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A SIMULATION STUDY OF AN ASYMMETRIC EXCLUSION MODEL WITH OPEN AND PERIODIC BOUNDARIES

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ABSTRACT

Using numerical simulations we study the effect of the jumping rate on the density, current and phase diagram in the open boundaries case, and on the velocities of particles in the case of one and two species of particles on a ring, of one dimensional asymmetric exclusion model. However, on the one hand, a passage from discontinuous to continuous transition occurs by decreasing the jumping rate in the open boundaries, on the other hand, for two species of particles on a ring the velocity of particle 1 increases while the velocity of particle 2 decreases as the jumping rate increases.

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I) Introduction:

The stochastic dynamics of interacting particles have been studied in the mathematical and physical literature [1-2]. In the case of 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 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]. Using a recursion relation [17] and a matrix formulation [18-19] for a steady state and an infinitesimal hopping rate, where only one particle can move in each time step, dt, an exact solution of this model is known. Our aim is to study, by numerical simulations, the effect of jumping probability on density, current and phase diagram in the open boundaries case and velocities of particles in the case of one and two species of particles on a ring.

II) Model:

We consider a one-dimensional lattice of N sites. Each lattice site is either occupied by one particle or empty [17-19]. Hence the state of the system is defined by a set of occupation numbers $\{\tau_1, \tau_2, \ldots, \tau_N\}$ while $\tau_i=1$ ($\tau_i=0$) means site i is occupied (empty). During every time interval Δt, each particle in the system has a probability, p, of jumping to the next site on its right if this site is empty (and does not move otherwise), hereafter we consider $p=\Delta t$. 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 $\{\tau_1(t), \tau_2(t), \ldots, \tau_N(t)\}$ at time t it will change at time $t+\Delta t$ to the following:

for $1<i<N$

$\tau_i(t+\Delta t)=1$ with probability $p_i=\tau_i(t)+\left[\tau_{i-1}(t)(1-\tau_i(t))-\tau_i(t)(1-\tau_{i+1}(t))\right]\Delta t$
$\tau_i(t+\Delta t)=0$ with probability $1-p_i$

for $i=1$

$\tau_1(t+\Delta t)=1$ with probability $p_1=\tau_1(t)+\left[\alpha(1-\tau_1(t))-\tau_1(t)(1-\tau_2(t))\right]\Delta t$
$\tau_1(t+\Delta t)=0$ with probability $1-p_1$

for $i=N$

$\tau_N(t+\Delta t)=1$ with probability $p_N=\tau_N(t)+\left[\tau_{N-1}(t)(1-\tau_N(t))-\beta\tau_N(t)\right]\Delta t$
$=0$ with probability $1-p_N$.

The dynamics of the system is given by the following equations:

For $1<i<N$

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

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 $i=N$

$$\frac{\Delta\langle\tau_N\rangle}{\Delta t}=\langle\tau_{N-1}(1-\tau_N)\rangle-\beta\langle\tau_N\rangle$$

III) Open boundaries:

Open boundary conditions mean 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). First we compare our numerical simulations with an exact solution [17-19], in this context we give some typical examples where $\rho(i)=\langle\tau_i\rangle$ (average occupation of site i) varied as a function of i $(1\leq i\leq N)$ for fixed values of α and β, and $\rho(\alpha)=\langle\tau_{(N+1)/2}\rangle$ (average occupation of middle site) varied as a function of α for fixed value of β, where we can see the effect of Δt on the variation of $\rho(\alpha)$ Fig. 1-a. Then we obtain three cases; the first case corresponds to small Δt where our results are in reasonable agreement with the exact solution [17-19], indeed for small α we have $\rho(\alpha)=\alpha$, and for large α, $\rho(\alpha)$ saturate at 0.5, in this case there is a continuous transition between these two behaviours. Increasing Δt leads to a slow increasing of $\rho(\alpha)$ with α but the saturation value does not change, 0.5. It changes only for large value of Δt, where it goes to 0.59, with a discontinuous transition. For small values of Δt, $\rho(i)$ has the same behaviour as that of the exact solution Fig. 1-b, while they are very different for large value of Δt, Fig. 1-b. The current through the bond (N+1)/2 is simply $J=\langle\tau_{(N+1)/2}(1-\tau_{(N+3)/2})\rangle$ a, because during a time Δt, the probability that a particle jumps from (N+1)/2 to (N+3)/2 is $\tau_{(N+1)/2}(1-\tau_{(N+3)/2})\,\Delta t$. In figures 2-b,3-b, and 4-b, we give the behaviour of the current through the bond (N+1)/2, it is maximal for large value of α, and this maximal value increases with increasing β. The maximal current increases also with increasing Δt. Depending on the values of the density, ρ, and the current, J, the system studied exhibits three phases; phase (I) low 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 β and Δt, indeed when β decreases the transition change from continuous to discontinuous one, Fig. 2-a for small value of Δt, and Figs. 3-a, 4-a for large values of Δt. Collecting these results we obtain the phase diagram shown in Fig. 5. 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 $\alpha=\beta=0.5$, in agreement with exact results Fig. 5-a, this value becomes 0.72 for $\Delta t=0.8$, Fig. 5-b, and 1 for $\Delta t=1$ Fig. 5-c, which means that for $\Delta t=1$ phase at maximal current exist only on the point $\alpha=\beta=1$.

IV) Periodic boundaries:

We consider the case of M particles on a ring of N sites. The exact expression for the average velocity of particles, v, is given by [20] $v=\frac{N-M}{N-1}$

This expression is a simple consequence of the fact that in the steady state all configurations with M particles have equal probabilities. The effect of hopping rate Δt, on the velocity v is shown in Fig. 6. It increases with increasing Δt , for fixed value of particles density, $\rho=M/N$.

V) Periodic boundaries with two species of particle:

We consider a ring of N sites with two species of particle represented by 1 and 2, and holes represented by 0 and in which the hopping rates are:

10----------->01 with rate 1

20----------->02 with rate p_{20}

12----------->21 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. 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. Using numerical simulations for N=101, the average velocity of particles 1, v_1 , and the average velocity of particle 2, v_2 , as a function of the density $\rho=M/N$, are given in Figs. 7-a and 7-b, respectively, for a specific parameter p_{20} and p_{12} . The velocity v_1 increases with increasing Δt for low density Fig. 7-a, while the velocity v_2 decreases with increasing Δt in a large domain of density Fig. 7-b. The numerical simulations for small Δt are in good agreement with known exact results [19].

V) Conclusion:

Using numerical simulations we have studied the effect of the hopping rate on the (α,β) phase diagram, so as Δt decrease the discontinuous transition between low and high densities phases disappears and is replaced by the continuous transition between these phases and a high current phase for high α and β. The case of one and two species of particles has been studied for periodic boundaries. The known exact results have been obtained for small hopping rate.

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Figure captions:

Fig1: For N=51 and β=0.7, the full line presents an exact solution and the numbers accompanying each curve denote the value of Δt.

a) Variation of $\rho(\alpha)$ as a function of α.

b) Variation of $\rho(i)$ as a function of i for α=0.6.

Fig.2: For Δt=0.1;

a) Variation of $\rho(\alpha)$ as a function of α.

b) Variation of J (current) as a function of α.

Fig.3: For N=101 and Δt=0.8; The numbers accompanying each curve denote the value of β .

a) Variation of $\rho(\alpha)$ as a function of α.

b) Variation of J (current) as a function of α.

Fig.4: For N=101 and Δt=1; The numbers accompanying each curve denote the value of β .

a) Variation of $\rho(\alpha)$ as a function of α.

b) Variation of J (current) as a function of α.

Fig.5: Phase diagram (α,β);

a) Δt=1.

b) Δt=0.8.

c) Δt=1.

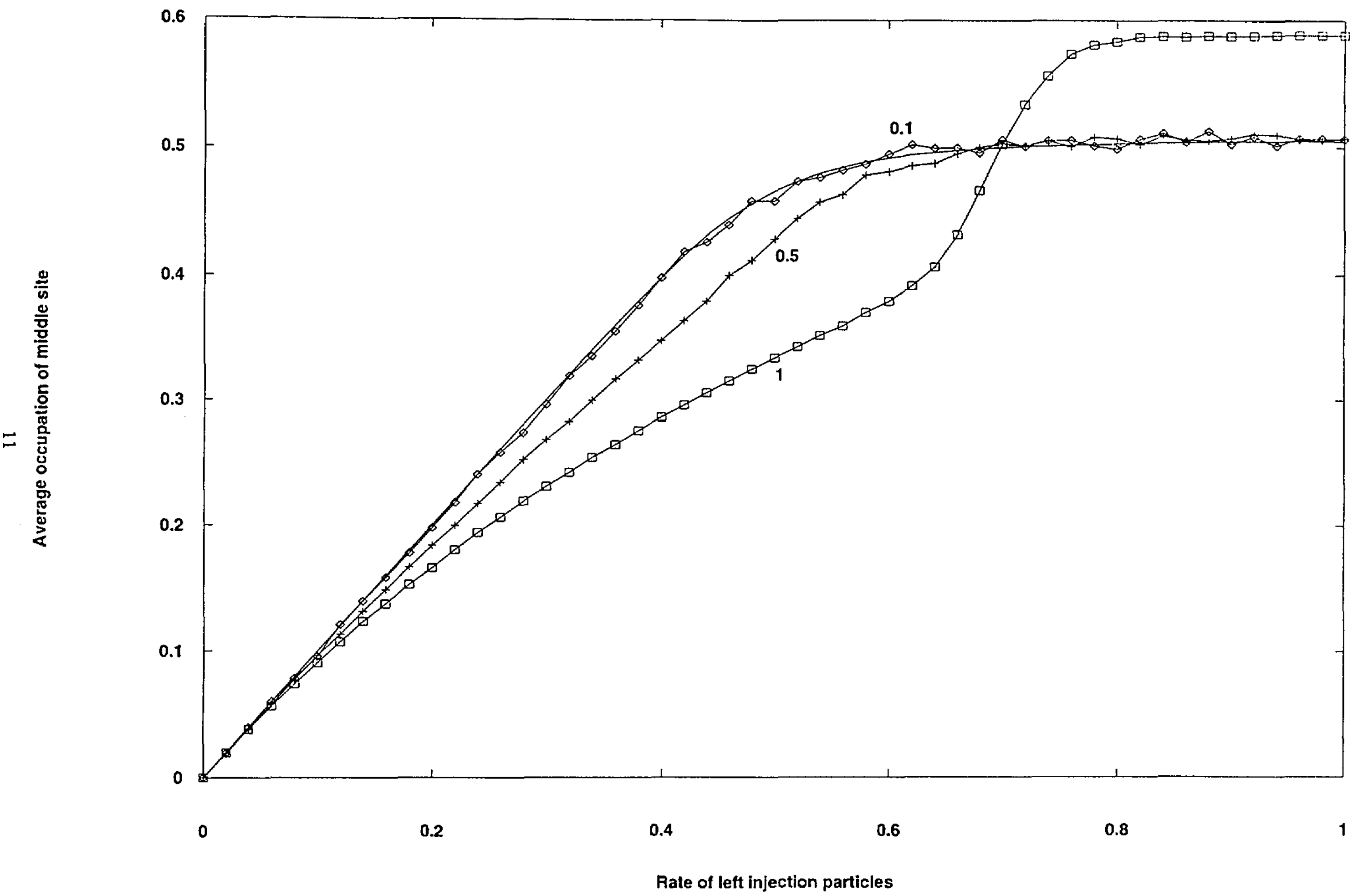
Fig.6: Variation of average velocity v of particles as a function of density. The numbers accompanying each curve denote the value of Δt. N=101.

Fig7: For p_{20}=0.15 and p_{21}=0.25; The numbers accompanying each curve denote the value of Δt . N=101.

a) Variation of average velocity v_1 as a function of density of particles 1.

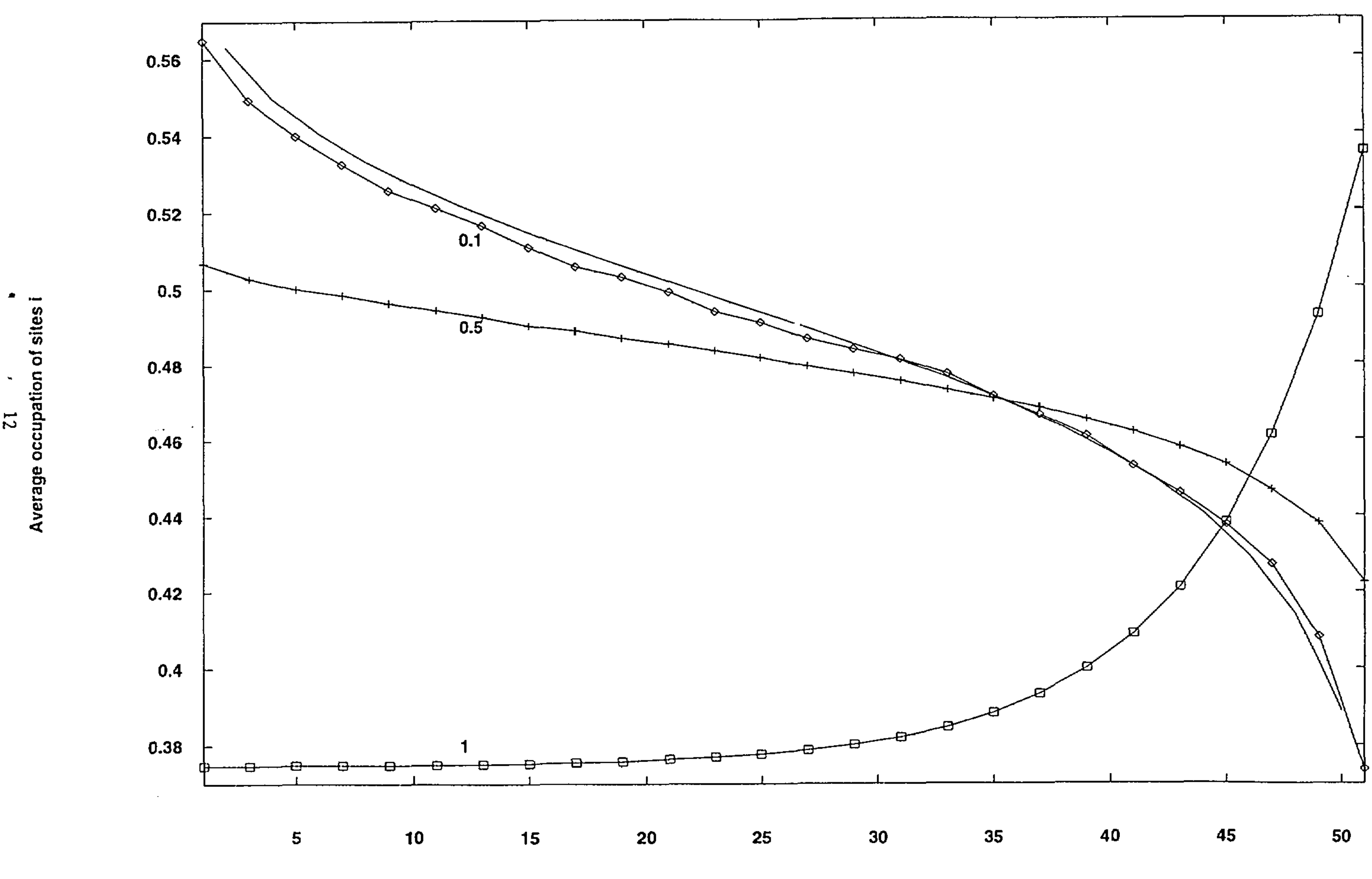
b) Variation of average velocity v_2 as a function of density density of particles 1.

Fig 1.a



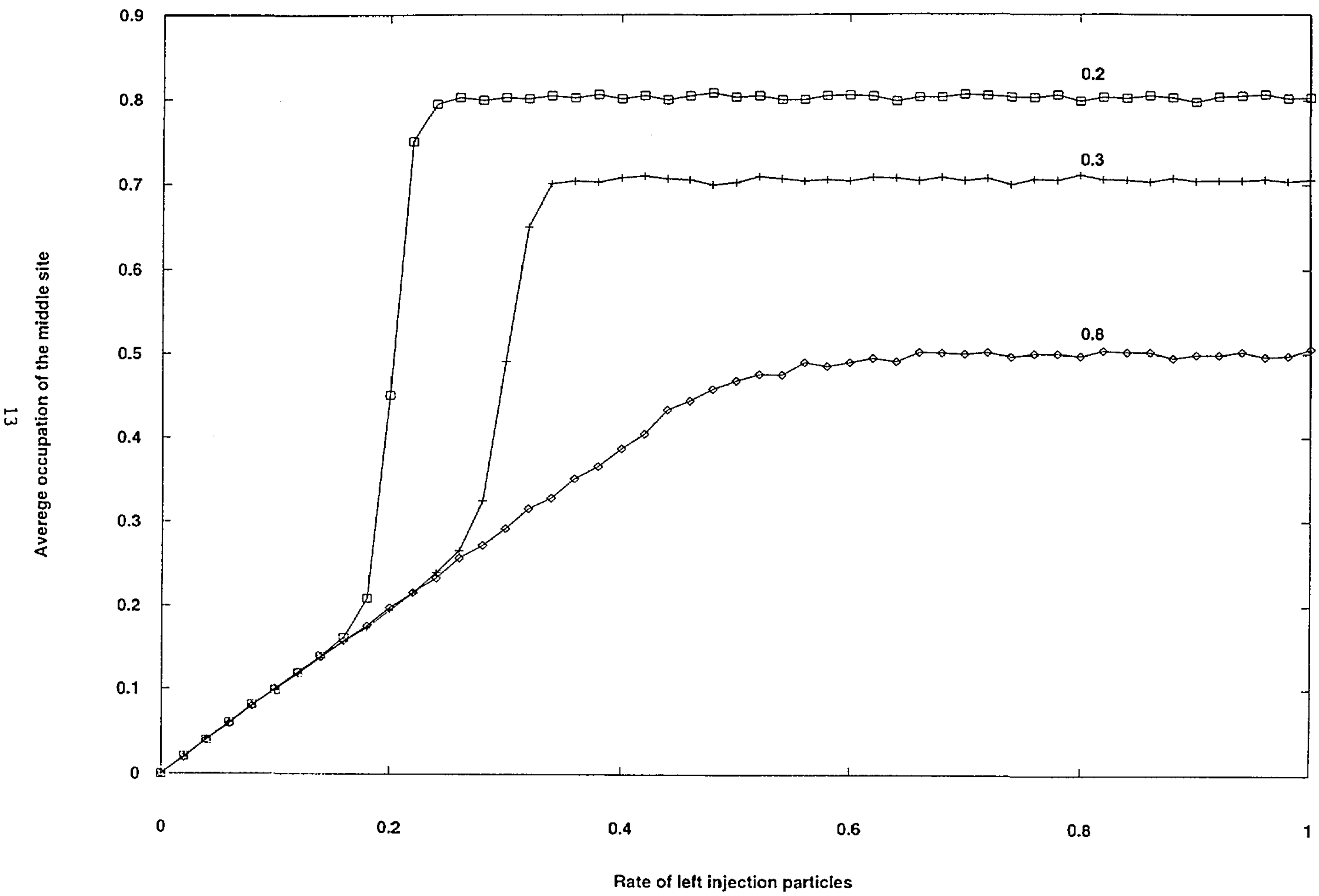
Average occupation of middle site
Rate of left injection particles
0.1
0.5
1

Fig 1.b



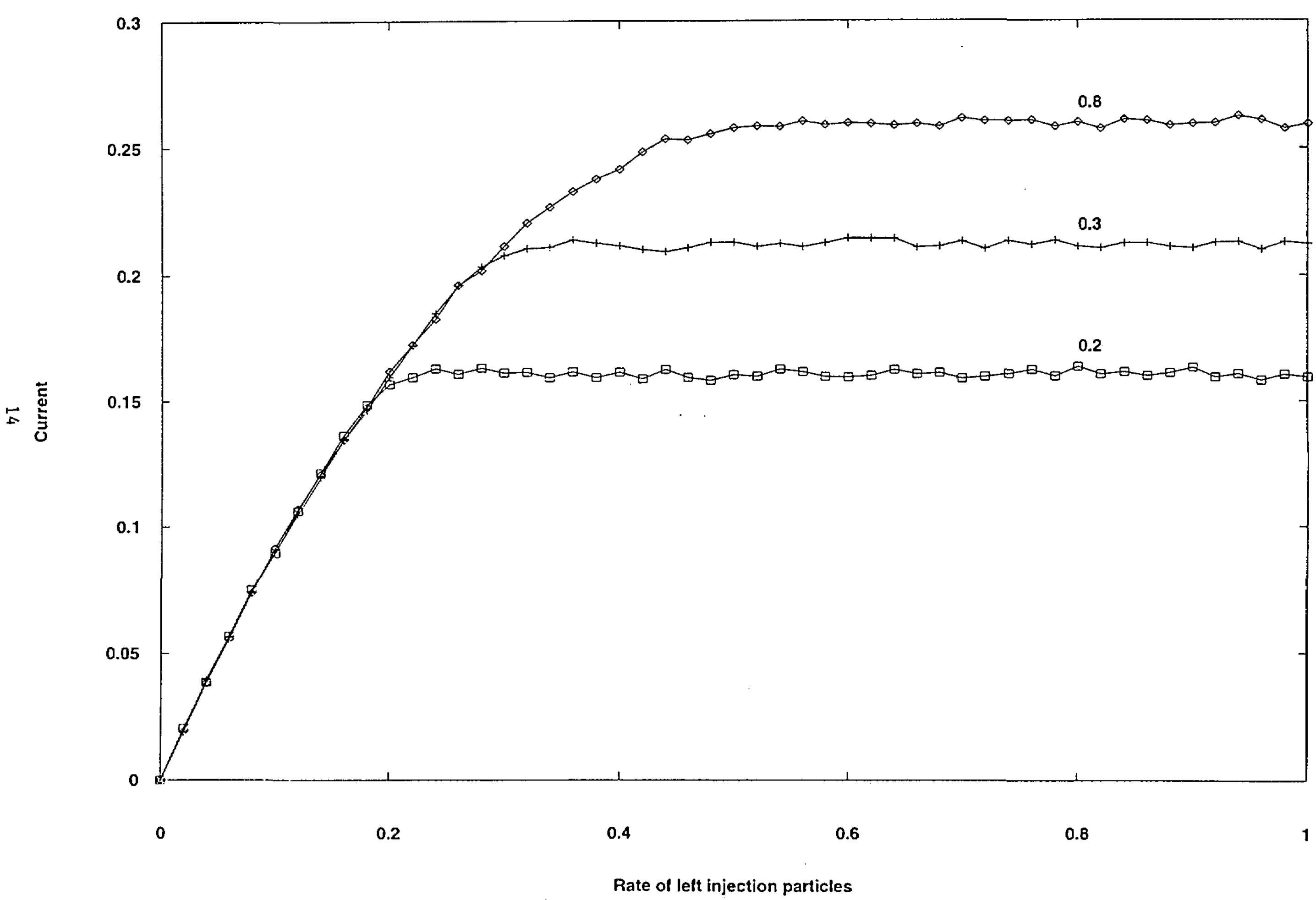
Average occupation of sites i
Position i
0.1
0.5
1

Fig 2.a



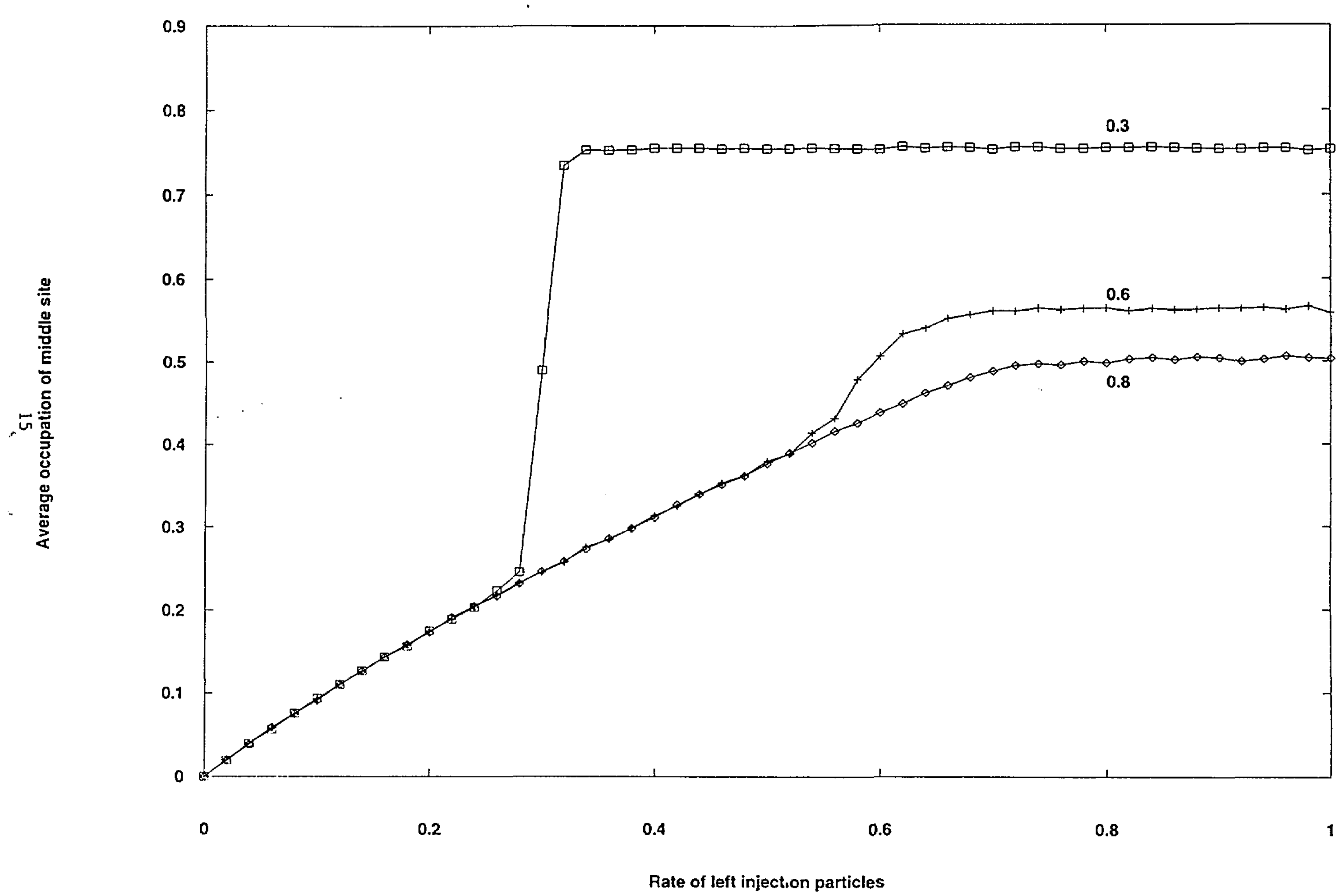
13
Averege occupation of the middle site
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.2
0.3
0.8
0
0.2
0.4
0.6
0.8
1
Rate of left injection particles

Fig 2.b



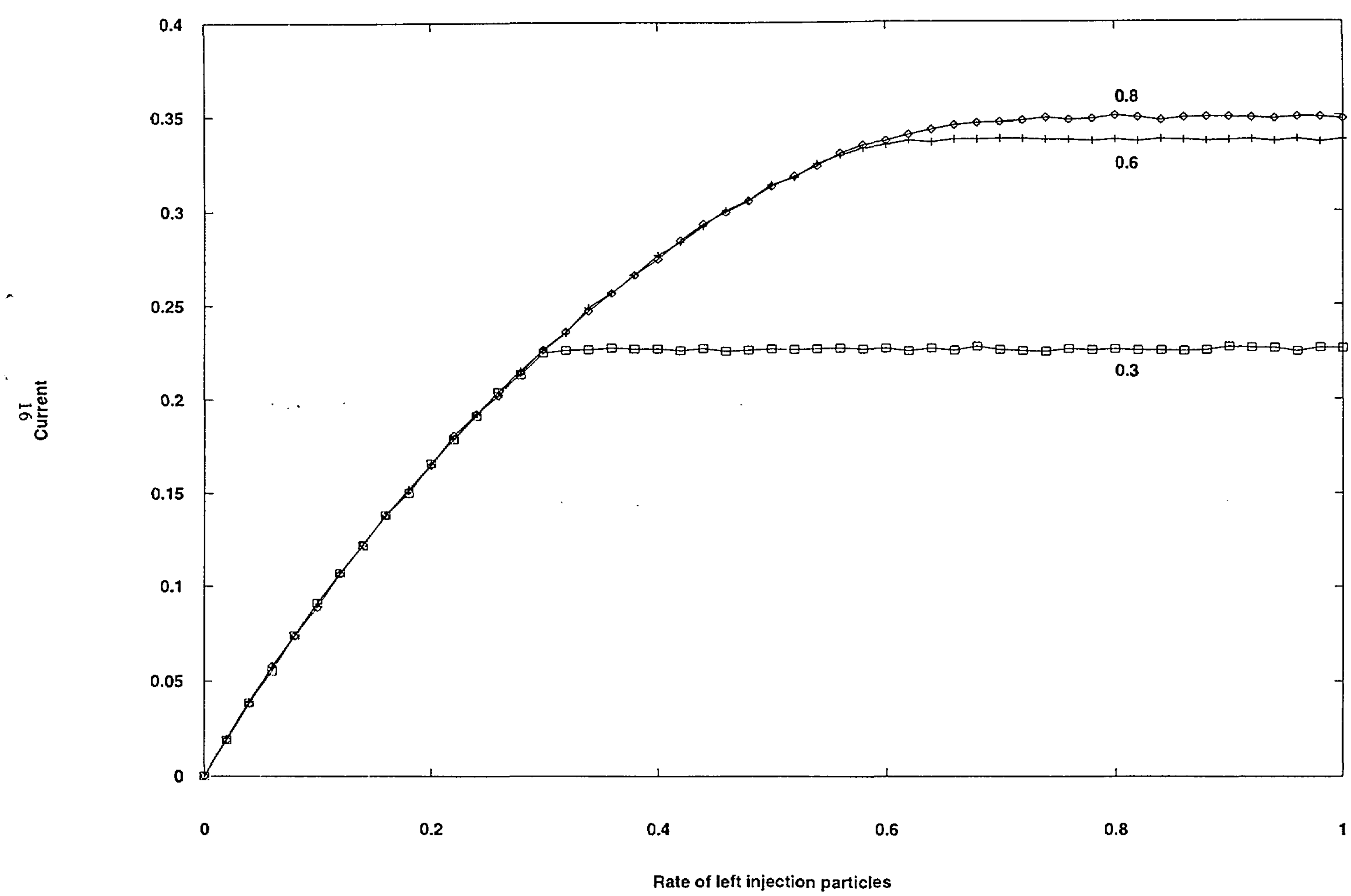
14
Current
0.3
0.25
0.2
0.15
0.1
0.05
0
0.8
0.3
0.2
0
0.2
0.4
0.6
0.8
1
Rate of left injection particles

Fig 3.a



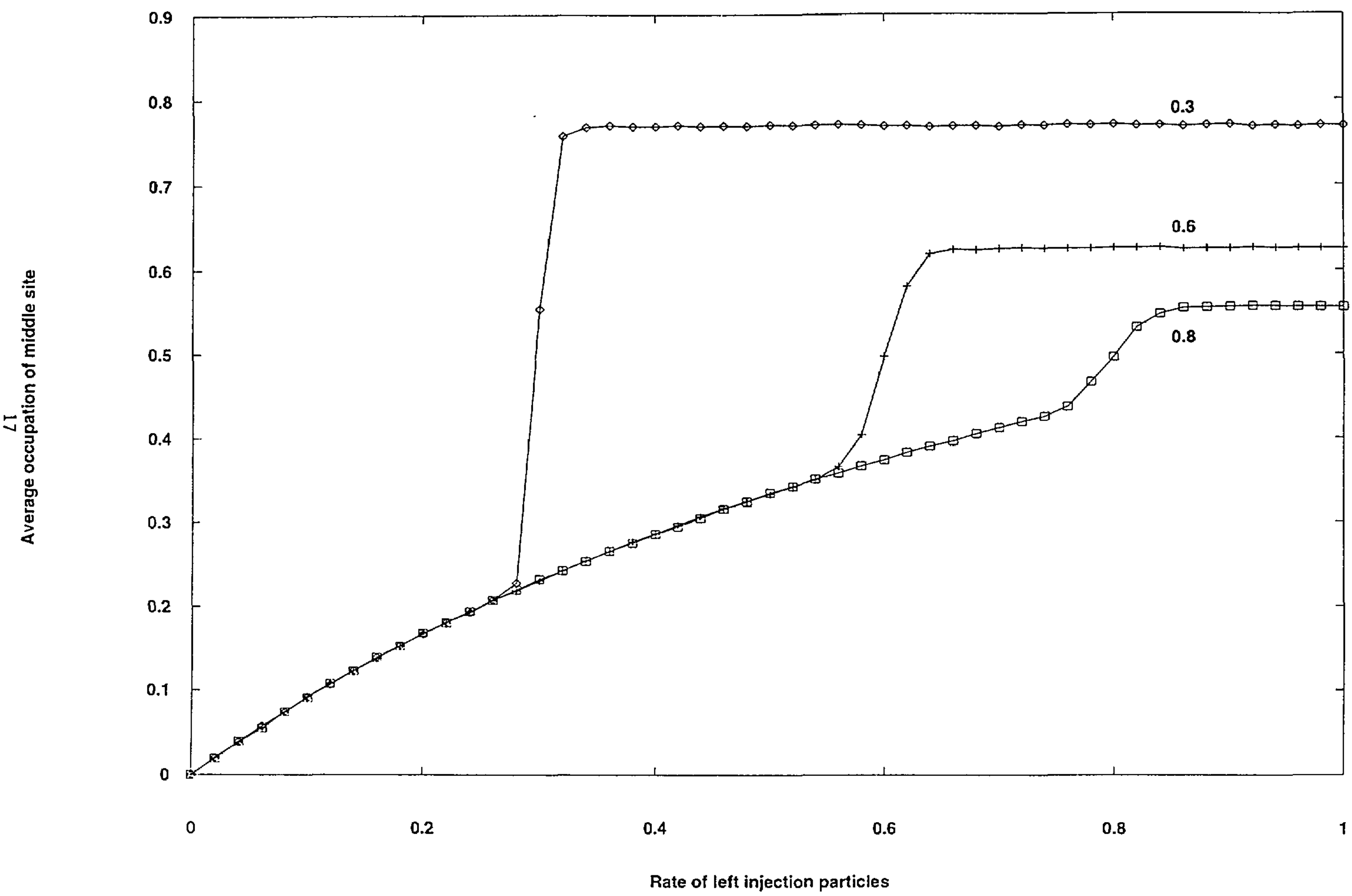
Average occupation of middle site
15
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.3
0.6
0.8
0
0.2
0.4
0.6
0.8
1
Rate of left injection particles

Fig 3.b



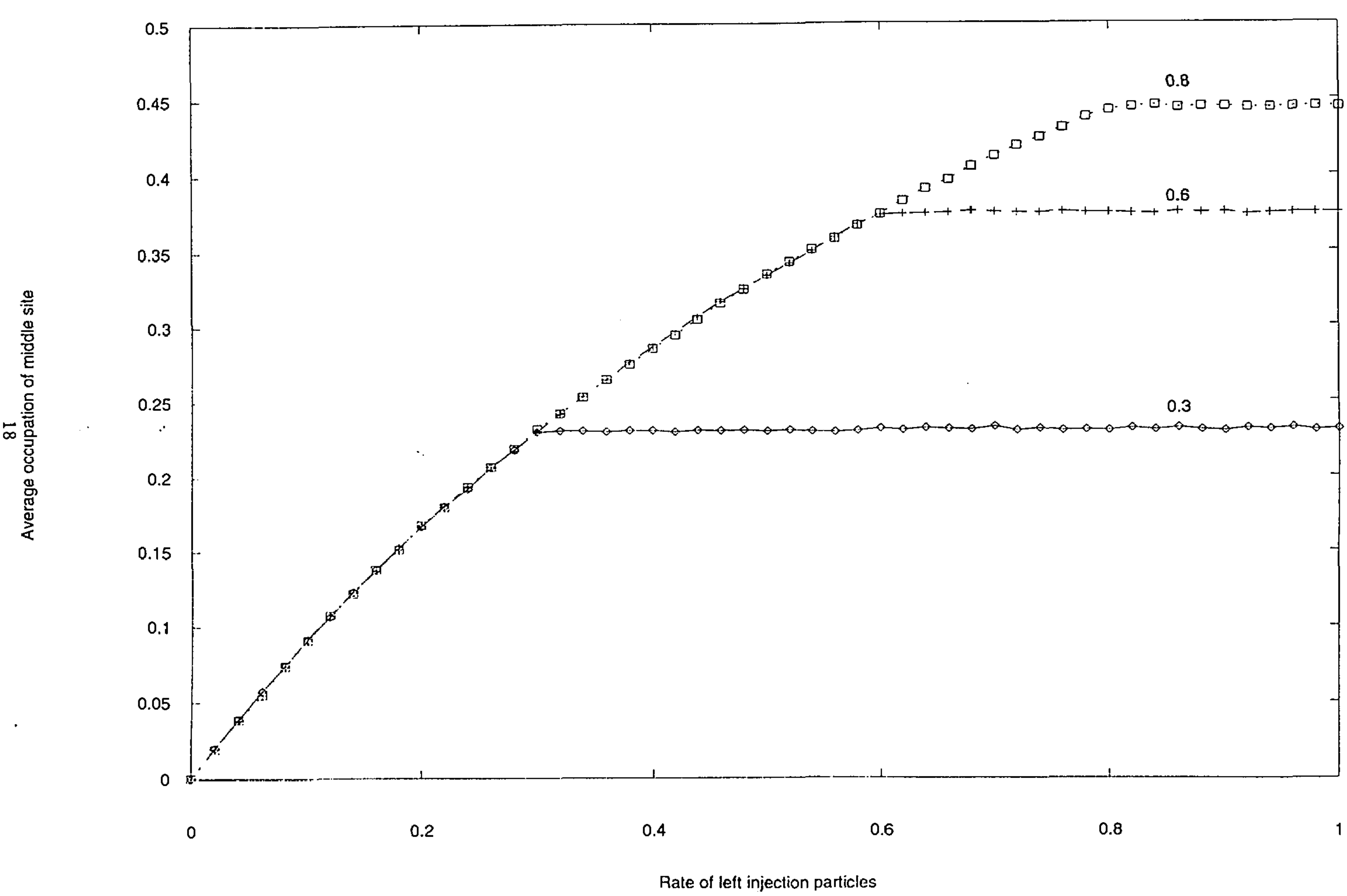
Current
16
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0.8
0.6
0.3
0
0.2
0.4
0.6
0.8
1
Rate of left injection particles

Fig 4.a



0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Average occupation of middle site
17
0
0.2
0.4
0.6
0.8
1
Rate of left injection particles
0.3
0.6
0.8

Fig 4.b



0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
Average occupation of middle site
18
0
0.2
0.4
0.6
0.8
1
Rate of left injection particles
0.8
0.6
0.3

Fig 5.a

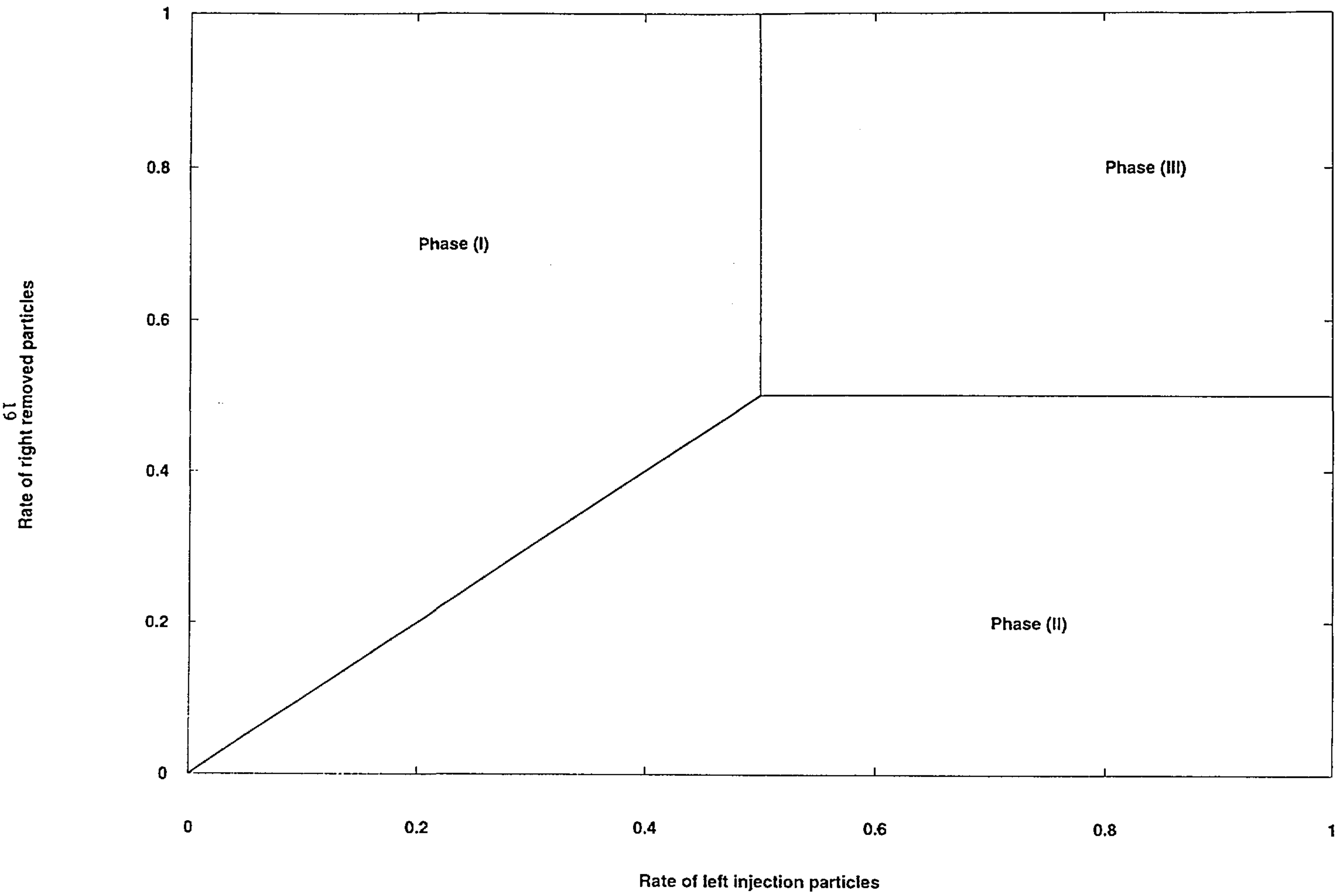

Phase (I)
Phase (III)
Phase (II)
Rate of right removed particles
Rate of left injection particles
0
0.2
0.4
0.6
0.8
1

Fig 5.b

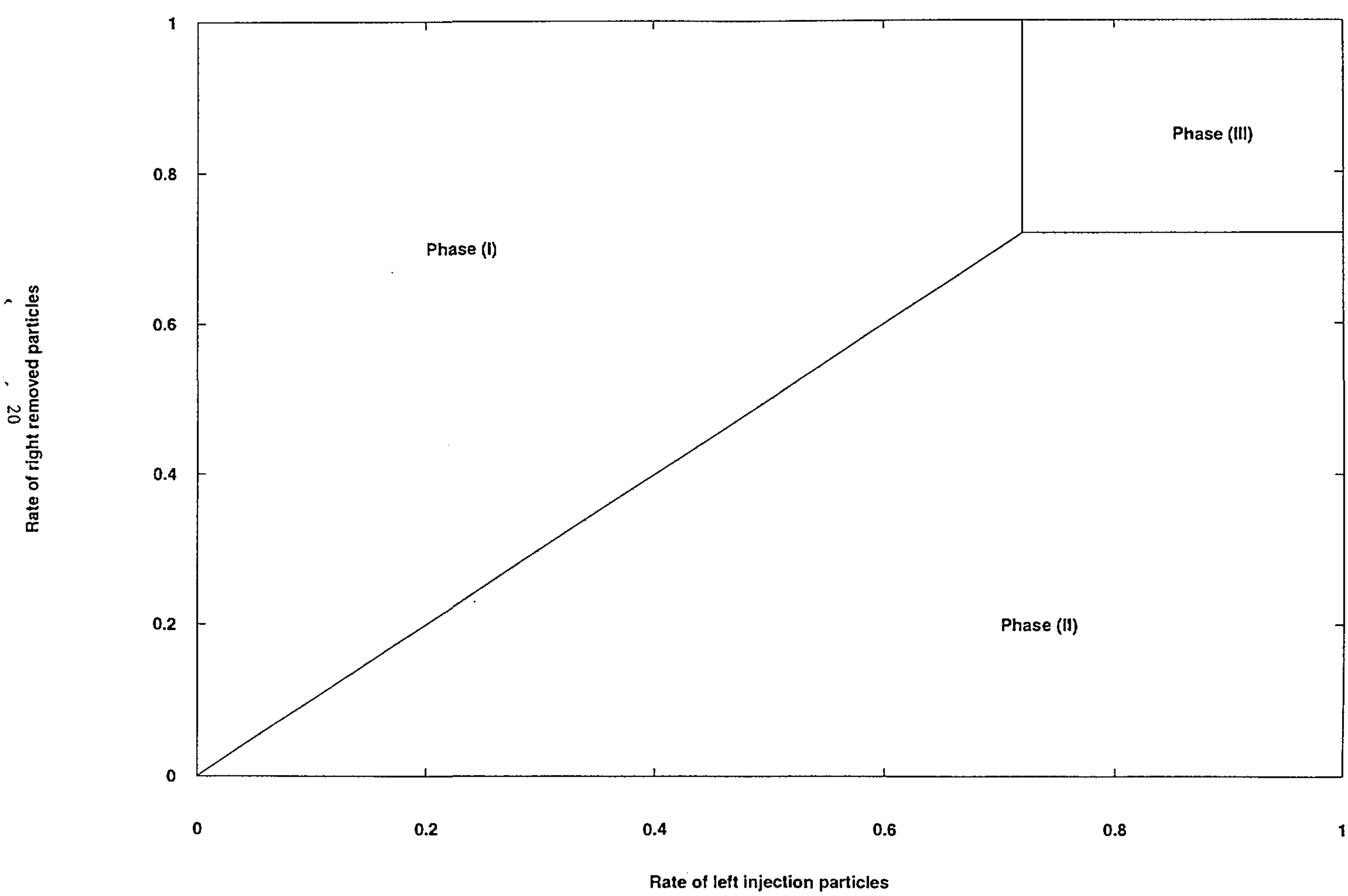

Phase (III)
Phase (I)
Phase (II)
Rate of right removed particles
Rate of left injection particles
0
0.2
0.4
0.6
0.8
1

Fig 5.c

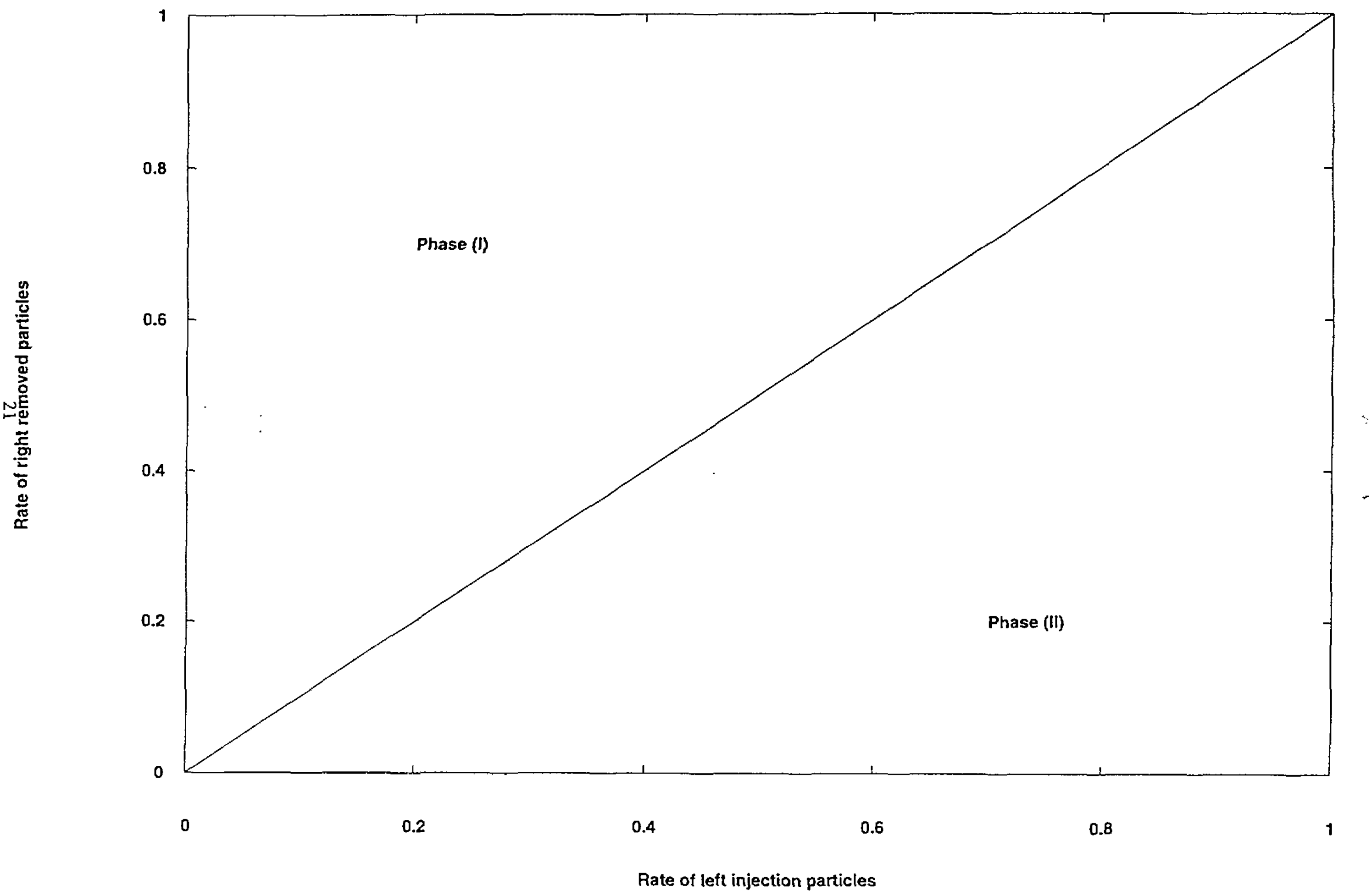

Phase (I)
Phase (II)
Rate of right removed particles
Rate of left injection particles
0
0.2
0.4
0.6
0.8
1

Fig 6

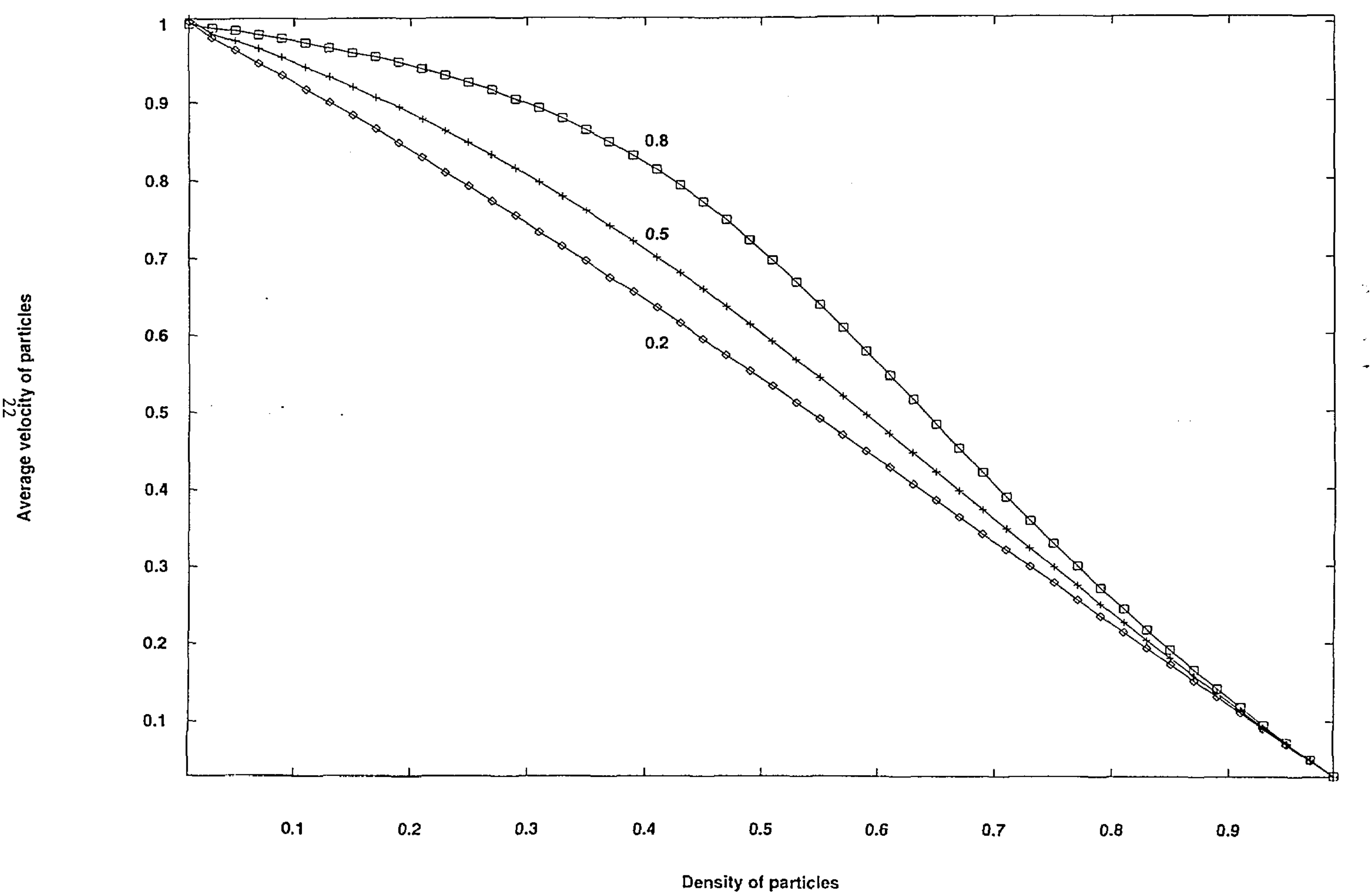
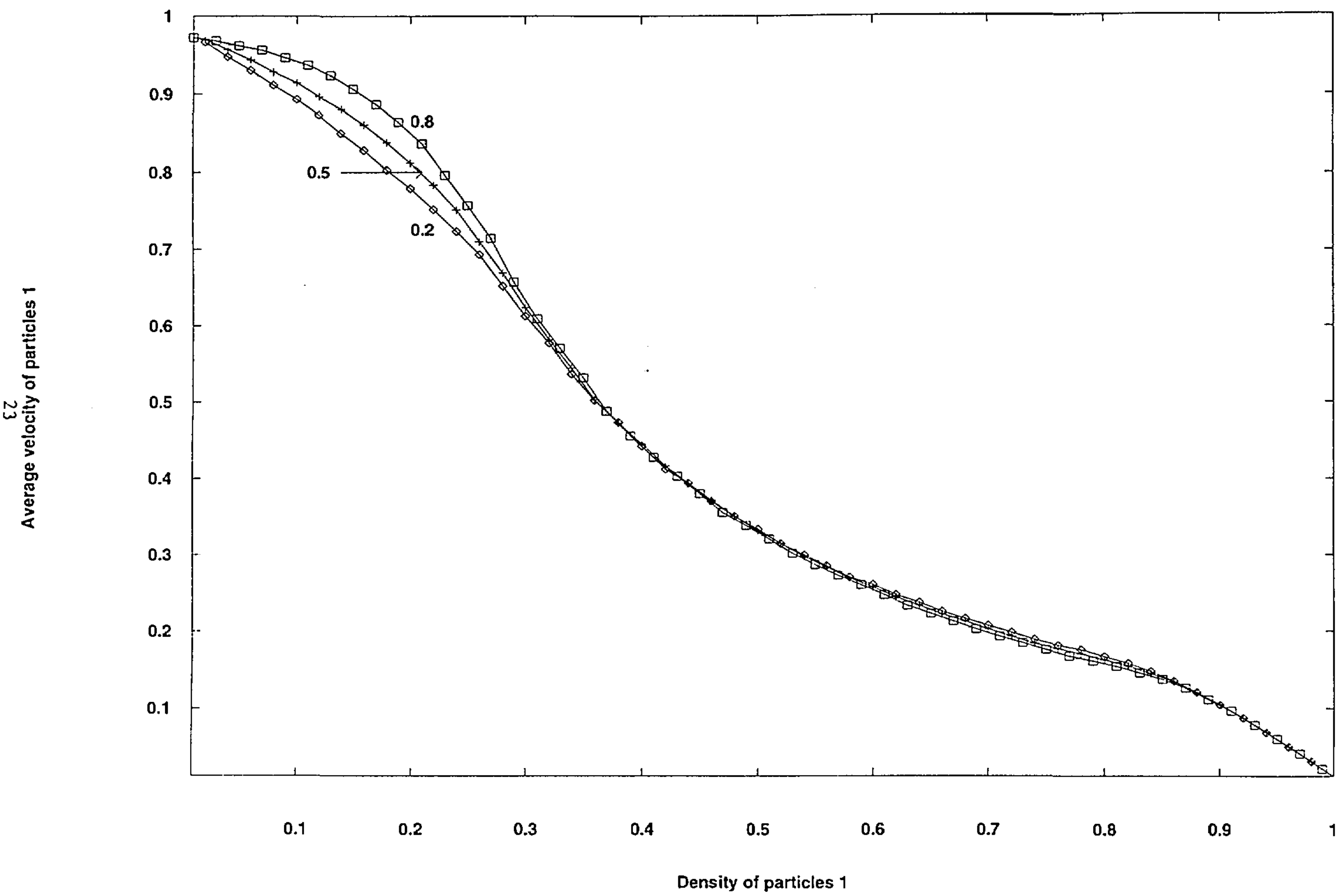
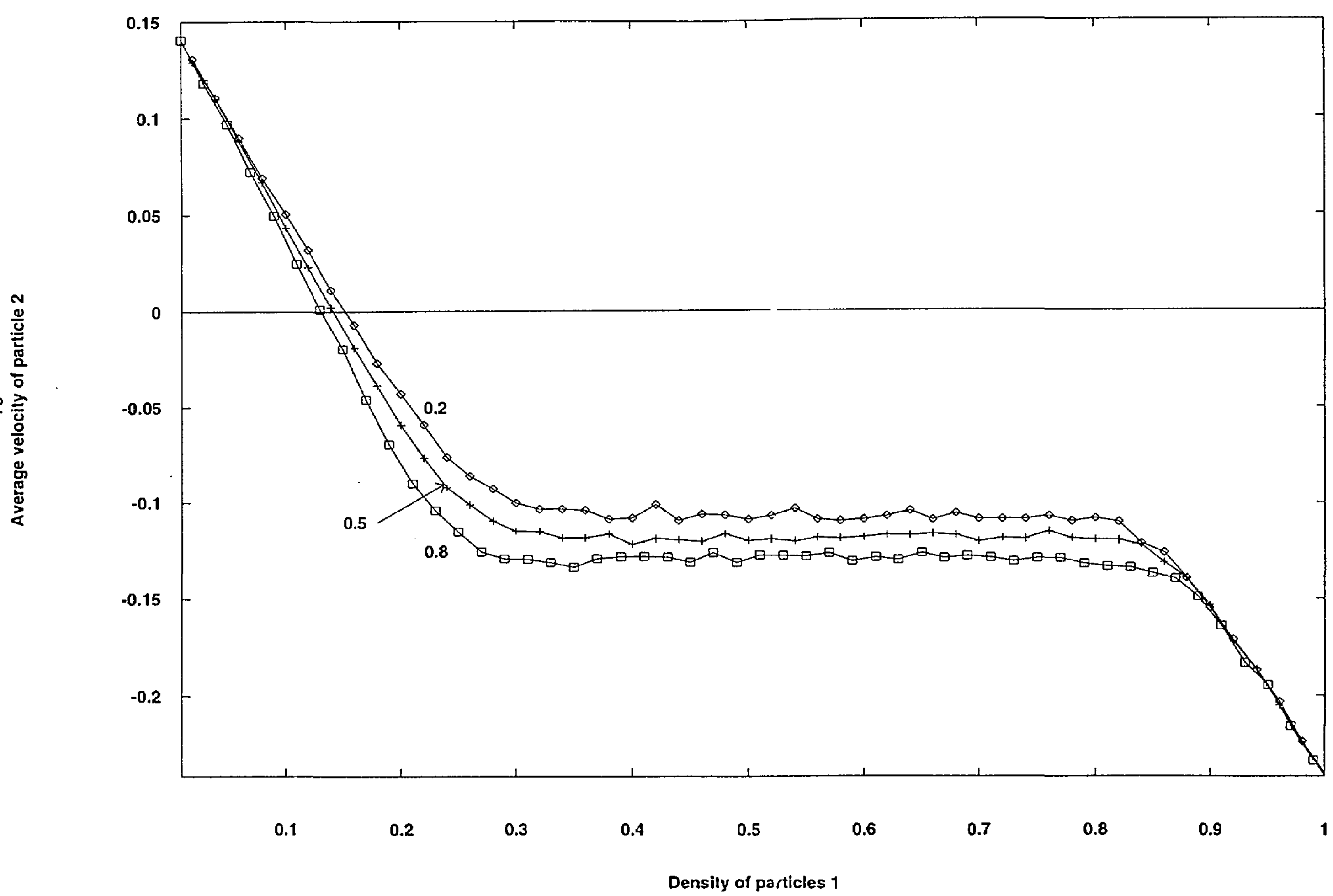

0.8
0.5
0.2
Average velocity of particles
Density of particles
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Fig 7.a



Average velocity of particles 1
23
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.8
0.5
0.2
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Density of particles 1

Fig 7.b



Average velocity of particle 2
24
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
0.2
0.5
0.8
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Density of particles 1