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A simulation study of an asymmetric exclusion model with open and periodic boundaries for parallel dynamics

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Abstract. The effect of jumping rate probability on the phase diagram of an asymmetric exclusion model is studied by numerical simulations. Density, current and velocity of particles are calculated for parallel dynamics. In the open boundaries case for one species of particles (particles 1), a passage from first to second order transition occurs by decreasing the jumping rate. In the periodic boundaries case, by introducing another species of particle (particle 2) which plays the role of obstacle for particles 1, the average velocity of particles 1 increases with increasing the jumping rate for small density. While the average velocity of particle 2 decreases for small and intermediate densities.

PACS. 05.40.+j Fluctuation phenomena, random processes, and Brownian motion – 02.50.-r Probability theory, stochastic processes, and statistics – 89.40.+k Transportation

1 Introduction

The stochastic dynamics of interacting particles have been studied in the mathematical and physical literature [1, 2]. In the case of the mathematical literature it allows an understanding of the asymptotic measures [3,4], the fluctuations of tagged particles [5,6], and the microscopic structure of shocks [7–9]. In the case of the physical literature, driven lattice gases with hard core repulsion provide models for the diffusion of particles through narrow pores and for hopping conductivity [10], and belong to the general class of non-equilibrium models which includes driven diffusing systems [11,12]. They are closely linked to growth processes [13–16], and can also be formulated as traffic jam or queuing problems [5]. The fully asymmetric exclusion model corresponds to the case where particles hop only in one direction. During any time interval Δt each particle has a probability Δt of jumping to its right-hand neighbour if this neighbouring site is empty. This model has been solved exactly in one dimension with open boundary conditions [17–20]. A simple way of obtaining the solution consists of representing the weights of configurations in the steady state as products of non commuting matrices [19,20]. Several phase transitions were found for this model. This method has been extended to the case of a system consisting of one species [21] and two species [22–25] of particles on a ring. The exact results are illustrated for continuous time dynamics (*i.e.* infinitesimal Δt), where only one particle can move during each time interval Δt. The parallel update of the asymmetric exclusion model can be introduced to obtain the phase diagram using Monte-Carlo simulations [26]. The aim of this paper is to study the effect of jumping rate Δt on density, current and the phase diagram in the open boundaries case and on velocities of particles in the case, of two species of particles on a ring by numerical simulations.

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2 Model

We consider a one-dimensional lattice of length L. Each lattice site can be empty or occupied by one particle. Hence the state of the system is defined by a set of occupation numbers $\{\tau_1, \tau_2, ..., \tau_L\}$ while $\tau_i = 1\,(\tau_i = 0)$ means that site i is occupied (empty). During each time interval Δt, each particle in the system has a probability, p, of jumping to the empty adjacent site on its right (and does not move otherwise), hereafter we consider $p = \Delta t\,(0 \leq p \leq 1)$. Particles are injected at the left boundary with a rate $\alpha\Delta t$ and removed on the right with a rate $\beta\Delta t$. Thus if the system has the configuration $\{\tau_1(t), \tau_2(t), ..., \tau_L(t)\}$ at time t it will change at time $t + \Delta t$ to the following:

For $1 < i < L$,

$\tau_i(t+\Delta t) = 1$ with probability
$$p_i = \tau_i(t) + [\tau_{i-1}(t)(1-\tau_i(t)) - \tau_i(t)(1-\tau_{i+1}(t))]\Delta t$$

$\tau_i(t+\Delta t) = 0$ with probability $1 - p_i$;

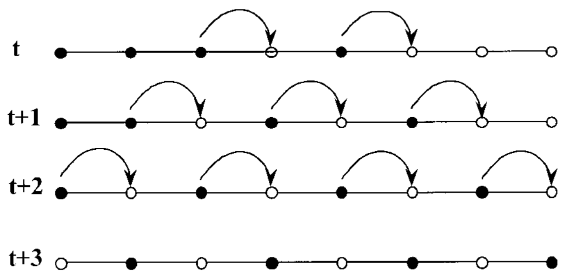

Fig. 1. Example of configurations obtained after even steps for system size $L = 8$, for jumping rate $\Delta t = 1$. $(\bullet)$, means an occupied site. $(\circ)$ means an empty site.

For $i = 1$,

$$\tau_1(t + \Delta t) = 1 \text{ with probability}$$
$$p_1 = \tau_1(t) + [\alpha(1 - \tau_1(t)) - \tau_1(t)(1 - \tau_2(t))]\Delta t$$

$$\tau_1(t + \Delta t) = 0 \text{ with probability } 1 - p_1;$$

For $i = L$,

$$\tau_L(t + \Delta t) = 1 \text{ with probability}$$
$$p_L = \tau_L(t) + [\tau_{L-1}(t)(1 - \tau_L(t)) - \beta\tau_L(t)]\Delta t$$

$$\tau_L(t + \Delta t) = 0 \text{ with probability } 1 - p_L.$$

The dynamics of the system are given by the following equations: For $1 < i < L$,

$$\frac{\Delta\langle\tau_i\rangle}{\Delta t} = \langle\tau_{i-1}(1 - \tau_i)\rangle - \langle\tau_i(1 - \tau_{i+1})\rangle;$$

For $i = 1$,

$$\frac{\Delta\langle\tau_1\rangle}{\Delta t} = \alpha\langle(1 - \tau_1)\rangle - \langle\tau_1(1 - \tau_2)\rangle;$$

For $i = L$,

$$\frac{\Delta\langle\tau_L\rangle}{\Delta t} = \langle\tau_{L-1}(1 - \tau_L)\rangle - \langle\beta\tau_L\rangle.$$

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 $\langle\tau_i\rangle$ requires the knowledge of the two point functions $\langle\tau_i\tau_{i+1}\rangle$ and $\langle\tau_{i-1}\tau_i\rangle$. The problem is an N-body problem in the sense that the calculation of any correlation function requires the knowledge of all the others, this makes the problem intractable.

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 of the time steps, each particle moves one site unless the site on its right-hand side is occupied by another particle. Figure 1 shows such a parallel updating process. In order to compute the average of any parameter u ($\langle u\rangle$), the values of $u(t)$ ($t = n\Delta t$, n is an integer) obtained from 5×10^4 to 10^5 time steps are averaged. Starting the simulations from random configurations, the system reaches a stationary state after a sufficiently large number of time steps. In all our simulations we averaged over 50–100 initial configurations.

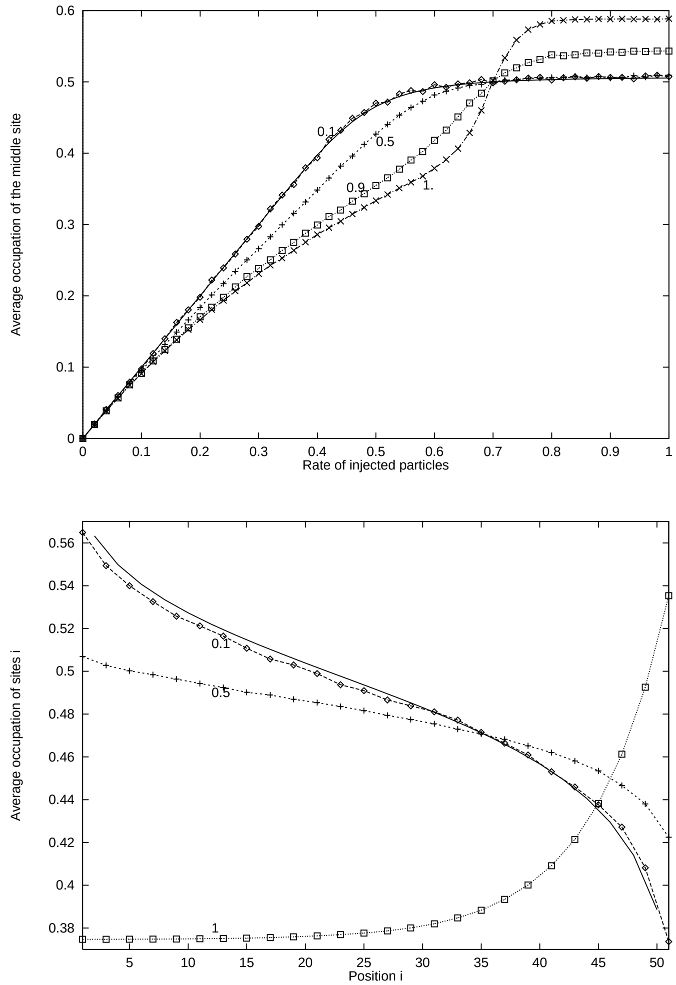

Fig. 2. For $N = 51$ and $\beta = 0.7$, the full line present an exact solution and the number accompanying each curve denote the value of Δt. (a) The variation of the average occupaition of the middle site ρ as a function of the rate of injected particles α. (b) The variation of the average occupation of sites $i(\rho(i))$ as a function of i for $\alpha = 0.6$.

3 Open boundaries with one species of particles

Open boundary conditions means that particles are injected at one end of the lattice and are removed at the opposite end. The asymmetric exclusion model with open boundaries exhibits phase transitions. In this section we study the influence of Δt defined in the preceding section on the phase diagram (α, β). Figure 2a shows the plot of the average occupation of the middle site, $\rho = \langle \tau_{(N+1)/2} \rangle$, *versus* α for various values of Δt and fixed value of $\beta\,(\beta = 0.7)$. We distinguish two regions when α is varied, a region in which ρ increases with α ($\rho(\alpha) = \alpha$ for $\Delta t = 0.1$) when $\alpha < \beta$, and a region in which ρ does not depend upon α when $\alpha > \beta$. By increasing Δt, ρ decreases in the first region, while it increases in the second region for sufficiently large values of Δt (ρ remains unchanged for low values of Δt). The transition between these regions is continuous for low Δt, and exhibits an inflection point at $\alpha = \beta$ for high values of Δt which means that the system is in unstable equilibrium state. So, the difference between injected and removed rates of particles ($(\alpha - \beta)\Delta t$) increases (decreases) for $\alpha > \beta$ ($\alpha < \beta$) with increasing Δt. Moreover, for low values of α ($\alpha < \beta$), when Δt increases most particles can move and change their location in each time step which reduces the interactions between particles. Therefore, the current increases which forces the particles to leave the lattice. For high values of α ($\alpha > \beta$), a few particles move using newly created vacancies while most particles remain immobile, patches of local queues of particles cover the whole system. There is no apparent global structure. By increasing Δt, the particles participate in collective moves, which allows an increase of queue sizes in the right side.

In order to investigate the contribution that the jumping rate, Δt, affects upon the density inside the chain, Figure 2b gives for fixed values of α and β, an indication of how much the average occupation of each position $i\,(\rho(i) = \langle \tau_i \rangle)$ changes as Δt is modified. The full line represents the calculated $\langle \tau_i \rangle' s$ matrix formulation [19,20], while the dashed lines show the effect of Δt. The observed shifts may be interpreted as follows. For very large values of $\Delta t\,(\Delta t = 1)$, the average occupation increases monotonously as a function of increasing the position. The rate of increase depends on the magnitude of the position: the higher the position, the larger the rate. Indeed, for high values of jumping rate the particles have a tendency to move toward the right of the chain, then the density in the right side is greater than the left one. For average values of $\Delta t\,(\Delta t = 0.5)$, the average occupation decreases almost linearly in low positions, with a relatively slow decay in high positions. For low values of $\Delta t\,(\Delta t = 0.1)$, a slow decay of the average occupation in low positions is followed by a linear decrease regime in average positions and rapid decay in high positions. In these cases, as Δt decreases, the particles do not move more rapidly, this implies an increase (reduction) of density in low (high) position sites. The system exhibits first and second order transitions. Figure 2a shows that the order parameter (average occupation of the middle site ρ) does not exhibit a sharp transition. The situation is quite similar to the behavior of the order parameter in finite systems [27]. In order to have a suitable criterion for the determination of the transition; we identify the first order transition for the system size L by the appearance of the peak in the derivative of $\rho(\alpha)$ function with respect to ρ, otherwise, the derivative will undergo a jump at the second order transition. The size independence of the position

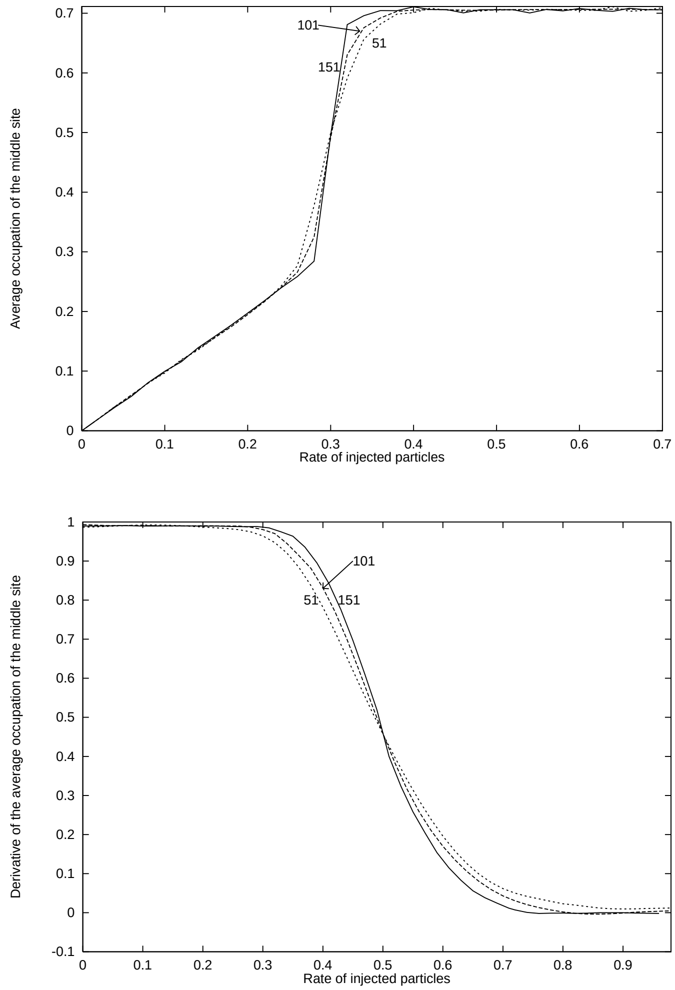

Fig. 3. (a) The average occupation of the middle site ρ *versus* α, for $\beta = 0.3$ and various system sizes L. (b) The fit of the derivative of ρ *versus* α, for $\beta = 0.8$ and various system sizes L.

of these transitions, allows us to define the first order (second order) transition point α_c by the intersection of the $\rho(\alpha) (d\rho(\alpha)/d\alpha)$ curves plotted for various sizes. The numerical derivation amplifies the errors of the data so we had to smooth the curves before further calculations. Figures 3a and 3b show, respectively, the plot of $\rho(\alpha)$ and $d\rho(\alpha)/d\alpha$ curves, run at various values of L. For $\beta = 0.3$ and $\Delta t = 0.1$; Figure 3a exhibits a first order transition at $\alpha_c = 0.3 \pm 0.02$. For $\beta = 0.8$ and $\Delta t = 0.1$; Figure 3b exhibits a second order transition at $\alpha_c = 0.5 \pm 0.02$. The current through the bond $((N+1)/2,\, (N+3)/2)$ is simply $J = \langle \tau_{(N+1)/2} (1 - \tau_{(N+3)/2}) \rangle$, because during the time Δt the probability that a particle jumps from $(N+1)/2$ to $(N+3)/2$ is $\tau_{(N+1)/2} (1 - \tau_{(N+3)/2}) \Delta t$. Figure 4b (for $\Delta t = 0.1$) shows the behavior of the current through the bond $((N+1)/2,\, (N+3)/2)$, it is maximal for large α, and this maximal value increases with increasing β. Depending on the values of the density, ρ, and the current, J, the system studied exhibits three phases; phase (I) low

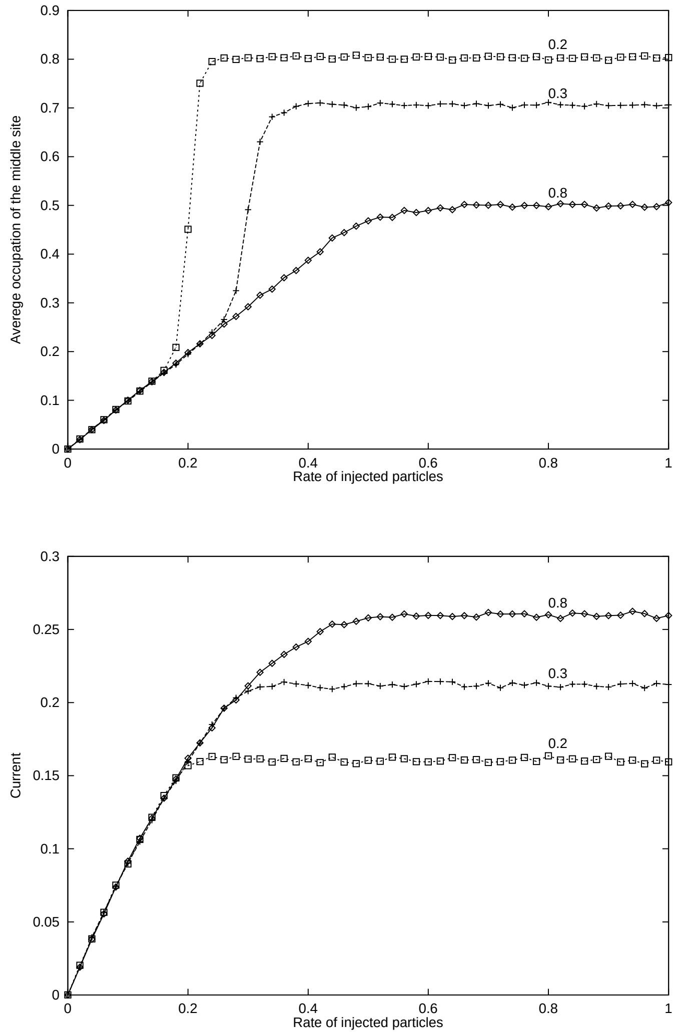

Fig. 4. For $\Delta t = 0.1$; (a) Variation of ρ as a function of α. (b) Variation of J (current) as a function of α. The number accompanying each curve in Figures 4a and 4b denotes the value of β for $N = 101$.

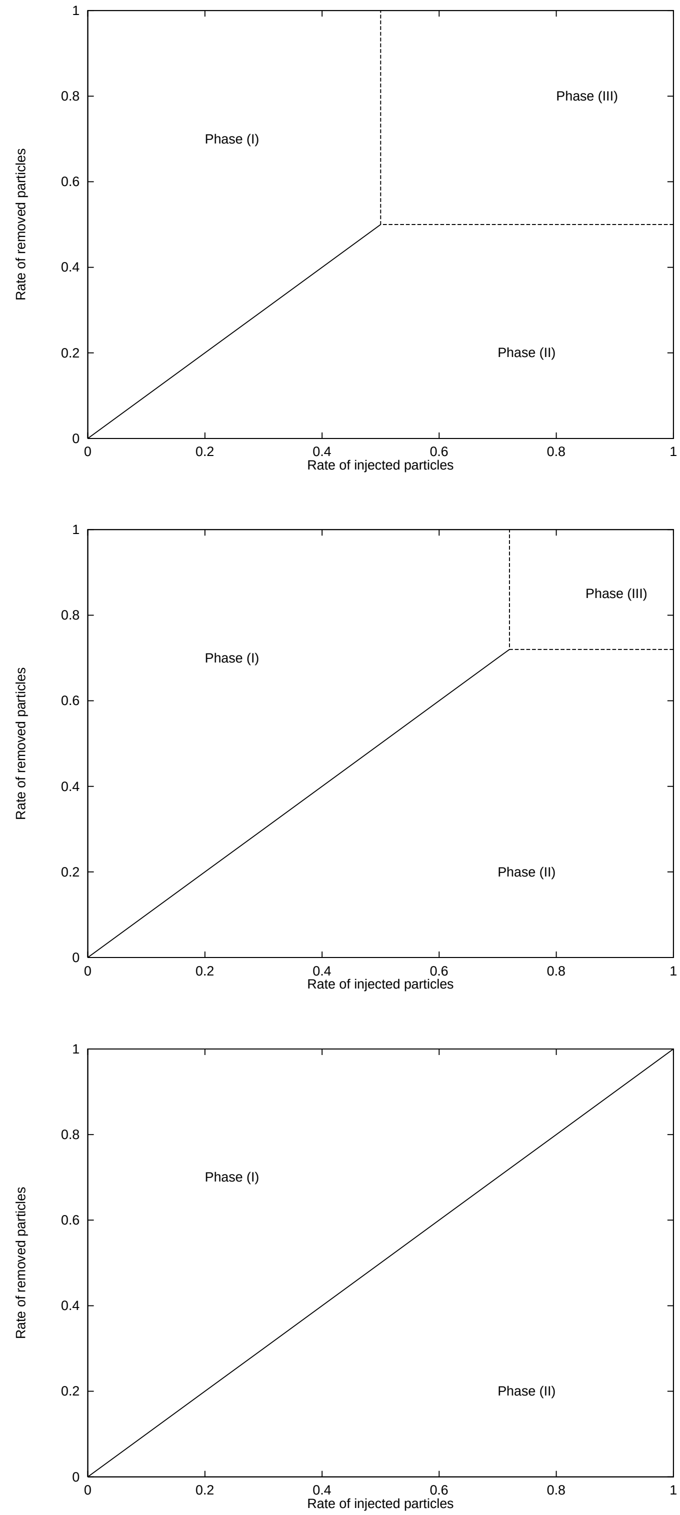

Fig. 5. Phase diagram (α, β); (a) $\Delta t = 0.1$; (b) $\Delta t = 0.8$; (c) $\Delta t = 1$.

density phase, phase (II) high density phase and phase (III) maximal current phase. The nature of the transition between these phases depends upon the values of α, β and Δt. In this sense we give a typical example where ρ varies as a function of α for fixed value of β. Indeed, when β increases, the transition changes from a first to second order transition, as illustrated in Figure 4a for small value of Δt. Collecting these results we obtain the phase diagram as shown in Figure 5a. The low and high density phases are separated by a first-order transition line. Each of these phases undergoes continuous transitions to the phase at maximal current. To illustrate the effect of Δt we give the phase diagrams for three values of Δt. For $\Delta t = 0.1$, the first order transition line between phases (I) and (II) reaches $\alpha = \beta = 0.5$ (see Fig. 5a), in agreement with matrix formulation results [19,20]. This value becomes 0.72 for $\Delta t = 0.8$ (see Fig. 5b), and 1 for $\Delta t = 1$ (see Fig. 5c), which means that for $\Delta t = 1$ the phase at maximal current exists only at the point $\alpha = \beta = 1$ [28].

4 Periodic boundaries with two species of particles

The implementation of the periodic boundaries means that upon leaving the lattice re-enters on the opposite side. The periodic boundary condition with one species of particles on a ring has been studied exactly by Schadschneider and Schreckenberg [29]. Here we consider a ring of N sites with two species of particles represented by 1 and 2, and holes represented by 0 in which the hopping rates are:

$$10 \longrightarrow 01 \text{ with rate } 1$$

$$20 \longrightarrow 02 \text{ with rate } p_{20}$$

$$12 \longrightarrow 21 \text{ with rate } p_{12}.$$

To illustrate a situation with two species, let us consider on a ring of N sites a single particle 2 and M particles 1. In order to compute the average velocity v of any species of particles at a given density, we denote $v(t)$ the average velocity per particle at time t, *i.e.*, the ratio of the average jumps per particle to the unit time steps Δt. The values of the average velocity $v(t)$ ($t = n\Delta t$, n is an integer) of particles obtained from 5×10^4 to 10^5 time steps are averaged. The parameters p_{20} and p_{12} are chosen such that:

$$p_{12} < 1 - p_{20}.$$

This implies in particular that $p_{20} < 1$ and $p_{12} < 1$, since particle 2 is slower than particles 1 and as $p_{12} < 1$, it plays the role of a moving obstacle. Both first and second class of particles hop forward when they have a hole to their right, but when a first class particle has a second class particle on its right the two particles interchange positions. Therefore a second class particle tends to move backwards in an environment of a high density and tends to move forwards in an environment of a low density. Using numerical simulations for $N = 101$, the average velocity of particles 1, v_1, and the average velocity of particle 2, v_2, *versus* the density of particles 1, $\rho = M/N$, are given, respectively, in Figures 6a and 6b for specific parameters p_{20} and p_{12}, and various values of Δt. The various behaviors can be classified as follows [22–25]. For small values of density ($p \lesssim 0.25$), both v_1 and v_2 decrease on increasing ρ. Although, the jumping rate has an opposite effect on these velocities. The average velocity v_1 increases with Δt as this is the case of one species of particles [29], while v_2 decreases as the jumping rate increases. Since the increase of the jumping rate allows a uniform distribution of particles 1, the particle 2 undergoes more and more backward moves in an environment.

For intermediate densities ($0.25 \lesssim \rho \lesssim 0.85$), the average velocity of particles 1 decreases as the density ρ increases while the average velocity of particle 2 does not depend upon the density ρ. This means that the particle 2 moves as if the site ahead of it was always empty and the site behind it always occupied. In this stage the ring exhibits two macroscopic regions: a region of high density following the particle 2 and a region of low density.

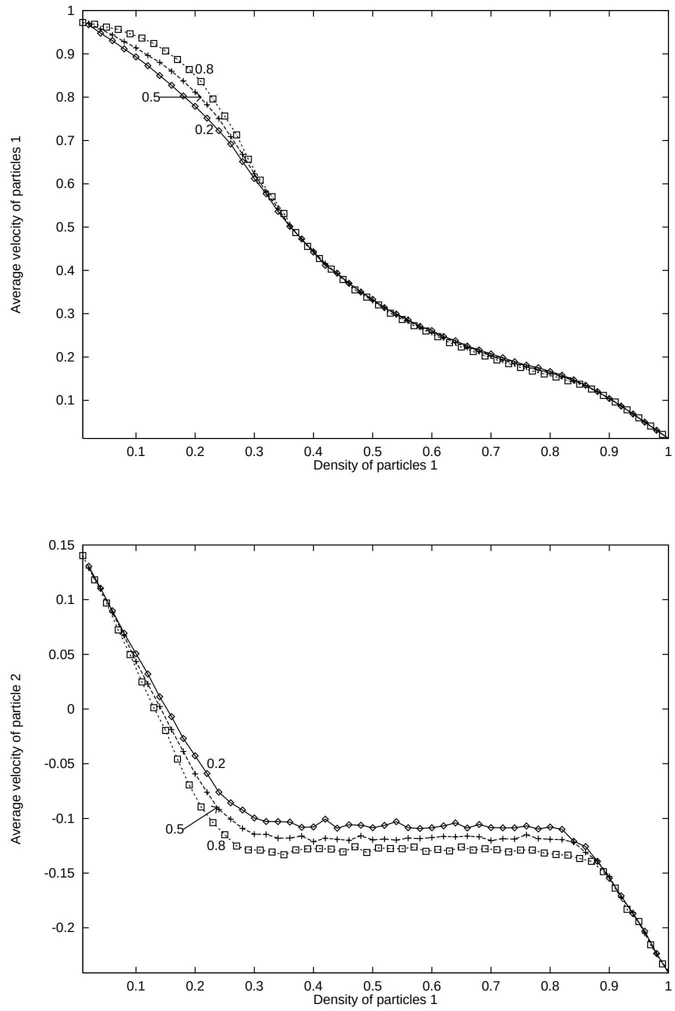

Fig. 6. For $p_{20} = 0.15$ and $p_{12} = 0.25$; (a) Variation of average velocity v_1 as a function of density of particles 1; (b) Variation of average velocity v_2 as a function of density of particles 1. The number accompanying each curve in Figures 6a and 6b denotes the value of Δt for $N = 101$.

Like in the case of the low density, the increase of Δt leads to the growth of backwards movement of the particle 2: This suggest that as the particle 2 blocks the particles 1 behind it, an increase of the jumping rate strengthens this blockage, and since $p_{21} > p_{20}$, we have the growth of the backwards movement of the particle 2. For high density ($\rho \gtrsim 0.85$), the average velocities v_1 and v_2 continue their decrease, both velocities are insensitive to the variation of the jumping rate. Indeed, the blockage undergone by the particles 1 behind the particle 2 plays an opposite role of the one played by the jumping rate Δt, this is true for intermediate and high densities. Concerning the particle 2, the regions behind and ahead of it tend to have the same density, and as the distribution of particles 1 along the lattice remains qualitatively unchanged on varying Δt, the average velocity v_2 does not depend upon the jumping rate Δt.

5 Conclusion

A computer-simulation is introduced to study the contribution of the jumping rate Δt on the (α, β) phase diagram in the case of open boundaries. The jumping rate Δt has for effect to investigate the difference between the sequential movement and the parallel movement which in general produce stronger correlation. So, as Δt decreases, the first order transition between low and high density phases disappears and is replaced by the continuous transition between these phases and the maximal current phase for high values of α and β. Measurements of the order parameter show that the maximal current phase only occurs on the point $\alpha = \beta = 1$ at $\Delta t = 1$. Another interesting aspect is the dependence of the average velocity of particles on the variation of Δt in the periodic boundaries case, where the average velocity of particles increases with Δt. Studying the effect of Δt on the velocities of the two species of particles on a ring, the jumping rate acts are seen only at small density on particles 1, while it is manifested on particle 2 for small and intermediate densities of particles 1. Increasing Δt, the average velocity of particles 1 (particle 2) increases (decreases). The known exact results have been obtained for small jumping rate [17–25].

The interpolation between the discrete and continuous time dynamics presented above could be extent to some results; such as partial asymmetry [19,30], the diffusion constant in systems with open boundary conditions [31], transient properties [32]. However there remains a number of simple generalizations of the asymmetric exclusion model such as the case of a fixed blockage [33], two species of particles with open boundaries [34,35] and the application to traffic flow [36,37].

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