Approximation (SBA).

The transport capacity $J^*$ of a disordered system with randomly distributed defects is the same as the transport capacity $J^*_{SBA}$ of a system with a single bottleneck if the length of this bottleneck is the same as that of the longest bottleneck in the disordered system.

A similar conjecture has been made by Krug for periodic systems [24].

The SBA reduces the problem to the much simpler one of a single bottleneck in a system. In particular for the TASEP, efficient methods have been developed recently, namely the finite segment mean field theory (FSMFT) [33] and the interaction subsystem approximation (ISA) [36].

We expect the SBA to work for generic driven lattice gases, especially for low defect density $\phi$, where the average distance between defects is large and their interactions can be neglected. As an example we have tested it not only for the TASEP, but also the disordered NOSC model in the limit of vanishing Langmuir kinetics. In both systems the average velocity of the particles is dependent on one or more transition rates. In the TASEP the hopping rate $p$ is such a parameter, while in the NOSC model the forward-rebinding rate $\omega_f$ is a parameter controlling the average velocity.

First we consider a fixed realization of disorder with small defect density $\phi$. In this case we have a system with dilutely distributed bottlenecks of different lengths. We want to test the SBA for the disordered TASEP and the NOSC model. For this purpose we simulated systems with different disorder samples and compared the results for the transport capacity $J^*$ with numerical and analytical results of systems with single bottlenecks in tables 1 and 2. For each sample we identified the longest bottleneck $l^*$ and calculated the transport capacity $J^*_{SBA}(l^*)$ in a single-bottleneck system with just one bottleneck of size $l^*$. One observes a quite good agreement, although the SBA seems to overestimate the transport capacity systematically. This is not surprising since effective interactions of the bottlenecks will lead to an additional decrease of the current. From the results in [36] we expect that the main effect comes from bottlenecks near the longest
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Table 2. Same as in table 1, but for the NOSC model without Langmuir kinetics. The forward hopping rate is inhomogeneous with $\omega_{f, fast} \Delta t = 0.58$ and $\omega_{f, slow} \Delta t = 0.32$. The other parameters are fixed: $\omega_{h} \Delta t = 0.8$, $\omega_{s} \Delta t = 0.22$, $\omega_{b} = 0$.

| $L$ | $\phi$ | $t^*$ | Distance | Length | $J^*_MC$ | $J^*_SBA$ |
|-----|--------|-------|----------|--------|----------|----------|
| 1000 | 0.05  | 2     | 4        | 1      | 0.07923  | 0.08179  |
| 1000 | 0.1   | 3     | 2        | 1      | 0.07451  | 0.07643  |
| 1000 | 0.2   | 6     | 3        | 1      | 0.06659  | 0.06717  |
| 3000 | 0.1   | 4     | 6        | 1      | 0.07205  | 0.07213  |
| 3000 | 0.2   | 6     | 3        | 1      | 0.06677  | 0.06717  |

one. There it was shown that, for systems with two bottlenecks, although the main reduction of the transport capacity comes from the longer one, the transport capacity will be further reduced if the distance between the bottlenecks is small. To illustrate this effect we included the distance of the nearest bottleneck in tables 1 and 2. Since it is more probable to find a bottleneck close to the longest one for larger defect density $\phi$, the results tend to be less accurate with increasing $\phi$.

Surprisingly it seems that the values $J^*_ISA$ obtained by the semi-analytical ISA method [36] are more accurate than the numerical ones ($J^*_SBA$) of the single-bottleneck system. This is because ISA usually underestimates the value of $J^*(l)$ in the TASEP with one bottleneck, while SBA overestimates the current. Thus errors cancel.

4. Probability distributions and expectation values in SBA

As we have seen, the transport capacity depends quite strongly on the particular sample of the defect distribution, i.e. the size of the longest bottleneck. Usually in real systems the exact distribution of defect sites is not known, particularly the size and position of the longest defect cannot be identified. Then a statistical treatment, i.e. considering an ensemble of systems with fixed defect density, is more appropriate. It allows us to determine expectation values for quantities like currents and effective boundary rates (see section 6.1). This is especially relevant for applications, e.g. to intracellular transport on cell filaments. Each cell consists of a large number of filaments that serve as tracks for motor proteins, and often inhomogeneities play an important role [26]. Therefore each filament can be modelled by a driven lattice gas on a linear chain [38, 40] and the quantities of interest are averages rather than the properties of individual chains.

In this section we want to approximate the expectation value of the transport capacity $J^*(q, \phi, L)$ for fixed defect density $\phi$ and finite but large system size $L$. In the last section we have shown that for small $\phi$ the capacity depends approximately on the size of the longest defect. Therefore we first determine the expectation value for the size of the longest defect in such a system.

We now consider a given sample at defect density $\phi$ and system size $L$. The $k$th bottleneck has length $l_k$ and in the following two consecutive fast sites $j, j + 1$ will be interpreted as a bottleneck of length $l = 0$ located at site $j$. This implies that the number $N_b$ of bottlenecks is equal to the number $N_f$ of fast sites, since each bottleneck is followed
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by a fast site. The bottleneck length \( l \) is a random variable with distribution

\[
P_\phi(l) = \phi^l (1 - \phi).
\]

Since on average the fraction of fast sites is \((1 - \phi)\), the mean number of fast sites is \( N_f = (1 - \phi)L \). The length of the longest bottleneck is \( l^* = \max\{l_k | k = 1, \ldots, N_f\} \).

The statistics of the maximum of independently distributed random values is governed by extreme value statistics [41]. It says that for a continuous probability distribution \( P(l) \) that decays exponentially or faster for \( l \to \infty \), the probability density of \( l^* \) being the maximum value of \( N \) independently distributed random values is, for large \( N \), asymptotically described by the Gumbel distribution [41]:

\[
G(u) = e^{-u} e^{-e^{-u}}
\]

where \( u = u(l^*) \) is a rescaled and shifted function of \( l^* \) depending on the details of the probability distribution \( P(l) \).

However, since in our case the probability distribution is discrete we need to be careful. Therefore, following the derivation used in [41] for continuous distributions, we derive the probability distribution of the maximal bottleneck length explicitly in order to control errors made by approximations. This will also provide an explicit expression for \( u(l^*) \). The probability of a bottleneck being shorter than \( l' \) is

\[
P_<(l') = \sum_{l=0}^{l' - 1} P_\phi(l) = 1 - \phi^{l'}.
\]

Since the \( l_k \) are independently distributed, we have the probability that all \( l_k \) are smaller than \( l' \):

\[
H_<(l') = P_<(l')^N_f = \exp \left( N_f \ln(1 - \phi^{l'}) \right) = \exp \left( (1 - \phi)L \ln(1 - \phi^{l'}) \right).
\]

For large \( L \) this probability is significantly larger than zero only for \( \phi \ll 1 \) and we can use the approximation \( \ln(1 - \phi^{l'}) \approx -\phi^{l'} \). Thus

\[
H_<(l') \approx \exp(-\phi^{l'} (1 - \phi)L).
\]

As was shown in [41], the error of this correction is \( O(1/L^2) \) for exponential \( P(l) \). Thus we can neglect finite-size corrections. The probability that all values are smaller than \( l' \) is equal to the probability that the maximum \( l^* \) is smaller than \( l' \):

\[
H_<(l') = \sum_{l^*=0}^{l'-1} P(l^*).
\]

\footnote{We neglect the possible exception at the right boundary.}
\( \mathcal{P}(l^*) \) is the probability that the longest bottleneck has length \( l^* \) which is explicitly given by

\[
\mathcal{P}(l^*) = H_<(l^* + 1) - H_<(l^*) \quad (10)
\]

\[
= H'_<(l^* + \frac{1}{2}) + \mathcal{O}((\Delta l^*)^3)
\]

\[
\approx L(1 - \phi)\theta_{l^*+\frac{1}{2}}\ln\phi \exp\left(-\theta_{l^*+\frac{1}{2}}(1 - \phi)L\right)
\]

\[
= -\ln\phi e^{-u}e^{-\sigma^2} = -\ln\phi G(u),
\]

where \( G(u) \) is the Gumbel distribution (5) and we have introduced the function

\[
u(l^*) = -(l^* + \frac{1}{2})\ln\phi - \ln(1 - \phi) - \ln L.
\]

(12)

The expectation value of the Gumbel distribution is known to be \( \langle u \rangle = \gamma_e \) [42], where \( \gamma_e = 0.5772 \) is the Euler–Mascheroni constant. Using (12) we have

\[
\gamma_e = \langle u \rangle = -\ln\phi \langle l^* \rangle - \frac{1}{2}\ln\phi - \ln(1 - \phi) - \ln L,
\]

(13)

which can be solved for \( \langle l^* \rangle \) to obtain

\[
\langle l^* \rangle = \frac{\ln L + \ln(1 - \phi) + \gamma_e - \frac{1}{2}}{\ln(1/\phi)}
\]

(14)

\( \langle l^* \rangle \) diverges for infinite systems, as expected. However, it grows only of order \( \mathcal{O}(\ln L) \), so that we have to keep this term in finite but large systems. The variance of the Gumbel distribution \( G(u) \) is \( \sigma^2(u) = \pi^2/6 \) [42]. Since \( \sigma^2(l^*) = (du/dl^*)^{-2}\sigma^2(u) \) (linear transformation) this yields the variance

\[
\sigma^2(l^*) = \frac{\pi^2}{6\ln^2(1/\phi)}
\]

(15)

of the longest bottleneck distribution \( \mathcal{P}(l^*) \). Hence \( \sigma^2(l^*) \) does not depend on the system size. In figure 1, the dependence of the expectation value and variance of the longest bottleneck on the defect density is compared to Monte Carlo results. The expectation value exhibits a very good agreement with averages obtained by simulations. The variance seems to slightly deviate from the simulation results for low \( \phi \), which is due to errors of the continuous approximation. However, it is confirmed that the variance does not depend on the system size.

If we approximate the transport capacity \( J^*(\phi) \) for small \( \phi \) by the corresponding current \( J_{\text{SBA}}^* \) of a system with one bottleneck, the expectation value is given by \( \langle J^*(\phi) \rangle = \sum_{l^*=0}^{\infty} J_{\text{SBA}}^*(l^*) \mathcal{P}(l^*) \). Due to the approximation by a continuous function, the norm \( \sum_{l^*=0}^{\infty} \mathcal{P}(l^*) \neq 1 \) can significantly deviate from one. In order to reduce this error we divide the result by \( \sum_{l^*=0}^{\infty} \mathcal{P}(l^*) \):

\[
\langle J_{\text{SBA}}^* \rangle (\phi) = \frac{\sum_{l^*=0}^{\infty} J_{\text{SBA}}^*(l^*) \mathcal{P}(l^*)}{\sum_{l^*=0}^{\infty} \mathcal{P}(l^*)}.
\]

(16)

We can now either take numerical values for \( J^*(l^*) \) or (semi-) analytical ones from [36] or [33]. Since \( \mathcal{P}(l^*) \) decays fast around \( \langle l^* \rangle \) it is sufficient to take into account only a few terms in (16) in the vicinity of \( \langle l^* \rangle \).

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Figure 1. Average longest bottleneck $\langle l^* \rangle$ and variance $\sigma^2(l^*)$ in dependence of the defect density $\phi$, for $L = 1000$ and 5000. Results obtained by averaging over 1000 samples in Monte Carlo computations are compared with analytical results obtained by (14) and (15). One observes a good agreement in both cases, while the variance is slightly underestimated by analytical results.

Since the asymptotic behaviour of the transport capacity in the TASEP is $J^*(l^*) = q/4 + O(1/l^*)$ [24, 36], we can state by using (16) that $J^*(\phi, L) = q/4 + O((\ln(1/\phi))/(\ln L))$ in the disordered TASEP. The variance $\sigma^2(l^*)$ is independent of the system size. Thus the variance of the transport capacity $\sigma^2(J^*) = O((dJ^*/dl^*)^2\sigma^2(l^*)) = O(1/(\ln L)^2)$ vanishes logarithmically in the thermodynamic limit $L \to \infty$.

In order to display the generic character of the SBA, we show results for the transport capacity not only for the TASEP but also for the disordered NOSC model without Langmuir kinetics (tables 3 and 4). We observe a good agreement in both systems.
Table 3. Comparison of disorder averages in MC results and SBA results for the expectation value of the transport capacity. The defect hopping rate is \( q = 0.6 \). Column 4 shows the numerical results from MC simulations of the disordered TASEP. Column 5 displays results by SBA using the probability distribution (11) and column 6 shows the variance of the current obtained in the simulations.

| \( L \) | \( \phi \) | No. of samples | \( \langle J^* \rangle_{MC} \) | \( \langle J^* \rangle_{SBA,MC} \) | \( \sigma^2(J^*) \) |
|---|---|---|---|---|---|
| 500 | 0.1 | 200 | 0.2098 | 0.2244 | \( 3.2 \times 10^{-5} \) |
| 1000 | 0.2 | 100 | 0.1918 | 0.2024 | \( 1.7 \times 10^{-5} \) |
| 3000 | 0.1 | 100 | 0.2016 | 0.2110 | \( 2.0 \times 10^{-5} \) |
| 3000 | 0.2 | 50 | 0.1878 | 0.1960 | \( 1.2 \times 10^{-5} \) |

Table 4. Same as in table 3 but for the NOSC model without Langmuir kinetics. The forward hopping rate is inhomogeneous with \( \omega_f^{\text{fast}} \Delta t = 0.58 \) and \( \omega_f^{\text{slow}} \Delta t = 0.32 \). The other parameters are fixed: \( \omega_h \Delta t = 0.8 \), \( \omega_s \Delta t = 0.22 \), \( \omega_b = 0 \).

| \( L \) | \( \phi \) | No. of samples | \( \langle J^* \rangle_{MC} \) | \( \langle J^* \rangle_{SBA,MC} \) | \( \sigma^2(J^*) \) |
|---|---|---|---|---|---|
| 500 | 0.1 | 200 | 0.07453 | 0.08010 | \( 5.9 \times 10^{-5} \) |
| 1000 | 0.2 | 100 | 0.06852 | 0.07258 | \( 5.8 \times 10^{-5} \) |
| 3000 | 0.1 | 100 | 0.07438 | 0.07553 | \( 1.0 \times 10^{-4} \) |
| 3000 | 0.2 | 50 | 0.06628 | 0.07258 | \( 9.1 \times 10^{-5} \) |

while the errors are of the same magnitude as for individual samples. This indicates that the probability distribution function for the longest bottlenecks is an appropriate approximation.

5. Corrections to SBA

In the following we consider corrections to the SBA and check the quality of this approximation and the range of its validity by statistical means.

In principle, corrections to the transport capacity could come from the following effects.

- The longest bottleneck (length \( l^* = \text{max}\{l_1, l_2, \ldots\} \)) is located near the boundary, not in the bulk as assumed in the SBA. Since the probability that a bottleneck at a given site is smaller than \( l \) is \( P_\phi(l) = 1 - \phi^l \) (see (6)), the probability of finding the first longest bottleneck \(^7\) of length \( l \) at distance \( x \) from a boundary is \( P(x) = (1 - \phi^l)^x \phi^l \). Therefore the average distance of the longest bottleneck can be approximated as

\[
\langle x \rangle \approx \frac{1}{\phi^l \Gamma(l)} \int_0^\infty x (1 - \phi^l)^x \phi^l \, dx = \frac{\phi^l}{(\ln(1 - \phi^l))^2}\]

\[
\approx \phi^{-l} = \phi^{1/2} L (1 - \phi) e^{-\gamma} = \mathcal{O}(L),
\]

where we approximated the longest bottleneck by its expectation value (14). That means for large systems the longest bottleneck is, on average, far from the boundaries.

\(^7\) There can be more than just one longest bottleneck.
However, we see that, for finite systems and small defect densities $\phi \ll 1$, $\langle x \rangle$ is becoming small, so that the boundaries might affect the transport capacity. This is due to a kind of ‘degeneracy’ of the longest bottleneck, since for small defect densities the probability that there are many longest bottlenecks is high (e.g. for $l^* = 1$ this degeneracy is $O(L)$); thus, contributions of samples with a longest bottleneck near a boundary are relevant. We therefore expect deviations from the SBA for very small defect densities in finite systems. The effect should vanish in the limit $L \to \infty$ for fixed $\phi$.

- Other smaller bottlenecks near the boundary can be treated by introducing effective boundary rates (see section 6).
- Corrections from other bulk defects, i.e. ‘defect–defect interactions’. Candidates for the leading contribution from this type of correction would be (a) other long defects, i.e. defects of length $l \leq l^*$, and (b) defects (of arbitrary length) located in the neighbourhood of the longest one. The results of [36] indicate that the second correction is more important.

In order to estimate the corrections we consider an ensemble of systems which all have a longest bottleneck of length $l^*$ and defect density $\phi$. The slow hopping rate $q$ is considered to be fixed. The longest bottleneck (or one of them in the case of degeneracy) is located at an arbitrary position and the distribution of the other defect sites is not restricted. For this ensemble the average transport capacity is given by

$$\langle J^* \rangle(\phi, L, l^*) = \sum_{\mathbf{x}} J^*_p(\mathbf{x}) P_\phi(\mathbf{x}), \quad (18)$$

where $\mathbf{x} = (x_1, \ldots, x_N)$ denotes a defect configuration with defects at sites $x_j$. The sum is restricted to such configurations for which the longest bottleneck has length $l^*$ (and therefore $N \geq l^*$). $P_\phi(\mathbf{x})$ is the probability to find the configuration $\mathbf{x}$.

Denoting the transport capacity in the SBA by $J^*_{\text{SBA}}$ we have

$$\langle J^* \rangle(\phi, L, l^*) = J^*_{\text{SBA}}(l^*) + \sum_{\mathbf{x}} \Delta J^*_p(\mathbf{x}) P_\phi(\mathbf{x}) \quad (19)$$

with $\Delta J^*_p(\mathbf{x}) = J^*_p(\mathbf{x}) - J^*_{\text{SBA}}(l^*)$. The expectation value for the corrections to the SBA is then

$$\langle \Delta J^* \rangle(\phi, L, l^*) = \sum_{\mathbf{x}} \Delta J^*_p(\mathbf{x}) P_\phi(\mathbf{x}) = \sum_{N^*} \sum_{\mathbf{x}_{N^*}} \Delta J^*_p(\mathbf{x}_{N^*}) P_\phi(\mathbf{x}_{N^*}), \quad (20)$$

where $N^* = N - l^*$ is the number of defects besides $l^*$ and $\mathbf{x}_{N^*}$ denotes the positions of these defects. In the case of a degeneracy one of the longest bottlenecks is chosen arbitrarily.

Since $P_\phi(\mathbf{x}_{N}) = \phi^N (1 - \phi)^{L-N} = O(\phi^N)$, the leading correction in $O(\phi)$ comes from configurations with one additional defect:

$$\langle \Delta J^* \rangle(\phi, L, l^*) \approx \sum_{x_1} \Delta J^*_p(x_1) P_\phi(x_1) = \left( \sum_{x_1} \Delta J^*_p(x_1) \right) P_\phi(x_1), \quad (21)$$

where we have used that $P_\phi(x_1)$ does not explicitly depend on $x_1$ (all allowed defect positions are equally probable).
As long as the longest bottleneck is far from the boundaries, which can be assumed for large systems, the transport capacity does not depend explicitly on its position \[36\]. Hence, instead of \(x_1\), we can also use the relative position \(d\) of the additional defect to the longest bottleneck to characterize the configuration. If the defect is right of the longest bottleneck, we have \(d > 0\), else \(d < 0\). Then we obtain the following necessary condition for the SBA to work for large systems \((L \rightarrow \infty)\):

\[
\sum_{d=-\infty}^{\infty} \Delta J^*_l(d) < \infty. \tag{22}
\]

This condition is fulfilled if the ‘bottleneck–bottleneck interaction’ \(\Delta J^*_l(d)\) decays faster than \(|d|^{-1}\) for large \(|d|\), which is a restriction on the interaction strength of defects. In \[36\] it was shown numerically that in the TASEP this function indeed decays faster than \(|d|^{-2}\), so that (22) is fulfilled for the TASEP.

We can further quantify the contribution of the first defect near the longest bottleneck as \(P_\phi(x_1) = \phi(1 - \phi)^{L-N} = \phi + O(\phi^2)\). Since we have to take into account defects to the right and the left of the longest bottleneck, we obtain in leading order

\[
\langle J^* \rangle(\phi, l^*) \approx \left[ \sum_d \Delta J^*_l(d) \right] \phi, \tag{23}
\]

where contributions with a defect on an adjacent site of the bottleneck (i.e. \(d = 1\) and \(d = -1\)) do not appear in the sum, since they belong to longer bottlenecks. Note that this approximation does not depend on \(L\).

Unfortunately currently no analytical results for \(\Delta J^*_l(d)\) are available. Therefore we have to rely on the results of MC simulations to test the considerations made in this section. We simulated systems with one bottleneck at a position far from the boundaries (>200 sites) and one single defect for several bottleneck lengths \(l^*\) and defect position \(d\) relative to the bottleneck to obtain \(J^*_l(d)\). The interaction function is then obtained as \(\Delta J^*_l(d) = J^*_l(d) - J^*_l\), where \(J^*_l\) is the transport capacity of a single bottleneck. Since \(\Delta J^*_l(d)\) should decay fast with increasing \(|d|\) (see also \[36\]), it is sufficient to take into account only defects within a finite distance to the bottleneck. In order to obtain the expectation value \(\langle J^* \rangle(\phi)\) for arbitrary configurations, one has to average over \(l^*\) in the same manner as in equation (16).

In figure 2 we have plotted average values of the transport capacity obtained by MC simulations in dependence of the defect density as well for the disordered TASEP and the NOSC model. Each data point has been obtained by simulating 50 samples. For comparison the results in SBA and the leading-order corrections obtained by (23) are included. We see that, while already the SBA appears to be a good approximation, the accuracy of the corrections over a wide range of defect densities is striking. It comes as a surprise that in the TASEP for larger defect densities the leading-order correction, which takes into account only one additional defect, is extremely accurate. This is not expected since for larger \(\phi\) there is a higher probability of having more than one defect in the vicinity of the longest bottleneck. However, these results indicate that the position of other defects beyond the first one does not significantly contribute to the transport capacity.

\[8\] In our computations we simulated systems from \(d = -20\) to 20.
Figure 2. First-order corrections to SBA as a function of the defect density $\phi$ for the disordered TASEP (top) and the disordered NOSC models (bottom) using the probability distribution (10) for averaging over $t^*$. The slow hopping rates are $q = 0.6$ in the TASEP and $\omega^\text{slow}_t \Delta t = 0.32$ in the NOSC models. The system size is $L = 1000$ in each case.

Furthermore we see that the deviation of the SBA approaches a rather constant value for larger $\phi$, despite the factor $\phi$ in (23). This indicates that, for larger bottlenecks, the influence of single defects on the transport capacity is weaker than for small bottlenecks, which is consistent with results in [36]. For small defect densities configurations where the longest bottleneck is near a boundary bottlenecks become relevant, as was argued in the beginning of the section. Thus a deviation of the SBA arises in this region, although the distance of other defects from the longest bottleneck is large on average.
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6. The phase diagram of disordered driven lattice gases

The phase diagrams of driven lattice gases that have exactly one maximum all have the same topology. This is based on a maximum current principle and shock dynamics [2, 43, 44]. The class of driven lattice gases meeting this condition includes many weakly interacting lattice gases, e.g. the TASEP and the NOSC models [38, 39]. If disorder is included, some conceptual problems with the expression phase diagram arise. Usually a phase transition is identified by a non-analytic behaviour of a macroscopic quantity. In driven lattice gases these can be discontinuities in the density (first-order transitions) or kinks in the dependence of the current on the system parameters (second-order transition). Strictly speaking these transitions only occur in infinite systems, since non-analyticities are only present in the thermodynamic limit. In disordered systems, however, there is no unique way of taking the limit \( L \to \infty \) since this cannot be done with a fixed defect sample and, as we have seen, macroscopic quantities like the transport capacity may be sample-dependent. Indeed, the process of taking the thermodynamic limit has to be specified, since it is ambiguous how the ‘new defect sites’ by increasing \( L \) are included. Enaud et al [37], for example, discussed two possibilities of defining a limit \( L \to \infty \) and showed that, if this limit is taken by including sites at the boundaries, there actually is no unique phase transition point if the exit rate \( \beta \) is fixed and \( \alpha \) is varied.

For infinite systems, according to equation (14), the length of the maximum bottleneck is infinite and thus the transport capacity would be the same as the one of a pure system with hopping rate \( q \), \( J^* = q/4 \). In this work, however, we are explicitly interested in ‘finite but large systems’ and we are considering ensembles, not individual samples. Since the longest bottleneck increases as \( \mathcal{O}(\ln L) \), the transport capacity approaches its asymptotic value only logarithmically: \( J^*(L) = q/4 + \mathcal{O}(1/\ln L) \) (see also [24]). For finite but large systems we have to take into account terms of the order \( \mathcal{O}(1/\ln L) \). Hence in this view, we want to consider an explicit dependence on the system size and cannot take the thermodynamic limit to obtain phase transitions.

In [36] it is shown that, if a single bottleneck is near a boundary, phase separation cannot occur. Then the character of phase transitions is different, since the current is not limited by the bottleneck anymore but by the bulk exclusion like in the pure system. In this case the phase transition is of second order. On the other hand, if the bottleneck is far from the boundaries at a distance \( d = \mathcal{O}(L) \) there is not only a sharp kink, but also macroscopic phase separation occurs accompanied by a steep increase of the average density, indicating a first-order transition. This corresponds to the phase separating transition that can already be observed for single defects [22].

In section 5 we have seen that the average distance of the longest bottleneck from the boundaries is \( \mathcal{O}(L) \). Hence on average we have a sharp transition for large \( L \). Therefore we call this a phase transition for finite but large systems at the critical point \( \alpha_c \) where the current reaches \( J^* \), although this point depends on the system size.

6.1. Effective boundary rates

Investigations in a TASEP with one and two bottlenecks far from the boundaries (distance \( \mathcal{O}(L) \)) [36, 34] showed that the transport capacity only depends on the longer bottleneck, while outside of the maximum current phase the current only depends on the position.

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of a bottleneck that is near a boundary. This \textit{(negative) edge effect} is considerable for defects not more than \(\sim 20\) sites away from the boundaries. The observation of this effect motivates the concept of \textit{effective boundary rates}: if the system is not in the maximum current phase, it can be treated as a pure TASEP with effective boundary rates \(\alpha_{\text{eff}}, \beta_{\text{eff}}\) that depend on the distance and size of a bottleneck from the boundary and differ from the real boundary rates \(\alpha\) and \(\beta\). The concept was tested in [36] for single bottlenecks and yielded good results. The transition from low- to high-density phase was shown to be at the line \(\alpha_{\text{eff}} = \beta_{\text{eff}}\) which, in general, does not correspond to the diagonal \(\alpha = \beta\) in the phase diagram. The observations of Enaud \textit{et al.} [37] in the disordered TASEP for different defect samples indicate that the concept of effective boundary rates can also be applied for the disordered TASEP.

Taking into account defects near the boundary, we can write the current in the form
\[
J(\alpha) = \alpha(1 - \alpha) + \Delta J_\alpha(x).
\]
Here \(\alpha\) is the entry rate in the low-density phase. However, due to particle–hole symmetry\(^9\) we can transfer this result to \(\beta\) and the high-density phase.

The defect configuration \((x_1, x_2, \ldots)\) is defined in the same manner as in section 5. Indeed, taking the expectation value we can proceed as in the last section to obtain the average corrections in leading order:
\[
\langle \Delta J_\alpha \rangle(\phi) \approx \phi \left[ \sum_{d_1} \Delta J_\alpha(d_1) \right],
\]

where \(d_1\) is the position of the first defect and \(\Delta J_\alpha(d_1) = J_\alpha(d_1) - \alpha(1 - \alpha)\). Thus the corrections by defects near the boundaries are of the same magnitude as the corrections to the SBA, while the ‘defect–boundary interaction’ \(\Delta J_\alpha(d_1)\) is, in general, not the same as the ‘defect–defect interaction’ \(\Delta J_\alpha(d_1)\).

Figure 3 shows that results obtained by (24) yield an accurate approximation for the expectation value of the current for low entry rates, though for larger \(\phi\) they appear to slightly overestimate the MC values.

The expectation value of the effective entry rate can then be obtained if the current density relation of the pure system \(J(\rho)\) is known.

If the relations \(\alpha_{\text{eff}}(\alpha), \beta_{\text{eff}}(\beta)\) and their inverses \(\alpha^{-1}(\alpha_{\text{eff}})\) and \(\beta^{-1}(\beta_{\text{eff}})\) are known as well as the transport capacity \(J^*\), we are in principle able to map the problem of determining the phase diagram of a disordered system on a pure system with a known dependence on the current on the boundary rates \(J(\alpha, \beta)\).

(i) If the system current \(J(\alpha_{\text{eff}}, \beta_{\text{eff}}) < J^*\) the system globally has the same properties as the pure one if one replaces the real boundary rates by the effective ones.

(ii) At the points in the \(\alpha–\beta\) space where \(J(\alpha_{\text{eff}}, \beta_{\text{eff}}) = J^*\), a phase transition to a phase-separated phase occurs in which the current is independent of the boundary rates and maximal.

In particular in the TASEP we can determine the expectation value of the effective boundary rates:
\[
\langle \alpha_{\text{eff}} \rangle = \frac{1}{2} - \sqrt{\frac{1}{4} - \langle J_\alpha \rangle}.
\]

\(^9\) Note that, for individual defect samples, particle–hole symmetry is broken, but for large ensembles it is restored.
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Figure 3. Disorder average of the current in dependence of the defect density in the disordered TASEP with $q = 0.6$, $\alpha = 0.2$ (top) and the disordered particle-conserving NOSC model with $\omega_{\text{slow}} \Delta t = 0.32$ (bottom). MC simulations are compared with leading-order corrections to the pure current obtained by (24). Entry rates are chosen to be small enough so that $J < J^*$. 

There is a phase transition from a low-density to high-density phase for $\alpha_{\text{eff}}(\alpha') = \beta_{\text{eff}}(\beta') \Leftrightarrow \alpha' = \alpha_{\text{eff}}^{-1}(\beta_{\text{eff}}(\beta))$ which, in general, is not on the diagonal $\alpha = \beta$. Nonetheless we have on average due to particle–hole symmetry $\langle J_{\alpha} \rangle = \langle J_{\beta} \rangle$ that leads to $\alpha' = \beta'$ on average. The transition to the phase-separated phase is determined by $\alpha_c(1 - \alpha_c) = J^*$ or $\beta_c(1 - \beta_c) = J^*$. Unfortunately, we are not able to determine the functions $\alpha_{\text{eff}}(\alpha)$, $\beta_{\text{eff}}$ explicitly, since for each $\alpha$, $\beta$ we need to obtain a set of functions $\Delta J_{\alpha,\beta}$ which requires much computational effort, as long as no analytical results are available. Nonetheless, the concept of effective boundary rates can be used to extract some qualitative properties of the phase diagram, though obtaining quantitative results is difficult.
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Figure 4. Mean density $\langle \rho \rangle$ and current $J$ in dependence of $\alpha$ for fixed $\beta = 0.9$, $q = 0.6$ and $\phi = 0.05$ obtained by MC simulation of a system with $L = 2000$ and fixed defect sample. One observes a steep increase at the same point where the current reaches the plateau.

However, since corrections of the SBA are of the same order as corrections to the boundary rates, we can approximate $\alpha_{\text{eff}} \approx \alpha$ and $\beta_{\text{eff}} \approx \beta$ in order to find $\alpha_c$ and $\beta_c$. In figure 4 we plotted the current and the average density in dependence of the entry rate $\alpha$. One observes a steep increase in the average density at the point where the plateau begins. Thus we can characterize this transition as a first-order phase transition.

Figure 5 displays a sketch of the phase diagram of an individual defect sample in the disordered TASEP. The transition line between HD and LD is distorted compared to the homogeneous case. On average, the transitions are again on the diagonal line $\alpha = \beta$. In contrast to the pure TASEP, the maximum current phase is not induced by bulk exclusion and no long-range boundary layers occur. Instead phase separation, induced by the longest bottleneck, is observed. Therefore this is called a phase-separated phase (PS) which covers a larger area of the $\alpha$–$\beta$ plane than the maximum current phase of the pure TASEP (M). In contrast to the pure system, the transition to this phase can be characterized as a first-order phase transition, since a jump of the average density occurs at the transition line.

7. Discussion and outlook

We have investigated disorder effects in driven lattice gases using the TASEP with binary hopping rates as a paradigmatic example. Our results indicate that good approximations for the expectation value of the transport capacity (and other quantities) of an ensemble of driven diffusive lattice gas systems can be obtained with low effort (no averaging over disorder distribution).

The basic idea stems from the observation that the longest bottleneck (consecutive string of slow sites) is the current limiting factor. This suggests the possibility of
Figure 5. Schematic phase diagram of the disordered TASEP for a single defect sample. It is obtained by taking the phase diagram of the TASEP in dependence of $\alpha_{\text{eff}}$ and $\beta_{\text{eff}}$ with one bottleneck that corresponds to the longest one and rescale the axis by $\alpha_{\text{eff}} \rightarrow \alpha$, $\beta_{\text{eff}} \rightarrow \beta$. For comparison we included the phase transitions of the homogeneous TASEP with $p = 1$ (dashed lines).

calculating the transport capacity of given defect samples by the single-bottleneck approximation (SBA). It allows us to use known results for systems with only one bottleneck, which are usually much better understood than the disordered ones, as an efficient and accurate description. With the help of extreme value statistics one obtains the probability distribution for the longest bottleneck from which the expectation value of the transport capacity in the SBA can be determined. Since for finite systems only a small range of bottleneck lengths gives relevant contributions to the expectation value, it is sufficient to have the results for a small number of single-bottleneck systems. So, even for systems for which no analytical results are available, one can get SBA results by once simulating a small number of single-bottleneck systems. Using these data approximations of the transport capacity for arbitrary system size and defect density (but fixed transition rates $p, q$) can be obtained.

We emphasize that the results obtained here are useful in two different situations: (a) for a fixed realization of disorder, if the longest bottleneck can be identified, and (b) for ensembles of systems with fixed density. In the first case, one can directly identify the disordered system with the appropriate single-bottleneck case. In the second case, which is also relevant for many realistic scenarios, one can use the statistical description developed here to obtain predictions for the ensemble.
The accuracy of the SBA can be systematically improved by taking into account various corrections. We found that, for small defect densities, the most important correction is due to the first defect next to the longest bottleneck. It can be expressed in terms of functions $\Delta J^*(x_1)$ that measure the contribution of a single defect at position $x_1$ relative to the bottleneck. A rather general argument indicates that the SBA is applicable to a generic driven lattice gas if these functions decay faster than $d^{-1}$ with increasing distance. Indeed for both cases studied here explicitly, the disordered TASEP and the NOSC model with vanishing Langmuir kinetics, the SBA yields good results and thus we can expect it to work even for generic driven lattice gases. Surprisingly, the leading-order corrections appear to be quite accurate in both systems also for larger defect densities $\phi \approx 0.5$. This indicates that other defects than the first one only have a very small influence on the transport capacity if large bottlenecks are present\textsuperscript{10}. However, for finite systems at small defect densities, deviations from the SBA occur that cannot be explained by defects near the longest bottleneck. Here, interactions of the boundaries with (one of) the longest bottleneck cannot be neglected, which lead to relevant deviations (see section 5).

We observed that deviations from the current of the pure system also occur if the current is less than the transport capacity. However, these deviations are smaller in magnitude. This effect is due to defects near the boundaries, which was already shown before in systems with single bottlenecks [36,34]. They can be treated in the same manner as corrections to the SBA and we see that in this case the first defect near the boundary is the most relevant contribution as expected from the results before. The effect can be encompassed in terms of effective boundary rates. In principle, for known relations between boundary rates and transport capacity, the problem of determining the phase diagram can be mapped on a pure system using these quantities instead of the ones of the pure system\textsuperscript{11}. Though usually it is difficult to determine effective boundary rates explicitly that concept is useful to obtain qualitative properties of the phase diagram.

From a theoretical point of view the SBA and its corrections as well as the effective boundary rates are interesting since by these concepts disordered systems can be treated in terms of systems with single bottlenecks and two-bottleneck systems. These are much easier to investigate since one has to consider fixed defect configurations. This follows the tradition of statistical physics since microscopic properties of particles as well as particle–particle interactions (here ‘bottleneck–bottleneck interactions’ in the form of the functions $\Delta J(x)$) are used to obtain macroscopic quantities using statistics. The concept presented in this work is rather generic provided that microscopic properties can be obtained. This can be done by numerical simulations, for example.

Driven diffusive systems are used as models for active intracellular transport processes. These are characterized by the directed motion of motor proteins on microtubules. However, usually the microtubuli are not homogeneous, but there are other microtubule associated proteins (MAPs) that are attached to the microtubules and can form obstacles that correspond to defects on the modelling level, impeding forward movement of motor proteins. One example is the aggregation of tau proteins in neurons of organisms suffering from Alzheimer’s disease [45]. Furthermore there are experiments that show

\textsuperscript{10} The average length of the longest bottleneck increases with increasing defect density.

\textsuperscript{11} One still has to be careful since the characteristics of the phases can be different in the disordered system, although the topology is the same.
that modified kinesin molecules can immobilize moving kinesins which thus form obstacles on the microtubule track [46]. For living organisms the current of transported objects is a measure for the performance of the transport system, which may not fall below a threshold for maintaining cell metabolism and enable cell division. Hence, the maximum current is a measure for the transport capacity of a microtubule. Since binding and unbinding of molecules to microtubules and kinesin occurs stochastically, depending on temperature and concentration, this system meets the criterion of a randomly disordered system. In a living organism there can be trillions of microtubules; thus the expectation value of the maximum current is a crucial quantity. The defect density rather than the individual sample of defects on a microtubule is a measurable quantity determined by the concentration of defect molecules and temperature.

Nonetheless systems with particle conservation in the bulk are not sufficient to serve as models for intracellular transport. One crucial property intracellular transport exhibits is the attachment and detachment of motor proteins. That means that one has to include these effects in the models allowing particle creation and annihilation that leads to a spatially varying current. The so-called PFF model [5] includes Langmuir kinetics to the TASEP and virtually takes into account the attachment and detachment of motor proteins. In [40] this model was investigated with one defect site. The NOSC model in its original form [38] also includes creation and annihilation of particles and was used to model the dynamics of the KIF1A motor protein using some kind of Brownian ratchet to perform directed movement. The success of the SBA provokes the assumption that the defects locally impose a maximum transport capacity, so that the spatial varying current may not exceed the transport capacity at any point. This problem is currently under investigation and the results may help to improve our understanding of intracellular transport with particle creation and annihilation in the presence of defects or disorder.

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Appendix. The NOSC model

The NOSC model is used for modelling the dynamics of KIF1A motor proteins on microtubules. These motor proteins can be in a strongly bound state (1) where movement parallel to the microtubule is not possible, and a weakly bound state (2) where it can diffuse along the microtubule. Cyclic transitions between these states lead to a directed net motion using a Brownian ratchet due to an asymmetric binding potential. The transitions rules are in the bulk

Transition to weakly bound state (hydrolysis): \( 1 \rightarrow 2 \) with probability \( \omega_h \Delta t \).
Transition to strongly bound state on site \( i \): \( 2 \rightarrow 1 \) with probability \( \omega_s \Delta t \).
Transition to strongly bound state on site \( i + 1 \): \( 02 \rightarrow 01 \) with probability \( \omega_l \Delta t \).
Diffusion to the right: \( 20 \rightarrow 02 \) with probability \( \omega_h \Delta t \).
Diffusion to the left: \( 02 \rightarrow 20 \) with probability \( \omega_b \Delta t \).
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At the right boundary (site 1):

Entry at the left boundary: $0 \rightarrow 1$ with probability $\alpha \Delta t$.

Detachment: $1 \rightarrow 0$ never.

Diffusion out of the system: $2 \rightarrow 0$ never. \hfill (A.2)

At the left boundary (site $L$):

Exit $1 \rightarrow 0$ with probability $\beta \Delta t$.

Attachment $0 \rightarrow 1$ never.

Diffusion out of system $2 \rightarrow 0$ never. \hfill (A.3)

In the original NOSC model [38] also creation and annihilation of particles, i.e. Langmuir kinetics, is included:

Creation: $0 \rightarrow 1$ with probability $\omega_a \Delta t$.

Annihilation: $1 \rightarrow 0$ with probability $\omega_d \Delta t$, \hfill (A.4)

but here we focus on the case $\omega_a = \omega_d = 0$. In our simulations we have considered disorder in the forward-rebinding rate $\omega_f$ which is one of the parameters that control the average velocity of a particle. The standard parameter values are $\omega_f^\text{fast} = 0.145 \text{ m s}^{-1}$ for the fast rate and $\omega_f^\text{slow} = 0.08 \text{ m s}^{-1}$ for the slow rate. In this work we used a timestep of $\Delta t = 4 \text{ ms}$; thus the transition probabilities are obtained by four times the rates.

References

[1] Schmittmann B and Zia R K P, *Statistical mechanics of driven diffusive systems*, 1995 *Phase Transitions and Critical Phenomena* vol 17, ed C Domb and J L Lebowitz (New York: Academic)

[2] Schütz G M, *Exactly solvable models for many-body systems far from equilibrium*, 2000 *Phase Transitions and Critical Phenomena* vol 19, ed C Domb and J L Lebowitz (New York: Academic)

[3] Chowdhury D, Santen L and Schadschneider A, *Statistical physics of vehicular traffic and some related systems*, 2000 Phys. Rep. 329 199

[4] Chowdhury D, Nishinari K, Santen L and Schadschneider A, 2008 *Stochastic Transport in Complex Systems: From Molecules to Vehicles* (Amsterdam: Elsevier)

[5] Parmeggiani A, Franosch T and Frey E, *Phase coexistence in driven one dimensional transport*, 2003 Phys. Rev. Lett. 90 086601

[6] Lipowsky R, Kluwick S and Nieuwenhuis T M, *Random walks of cytoskeletal motors in open and closed compartments*, 2001 Phys. Rev. Lett. 87 108101

[7] Chowdhury D, Schadschneider A and Nishinari K, *Physics of transport and traffic phenomena in biology: from molecular motors and cells to organisms*, 2005 Phys. Life Rev. 2 318

[8] MacDonald C, Gibbs J and Pipkin A, *Kinetics of biopolymerization on nucleic acid templates*, 1968 Biopolymers 6 1

[9] Derrida B, Evans M R, Hakim V and Pasquier V, *Exact solution of a 1D asymmetric exclusion model using a matrix formulation*, 1993 J. Phys. A: Math. Gen. 26 1493

[10] Schütz G M and Domany E, *Phase transitions in an exactly soluble one-dimensional exclusion process*, 1993 J. Stat. Phys. 72 277

[11] Krug J, *Boundary-induced phase transitions in driven diffusive systems*, 1991 Phys. Rev. Lett. 67 1882

[12] Evans M R, *Bose-Einstein condensation in disordered exclusion models and relation to traffic flow*, 1996 Europhys. Lett. 36 13

[13] Krug J and Ferrari P A, *Phase transitions in driven diffusive systems with random rates*, 1996 J. Phys. A: Math. Gen. 29 L465

[14] Evans M R, *Exact steady states of disordered hopping particle models with parallel and ordered sequential dynamics*, 1997 J. Phys. A: Math. Gen. 30 5669

[15] Evans M R and Hanney T, *Nonequilibrium statistical mechanics of the zero-range process and related models*, 2005 J. Phys. A: Math. Gen. 38 R195
Driven lattice gases with disorder and open boundary conditions

[16] Jain K and Barma M, *Dynamics of a disordered, driven zero range process in one dimension*, 2003 Phys. Rev. Lett. 91 135701
[17] Juhász R, Santen L and Iglói F, *The partially asymmetric zero range process with quenched disorder*, 2005 Phys. Rev. E 72 72
[18] Schütz G M, *Generalized Bethe ansatz solution of an one-dimensional asymmetric exclusion process on a ring with a blockage*, 1993 J. Stat. Phys. 71 471
[19] Schütz G M, *Time-dependent correlation functions in a one-dimensional asymmetric exclusion process*, 1993 Phys. Rev. E 47 4265
[20] Hinrichsen H and Sandow S, *Deterministic exclusion process with a stochastic defect: matrix product ground states*, 1997 J. Phys. A: Math. Gen. 30 2745
[21] Barma M, *Driven diffusive systems with disorder*, 2006 Physica A 372 22
[22] Janowsky S A and Lebowitz J L, *Finite-size effects and shock fluctuations in the asymmetric simple-exclusion process*, 1992 Phys. Rev. A 45 618
[23] Janowsky S A and Lebowitz J L, *Exact results for the asymmetric simple exclusion process with a blockage*, 1994 J. Stat. Phys. 77 35
[24] Krug J, *Phase separation in disordered exclusion models*, 2000 Braz. J. Phys. 30 97
[25] Stinchcombe R, *Disorder in non-equilibrium models*, 2002 J. Phys.: Condens. Matter 14 1473
[26] Kafri Y and Nelson D R, *Sequence heterogeneity and the dynamics of molecular motors*, 2005 J. Phys.: Condens. Matter 17 S3871
[27] Tripathy G and Barma M, *Steady state and dynamics of driven diffusive systems with quenched disorder*, 1997 Phys. Rev. Lett. 78 3039
[28] Tripathy G and Barma M, *Driven lattice gases with quenched disorder: exact results and different microscopic regimes*, 1997 Phys. Rev. E 58 1911
[29] Fouladvand M E, Chaaboki S and Saalehi M, *Characteristics of the asymmetric simple exclusion process in the presence of quenched spatial disorder*, 2007 Phys. Rev. E 75 011127
[30] Juhász R, Santen L and Iglói F, *Partially asymmetric exclusion processes with quenched disorder*, 2005 Phys. Rev. Lett. 94 010601
[31] Harris A B, *Effect of random defects on the critical behaviour of Ising models*, 1974 J. Phys. C: Solid State Phys. 7 1671
[32] Kolomeisky A B, *Asymmetric simple exclusion model with local inhomogeneity*, 1998 J. Phys. A: Math. Gen. 31 1153
[33] Chou T and Lakatos G W, *Clustered bottlenecks in mRNA translation and protein synthesis*, 2004 Phys. Rev. Lett. 93 198101
[34] Dong J J, Schmittmann B and Zia R K P, *Towards a model for protein production rates*, 2007 J. Stat. Phys. 128 21
[35] Dong J J, Schmittmann B and Zia R K P, *Inhomogeneous exclusion processes with extended objects: the effect of defect locations*, 2007 Phys. Rev. E 76 051113
[36] Greulich P and Schadschneider A, *Phase diagram and edge effects in the ASEP with bottlenecks*, 2008 Physica A 387 1972
[37] Enaud C and Derrida B, *Sample-dependent phase transitions in disordered exclusion models*, 2004 Europhys. Lett. 66 83
[38] Nishinari K, Okada Y, Schadschneider A and Chowdhury D, *Intra-cellular transport of single-headed molecular motors KIF1A*, 2005 Phys. Rev. Lett. 95 118101
[39] Greulich P, Garai A, Nishinari K, Schadschneider A and Chowdhury D, *Intra-cellular transport by single-headed kinesin KIF1A: effects of single-motor mechano-chemistry and steric interactions*, 2007 Phys. Rev. E 75 041905
[40] Pierobon P, Mobilia M, Kouyos R and Frey E, *Bottleneck-induced transitions in a minimal model for intracellular motor*, 2006 Phys. Rev. E 74 031906
[41] Sornette D, 2000 *Critical Phenomena in Natural Sciences* (Berlin: Springer)
[42] Graf U, Henning H-J, Stange K and Wilrich P-T, 1987 *Formeln und Tabellen der angewandten Mathematischen Statistik* (Berlin: Springer)
[43] Popkov V and Schütz G M, *Steady-state selection in driven diffusive systems with open boundaries*, 1999 Europhys. Lett. 48 257
[44] Greulich P, 2006 *Diploma Thesis* Cologne University
[45] Mandekelow E-M, Stamer K, Vogel R, Thies E and Mandekelow E, *Clogging of axons by tau, inhibition of axonal traffic and starvation of synapses*, 2003 Neurobiol. Aging 24 1079
[46] Böhm K J, 2007 private communication

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