Journal of Statistical Physics, Vol. 110, Nos. 3–6, March 2003 (© 2003)

Effect of Detachments in Asymmetric Simple Exclusion Processes[1]

Nikolay Mirin[2] and Anatoly B. Kolomeisky[2]

Received October 3, 2001; accepted January 25, 2002

Asymmetric simple exclusion processes are important for understanding low-dimensional multi-particle dynamic phenomena. The effect of irreversible detachments of particles on dynamics of asymmetric simple exclusion processes is studied using analytical and computer simulation techniques. In the simplest model, where particles can only detach from a single site in the bulk of the system, a theory is presented and used to calculate explicitly phase diagrams and particle density profiles. The complexity of the phase behavior is discussed in terms of a recent domain-wall theory for driven lattice systems. The theoretical results qualitatively and quantitatively agree with computer Monte Carlo simulations.

KEY WORDS: Asymmetric simple exclusion processes; nonequilibrium phase transitions.

1. INTRODUCTION

Asymmetric simple exclusion processes (ASEPs) have attracted a lot of attention in recent years.[1–4] They are important in studies of one-dimensional multi-particle dynamic phenomena such as kinetics of biopolymerization,[5] reptation dynamics of entangled polymers,[6] diffusion through biological membrane channels,[7] and traffic problems.[8] ASEPs are lattice gas models where particles diffuse mainly in one direction and interact with hard-core exclusion. Some simple versions of these models have been solved exactly.[2–4]

[1] Dedicated to Michael E. Fisher with admiration and affection.

[2] Department of Chemistry, Rice University, Houston, Texas 77005-1892; e-mail: tolya@rice.edu

The characteristic feature of ASEPs is the occurrence of boundary-induced phase transitions between nonequilibrium stationary states that do not have analogs in equilibrium systems.[3,4,9] The microscopic nature of these phase transitions can be explained using a phenomenological domain-wall theory.[9] According to this theory, for the ASEP with open boundaries, the entrance, the exit and the bulk of the system enforce their own domains, i.e., homogeneous parts of the system with a uniform density and current. At any given time two domains coexist in the system, which implies the existence of a domain wall, or a shock, in the boundary region between these two domains. This domain wall is moving as a random walker with rates determined by currents and densities of domains, and in the limit of large times one of the domains is winning over the other. Thus, in a stationary state the domain wall will be found fluctuating near one of the boundaries. Note, however, that the domain wall picture fails in maximal-current phase, i.e., when the properties of the system are determined by bulk dynamics alone.[9] This theory has been applied successfully to explain the behavior of asymmetric exclusion processes with both complex dynamics and symmetry.[10–12]

Most theoretical investigations of asymmetric simple exclusion processes concentrate on translationally invariant systems where particles can always be found on the lattice.[3,4] However, some experimental observations, such as frequent irreversible detachments of particles during biological transport phenomena,[13] demand an extension of basic asymmetric simple exclusion processes. The effect of dissociation from linear tracks, which is important for the motion of motor proteins,[13,14] has been investigated recently in detail for the transport of single particles.[15] However, the effect of irreversible detachments on dynamics of multi-particle systems does not appear to have been studied yet in a systematic way.

In this paper, we study the effect of detachments in ASEPs and investigate, specifically, the simplest situation where irreversible dissociations may play a role in the dynamics of asymmetric simple exclusion processes. We consider a one-dimensional lattice model with N sites where particles enter the system with rate α, $0 \leqslant \alpha \leqslant 1$, (if there is no particle at the first site) and leave the system with rate β, $0 \leqslant \beta \leqslant 1$, (if there is a particle at the last site) as shown in Fig. 1. In this model each lattice site i, $1 \leqslant i \leqslant N$, is either occupied by a particle, or empty, and the only allowed motion is that of particles hopping from site i one step forward to site $i+1$ with unit rate if site $i+1$ is empty. In addition, particles can dissociate irreversibly with rate q from a bulk site k far away from boundaries (see Fig. 1), i.e., $1 \ll k \ll N$. Without detachments, our model is reduced to a totally asymmetric simple exclusion model for which the exact solution is known.[3,4] For this reason, the totally asymmetric simple exclusion model

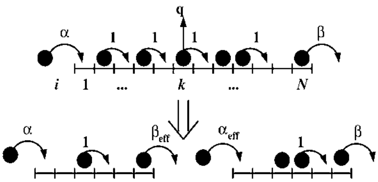


Fig. 1. The totally asymmetric exclusion model with irreversible detachments from a specific site in the middle of the lattice. The model can be mapped into two coupled totally asymmetric exclusion models without detachments (see text for details).

will be used in our analysis as a reference model, and the effect of detachments will be evaluated by comparison with the properties of this model.

A possible method of solution of ASEPs is based on the matrix-product ansatz,[2–4] which requires translational symmetry in the bulk of the system. However, in the present model the possibility of detachment from the single site in the bulk breaks this symmetry and thus only approximate solutions are possible. To investigate the effect of detachments on dynamics of asymmetric exclusion processes, we will present an approximate theory similar to one which has been used successfully for ASEPs with local inhomogeneity.[16] The results will be verified with Monte Carlo computer simulations.

Note that this system, as well as many other ASEPs, has a special particle-hole symmetry, where holes can be viewed as new "particles," while particles become new "holes." Then this model can be viewed as an asymmetric simple exclusion process, although with particles moving now from right to left, and with irreversible attachments at site k. Our analysis thus also describes the effect of irreversible associations on dynamics of ASEPs.

2. APPROXIMATE SOLUTIONS

2.1. General Scheme

To simplify the calculations we assume that the lattice size N is a large even number and we put the special site k from which dissociations are possible at the middle of the lattice, i.e., $k = N/2$. It is reasonable to expect that the exact position of this special site will not influence qualitatively our arguments, as long as this site is far away from the boundaries.[16] Before presenting the solution for the asymmetric exclusion model with irreversible detachments, we review some results for the totally asymmetric exclusion model without dissociations, which will be used in the present theory.

The totally asymmetric simple exclusion model at the thermodynamic limit $N \to \infty$ can be found in three stationary phases depending on the values of the entrance rate α and the exit rate β. When $\alpha \geqslant 1/2$ and $\beta \geqslant 1/2$, a maximal-current (mc) phase dominates, for which

$$\begin{aligned} \rho_1 &= 1 - \frac{1}{4\alpha}, & \rho_N &= \frac{1}{4\beta}, \\ \rho_{\text{bulk}} &= 1/2, & J &= 1/4, \end{aligned} \tag{1}$$

where ρ_i is the particle density at site i, ρ_{bulk} is the density in the bulk of the system and J is the stationary particle current. The conditions $\alpha > \beta$ and $\beta < 1/2$ define a high-density (hd) phase for which

$$\begin{aligned} \rho_1 &= 1 - \frac{\beta(1-\beta)}{\alpha}, & \rho_N &= 1-\beta, \\ \rho_{\text{bulk}} &= 1-\beta, & J &= \beta(1-\beta). \end{aligned} \tag{2}$$

A low-density (ld) phase exists when $\alpha < \beta$ and $\alpha < 1/2$. This phase can be described by

$$\begin{aligned} \rho_1 &= \alpha, & \rho_N &= \frac{\alpha(1-\alpha)}{\beta}, \\ \rho_{\text{bulk}} &= \alpha, & J &= \alpha(1-\alpha). \end{aligned} \tag{3}$$

The special site k, from which irreversible detachments are possible, breaks the original translational invariance of the totally asymmetric exclusion model. However, it also divides the lattice of size N into two translationally invariant sublattices of size $N/2$. Thus, we can think of our system as two totally asymmetric exclusion models coupled at the site k (see Fig. 1), and stationary particle currents through sublattices are related by their special condition. According to this requirement, the current through the right lattice should be equal to the current through the left lattice minus the current lost due to irreversible dissociations from site k. Thus we can use known results for the totally asymmetric exclusion model for each sublattice in order to determine the properties for the overall system. A similar approach has been used successfully in the investigation of the asymmetric simple exclusion model with local inhomogeneity.[16]

Following the idea that the system with detachments can be viewed as two coupled lattices without detachments, the left sublattice will have the entrance rate α and the effective exit rate β_{eff}, which can be defined as

$$\beta_{\text{eff}} = q + (1 - \rho_{k+1}). \tag{4}$$

This expression reflects the fact that particles can leave the left lattice in two ways: they can move into the right lattice with rate 1 (if there is no particle at the site $k+1$), or they can dissociate irreversibly with rate q. Similarly, the right sublattice will have the exit rate β and the effective entrance rate α_{eff}, which is defined as

$$\alpha_{\mathrm{eff}} = \rho_k. \tag{5}$$

By defining the effective entrance and exit rates through expressions (4) and (5), it is assumed that particles can occupy the two neighboring sites k and $k+1$ independently from each other, i.e., the probability that particles occupy sites k and $k+1$ simultaneously is equal to the product of the probabilities that particles occupy each site independently. Obviously, this is not the case in real systems.

2.2. Phase Diagram and Density Profiles

Since each sublattice can be viewed independently as a totally asymmetric simple exclusion model, it may exist in three different stationary states. There are then 9 possible phases for the overall asymmetric exclusion model with irreversible detachments. However, because particles can dissociate from site k, the current in the right subsystem cannot reach its maximal value, and thus three phases which support the maximal current in the right lattice, i.e., low-density/maximal-current (ld/mc), high-density/maximal-current (hd/mc) and maximal-current/maximal-current (mc/mc), do not exist. The conditions for existence of the other 6 phases can be found using the properties of the totally asymmetric exclusion model and expressions (4) and (5).

The maximal-current/high-density (mc/hd) phase is determined by the following general conditions

$$\begin{aligned} \alpha > 1/2, \qquad & \beta_{\mathrm{eff}} > 1/2, \\ \alpha_{\mathrm{eff}} > \beta, \qquad & \beta < 1/2. \end{aligned} \tag{6}$$

In addition, densities at sites k and $k+1$ are given by

$$\rho_k = \frac{1}{4\beta_{\mathrm{eff}}}, \qquad \rho_{k+1} = 1 - \frac{\beta(1-\beta)}{\alpha_{\mathrm{eff}}}. \tag{7}$$

However, we would like to describe the conditions for the existence of this phase only in terms of parameters α, β and q. From Eqs. (4), (5) and (7), we derive the effective exit rate from the left lattice and the effective entrance rate to the right lattice, namely,

$$\alpha_{\text{eff}} = \frac{(1-2\beta)^2}{4q}, \qquad \beta_{\text{eff}} = \frac{q}{(1-2\beta)^2}. \tag{8}$$

Because these rates should satisfy the general conditions (6), we finally obtain the parameter ranges for α, β and q,

$$\frac{1-\sqrt{2q}}{2} < \beta < \frac{1+q-\sqrt{(1+q)^2-1}}{2}, \qquad \alpha > 1/2, \tag{9}$$

for the case in which the asymmetric simple exclusion model with irreversible detachments can be found in the mc/hd phase.

Similar calculations can be performed for the maximal-current/low-density (mc/ld) phase, which exists when

$$\begin{aligned} \alpha > 1/2, \qquad & \beta_{\text{eff}} > 1/2, \\ \alpha_{\text{eff}} < \beta, \qquad & \alpha_{\text{eff}} < 1/2. \end{aligned} \tag{10}$$

Particle densities at special sites k and $k+1$ are given by

$$\rho_k = \frac{1}{4\beta_{\text{eff}}}, \qquad \rho_{k+1} = \alpha_{\text{eff}}. \tag{11}$$

Combining Eq. (11) with Eqs. (4) and (5) leads to the following expressions for the effective rates

$$\alpha_{\text{eff}} = \frac{1+q-\sqrt{(1+q)^2-1}}{2}, \qquad \beta_{\text{eff}} = \frac{1+q+\sqrt{(1+q)^2-1}}{2}. \tag{12}$$

Substituting these results into Eq. (10) yields the following parameter ranges for mc/ld phase

$$\beta > \frac{1+q-\sqrt{(1+q)^2-1}}{2}, \qquad \alpha > 1/2. \tag{13}$$

The case with the high-density/high-density (hd/hd) phase is more complicated. It can be generally described by the following conditions

$$\begin{aligned} \alpha > \beta_{\text{eff}}, \qquad & \beta_{\text{eff}} < 1/2, \\ \alpha_{\text{eff}} > \beta, \qquad & \beta < 1/2, \end{aligned} \tag{14}$$

and

$$\rho_k = 1 - \beta_{\text{eff}}, \qquad \rho_{k+1} = 1 - \frac{\beta(1-\beta)}{\alpha_{\text{eff}}}. \tag{15}$$

Substituting this last equation into (4) and (5) yields the effective entrance and exit rates

$$\alpha_{\text{eff}} = \frac{1-q+\sqrt{(1-q)^2-4\beta(1-\beta)}}{2}, \qquad \beta_{\text{eff}} = \frac{1+q-\sqrt{(1-q)^2-4\beta(1-\beta)}}{2}. \tag{16}$$

Comparing these expressions with the inequalities (14) we obtain for $\alpha > 1/2$

$$\beta < \frac{1-\sqrt{1+4(1-\alpha)(q-\alpha)}}{2}, \qquad q < \alpha, \tag{17}$$

while for $\alpha < 1/2$

$$\beta < \frac{1-\sqrt{2q}}{2}. \tag{18}$$

Equations (17) and (18) determine the conditions for the existence of the hd/hd phase. From the last equation we can also conclude that this phase exists only for $q < 1/2$.

The high-density/low-density (hd/ld) phase is defined by

$$\begin{aligned} \alpha > \beta_{\text{eff}}, \qquad & \beta_{\text{eff}} < 1/2, \\ \alpha_{\text{eff}} < \beta, \qquad & \alpha_{\text{eff}} < 1/2. \end{aligned} \tag{19}$$

Particle densities at sites k and $k+1$ are given by

$$\rho_k = 1 - \beta_{\text{eff}}, \qquad \rho_{k+1} = \alpha_{\text{eff}}. \tag{20}$$

However, in contrast to the case of the previous phases, comparison of these equations with (4) and (5) shows that conditions (19) cannot be satisfied for any values of the parameters α, β and q. Thus the hd/ld phase does not exist at stationary conditions.

For the low-density/high-density (ld/hd) phase, which is defined for

$$\begin{aligned} \alpha < \beta_{\text{eff}}, \qquad & \alpha < 1/2, \\ \alpha_{\text{eff}} > \beta, \qquad & \beta < 1/2, \end{aligned} \tag{21}$$

and

$$\rho_k = \frac{\alpha(1-\alpha)}{\beta_{\mathrm{eff}}}, \qquad \rho_{k+1} = 1 - \frac{\beta(1-\beta)}{\alpha_{\mathrm{eff}}}, \tag{22}$$

we can perform similar calculations, and find that this phase exists when

$$\frac{1-\sqrt{1+4(1-\alpha)(q-\alpha)}}{2} < \beta < \frac{1+q-\sqrt{(1+q)^2-4(1-\alpha)(1-\alpha)}}{2}, \quad \alpha < 1/2. \tag{23}$$

Finally, for the low-density/low-density (ld/ld) phase, for which

$$\begin{aligned} \alpha < \beta_{\mathrm{eff}}, \qquad & \alpha < 1/2, \\ \alpha_{\mathrm{eff}} < \beta, \qquad & \alpha_{\mathrm{eff}} < 1/2, \end{aligned} \tag{24}$$

and

$$\rho_k = \frac{\alpha(1-\alpha)}{\beta_{\mathrm{eff}}}, \qquad \rho_{k+1} = \alpha_{\mathrm{eff}}, \tag{25}$$

the existence conditions are given by

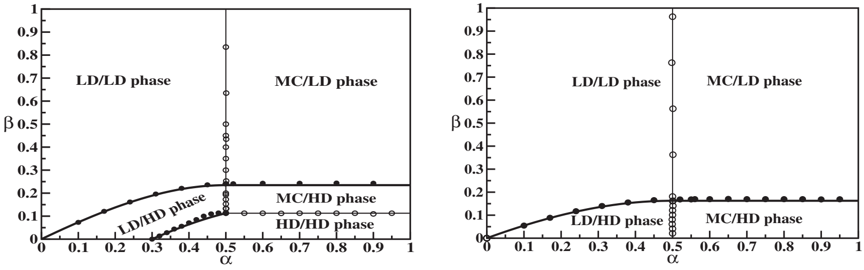
$$\beta > \frac{1+q-\sqrt{(1+q)^2-4(1-\alpha)(1-\alpha)}}{2}, \qquad \alpha < 1/2. \tag{26}$$

Thus the phase diagram consists of four (for $q > 1/2$) or five (for $q < 1/2$) stationary phases, as shown in Fig. 2. Density profiles in all phases can be easily constructed from the corresponding density profiles at each sublattice using the exact expressions given in refs. 2 and 3.

3. MONTE CARLO SIMULATIONS AND DISCUSSION

In the limit of $q \to 0$, the present model with detachments reduces to the totally asymmetric exclusion model, and it can be easily checked that the results obtained using our approximate theory agree perfectly with the known exact solution.[3] To investigate the validity of our theoretical approach for general values of q, we performed Monte Carlo computer simulations.

In our computer simulations we considered a lattice with $N = 200$ sites. Since our theory is valid only at the thermodynamic limit $N \to \infty$, there are deviations from theoretical predictions for finite-size lattices;



(a) (b)

Fig. 2. Phase diagrams for the asymmetric exclusion model with irreversible detachments: (a) for $q = 0.3$; (b) for $q = 0.7$. Solid lines correspond to results obtained from approximate solutions. Thick solid lines indicate the position of first-order phase boundaries, while thin solid lines denote second-order phase transitions. The circles show the results from Monte Carlo computer simulations. Filled circles show first-order phase boundaries, and empty circles display second-order phase boundaries.

however, as we checked for the totally asymmetric simple exclusion model, $N = 200$ is large enough to neglect these deviations. Similar lattice sizes have been used successfully in computer analysis of local inhomogeneities in ASEPs.[16] In addition, in our simulations we assumed that the system reaches a stationary state when more than 20000 particles pass through the lattice starting from the initial moment. Each density profile was calculated by averaging over 10^9 Monte Carlo steps. Boundaries in phase diagrams were determined by analyzing the changes in density profiles in corresponding sublattices: see Fig. 4.

For $q < 1/2$, our approximate theory predicts that there are five possible stationary phases, while for $q > 1/2$ the number of available phases decreases by one. We also predict that there are two types of phase transitions in the system: first-order phase transitions (thick solid lines in Fig. 2) involve a jump in the particle density in one of the sublattices, while for second-order phase transitions (thin solid lines in Fig. 2) the density profiles change continuously. These results are well supported by extensive computer simulations as illustrated in Fig. 2. The phase boundaries obtained from Monte Carlo simulations are in excellent agreement with theoretically calculated boundaries, although there are small deviations at first-order phase boundaries.

Similarly, as shown in Fig. 3, there is a very good qualitative and quantitative agreement between the density profiles calculated from our approximate approach and those obtained by Monte Carlo simulations. However, there are differences in the region near the special site k from which irreversible detachments may occur. This is a consequence of the

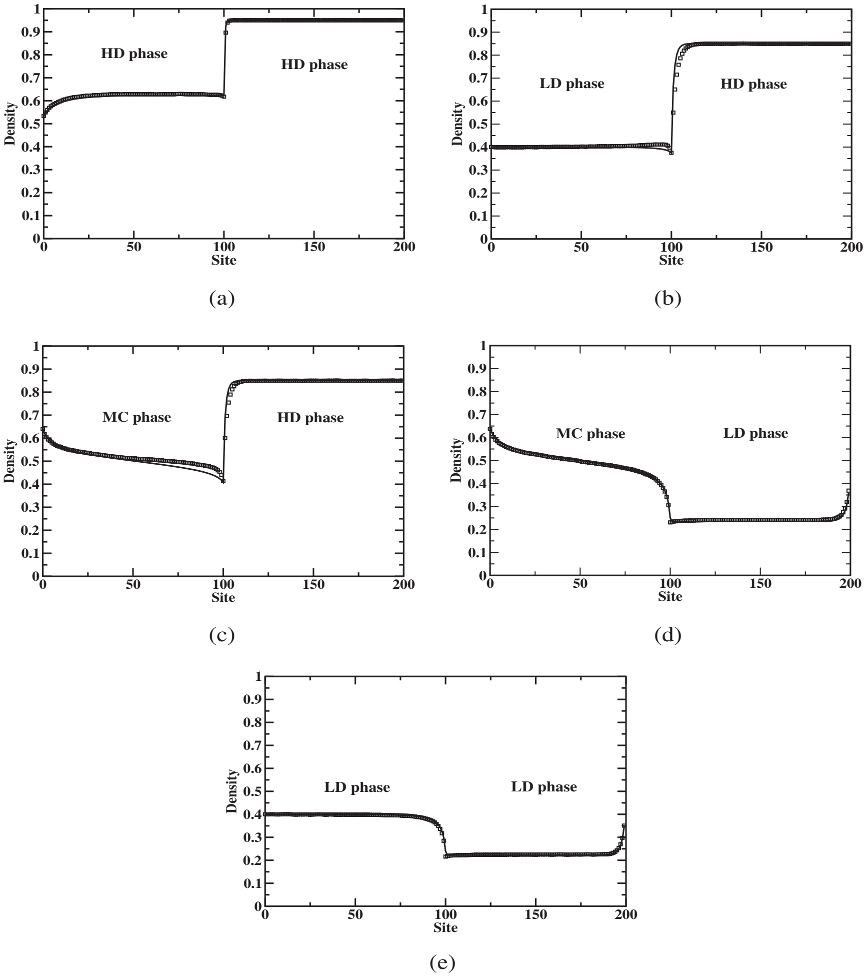


Fig. 3. Density profiles for the system of size $N = 200$ with $q = 0.3$. The squares indicate the Monte Carlo simulation results. Solid lines show the present theoretical results. Equations (39), (43) and (44) of ref. 2 have been used in the calculation of approximate density profiles. Monte Carlo densities are obtained by averaging over 10^9 Monte Carlo steps. (a) hd/hd phase with $\alpha = 0.5$, $\beta = 0.05$; (b) ld/hd phase with $\alpha = 0.4$, $\beta = 0.15$; (c) mc/hd phase with $\alpha = 0.7$, $\beta = 0.15$; (d) mc/ld phase with $\alpha = 0.7$, $\beta = 0.5$; (e) ld/ld phase with $\alpha = 0.4$, $\beta = 0.5$.

approximation which neglects the density correlations near the special site k. In real systems these correlations are significant and determine the behavior of the system near the boundary between two sublattices. This effect is clearly seen in the failure of our theory to locate exactly the positions of phase transitions (see Fig. 4), especially first-order phase boundaries.

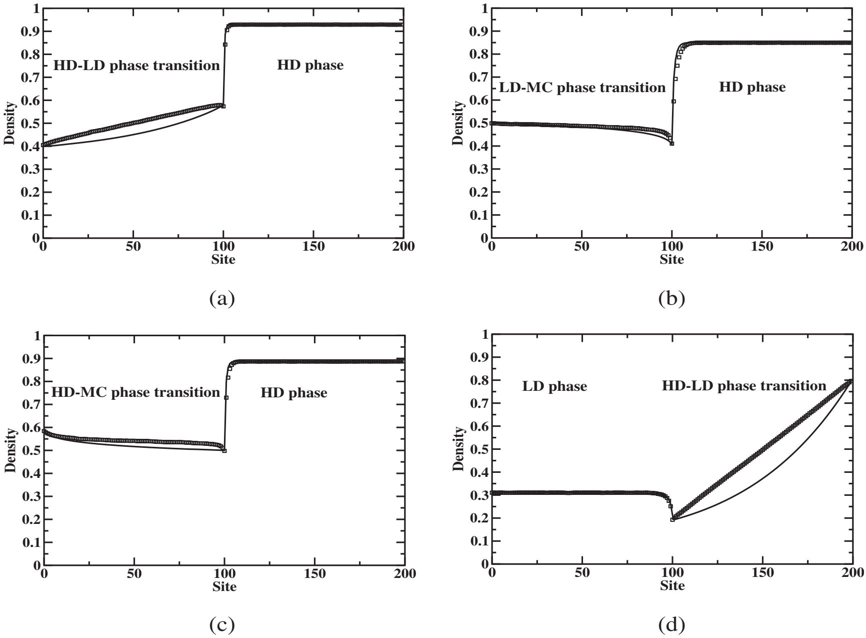


Fig. 4. Density profiles near phase boundaries for the system of size $N = 200$ with $q = 0.3$. The squares indicate the Monte Carlo simulation results. Solid lines show the present theoretical results. Equations (39), (43) and (44) of ref. 2 have been used in the calculation of the approximate density profiles. Monte Carlo densities are obtained by averaging over 10^9 Monte Carlo steps. (a) $\alpha = 0.4$, $\beta = 0.071$; (b) $\alpha = 0.5$, $\beta = 0.15$; (c) $\alpha = 0.6$, $\beta = 0.113$; (d) $\alpha = 0.31$, $\beta = 0.196$.

Our approximate theory is based on the representation of the system with irreversible detachments as two coupled totally asymmetric exclusion models. This suggests that there are 9 possible stationary phases; however, three phases cannot occur due to the fact that the particle current in the right sublattice cannot reach its maximal value. In addition, our theoretical calculations, supported by computer simulations, indicate that the hd/ld phase also cannot be found at stationary conditions. However, the reason for this is not understood. To explain the microscopic nature of this phenomenon we invoke the domain-wall theory.[9] At large times, the domain walls will be found near corresponding boundaries of sublattices, as shown in Fig. 5. In all existing stationary phases, one or two domain walls are found near the boundary between sublattices, however in the possible hd/ld phase the region near site k does not contain the domain walls. This means that any density fluctuation in this region will destroy the density gradient between the left and the right sublattices and eventually, at large

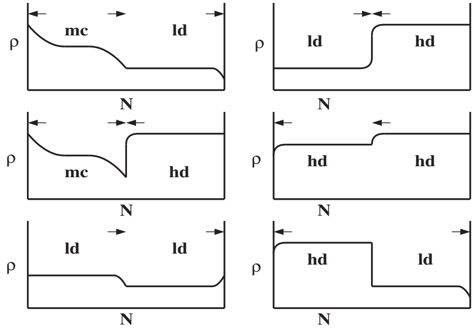


Fig. 5. Schematic density profiles for possible stationary phases in the asymmetric exclusion model with irreversible detachments. Arrows indicate the approximate positions and directions of the motion of domain walls.

times, this phase will not occur. In contrast, all other phases will be stable with respect to any density fluctuation.

4. SUMMARY AND CONCLUSIONS

We investigated the effect of irreversible detachments of particles on the dynamics of asymmetric simple exclusion processes. We specifically considered the simple model with only dissociations from a single site in the bulk of the system. The model was solved analytically using a simple approximate theory. Our method is based on two assumptions. First, we mapped our model with irreversible detachments into two coupled totally asymmetric exclusion processes without detachments. In the second assumption, we treated the particle occupancies of site k (where detachments take place) and site $k+1$ in a mean-field fashion, i.e., we neglected the density correlations near the boundary between two sublattices. Using these assumptions we showed that irreversible detachments, even from the single site far away from the boundaries, strongly influence the density profiles and phase behavior in ASEPs. These results are generally supported by computer Monte Carlo simulations. Some observed deviations between theory and computer simulations are attributed to the mean-field assumption for densities near the special site with detachments. The microscopic origins of complex phase behavior was analyzed using a phenomenological domain-wall theory. This analysis concludes that existing stationary phases should contain the domain walls in the boundary region between sublattices.

Due to particle-hole symmetry, our analytical and computational analysis is also valid for the description of effects of attachments on the dynamics of ASEPs. This leads to an interesting problem of how *both* attachments and detachments may influence the dynamics of asymmetric simple exclusion processes. It is reasonable to suggest that our simple approximate method, along with computer simulations, is a promising approach to tackle these complex problems of low-dimensional multi-particle transport.

ACKNOWLEDGMENTS

The critical reading of the manuscript by Prof. M. Robert is highly appreciated. The financial support of the Camille and Henry Dreyfus New Faculty Awards Program (under Grant NF-00-056) is gratefully acknowledged.

REFERENCES

1. B. Schmittmann and R. K. P. Zia, in *Phase Transitions and Critical Phenomena*, C. Domb and J. Lebowitz, eds. (Academic, New York, 1995), Vol. 17.
2. B. Derrida, M. R. Evans, V. Hakim, and V. Pasquier, *J. Phys. A: Math. Gen.* **26**:1493 (1993).
3. B. Derrida, *Phys. Rep.* **301**:65 (1998).
4. G. M. Schütz, in *Phase Transitions and Critical Phenomena*, C. Domb and J. Lebowitz, eds. (Academic, London, 2000), Vol. 19.
5. J. T. MacDonald, J. H. Gibbs, and A. C. Pipkin, *Biopolymers* **6**:1 (1968).
6. G. M. Schütz, *Europhys. Lett.* **48**:623 (1999).
7. T. Chou, *Phys. Rev. Lett.* **80**:85 (1998).
8. V. Popkov, L. Santen, A. Schadschneider, and G. M. Schütz, *J. Phys. A: Math. Gen.* **34**:L45 (2001).
9. A. B. Kolomeisky, G. M. Schütz, E. B. Kolomeisky, and J. P. Straley, *J. Phys. A: Math. Gen.* **31**:6911 (1998).
10. V. Popkov and G. M. Schütz, *Europhys. Lett.* **48**:257 (1999).
11. C. Pigorsch and G. M. Schütz, *J. Phys. A: Math. Gen.* **33**:7919 (2000).
12. J. S. Hager, J. Krug, V. Popkov, and G. M. Schütz, *Phys. Rev. E* **63**:056110 (2001).
13. M. J. Schnitzer, K. Visscher, and S. M. Block, *Nature Cell Biology* **2**:718 (2000).
14. M. E. Fisher and A. B. Kolomeisky, *Proc. Natl. Acad. Sci USA* **98**:7748 (2001).
15. A. B. Kolomeisky and M. E. Fisher, *Physica A* **279**:1 (2000).
16. A. B. Kolomeisky, *J. Phys. A: Math. Gen.* **31**:1153 (1998).