Hopping motion of lattice gases through nonsymmetric potentials under strong bias conditions

K. W. Kehr[1] and Z. Koza[1,2]
[1]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany
[2]Institute of Theoretical Physics, University of Wrocław, pl. Maxa Borna 9, PL-50204 Wrocław, Poland
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The hopping motion of lattice gases through potentials without mirror-reflection symmetry is investigated under various bias conditions. The model of two particles on a ring with four sites is solved explicitly; the resulting current in a sawtooth potential is discussed. The current of lattice gases in extended systems consisting of periodic repetitions of segments with sawtooth potentials is studied for different concentrations and values of the bias. Rectification effects are observed, similar to the single-particle case. A mean-field approximation for the current in the case of strong bias acting against the highest barriers in the system is made and compared with numerical simulations. The particle-vacancy symmetry of the model is discussed.

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I. INTRODUCTION

The motion of particles in potentials that do not have mirror reflection symmetry has attracted much attention in the last years for several reasons. The interest extends from fundamental problems concerning the validity of the second law of thermodynamics [1,2] to applications in biological [3–7] and chemical systems [8], as well as for solid-state devices [9,10]. Major efforts have been devoted to an understanding of molecular motors, where proteins move in nonsymmetric potentials under the influence of stochastic and/or other forces. One specific observation for transport in nonsymmetric potentials is the possibility of rectification effects if the forces on the particles are beyond the regime where linear-response theory is applicable [11]. Rectification effects have been discussed in continuous [12] as well as in hopping systems [4,11]. If applications of effects of particle motion in nonsymmetric potentials are envisaged, then the question arises as to the influence of many-particle effects. The limit of single-particle motion is rarely realized; in real systems many particles are present that compete about the sites that can be occupied. Many-particle effects have been studied in continuous nonsymmetric periodic potentials in Ref. [13], where interesting dependencies of the current on particle concentration and size were found. In this paper we will investigate hopping motion of lattice-gas particles in nonsymmetric hopping potentials under the influence of strong bias. We utilize the simple site exclusion model where multiple occupancy of sites is excluded and direct our attention to nonlinear effects on the particle current.

The stationary current of a single particle performing a hopping motion in a nonsymmetric potential under an arbitrary bias is known exactly [11]. The calculation of the stationary current of site-exclusion lattice gases in nonsymmetric potentials that lead to rectification effects in the single-particle case is a difficult problem. Extensive work has been devoted to the asymmetric site-exclusion process including the totally asymmetric site-exclusion process (TASEP) where the particles can only hop in one direction, corresponding to very strong bias. The case of uniform hopping potentials is now well understood [14], but the case of nonuniform potentials is not generally solved. Recent work has been devoted to the TASEP with disordered potentials [15–20]. For the general asymmetric case one has to resort to numerical simulations; we are going to present simulation results for the stationary current of lattice-gas particles in nonsymmetric potentials, for various concentrations and values of the bias.

Nonetheless, some analytical treatment can be given. First, the case of very small periodic systems can be treated explicitly: the motion of two particles on a ring of period 4 can be solved by elementary means. Although this is a very simple system, conclusions can be drawn in the limit of very strong bias that are of interest for the totally asymmetric site-exclusion process. The nonlinear current of site-exclusion lattice gases in extended systems with periodic repetitions of nonsymmetric segments can be derived in a mean-field approximation for strong bias conditions. Interesting symmetry properties have been pointed out for the TASEP in disordered hopping potentials [18–20]. While a particle-vacancy symmetry is also present in our model, the case of inversion of the bias direction is different here.

In the following section the hopping motion of two particles on a ring of period 4 is solved and analyzed. In Sec. III a mean-field approximation for the stationary current of lattice gases under strong bias in nonsymmetric hopping potentials is presented and compared with simulation results in a sawtooth potential. The symmetry properties of the model are discussed in Sec. IV and concluding remarks are given in Sec. V.

II. TWO PARTICLES ON RING WITH FOUR SITES

A. Solution of the stationary master equations

A very simple yet nontrivial model is given by a ring with four sites and two particles; cf. Fig. 1. The basic quantities for the description of the system are the joint probabilities $P(i,j;t)$ $(i \neq j)$ of finding one particle at site i and the other particle at site j, at time t, for specified initial conditions. Since the particles are considered as indistinguishable, $P(i,j;t) = P(j,i;t)$. There are six different joint two-particle probabilities on the ring consisting of four sites [generally $L(L-1)/2$ on rings with L sites]. Higher-order joint probabilities do not occur for two particles.

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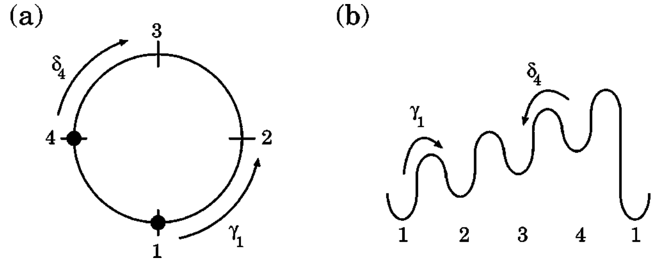

FIG. 1. (a) Ring of four sites with two particles. (b) Sawtooth potential with period 4 without bias ($b=1$) with two transition rates indicated.

The probabilities $P(i;t)$ of finding a particle at site i at time t are given by

$$P(i;t)=\sum_{j\neq i} P(i,j;t). \tag{1}$$

For two particles they are normalized to

$$\sum_{i=1}^{4} P(i;t)=2. \tag{2}$$

This condition implies

$$\sum_{i<j} P(i,j;t)=1. \tag{3}$$

The master equations for the joint probabilities are easily written down,

$$\begin{aligned}
\frac{d}{dt}P(1,2;t)&=\delta_3 P(1,3;t)+\gamma_4 P(2,4;t)-(\gamma_2+\delta_1)P(1,2;t),\\
\frac{d}{dt}P(2,3;t)&=\delta_4 P(2,4;t)+\gamma_1 P(1,3;t)-(\gamma_3+\delta_2)P(2,3;t),\\
\frac{d}{dt}P(3,4;t)&=\delta_1 P(1,3;t)+\gamma_2 P(2,4;t)-(\gamma_4+\delta_3)P(3,4;t),\\
\frac{d}{dt}P(1,4;t)&=\delta_2 P(2,4;t)+\gamma_3 P(1,3;t)-(\gamma_1+\delta_4)P(1,4;t),\\
\frac{d}{dt}P(1,3;t)&=\gamma_2 P(1,2;t)+\delta_2 P(2,3;t)+\gamma_4 P(3,4;t)\\
&\quad+\delta_4 P(1,4;t)-(\gamma_1+\delta_1+\gamma_3+\delta_3)P(1,3;t),\\
\frac{d}{dt}P(2,4;t)&=\delta_1 P(1,2;t)+\gamma_3 P(2,3;t)+\delta_3 P(3,4;t)\\
&\quad+\gamma_1 P(1,4;t)-(\gamma_2+\delta_2+\gamma_4+\delta_4)P(2,4;t).
\end{aligned} \tag{4}$$

The sum of the six master equations leads to the conservation law

$$\frac{d}{dt}\left(\sum_{i<j} P(i,j;t)\right)=0, \tag{5}$$

consistent with the relation (3) given above.

We are interested in the stationary solution of the system of master equations (4). The stationary values $P(i,j;t\rightarrow\infty)$ will be denoted by P_{ij}. The stationary joint probabilities for adjacent sites, e.g., P_{12}, can all be expressed by the stationary joint probabilities P_{13} and P_{24}. For instance, the first line of Eq. (4) yields

$$P_{12}=\frac{1}{\gamma_2+\delta_1}(\delta_3 P_{13}+\gamma_4 P_{24}). \tag{6}$$

Three analogous relations follow from Eqs. (4); they can be obtained by cyclically increasing the indices in Eq. (6). If the joint probabilities for adjacent sites are eliminated from the stationary master equations, two homogeneous equations remain that are equivalent. We write this equation as

$$a_{11}P_{13}+a_{12}P_{24}=0, \tag{7}$$

with the coefficients

$$\begin{aligned}
a_{11}&=-\left(\frac{\delta_1\delta_3}{\gamma_2+\delta_1}+\frac{\gamma_1\gamma_3}{\gamma_3+\delta_2}+\frac{\delta_1\delta_3}{\gamma_4+\delta_3}+\frac{\gamma_1\gamma_3}{\gamma_1+\delta_4}\right),\\
a_{12}&=\frac{\gamma_2\gamma_4}{\gamma_2+\delta_1}+\frac{\delta_2\delta_4}{\gamma_3+\delta_2}+\frac{\gamma_2\gamma_4}{\gamma_4+\delta_3}+\frac{\delta_2\delta_4}{\gamma_1+\delta_4}.
\end{aligned} \tag{8}$$

The second equation for P_{13} and P_{24} is obtained from the normalization condition, Eq. (3), after elimination of the joint probabilities of adjacent sites. It reads

$$a_{21}P_{13}+a_{22}P_{24}=1, \tag{9}$$

with the coefficients

$$\begin{aligned}
a_{21}&=\frac{\delta_3}{\gamma_2+\delta_1}+\frac{\gamma_1}{\gamma_3+\delta_2}+\frac{\delta_1}{\gamma_4+\delta_3}+\frac{\gamma_3}{\gamma_1+\delta_4}+1,\\
a_{22}&=\frac{\gamma_4}{\gamma_2+\delta_1}+\frac{\delta_4}{\gamma_3+\delta_2}+\frac{\gamma_2}{\gamma_4+\delta_3}+\frac{\delta_2}{\gamma_1+\delta_4}+1.
\end{aligned} \tag{10}$$

The solution of the two linear equations is

$$\begin{aligned}
P_{13}&=\frac{-a_{12}}{a_{11}a_{22}-a_{12}a_{21}},\\
P_{24}&=\frac{a_{11}}{a_{11}a_{22}-a_{12}a_{21}}.
\end{aligned} \tag{11}$$

Since the joint probabilities for adjacent sites are obtained from the P_{13}, P_{24}, and the one-site stationary probabilities $P_i\equiv P(i;t\rightarrow\infty)$ from Eq. (1), Eq. (11) represents the complete solution of the stationary problem.

We derive the stationary current in the system by considering the bond connecting sites 1 and 2. The stationary current is given by

$$J=\gamma_1(P_1-P_{12})-\delta_2(P_2-P_{12}). \tag{12}$$

The joint probabilities in Eq. (12) ensure exclusion of double occupancy of sites. Using Eq. (1) the current is expressed in terms of the joint probabilities,

$$J=\gamma_1(P_{13}+P_{14})-\delta_2(P_{23}+P_{24}). \tag{13}$$

Insertion of the stationary solution for the joint probabilities gives

$$J=\frac{\gamma_1+\gamma_3+\delta_2+\delta_4}{(\gamma_1+\delta_4)(\gamma_3+\delta_2)}(\gamma_1\gamma_3P_{13}-\delta_2\delta_4P_{24}). \tag{14}$$

The current may also be derived by considering the other bonds of the ring. Two equivalent forms of the current result; the second (equivalent) form reads

$$J=\frac{\gamma_2+\gamma_4+\delta_1+\delta_3}{(\gamma_2+\delta_1)(\gamma_4+\delta_3)}(\gamma_2\gamma_4P_{24}-\delta_1\delta_3P_{13}). \tag{15}$$

It can be shown that the current vanishes if the right and left transition rates fulfill the following condition:

$$\gamma_1\gamma_2\gamma_3\gamma_4=\delta_1\delta_2\delta_3\delta_4, \tag{16}$$

corresponding to a detailed balance relation over the ring.

B. Solution for the sawtooth potential

The sawtooth potential including bias on a four-site ring is defined by choosing

$$\gamma_1=\gamma_2=\gamma_3=\gamma_4=b\gamma,$$
$$\delta_1=b^{-1}\gamma^4, \tag{17}$$
$$\delta_2=\delta_3=\delta_4=b^{-1},$$

where b represents the bias and $\gamma<1$ is a constant representing a transition rate to the right in the absence of a bias; cf. Fig. 1(b). Note that the right transition rates are explicitly multiplied by the bias factor b and the left transition rates by b^{-1}, respectively. Physically, $b=\exp(\Delta U/2k_BT)$, where ΔU represents the potential drop between two neighboring sites under the influence of the bias. For $b=1$ the system satisfies the detailed balance condition and the current J vanishes. In what follows the current obtained in a system with M particles will be denoted as J_M.

In Fig. 2 we present a plot of J_1 and J_2 as functions of the bias b for the ring with four sites and $\gamma=\exp(-2)$. The result for the two-particle system was obtained using Eq. (15), and for a single-particle system we employed the exact solution derived in Ref. [11]. We can see that the behavior of the currents of one- and two-particle systems are qualitatively similar. Of course, the current J_2 of two particles is larger than the one-particle current J_1. The inset shows the behavior of the current for smaller bias. The curves for the bias to the right and to the left become equal in the limit $b\to1$, i.e., in the linear-response regime for two particles on the ring with four sites and also for one particle on this ring. However, the two-particle current is about 17% larger than the one-particle current.

In the case of a strong bias to the right, $b\gg1$, the two-particle current J_2 differs from J_1 by a constant factor. For the sawtooth potential this behavior can be understood as follows. If $b\gg1$, only transitions to the right are important, and backward transitions can be neglected. In our model the transition rates to the right are all equal, $\gamma_i=b\gamma$ for $i=1,\dots,4$.

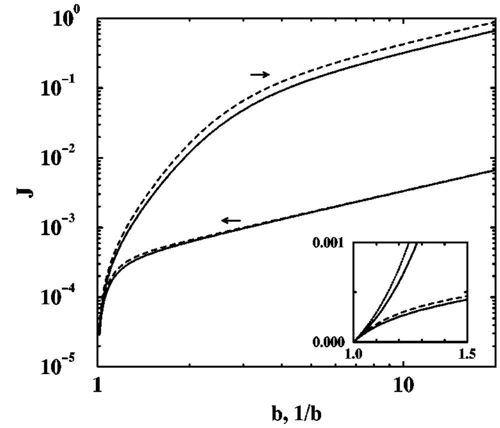

FIG. 2. Particle current J (arbitrary units) as a function of the dimensionless bias parameter. Upper curves, bias to the right, abscissa indicates b; lower curves, bias to the left, abscissa indicates $1/b$. Dashed lines, two particles on the ring with four sites; full lines, single particle on the ring. Inset, behavior for small bias (linear axes).

Hence for $b\gg1$ all stationary site occupation probabilities become equal, $P_i=1/2$ for the four-site ring and $P_i=2/L$ for a ring with L sites. In the limit of a strong bias to the right all stationary joint probabilities also become equal, i.e., $\forall_{i,j}\ P_{ij}=1/6$ for the four-site ring and, generally, $P_{ij}=2/L(L-1)$ (see Ref. [21]). Using expression (12) we thus expect that, for $b\gg1$,

$$J\approx b\gamma\left[\frac{2}{L}-\frac{2}{L(L-1)}\right]. \tag{18}$$

For $L=4$ there is thus $J_2=b\gamma/3$, which should be compared with the single-particle current $J_1=b\gamma/4$. Similarly, in the general case of an L-site ring we have

$$\lim_{b\to\infty}\frac{J_2}{J_1}=\frac{2(L-2)}{L-1}. \tag{19}$$

For the four-site ring this limiting behavior can be easily derived from the exact formula (15). Actually, for $L=4$, $\gamma=\exp(-2)$, and $b=10$ there is $J_2/J_1\approx1.3337$, in agreement with the above considerations.

Figure 2 also shows that J_2 becomes almost identical to J_1 in the case of a strong bias to the left, $b\ll1$. To understand this phenomenon assume that $\gamma\ll1$, so that $\delta_1\ll\delta_2=\delta_3=\delta_4$, i.e., site 1 acts as a ''bottle-neck.'' If $b\ll1$ the particles are driven against the high barrier at site 1, which has a relatively very small transition rate δ_1 to the left. The second particle on site 2 has to wait until the first particle has jumped over the high barrier, and only then can it make an attempt to jump over that barrier. Soon after the first particle has managed to pass the bottleneck at site 1, the second particle will jump from site 2 to 1 and the first particle will quickly line up behind the second particle, waiting for it to jump over the high barrier. Consequently, the current becomes practically equal to that of a single-particle system. It is evident that in the limit of a large bias to the left the system behaves as a TASEP on a ring with one defect. If the defect is characterized, in a discrete-time dynamics, by the transition probability $p \ll 1$, the current of M particles on a ring with L sites ($M < L$) will approach the one-particle current. The above reasoning is confirmed by an explicit calculation of the current J_2 in the limit $b \to 0$. Using Eq. (15), we conclude, after some algebra, that $J_2 \approx 2b^{-1}(1+\gamma^4)(5\gamma^4 + 2\gamma^{-4}+5)^{-1}$. Since for a single-particle system the current J_1, for $b \ll 1$, is approximately equal $b^{-1}\gamma^4(1+3\gamma^4)$ (see Ref. [11]), we find that

$$\lim_{b\to 0} \frac{J_2}{J_1} = \frac{2(1+\gamma^4)(1+3\gamma^4)}{5\gamma^8+5\gamma^4+2}. \tag{20}$$

For $\gamma \to 0$, i.e., for a growing asymmetry of the sawtooth potential, this limit actually approaches 1. In particular, for the value of $\gamma = \exp(-2)$ used in Fig. 2 there is $\lim_{b\to 0} J_2/J_1 \approx 1.0005$.

Note, however, that in contrast to the case $b \gg 1$, for $b \ll 1$ the current depends on the parameter γ characterizing the inhomogeneity of the sawtooth potential. In particular, for $\gamma = 1$, which corresponds to a fully homogeneous system, $\lim_{b\to 0} J_2/J_1 = 4/3$. Actually, for $\gamma = 1$, the ratio J_2/J_1 equals 4/3 irrespective of the bias b (see [21]).

III. EXTENDED NONSYMMETRIC POTENTIALS

A. The model

In this section lattice gases in extended potentials are considered that consist of periodic repetitions of nonsymmetric segments. First the situation of very strong bias is discussed and a mean-field approximation is given for the case where the particles experience periodically arranged high barriers. The analytical results are then compared with numerical simulations of the motion of lattice-gas particles in nonsymmetric hopping potentials for different concentrations and under various bias conditions. The hopping potential that is used in this section is the sawtooth potential shown in Fig. 1(b), except that it is periodically repeated with period L. The nearest-neighbor transition rates from site l to $l \pm 1$ are $\Gamma_{l,l\pm 1}$. As a short notation we use $\gamma_l \equiv \Gamma_{l,l+1}$ for the "right" and $\delta_l \equiv \Gamma_{l,l-1}$ for the "left" transition rates. Without additional bias, the transition rates between neighbor sites fulfill detailed balance. Bias is introduced by multiplying all right transition rates by b, $\gamma_l \to b\gamma_l$, and all left transition rates by b^{-1}, $\delta_l \to b^{-1}\delta_l$.

The linear chain on which the model is defined shall have $N = \nu L$ sites where we consider $\nu \gg 1$ in this section. Periodic boundary conditions are introduced and the sites are occupied by M particles. The concentration is then $\rho = M/N$. Multiple occupancy of the sites is excluded; no further interactions of the particles are taken into account.

B. Strong bias

1. The case $b \gg 1$

For $b \gg 1$ we can apply essentially the same reasoning as in the case of the two-particle system considered in Sec. II. In this limit transitions to the left are so rare that they can be ignored and the system essentially behaves like a TASEP with transitions $\gamma_i = b\gamma$, $i = 1, \ldots, N$. The current for such a system reads [21]

$$J = b\gamma M \frac{N-M}{N-1}. \tag{21}$$

For large system sizes $N \gg 1$ this formula can be rewritten as

$$J(\rho) = b\gamma\rho(1-\rho). \tag{22}$$

2. The case $b \ll 1$

For $b \ll 1$ we can neglect transition rates to the right, and so the system behaves like a TASEP with transition rates $\delta_i = b^{-1}\gamma^4$ if $i = 1 (\mathrm{mod}\, L)$ and $\delta_i = b^{-1}$ otherwise. If additionally $\gamma = 1$, all δ_i are equal to each other and the current is given simply by Eq. (21).

A more complicated situation appears for $\gamma \ll 1$, a condition that will be assumed henceforth. In this case, sites $i = 1, L+1, \ldots, N-L+1$ act on the flow of particles as "bottlenecks," for the mean time necessary to leave them is much larger than the time to leave any other site. Therefore the system, which consists of ν similar segments of length L, effectively behaves like a ring made up of ν similar "boxes," each able to contain up to L particles. A transition from a segment j to $j-1$ occurs with a rate $b^{-1}\gamma^4$, irrespective of the number of particles in each of the segments, provided, of course, that there is at least one particle in segment j and at most $L-1$ particles in segment $j-1$.

Let Q_n denote the probability that in the steady state there are n particles in a given segment ($n = 0, \ldots, L$). Let $Q_{m,n}$ denote the joint probability of finding, in the steady state, $0 \leq m \leq L$ particles at a given segment j and $0 \leq n \leq L$ particles at $j+1$. Of course, Q_n and $Q_{m,n}$ do not depend on j, and the Q_n satisfy

$$\sum_{n=0}^{L} Q_n = 1, \tag{23}$$

$$\sum_{n=0}^{L} nQ_n = L\rho. \tag{24}$$

Let us assume a mean-field approximation, $Q_{m,n} = Q_m Q_n$. In the stationary state the mean number $\mathcal{N}_n$ of segments occupied by n particles does not depend on time. As the particles hop between segments, $\mathcal{N}_n$ can decrease when one of the particles jumps from or to a segment occupied by n particles. The corresponding rates are $Q_n(1-Q_L)$ and $Q_n(1-Q_0)$, respectively. The number of segments containing n particles can also increase owing to jumps ending at segments containing $n-1$ particles or originating at segments with $n+1$ particles; the corresponding transition rates are $Q_{n-1}(1-Q_0)$ and $Q_{n+1}(1-Q_L)$, respectively. Consequently, the appropriate balance conditions read

$$(Q_n - Q_{n+1})(1-Q_L) = (1-Q_0)(Q_{n-1} - Q_n), \tag{25}$$

$$Q_1(1-Q_L) = (1-Q_0)Q_0, \tag{26}$$

$$Q_L(1-Q_L) = (1-Q_0)Q_{L-1}, \tag{27}$$

where $n=1,\ldots,L-1$ in Eq. (25), and in Eqs. (26) and (27) we have taken into account the fact that neither jumps from a segment containing 0 particles nor transitions to a segment with L particles are possible. Together with Eqs. (23) and (24) these relations form $L+3$ equations for $L+1$ variables Q_n, $n=0,\ldots,L$, with the concentration ρ being the only free parameter. This system of equations is easily shown to have a unique solution

$$Q_n=\frac{a^n}{1+a+\ldots+a^L}, \tag{28}$$

where the parameter a can be determined using

$$L\rho=\frac{\sum_{n=0}^{L} na^n}{\sum_{n=0}^{L} a^n}. \tag{29}$$

The concentration ρ is a monotonic function of a, increasing from 0 for $a=0$ to 1 in the limit $a\to\infty$. The value $a=1$ corresponds to $\rho=\frac{1}{2}$ and, generally,

$$\rho(a)=1-\rho(1/a). \tag{30}$$

Having obtained Q_n we can calculate the current as

$$J=b^{-1}\gamma^4(1-Q_0)(1-Q_L)$$

$$=b^{-1}\gamma^4\frac{a\left(\sum_{n=0}^{L-1} a^n\right)^2}{\left(\sum_{n=0}^{L} a^n\right)^2}. \tag{31}$$

Using (30) it is easy to see that

$$J(\rho)=J(1-\rho). \tag{32}$$

Because for $\rho\ll\frac{1}{2}$ Eq. (29) implies $a\approx\rho/L$, using our formula (31) we conclude that for small concentrations of particles the current J grows linearly with ρ,

$$J\approx b^{-1}\gamma^4L^{-1}\rho. \tag{33}$$

For $\rho=\frac{1}{2}$ the mean-field theory (31) predicts

$$J(0.5)=\frac{b^{-1}\gamma^4L^2}{(L+1)^2}. \tag{34}$$

C. Numerical simulations

In our simulations we used a lattice with $N=400$ sites consisting of $\mu=100$ segments, each of length $L=4$. We used a sawtooth potential with $\gamma=\exp(-2)\approx0.135$. The number of particles in the system varied from $M=1$ to $M=399$. We carried out our simulations for $t=10^6$ Monte Carlo time steps per particle and the results were averaged over ten different realizations of the process, which enabled us to estimate the statistical errors.

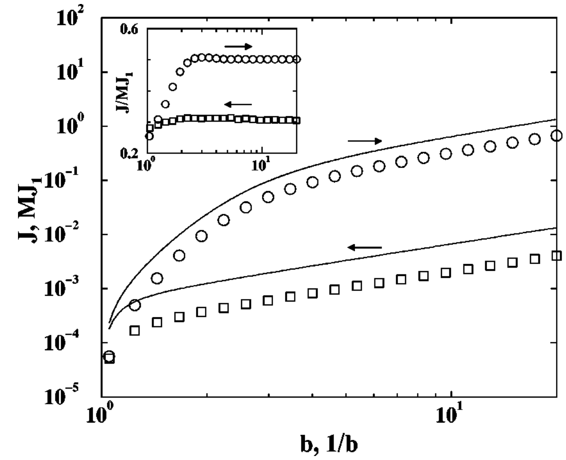

FIG. 3. Current J (arbitrary units) as a function of the dimensionless bias parameter for the concentration $\rho=0.5$. Upper curves, bias to the right, abscissa indicates b; lower curves, bias to the left, abscissa indicates $1/b$. Full lines, single-particle current J_1 of Ref. [11] multiplied by the number of particles M. Symbols, result of numerical simulations for $N=400$, $L=4$, $\gamma=\exp(-2)$, $t=10^6$. The (semilogarithmic) inset shows the ratio J/MJ_1.

We first present simulation results for the current at a fixed concentration $\rho=0.5$, or for $M=200$, as a function of the bias parameter b for bias to the right, and b^{-1} for bias to the left, respectively. Figure 3 shows the current J observed in simulations (symbols) together with a simple approximation obtained by multiplying a single-particle current J_1 [11] by the number M of particles in the system (free particle approximation). One observes that the current in the case of a system with a hard-core interactions is reduced as compared to the case of noninteracting particles, but the general behavior as a function of the bias parameter is practically the same. In particular, the rectification effects for particle motion in nonsymmetric potentials are qualitatively the same in both cases. The inset in Fig. 3 depicts the ratio J/MJ_1 as a function of the bias. Owing to Eq. (21) we expect that for $b\gg1$ $J/MJ_1=(N-M)/(N-1)\approx1-\rho$. For $b=20$ we found $J/MJ_1\approx0.5014\pm0.0001$, in excellent agreement with the theoretical value $200/399\approx050125$. For $b\ll1$ our mean-field approximation (34) predicts $J/MJ_1=L^2/2(L+1)^2=0.32$; for $b=1/20$ our simulations yielded a slightly smaller value 0.305 ± 0.001.

We now discuss the dependence of the current on concentration for selected values of the bias $b>1$, or $b<1$, respectively, and compare the results with the theoretical considerations of Sec. III B. In Fig. 4 we present results of our simulations for a bias to the right ($b=30$, 10, and 2). For a strong bias ($b=30$) the agreement with the theoretical prediction, Eq. (22), is very good.

The results obtained for a bias to the left ($b=0.001$, 0.1, 0.5, and 0.9) are depicted in Fig. 5. We can see that if the bias is strong ($b\leqslant0.1$), the agreement between the mean-field theory (solid line) and the simulation data (circles and crosses) is very good for concentrations close to 0 and 1. However, for $\rho\approx\frac{1}{2}$ we observe that the mean-field theory tends to overestimate the actual value of J by approximately 5%, which is much more than the statistical errors of our data (the relative standard deviation at $\rho=0.5$ is about 0.33%). We repeated our simulations for larger number of

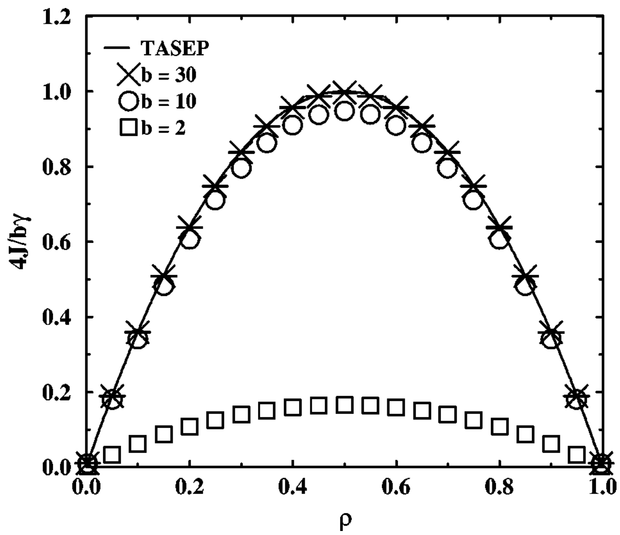

FIG. 4. The dimensionless current, $J/\frac{1}{4}b\gamma$, as a function of the dimensionless concentration ρ for the bias $b=30$ (crosses), 10 (circles), and 2 (squares). The solid line was computed using Eq. (22). The parameters are $N=400$, $L=4$, $\gamma=\exp(-2)$, and $t=10^6$. Results were averaged over 10 Monte Carlo simulations. The error bars are shown only for $b=30$; for other values of b they are similarly small.

Monte Carlo time steps ($t=5\times 10^6$) and for different values of the bias b, but the difference between simulations and the theory remained practically the same. We thus conclude that it is not a numerical artifact. A similar discrepancy was observed by Tripathy and Barma [18], who considered a TASEP with random transition rates. However, in their model the mean-field approach underestimated the magnitude of the current obtained in simulations for $\rho\approx 0.5$. Moreover, they found that $J(\rho)$ has quite a broad plateau around $\rho=0.5$. This phenomenon is not observed in our case because the transition rates in our model are not random.

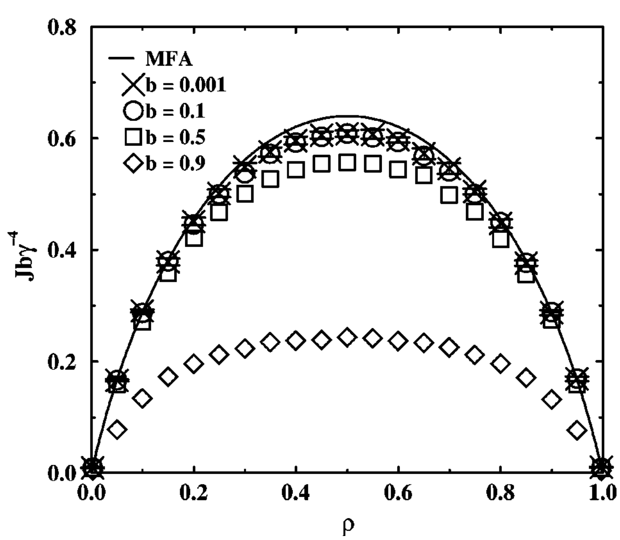

FIG. 5. The dimensionless current $J/b\gamma^{-4}$, as a function of the dimensionless concentration ρ for the bias $b=10^{-3}$ (crosses), 0.1 (circles), 0.5 (squares), and 0.9 (diamonds). The solid line was computed using Eq. (31). The parameters are the same as in Fig. 4. The error bars, shown only for $b=10^{-3}$, are of similar order for other values of b and represent the standard deviation.

IV. SYMMETRY PROPERTIES

In this section we discuss the symmetry properties of our lattice-gas model with nonsymmetric potentials and of related models. In the simulations, as well as in the mean-field approximation, the current exhibits a particle-vacancy symmetry,

$$J(\rho)=J(1-\rho). \tag{35}$$

The symmetry properties of the TASEP have been analyzed in [18–20] and the relation, Eq. (35), has been established in this context. However, the model employed in those references differs in important aspects from our model. Hence a detailed discussion is in order.

The particle-vacancy symmetry of the current for the TASEP has been shown in Refs. [18–20] for disordered hopping potentials where the transition rates are associated with the bonds between the sites. If the motion of the particles is reversed (symmetry operation T according to Refs. [18,20], the particles experience the same set of transition rates as before, only the order of the rates has been changed. If the vacancies are interpreted as particles (symmetry operation C), they experience the same transition rates as the particles after the operation T. The symmetry under CT is evident; the nontrivial statement is the symmetry of the current (up to a sign) under the operations C, or T, separately.

The class of models for the hopping potential that are considered here do not correspond to bond disorder. The set of ''right'' transition rates is different from the set of the ''left'' transition rates. If a strong bias $b\gg 1$ to the right is applied, leading approximately to a TASEP, the current is different from the case of strong bias to the left with $b^{-1}\gg 1$. In other words, the symmetry under reversal of motion T does not exist for the class of models leading to rectification, by their definition. If the vacancies are considered as particles, they experience the same set of transition rates as the original particles, see also below. We conjecture that symmetry under the operation C also exists for our models, if the limiting case of the TASEP is considered. Hence we expect Eq. (35) to be approximately valid for the models that lead to rectification effects, in the limit of very strong bias.

The sawtooth potential that is investigated in this paper has a special symmetry, which will be described now. In the limit of concentration of the lattice gas approaching 1, the particle problem is equivalent to the problem of hopping motion of single, independent vacancies. The hopping transitions of an isolated vacancy are reversed in comparison to the transitions of the particle that makes an exchange with the vacancy, e.g.,

$$\Gamma^{V}_{l,l+1}=\Gamma_{l+1,l}. \tag{36}$$

Using the rates, Eq. (36), it is easy to reconstruct the hopping potential for single vacancies. If this construction is done for the the extended sawtooth potential of Fig. 1(b), a sawtooth potential is obtained for the vacancy that is mirror-symmetric with respect to the original sawtooth potential; see Fig. 6. If a bias is applied to the particles, expressed by the factor b in the transition rates to the right, the factor b

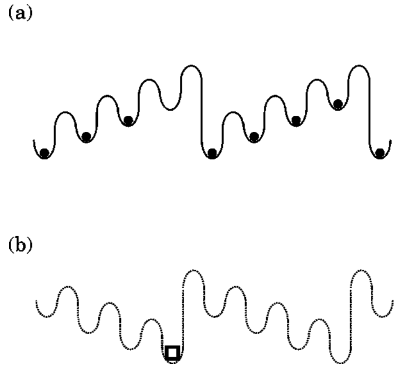

FIG. 6. (a) Repetition of the sawtooth potential of Fig. 1 with lattice-gas particles indicated. (b) Effective potential for a single vacancy, constructed according to Eq. (36).

appears in the transition rates of the vacancy to the left. It is evident from this consideration that the particle current for $\rho \to 0$ is identical to the one for $\rho \to 1$. It is obvious that a particle-vacancy symmetry pertains for the problem of motion of lattice gases in a sawtooth potential with the above symmetry property; hence we expect Eq. (35) to be valid for all values of the bias b.

We point out that the sawtooth potential represents a special case; general nonsymmetric potentials do not provide mirror-symmetric potentials for the vacancies in the limit $\rho \to 1$. For instance, if the potential corresponding to an Ehrlich-Schwoebel barrier (see, e.g., [22]) is transformed by using Eq. (36) in the corresponding hopping potential of a single vacancy, a different potential is obtained. As a consequence, the mobility of a single particle is different from the mobility of a single vacancy. Hence for this example $J(\rho) \neq J(1-\rho)$ for b close to 1. This example is sufficient to show that the particle-vacancy symmetry (35) cannot be generally valid for arbitrary b. Another counterexample is provided by the random-trap model; see Ref. ([23]).

V. CONCLUDING REMARKS

In this paper we investigated the motion of lattice-gas particles in hopping potentials that are composed of segments without mirror-reflection symmetry. We considered in particular the effects of exclusion of multiple occupancy of sites under various bias conditions. We first studied the case of two particles on a ring of four sites with a sawtooth potential. The explicit solution of this simple system can be given and interesting conclusions emerge in the limits of large bias to the right or to the left. We point out that the ring with four sites is a model case for the treatment of two site-exclusion particles on a finite ring; larger systems can be solved in a similar manner, e.g., by using symbolic formula manipulation programs.

We then investigated the case of many particles on extended systems that consist of periodic repetitions of sawtooth potentials. These systems behave, for strong bias in one direction, as uniform systems where the result for the current of lattice gases is known. For strong bias in the reverse directions, the extended sawtooth potential acts as a periodic arrangement of weak links. A mean-field expression for the current can be derived for this case from the cluster dynamics of the particles on the segments, which shows similarities to the cluster dynamics of the bosonic lattice gases of Refs. [24]. Good agreement with the numerical simulations was found for both cases under strong bias; deviations appear for smaller bias values. The results for the current exhibit a particle-vacancy symmetry as a consequence of a special particle-hole symmetry of the hopping processes in the sawtooth potential used.

Generally, the current per particle of a site-exclusion lattice gas shows the same qualitative behavior, as a function of the strength and the direction of the bias parameter, as the current of independent particles. This observation is important for possible applications; for instance, for transport through channels in membranes or through layered structures with suitable potential structures. It means that qualitative or even semiquantitative predictions of the effects of strong bias on the current can already be obtained from the single-particle description.

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[1] R. P. Feynman, R.B. Leighton, and M. Sands, *The Feynman Lectures in Physics* (Addison-Wesley, Reading, MA, 1966), Vol. 1, Chap. 46.
[2] M.O. Magnasco, Phys. Rev. Lett. **71**, 1477 (1993).
[3] J.E. Hall, C.A. Mead, and G. Szabo, J. Membr. Biol. **11**, 75 (1973).
[4] G. Stark, Biochim. Biophys. Acta **298**, 323 (1973).
[5] M.M. Millonas and D.R. Chialvo, Phys. Rev. Lett. **76**, 550 (1996).
[6] R.D. Astumian, Science **276**, 917 (1997).
[7] F. Jülicher, A. Ajdari, and J. Prost, Rev. Mod. Phys. **69**, 1269 (1997).
[8] H.X. Zhou and Y.D. Chen, Phys. Rev. Lett. **77**, 194 (1996).
[9] A. Lorke, S. Wimmer, B. Jager, J.P. Kotthaus, W. Wegscheider, and M. Bichler, Physica B **249-251**, 312 (1998).
[10] A.M. Song, A. Lorke, A. Kriele, J.P. Kotthaus, W. Wegscheider, and M. Bichler, Phys. Rev. Lett. **80**, 3831 (1998).
[11] K.W. Kehr, K. Mussawisade, T. Wichmann, and W. Dieterich, Phys. Rev. E **56**, R2351 (1997).
[12] G.A. Cecchi and M.O. Magnasco, Phys. Rev. Lett. **76**, 1968 (1996).
[13] I. Derenyi and T. Vicsek, Phys. Rev. Lett. **75**, 374 (1995).
[14] For a review and references see G.M. Schütz, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic, London, in press).
[15] S.A. Janowsky and J.L. Lebowitz, Phys. Rev. A **45**, 618 (1992).
[16] G.M. Schütz, J. Stat. Phys. **71**, 471 (1993).
[17] G. Tripathy and M. Barma, Phys. Rev. Lett. **78**, 3029 (1997).
[18] G. Tripathy and M. Barma, Phys. Rev. E **58**, 1911 (1998).

[19] S. Goldstein and E.R. Speer, Phys. Rev. E **58**, 4226 (1998).
[20] K.M. Kolwankar and A. Punnoose, e-print cond-mat/9807246.
[21] B. Derrida, Phys. Rep. **301**, 65 (1998).
[22] G. Ehrlich, and F.G. Hudda, J. Chem. Phys. **44**, 1039 (1966); R.L. Schwoebel and E.J. Shipsey, J. Appl. Phys. **37**, 3682 (1966).
[23] K.W. Kehr, O. Paetzold, and T. Wichmann, Phys. Lett. A **182**, 135 (1993).
[24] R. Kutner, K.W. Kehr, W. Renz, and R. Przenioslo, J. Phys. A **28**, 923 (1995).