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Phase Diagram of a Partially Asymmetric Exclusion Model with Open Boundaries: Numerical Study

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The effects of the right (left) jump p (q) and the probability of jumping At on densities, current and phase diagrams in the open boundaries of one dimensional partially asymmetric models are studied using the mean-field approximation and numerical simulations. However, for $p \neq q$ the system exhibits a first order transition between the low and high density phases, while for $p = q$ such transition disappears. Furthermore, when the rate of the injected particles at the left, α_1, is equal to the right one, α_2, and the rate of the removed particles at the left, β_1, is equal to the right one, β_2, the region of maximal current phase disappears. While in the general case $\alpha_1 \neq \alpha_2$ and $\beta_1 \neq \beta_2$, three phases are encountered namely a low density phase, a high density phase and a maximal current phase. The increase of At favours the first order transition and reduces the region of the maximal current phase. However, when At is sufficiently small the mean-field theory is in excellent agreement with simulations.

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I. Introduction

The one-dimensional asymmetric exclusion model (AEM) is a simple example for diffusion of interacting particles [1,2]. It is closely related to various other phenomena such as the fluctuations of tagged particles [3,4], the microscopic structure of shocks [5,6], interface growth [7,8], driven lattice gases with hard core repulsion, which provide models for the diffusion of particles through narrow pores and for hopping conductivity [9], and can also be formulated as traffic jam or queuing problems [3]. These models describe stochastic processes far away from thermal equilibrium, for which reason their stationary probability distribution cannot generally be derived from an energy function. For this reason different techniques are needed in order to determine the stationary properties. An exact method which proved to be very successful is the so-called matrix product formalism [10-21]. This formalism can be regarded as a generalisation of the stationary states with a product measure in which products of numbers are replaced by products of non-commutative algebraic objects. By representing these objects in terms of matrices, the stationary state and equal-time correlation functions can be derived exactly. So far this technique has been applied mainly to systems with sequential dynamics (continuous time evolution). However, many systems, are defined by parallel dynamics (discrete time evolution), for example traffic models [22-24], rather than sequential updates [25]. Exclusion models can be divided into four classes according to the dynamics (parallel or sequential) and the boundary conditions (periodic with conservation of the number of particles and (possibly) a defect or open with injection and absorption of particles). According to this classification we call them p-p models (parallel, periodic), p-o models (parallel, open), s-p models (sequential, periodic) and s-o models (sequential, open). A s-p model with a defect has been studied numerically by Janowsky ancl Lebowitz [26], without defect it was solved by a Bethe ansatz by Gwa and Spohn [27]. The s-o model was studied numerically by Krug [28], later the exact solutioll with the full phase diagram was found [14, 29]. The solution for the fully asymmetric process where particles hop only in one direction, using a recursion relations [30] and a matrix formulation [31-33] for a steady state is well known. The partially asymmetric process where particles are allowed to hop into both directions, but with different rates, is a generalisation of the fully asymmetric process.

In the present work we study a partially asymmetric one-dimensional exclusion model with open boundary conditions. In this model, particles hop in both directions but with different rates. At the right (left) end of the lattice, particles are injected with a rate $\alpha_2\Delta t$ ($\alpha_1\Delta t$) and removed with a rate $\beta_2\Delta t(\beta_2\Delta t)$. The parameter At allows us to interpolate between the cases of fully parallel At = 1) and random sequential updates (At $\to$ 0). For infinitesimal At such a model has been resolved exactly [15] using the algebraic ansatz introduced in [13] for a large lattice. Besides, also in the Fock representation of quadratic algebra, the problem of partially asymmetric diffusion with open boundaries has been studied [16]. With this representation, the density around the centre of the chain has a simple expression in terms of the parameters of the problem and it coincides with the mean-field results.

Our aim is to study the effects of the right (left) jump p (q) and the probability of jumping At on densities, current and phase diagram of such model using mean-field approximation (MFA) and numerical simulations.

The paper is organised as follows: In section II, the model is defined. The section III contains the methods: mean-field approximation and the numerical simulation. Results and discussions are given in section IV. Section V contains the conclusions.

II. Model

We consider a one-dimensional lattice of length N. Each lattice site can be occupied by one particle or, can be empty. Hence the state of the system is defined by a set of occupation numbers $\tau_1, \tau_2, \ldots, \tau_N$ while $\tau_i = 1$ (τ_i = 0) means that site i is occupied (empty). The particles are assumed to move stochastically on the lattice. During a time interval At, they hop to the right nearest neighbour site if this site is empty with a rate, and they hop to the left nearest neighbour site if this site is empty with a rate $q\Delta t(q = 1 - p)$. particles are injected with a rate $\alpha_2\Delta t(\alpha_1\Delta t)$ and extracted with a rate $\beta_2\Delta t(\beta_1\Delta t)$.

Thus, if the system has the configuration $\tau_1, \tau_2, \ldots, \tau_N$ at time t it will change to the following:

For $1 < i < N$

$$\tau_i(t+\mathrm{At})=1, \tag{1}$$

with probability ***Pi.***

$$\tau_i(t+\mathrm{At})=0, \tag{2}$$

with probability ***1 – Pi.*** where

$$\begin{aligned}P_i=\tau_i(t)+[(p\tau_{i-1}(t)+q\tau_{i+1}(t))(1-\tau_i(t))\\ -p\tau_i(t)(1-\tau_{i+1}(t))-q\tau_i(t)(1-\tau_{i-1}(t))]\Delta t\end{aligned} \tag{3}$$

For i = 1,

$$\tau_1(t+\mathrm{At}) = 1, \tag{4}$$

with probability P_1.

$$\tau_i(t+\mathrm{At})=0, \tag{5}$$

with probability $1-P_1$ where

$$P_1=\tau_1(t)+[(\alpha_1+q\tau_2(t))(1-\tau_1(t))-\tau_1(t)(p(1-\tau_2(t))+\beta_1)]\Delta t \tag{6}$$

For i $=N$,

$$\tau_N(t+\mathrm{At}) = \mathbf{1}, \tag{7}$$

with probability P_N.

$$\tau_N(t+\mathrm{At}) = 0, \tag{8}$$

with probability $1-P_N$. where

$$\begin{aligned}P_N=\tau_N(t)+[(\alpha_N \;\mathrm{t}\; p\tau_{N-1}(t))(1-\tau_N(t))\\ -q\tau_N(t)(1-\tau_{N-1}(t))+\beta_2\tau_N(t)]\Delta t\end{aligned} \tag{9}$$

These equations define the master equations of our system. The dynamic of the system is then done by the following equations: For **1 < i <** N,

$$\begin{aligned}\frac{\Delta<\tau_i>}{\mathrm{At}}=<p(1-\tau_i)\tau_{i-1}+q(1-\tau_i)\tau_{i+1}>\\ -<p\tau_i(1-\tau_{i+1})\;\mathrm{t}\;q\tau_i(1-\tau_{i-1})>\end{aligned} \tag{10}$$

For i = 1.

$$\frac{\Delta<\tau_1>}{\mathrm{At}}=<\alpha_1(1-\tau_1)\;\mathrm{t}\;q(1-\tau_1)\tau_2>-<p\tau_1(1-\tau_2)+\beta_1\tau_1> \tag{11}$$

For $i = N$

$$\frac{\Delta < \tau_N >}{\Delta t} =< \alpha_2(1 - \tau_N) + p(1-\tau_N)\tau_{N-1} > - < \beta_2\tau_N + q\tau_N(1-\tau_{N-1}) > . \quad (12)$$

Once these relations are written, one can calculate the time evolution of any quantity of interest. The problem however, is that the computation of the one point functions $< \tau_i >$ requires the knowledge of the two point functions $< \tau_i >< \tau_j >$, which themselves require the knowledge of higher correlation functions, this makes the problem intractable. Therefore, we use a mean-field approximation and numerical simulations in order to solve the model.

Then the quantities of interest are the average occupation of the middle site:

$$\rho =< \tau_{(N+1)/2} > \quad (13)$$

and the current through the middle site:

$$J =< p\tau_{(N+1)/2}(1 - \tau_{(N+1)/3}) - q\tau_{(N+1)/2}(1 - \tau_{(N-1)/2}) > \quad (14)$$

since the current through the bound $i, i+1 (i, i-1)$ is simply $J_+ =< p\tau_i(1-\tau_{i+1})>$ ($J_- =< q\tau_i(1-\tau_{i-1})>$), because during a time Δt, the probability that a particle jumps from i to $i+1$ (i to $i-1$) is $p\tau_i(1-\tau_{i+1})\Delta t\,(q\tau_i(1-\tau_{i-1})\Delta t)$, then the global current is $J = p\tau_i(1-\tau_{i+1}) - q\tau_i(1-\tau_{i-1})\Delta t$.

III. Methods

III-1. Mean-field approximation (MFA)

The mean field approximation ignores correlations, then we replace $<\tau_i\tau_j>$ by $<\tau_i><\tau_j>$ in the dynamic of the system, this dynamic is given in MFA by:

$$\begin{aligned}\rho_i(t+1) =< \tau_i(t+1) >=< \tau_i(t) > +(1 - \tau_i(t)[p < \tau_{i-1}(t) > + q < \tau_{i+1}(t) >] \\ -(\tau_i(t)[p(1- < \tau_{i+1}(t)) > + q(1- < \tau_{i-1}(t) >)]\end{aligned} \quad (15)$$

$$\begin{aligned}\rho_1(t+1) =< \tau_1(t+1) >=< \tau_1(t) > +(1 - \tau_1(t)[\alpha_1 + q < \tau_2(t) >] \\ -(\tau_1(t)[p(1- < \tau_2(t)) > + \beta_1]\end{aligned} \quad (16)$$

$$\begin{aligned}\rho_N(t+1) =< \tau_N(t+1) >=< \tau_N(t) > +(1 - \tau_N(t)[\alpha_2 + p < \tau_{N-1}(t) >] \\ -(\tau_N(t)[q(1- < \tau_{N-1}(t)) > + \beta_2]\end{aligned} \quad (17)$$

and the current through the site i becomes:

$$J =< p < \tau_i > (1- < \tau_{i+1} >) - q < \tau_i > (1- < \tau_{i-1} >) > \quad (18)$$

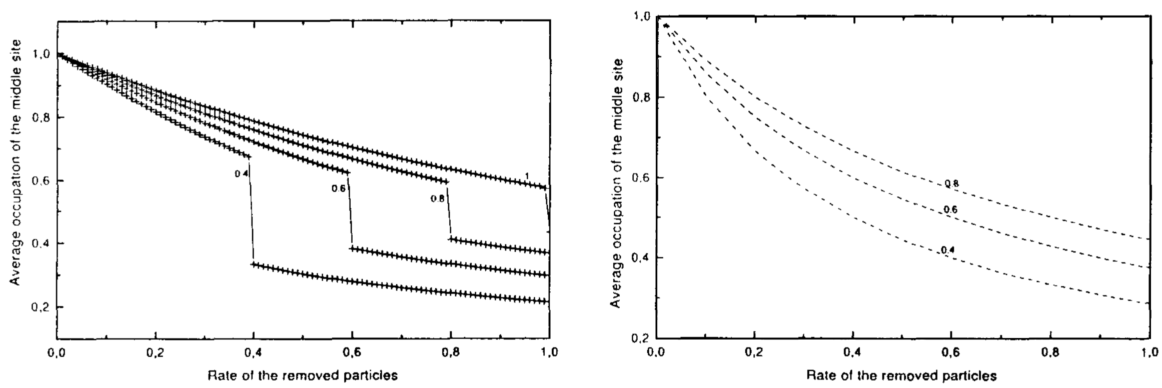
III-2. Numerical simulation

In our simulations the rule described above is updated in parallel, i.e., during one updating procedure the new particle positions do not influence the rest and only previous positions have to be taken into account. During each time step, each particle moves one site unless the site on its right-hand side is occupied by another particle. In order to compute theaverage of any parameter $w(<w>)$, the values of $w(t)(t = n\Delta t$, n is an integer) obtained from 2.10^5 to 10^6 time steps are averaged. Starting the simulations from random configurations, the system reaches a stationary state after a sufficiently large time steps. Furthermore, for At = 1 we rejoin the fully parallel dynamics and for At $\rightarrow$ 0 the dynamics becomes sequential, i.e. only one particle can hop at the time. In fact the jumping rate At has for effect to investigate the difference between parallel process and the sequential one which in general produce weaker correlation. In that sense, we be interested by the influence of jumping rate on the different quantities of interest.

IV. Results and discussions

IV-l. Particular case: $\alpha_1 = \alpha_2 = \alpha$ and $\beta_1 = \beta_2 = \beta$

Using mean-field approximation, we have studied both cases p $\neq q$ and $p = q$. The dependence on the rate of removed particles β of the average occupation of the middle site is given in Fig. la for $p \neq q$ and lb for p = q, for various values of rate of injection of particles α. In the first case (p $\neq q$), the system exhibits a first order transition between a low and a high density phases at $\alpha = \beta$. However, for p $= q$ the fist order transition between the low and a high density phases disappears. In order to complete this study, the current J through the middle site is given in Fig. 2 for the two cases p $= q$ and p $\neq q$. In the first case the right current passes through a maximum (curve at the top), while in the cases of p $\neq q$, the current passes through a maximum and present a peak at $\alpha = \beta$; this peak correspond to the first order transition. This phenomenon reveals the presence of shock between a region of low density and a region of high density.



(a) (b)

FIG. 1. The mean-field variation of the average occupation of the middle site as a function of the rate of removed particles β for N = 101. The number accompanying each curve denotes the value of the rate of the injected particles α. (a) p = 0.8, (b) y = 0.5.

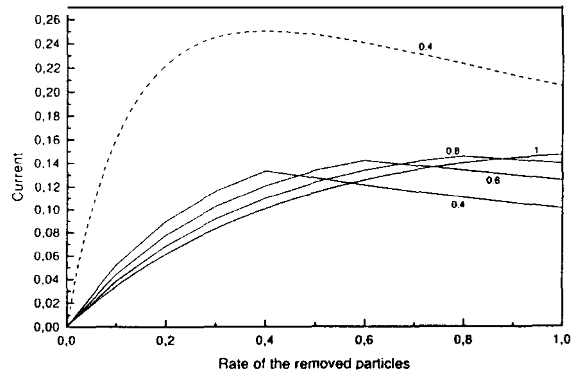
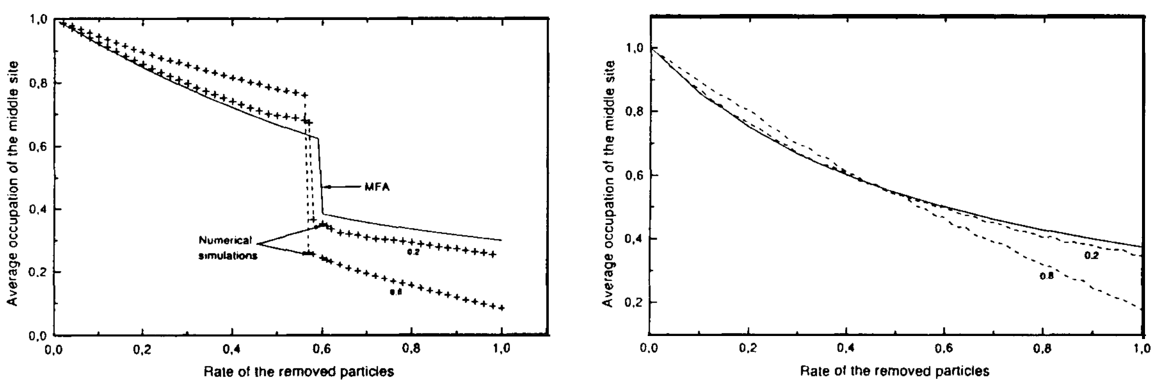


FIG. 2. The mean-field variation of the average current through the middle site as a function of the rate of removed particles β for N = 101. p = 0.5 (dashed line) and $p=$ 0.8 (solid lines). The number accompanying each curve denotes the value of the rate of injected particles α.



(a) (b)

FIG. 3. The simulation results of the variation of the average occupation of the middle site as a function of the rate of removed particles β for N = 101. The solid line denotes the mean-field approximation. The number accompanying each curve denotes the value of jumping rate At. (a) $p=$ 0.8, (b) $p=$ 0.5.

In order to examine the effect of the jumping rate At upon the average occupation of the middle site, the variation of the density as a function of the rate of extracted particles is studied by using the numerical simulations in the both cases $p \neq q$ (Fig. 3a) and $p = q$ (Fig. 3b). It is clear that the transition value β_c between the high and low density phases depend on the values of At and $\beta_c(\Delta t) < \beta_c$ ***(MFA),*** indeed $\beta_c(\Delta t)$ increases when decreasing At. The mean-field result, for which the first-order transition is being at the point $\alpha = \beta$, is also plotted (curve at the top), then $\beta_c(\Delta t) < \alpha$. However, for $p = q$ (Fig. 3b) the first order transition between low and high density phases disappears. By

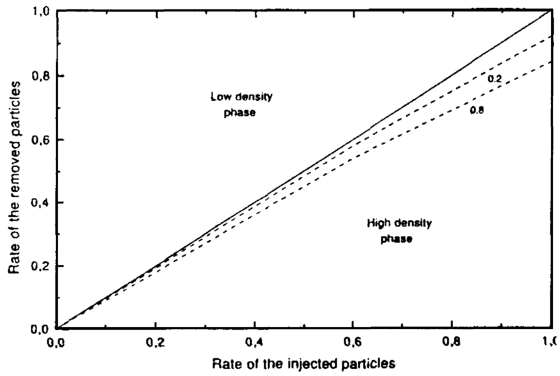


FIG. 4. Phase diagram in the (α,β) plane, for $N=101$ and p = 0.8. The solid line correspond to mean-field approximation, while dashed lines correspond to numerical simulations. The number accompanying each curve denotes the value of jumping rate At.

studying the variation of density ρ and the current J for other values of α and for p = q case, we complete the phase diagram (α,β) (Fig. 4) which contains two phases low density and high density separated by a first order transition line where the current reaches its maximal value. However, in our simulations when At decreases the results tend to MFA ones (Fig. 3a and 3b), since the correlations between sites are established by the move of particles, then when At decreases the correlations decrease.

In conclusion, for $p\neq q$, the first order transition correspond to a peak at the maximal current. Indeed, the maximal current correspond to the average value of the density where the particles have a large possibility to move. However, in the $p=q$ *case,* the system does not exhibit a first order transition, the whole current $J=J_+ - J_-$ take zero value while the right current take a maximum value which correspond to the average value of density.

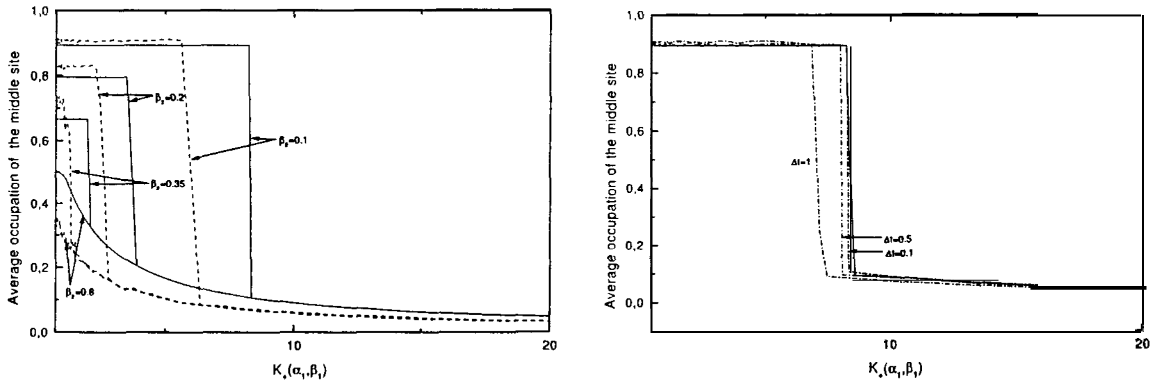
IV-2. General case: $\alpha_1\neq\alpha_2$ and $\beta_1\neq\beta_2$

In this case there are a large number of parameters namely, $p,\alpha_1,\alpha_2,\beta_1$ and β_2, so the problem is more difficult to solve, then to study the phase diagram, we consider the reduced parameters derived by Sandow [15], namely:

$$K_+(x,y)=\frac{1}{2x}\left[-x+y+p-q+\sqrt{(-x+y+p-q)^2+4xy}\right] \tag{19}$$

with $(x,y)=(\alpha_1,\beta_1)$ and (α_2,β_2).

In the case of $p\neq q$, using MFA we study the variation of the density as a function of $K_+(\alpha_1,\beta_1)$ for several values of $K_+(\beta_2,\alpha_2)$ (Fig. 5a), it is found that the system exhibits a first order transition between the low and high density phases at $K_+(\alpha_1,\beta_1)=K_+(\beta_2,\alpha_2)$. Furthermore, when the rate of the removed particles at the right (β_2) increases (and so $K_+(\beta_2,\alpha_2)$ decreases) the first order transition tends to disappear and the system reaches the maximal current phase. In order to study the effect of the probability of jumping At, we simulate the system for At = 1 (fully parallel updating) with $p\neq q$. However, in Fig. 5b, we give the variation of the average occupation of the middle site as a function of $K_+(\alpha_1,\beta_1)$



(a) (b)

FIG. 5. The variation of the average occupation of the middle site as a function of the parameter $K_+(\alpha_1,\beta_1)$ for $N=$ 101, $\beta_1=$ 0.3, α_2 = 0.3 and p = 0.8. Solid lines correspond to mean-field approximation. Dashed lines correspond to numerical simulations. (a) the rate of removed particles β_2 is varied. (b) the jumping rate At is varied.

for several values of β_2, it is clear that the three phases exist, namely low density phase, high density phase and maximal current phase. The low and high density are separated by a first order transition line where the density is discontinuous. This phenomenon has been investigated in the totally asymmetric case [13-14] and partially asymmetric case [15, 16]. Each of these phases undergoes a continuous transition to the phase of maximal current. Furthermore, it is clear that the critical value $K_+^c(\alpha_1,\beta_1)$ depends on the value of the jumping rate At and remains less than the one obtained from MFA. In fact, when the probability of jumping At decreases, the correlations between sites decreases and for At $\rightarrow$ 0 we reach the MFA results.

By fixing the direction of diffusion of particles (p > q), high density phase, low density phase and maximal current phase are recovered (Fig. 6). These results are in good agreement with the exact ones for sufficiently small At where using the matrix product formalism, the steady state current in each phase was computed and the phase diagram was derived in the thermodynamic limit [15] and by Fock representation of a general quadratic algebra [16], the exact expressions for density and correlation functions are derived.

Finally, we investigate the effects of the probability p and the jumping rate on the dependence of the current J on density ρ by using numerical simulations. By sampling the differents regions of the $(K_+(\beta_2,\alpha_2),\ K_+(\alpha_1,\beta_1))$-phase diagram, we collect pairs of values, which are depicted in Fig. 7. It is clear that the current is maximal at $\rho_{\mathbf{max}}=1/2$ for all values of p. This is due to the particle-hole symmetry. Furthermore, $J_{\mathbf{max}}$ increases with increasing p. However, in the case of a totally asymmetric exclusion model with periodic boundary conditions and using ordered sequential update [36], $\rho_{\mathbf{max}}$ increases with increasing p. Besides, it is found that the numerical result for small At (At = 0.1) are in good agreement with the exact results [15, 16]. However, when increasing At like At $=1$ (fully parallel update) the maximal current increases because of the strongest correlations in the parallel update, in particular for p = 1 the known result $J_{\mathbf{max}}=1/2$[36] is obtained.

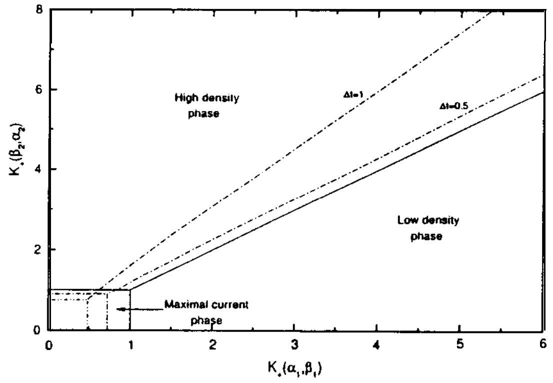


FIG. 6. Phase diagram in the $(K_+(\beta_2,\alpha_2), K_+(\alpha_1,\beta_1))$ space for N = 101. The number accompanying each dashed curve denotes the value of the jumping rate At. The solid curve corresponds to mean-field approximation.

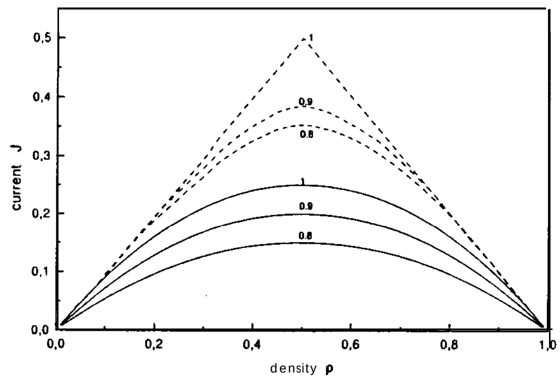


FIG. 7. The dependence of the current on density of the middle site for N = 101. The dashed lines correspond to At = 1, while the solid lines correspond to At = 0.1. The number accompanying each curve denotes the value of the right jump p.

V. **Conclusion**

We have studied the densities, current and phase diagrams in the case of open boundaries of the one dimensional partially asymmetric exclusion model. The three phases low density, high density and maximal current are encountered as for the fully asymmetric process for $p \neq q$. Moreover, for $p = q$ the first order line between the high and the low density phases is lost. We have also studied the effect of the jumping probability At on the (α, β)-phase diagram. It is found that the increase of At favours the first order transition and reduces the region of maximal current phase. Moreover, for At = 1 and for $p \neq q$, the maximal current phase persist, contrary to the totally asymmetric model [35] where the maximal current disappears for At = 1. When At is sufficiently small (random sequential updating) the mean-field theory is in excellent agreement with simulations. Furthermore, when the rate of the injected particles at the left α_1 is equal to the right one α_2 and the rate of the removed particles at the left β_1 is equal to the right one β_2, the region of maximal current disappears. While in the general case $\alpha_1 \neq \alpha_2$ and $\beta_1 \neq \beta_2$, three phases are encountered namely low density phase, high density phase and maximal current phase.

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