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Asymmetric simple exclusion model with local inhomogeneity

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Abstract. We study a totally asymmetric simple exclusion model with open boundary conditions and a local inhomogeneity in the bulk. It consists of a one-dimensional lattice with particles hopping stochastically with equal rates to the right at all lattice sites except one where the jump rate is different. Approximate stationary-state solutions and phase diagrams are obtained and compared with Monte Carlo simulation results.

1. Introduction

One-dimensional asymmetric simple exclusion processes (ASEPs) have received much attention recently [1]. ASEP is a lattice model of particles hopping stochastically and interacting through hard-core exclusion. It has been used to describe various physical phenomena such as gel electrophoresis [2, 3], interface growth [4], the formation of shocks [5, 11], biopolymerization [6, 7], and directed polymers in a random medium [8]. Exact solutions have been obtained for stationary states of some asymmetric exclusion models with various boundary conditions [9–14].

So far the stationary states have been calculated exactly for the asymmetric exclusion models with translational symmetry in the bulk. The introduction of a stationary defect, changing the rate of stochastic motion at one particular bond, makes the subject very complicated. Such models with periodic boundary conditions have been studied numerically [15, 16]. Also exact results exist for an exclusion model with stochastic defect, parallel dynamics, and deterministic hopping in the bulk [17, 18]. However, no exact solutions are known for the ASEPs with random sequential dynamics.

In this paper we consider a totally asymmetric exclusion model with open boundary conditions. Each site i of a one-dimensional lattice of size N is either occupied by a particle (occupation number $l_i = 1$), or empty ($l_i = 0$). During the infinitesimal time step $\mathrm{d}t$, each particle belonging to the sites $1 \leqslant i \leqslant N-1$ has a probability $\mathrm{d}t$ of jumping to the next right site if this neighbouring site is empty. The particles are injected at the left end ($i = 1$) with probability $\alpha\,\mathrm{d}t$ if site 1 is empty and removed from the right end ($i = N$) with probability $\beta\,\mathrm{d}t$ if this site is occupied. Furthermore, a defective bond is inserted between sites k and $k+1$ where the particles hop stochastically from k to $k+1$ with a probability $q\,\mathrm{d}t$. We consider both the cases $q < 1$ and $q \geqslant 1$. The former implies that the particles hop more slowly across the defect link, while the latter means that they hop faster. When $q = 1$ we have an ASEP solved exactly [9, 14]. In this paper we solve the introduced model approximately and compare our solution with exact results ($q = 0$, and $q = 1$) and Monte Carlo simulations.

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2. Approximate solutions

To simplify the calculations we assume that lattice size N is a large even number and we put a defect bond in the middle of the chain, i.e. we assume that the defect link connects the sites $k = N/2$ and $k+1 = N/2+1$. We expect the results for any position of the impurity a distance $O(N)$ from the ends will be qualitatively the same. Before solving the problem for general q we give the exact result for the limiting case $q = 0$ and quote the exact result for $q = 1$, which will be used as criteria of validity of our approximation scheme.

2.1. Exact results

When $q = 0$ the solution is trivial. In stationary state the current is not passing anywhere ($J = 0$) so that the density of the particles at the left half of the chain before the impurity is equal 1, and the density of the particles at the right half of the system after the impurity is 0. These results can be summarized as follows

$$\begin{aligned} &l_i = 1 \qquad 1 \leqslant i \leqslant k \\ &l_i = 0 \qquad k+1 \leqslant i \leqslant N \\ &J = 0. \end{aligned} \tag{1}$$

The case of $q = 1$ is exactly solvable and here we recall some of the results [9, 14] that will be used in the solution for general q. There are three phases in the limit of $N \to \infty$. When $\alpha \geqslant \frac{1}{2}$ and $\beta \geqslant \frac{1}{2}$ we have a maximal-current phase with

$$\begin{aligned} &l_1 = \frac{1}{4\beta} \\ &l_N = 1 - \frac{1}{4\alpha} \\ &J = \tfrac{1}{4} \\ &l_{\text{bulk}} = \tfrac{1}{2} \end{aligned} \tag{2}$$

where l_1 is the particle density at the first site and l_N is the particle density at the last site of the lattice, and l_{bulk} is the density in the bulk of the chain far away from the boundaries.

The conditions $\alpha > \beta$ and $\beta < \frac{1}{2}$ describe a high-density phase where

$$\begin{aligned} &l_1 = 1 - \beta(1-\beta)/\alpha \\ &l_N = 1 - \beta \\ &J = \beta(1-\beta) \\ &l_{\text{bulk}} = 1 - \beta. \end{aligned} \tag{3}$$

When $\alpha < \beta$ and $\alpha < \frac{1}{2}$ we have a low-density phase. The current and densities of the particles at the first and last sites are the following

$$\begin{aligned} &l_1 = \alpha \\ &l_N = \alpha(1-\alpha)/\beta \\ &J = \alpha(1-\alpha) \\ &l_{\text{bulk}} = \alpha. \end{aligned} \tag{4}$$

2.2. Approximate solution for general q

The one-dimensional lattice of size N with the defect bond in the middle can be thought of as two one-dimensional lattices each of size $N/2$ connected by the defect bond. Then the left part is a totally asymmetric exclusion model without impurity with the rate of injection of the particles α and the rate of removal of the particles β_{eff}, where

$$\beta_{\text{eff}} = q(1 - l_{k+1}). \tag{5}$$

Similarly, the right part is a totally asymmetric exclusion model without impurity with the rate of injection of the particles α_{eff} and the rate of leaving of the particles β, where

$$\alpha_{\text{eff}} = q l_k. \tag{6}$$

A similar idea has been successfully used recently in the investigation of the phase transitions in the one-dimensional reaction-diffusion model [19].

In the steady-state the current through the left lattice, right lattice, and defect bond should be the same. To find the current through the defect link we use a simple mean-field approximation which consists of the assertion that

$$J = q l_k (1 - l_{k+1}). \tag{7}$$

There is also a particle–hole symmetry in the system. Since particles are injected at the left end with probability α and removed at the right end with probability β, it is equivalent to say that holes are injected at the right end with probability β and removed at the left end with probability α. Because of this particle–hole symmetry, one always has

$$l_i(\alpha, \beta, q) = 1 - l_{N+1-i}(\beta, \alpha, q). \tag{8}$$

In our representation the kth site plays a role of the last site of the left lattice while the $(k+1)$th site is the first site of the right lattice. Then using equations (2)–(4), (7), (8), and exact large-N results for the left and right lattices one can find the following solutions.

When $q > 1$ we have the phase diagram shown in figure 1(a). Similarly to the case without local inhomogeneity ($q = 1$), it consists of three phases. The case $\alpha \geqslant \frac{1}{2}$ and $\beta \geqslant \frac{1}{2}$ corresponds to a maximal-current phase in which

$$\begin{aligned} l_k &= \frac{1}{2\sqrt{q}} \\ l_{k+1} &= 1 - \frac{1}{2\sqrt{q}} \\ J &= \tfrac{1}{4} \\ \alpha_{\text{eff}} &= \sqrt{q}/2 \\ \beta_{\text{eff}} &= \sqrt{q}/2 \\ l_{\text{bulk,left}} &= l_{\text{bulk,right}} = \tfrac{1}{2}. \end{aligned} \tag{9}$$

One can analyse the solution in the limiting case $q \to \infty$ where we have $l_k \to 0$ and $l_{k+1} \to 1$. These limits seem reasonable because in the maximal-current phase the system has enough time to empty the site before the defect bond and fill the site after the defect bond. Also, in the case $q = 1$ our solution gives $l_k = l_{k+1} = \frac{1}{2}$, the same results as in the case of exact solution for ASEP without defect bond [9, 14].

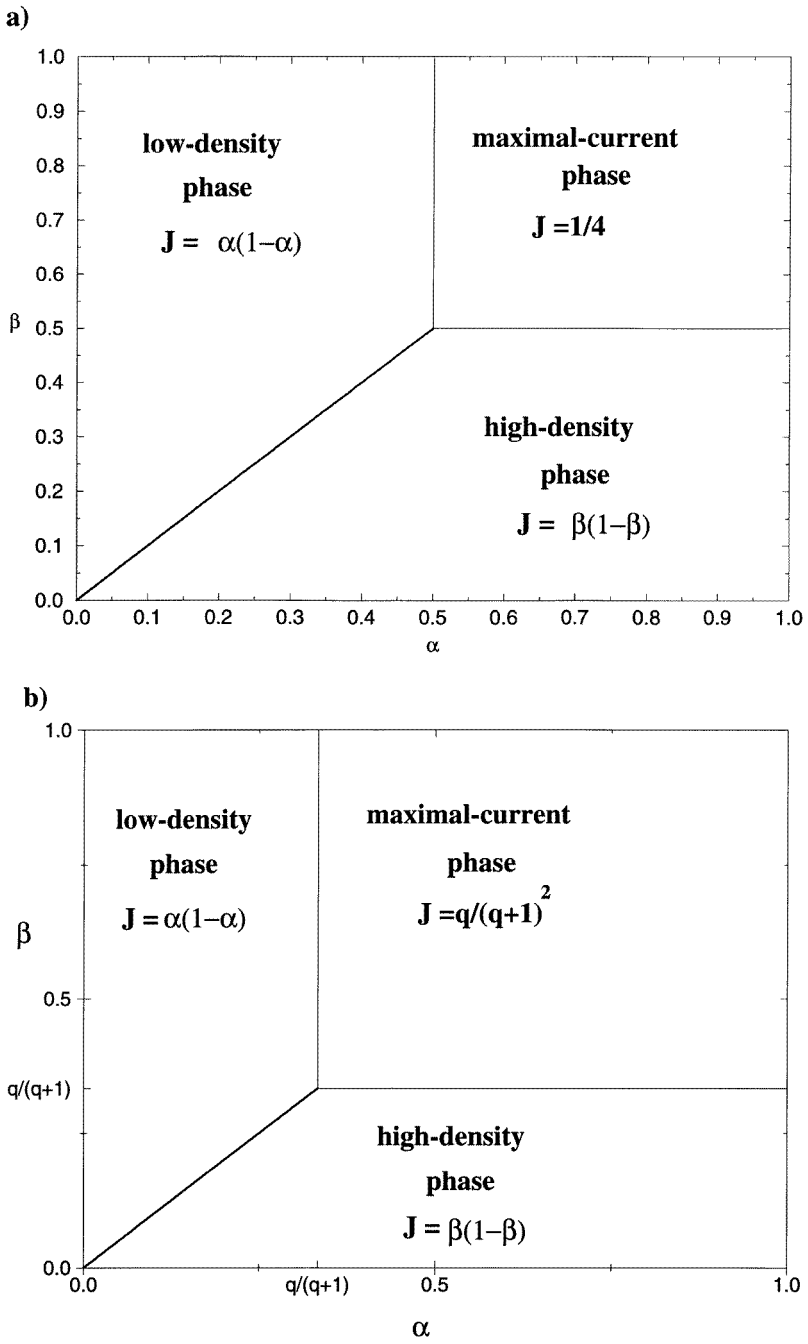

Figure 1. Phase diagrams obtained from the approximate solutions. Heavy full lines are first-order phase transition lines, light full lines are continuous transition lines. (*a*) $q > 1$; (*b*) $q < 1$.

The conditions $\alpha > \beta$ and $\beta < \frac{1}{2}$ describe a high-density phase, where

$$\begin{aligned} &l_k = 1-\beta \\ &l_{k+1} = 1-\beta/q \\ &J = \beta(1-\beta) \\ &\alpha_{\text{eff}} = q(1-\beta) \\ &\beta_{\text{eff}} = \beta \\ &l_{\text{bulk,left}} = l_{\text{bulk,right}} = 1-\beta. \end{aligned} \tag{10}$$

In the limit $q \to \infty$ the density at kth site is unchanged, but $l_{k+1} \to 1$. These limiting results can be understood as follows. In the high-density phase the slowest rate-determining process is the removal of the particles at the right end, that is why the site after the impurity will be filled, but the density at the site preceding the defect bond will not decrease to zero. In this phase the particles are 'stuck' inside the chain. Also, for $q = 1$ we have $l_k = l_{k+1} = 1-\beta$ which is in agreement with exact results for the asymmetric simple exclusion model without local inhomogeneity.

Similarly, $\beta > \alpha$ and $\alpha < \frac{1}{2}$ describe the low-density phase. One can find the following results in this phase

$$\begin{aligned} &l_k = \alpha/q \\ &l_{k+1} = \alpha \\ &J = \alpha(1-\alpha) \\ &\alpha_{\text{eff}} = \alpha \\ &\beta_{\text{eff}} = q(1-\alpha) \\ &l_{\text{bulk,left}} = l_{\text{bulk,right}} = \alpha. \end{aligned} \tag{11}$$

In the low-density phase the rate of injection of the particles is the limiting process, so there is a shortage of the particles inside the chain. Thus, in the limit $q \to \infty$ we have l_{k+1} unchanged and $l_k \to 0$. Also, for $q = 1$ we again reproduce the known exact results for the ASEP without impurity ($l_k = l_{k+1} = \alpha$).

The phase boundary $\alpha = \beta < \frac{1}{2}$ is a coexistence line of first-order phase transitions and we may expect a linear density profile (except in the area close to the local inhomogeneity), similarly to the case of the asymmetric exclusion model without a defect bond. The other phase boundaries correspond to continuous transitions.

The phase diagram for $q < 1$ is shown in figure 1(b). It also has three phases as in the case $q > 1$ but the locations of some phase boundaries are changed.

The conditions $\alpha \geqslant q/(q+1)$ and $\beta \geqslant q/(q+1)$ determine the maximal-current phase here. The solutions for this phase are the following

$$\begin{aligned} &l_k = 1/(q+1) \\ &l_{k+1} = q/(q+1) \\ &J = q/(q+1)^2 \\ &\alpha_{\text{eff}} = q/(q+1) \\ &\beta_{\text{eff}} = q/(q+1) \\ &l_{\text{bulk,left}} = 1/(q+1) \\ &l_{\text{bulk,right}} = q/(q+1). \end{aligned} \tag{12}$$

In the limit $q = 0$ the current goes to zero, $l_k = 1$ and $l_{k+1} = 0$, in agreement with the exact solutions (see equations (1)). When $q = 1$ we recover the exact results for the ASEP

without local inhomogeneity: $J = \frac{1}{4}$, $l_k = l_{k+1} = \frac{1}{2}$.

The high-density phase is defined here by $\alpha > \beta$ and $\beta < q/(q+1)$. The results in this phase are the same as for the high-density phase with $q > 1$:

$$\begin{aligned} l_k &= 1 - \beta \\ l_{k+1} &= 1 - \beta/q \\ J &= \beta(1-\beta) \\ \alpha_{\text{eff}} &= q(1-\beta) \\ \beta_{\text{eff}} &= \beta \\ l_{\text{bulk,left}} &= l_{\text{bulk,right}} = 1 - \beta. \end{aligned} \tag{13}$$

The results for the low-density phase (defined by $\beta > \alpha$ and $\alpha < q/(q+1)$) are also similar to those of the low-density phase with $q > 1$:

$$\begin{aligned} l_k &= \alpha/q \\ l_{k+1} &= \alpha \\ J &= \alpha(1-\alpha) \\ \alpha_{\text{eff}} &= \alpha \\ \beta_{\text{eff}} &= q(1-\alpha) \\ l_{\text{bulk,left}} &= l_{\text{bulk,right}} = \alpha. \end{aligned} \tag{14}$$

Also, the coexistence line $\alpha = \beta < q/(q+1)$ is the locus of first-order phase transitions. The other phase boundaries are continuous.

3. Monte Carlo simulations and discussion

So far our general approximate solution gave correct results at all limiting cases where exact results are known. To investigate the applicability of our approach for general q we tested our approximation with Monte Carlo simulations. First we compared our approximate solution with the exact solution for the asymmetric simple exclusion model without stochastic impurity ($q = 1$) (see figure 2). There is a slight deviation in our density profile from the exact density profile for $N = 200$, but as we checked for larger N this difference decreases and we expect that in the limit $N \to \infty$ our approximate solution gives the exact solution for the model without local inhomogeneity.

When $q > 1$ there is very good qualitative and quantitative agreement between the density profiles given by our approximation and Monte Carlo results in the high-density and low-density phases (see figures 3(a) and (b)). The results for the maximal-current phase ($q > 1$) are still qualitatively the same, but there are deviations in the region near the local inhomogeneity (figure 3(c)). That is a consequence of our mean-field treatment of correlations near the defect bond. Obviously, in reality the correlations are larger than predicted, and that makes the density in the left-hand part larger and that in the right-hand part smaller than our approximation predicts. The positions of the phase boundaries are determined exactly by our approach (figure 3(d)). Also, our approximation fails at the coexistence line ($\alpha = \beta < \frac{1}{2}$). Our approach predicts the existence of two discontinuities in the density profile, both of them are at the middle of the chain. One of them is a result of the local defect, another one is a jump in the bulk density between the left and right parts of the system (figure 3(d)). The latter discontinuity would exist even for the $q = 1$ case. The Monte Carlo density profile is linear (except close to the local inhomogeneity) due to

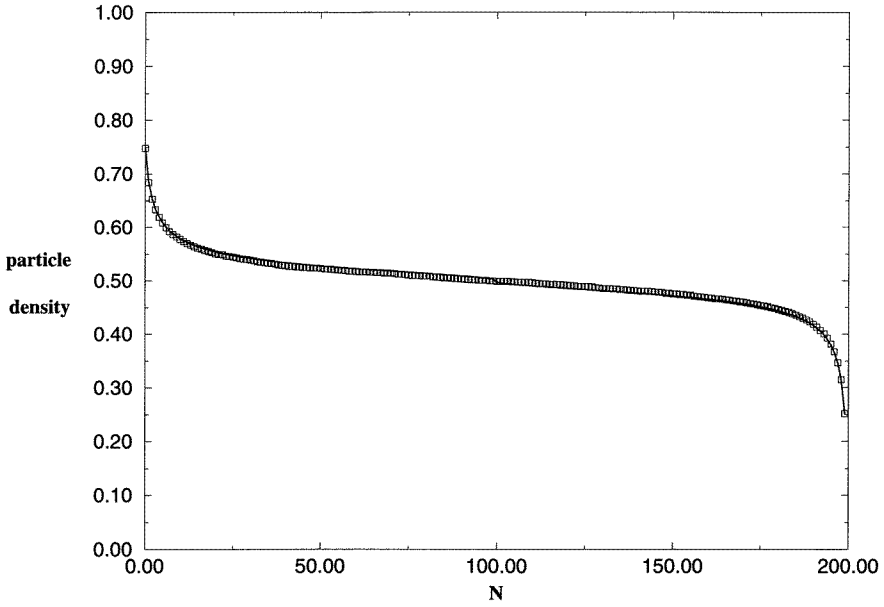

Figure 2. Density profiles for the system of size $N = 200$ without the defect bond and $\alpha = \beta = 1$. The squares are used to plot the density profile from Monte Carlo simulation which is the same as the exact density profile in this case. Monte Carlo densities are results of averaging over 5×10^9 Monte Carlo steps. Full curves are our approximation. The equations (43) and (44) of [9] have been used in the calculation of our approximate density profiles.

the fact that along the coexistence line, there is a superposition of states with the jump in the bulk density at an arbitrary position [9].

We have a similar picture for the case $q < 1$ (figures 4(a)–(d)). Again the agreement between our predictions and Monte Carlo simulations is quite good in the high- and low-density phases (but not as good as for the same phases in the case $q > 1$). The biggest deviations can be found in the maximal-current phase. For example, in the case $q = \frac{1}{2}$ we predict the phase boundary between the maximal-current phase and the high-density phase to be at $\beta = \frac{1}{3}$ while Monte Carlo simulations give $\beta \approx 0.38$. The reason for that is, probably, the fact that the density profile at all lattice sites is influenced by the behaviour of the system near the local inhomogeneity. In the case $q > 1$ only the density near the defect bond is influenced by the impurity, and that is why our approximation gives better results for $q > 1$. Despite these facts, our approach still calculates qualitatively correct density profiles.

4. Summary and conclusions

We presented a one-dimensional asymmetric simple exclusion model with open boundary conditions and with a stochastic impurity in the bulk. The model was solved using a simple approximation. Our scheme consisted of two parts. First, we represented our system as two systems without the stochastic defect, connected at the position of the local inhomogeneity. The second assumption was the approximation of mean-field behaviour for sites k and $k+1$ only (recall, that the defect bond is situated between these two sites) (equation (7)). We point out that the first statement alone suffices to obtain a qualitative picture, but to get

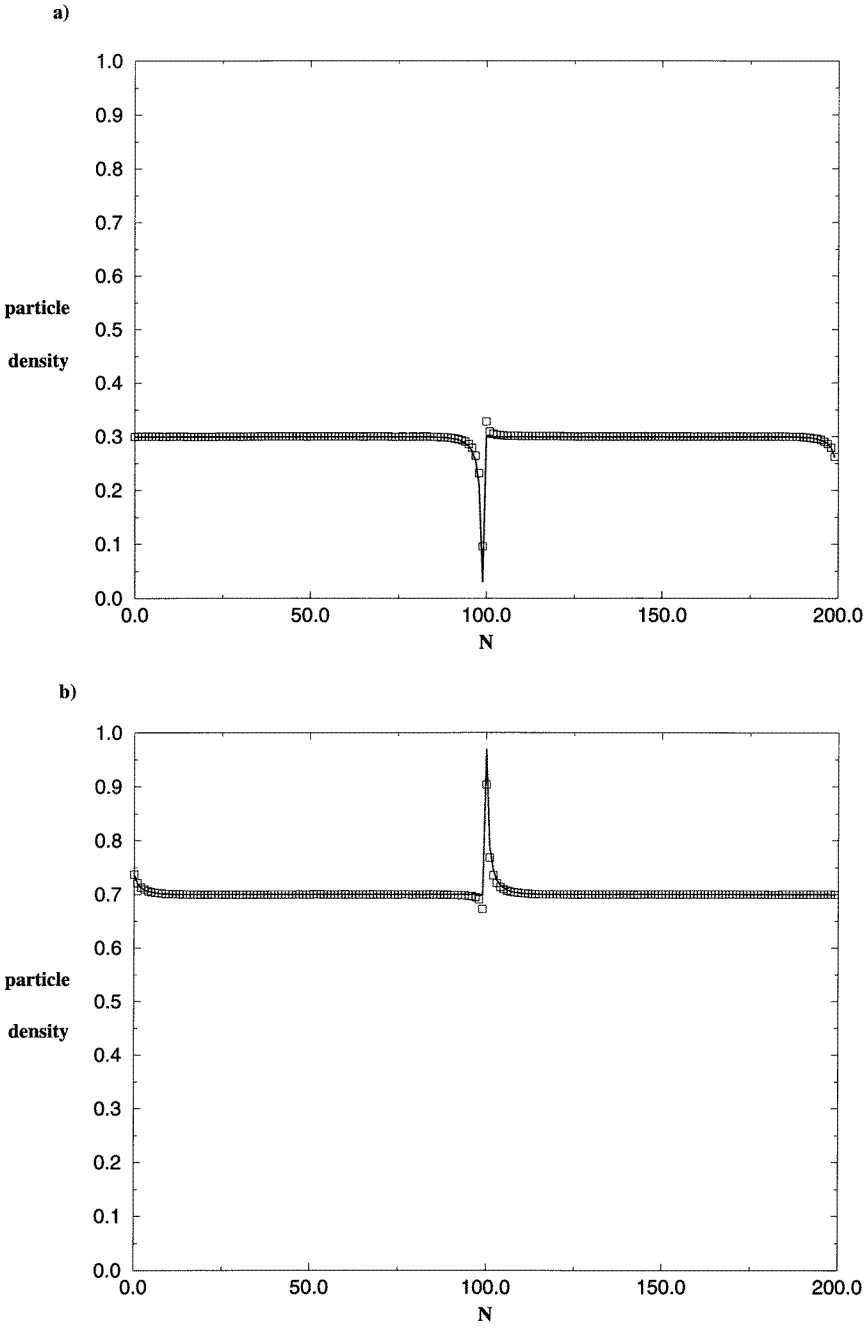

Figure 3. Density profiles for the system of size $N = 200$ with $q = 10$. The squares indicate the Monte Carlo simulation results. Full curves are our approximation. The equations (43) and (44) of [9] have been used in the calculation of our approximate density profiles. Monte Carlo densities are results of averaging over 5×10^9 Monte Carlo steps. (*a*) $\alpha = 0.3$, $\beta = 0.8$; (*b*) $\alpha = 0.8$, $\beta = 0.3$; (*c*) $\alpha = 0.8$, $\beta = 0.8$; (*d*) $\alpha = 0.3$, $\beta = 0.3$.

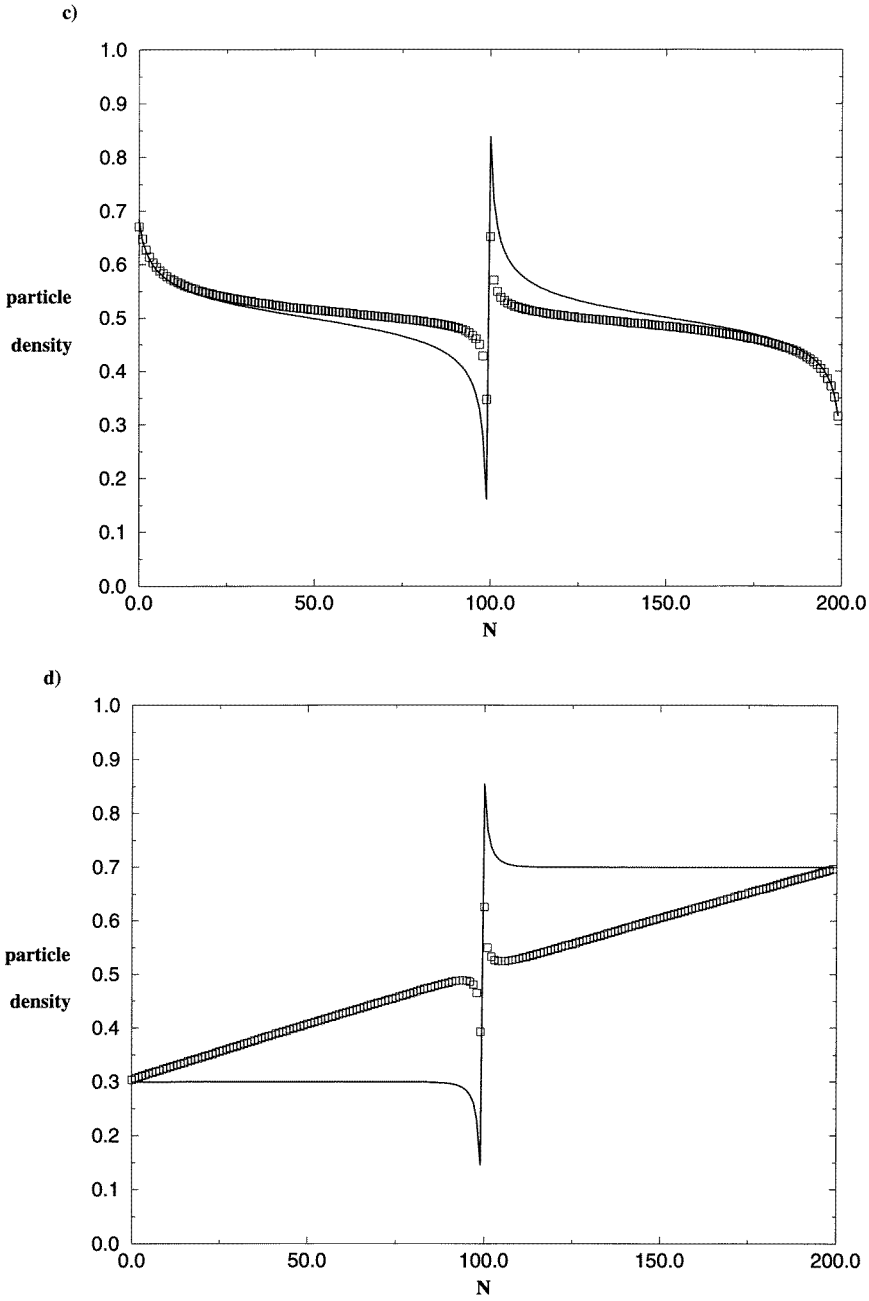

Figure 3. (Continued)

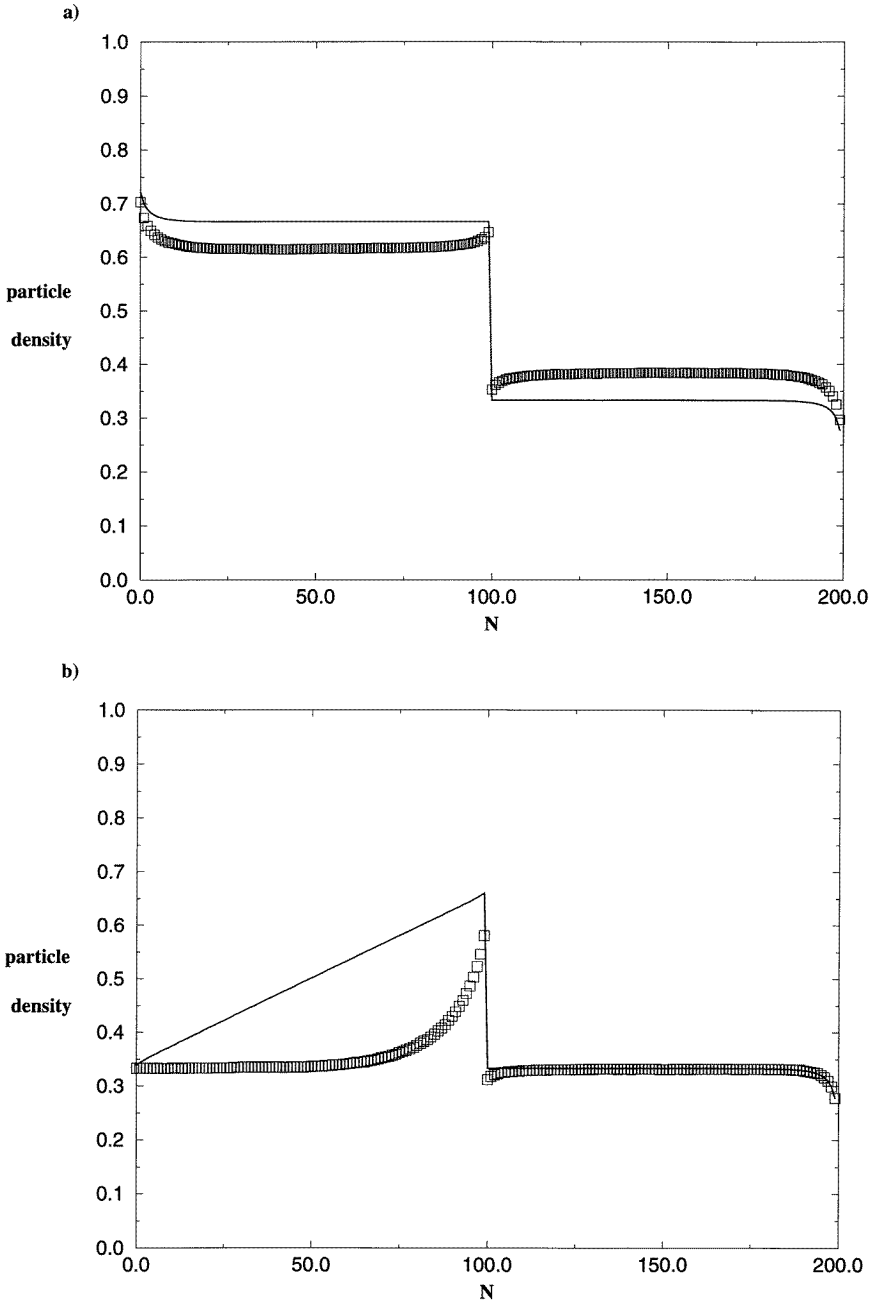

Figure 4. Density profiles for the system of size $N = 200$ with $q = 0.5$. The squares are the Monte Carlo simulation results. Full curves are our approximation. The equations (43) and (44) of [9] have been used in the calculation of our approximate density profiles. Monte Carlo densities are results of averaging over 10^9 Monte Carlo steps. (a) $\alpha = 0.8$, $\beta = 0.8$; (b) $\alpha = \frac{1}{3}$, $\beta = 0.8$; (c) $\alpha = 0.3$, $\beta = 0.3$; (d) $\alpha = 0.8$, $\beta = 0.38$.

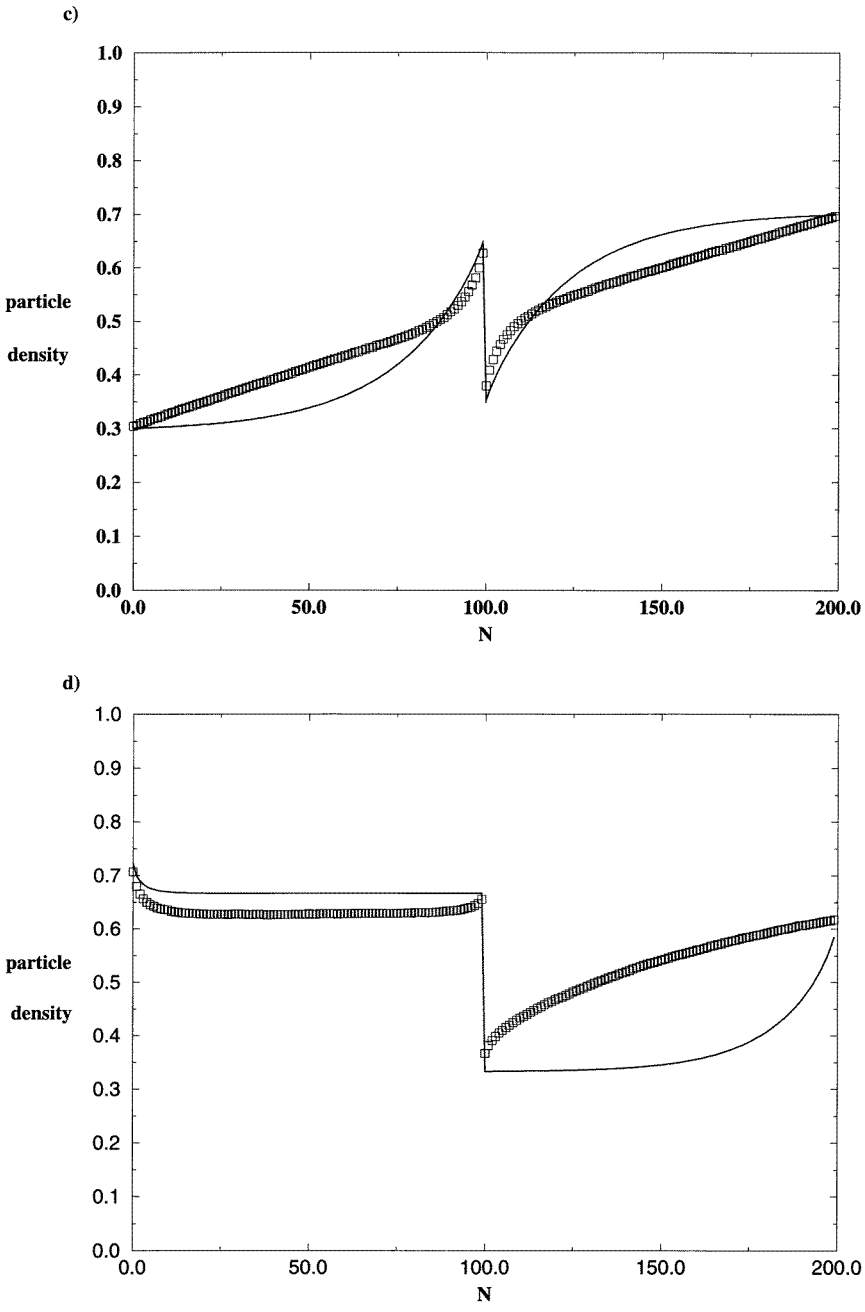

Figure 4. (Continued)

explicit formulae we had to make the second assumption. This second assumption is the real source of differences from Monte Carlo simulation results.

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