Repelling random walkers in a diffusion-coalescence system

F. H. Jafarpour[1,*] and S. R. Masharian[2]
[1]*Physics Department, Bu-Ali Sina University, Hamadan, Iran*
[2]*Institute for Advanced Studies in Basic Sciences, Zanjan, Iran*
(Received 10 December 2007; published 13 March 2008)

We have shown that the steady state probability distribution function of a diffusion-coalescence system on a one-dimensional lattice of length L with reflecting boundaries can be written in terms of a superposition of double-shock structures which perform biased random walks on the lattice while repelling each other. The shocks can enter into the system and leave it from the boundaries. Depending on the microscopic reaction rates, the system is known to have two different phases. We have found that the mean distance between the shock positions is of order L in one phase while it is of order 1 in the other phase.

DOI: 10.1103/PhysRevE.77.031115 PACS number(s): 02.50.Ey, 05.20.−y, 05.70.Fh, 05.70.Ln

Recently, the investigation of the microscopic structure and dynamics of shocks, defined as discontinuities in the space dependence of the densities of particles in one-dimensional driven diffusive systems, has drawn much attention [1–13]. It has been shown that the steady states of some of these systems can be explained in terms of collective excitations with one or more conservation laws.

In [4] three families of single-species driven diffusive systems are studied in which a traveling shock with a steplike density profile exists and behaves like a one-particle excitation in the system, provided that the microscopic hopping rates are fine tuned. This has also been observed in systems with more than one species of particles [5–10]. On the other hand, the steady states of these systems can be written in terms of a superposition of such product shock measures. In [6] and [11] the authors have shown that such steady states are associated with the existence of two-dimensional representations of the quadratic algebras of these systems when they are studied using the matrix product formalism (MPF) (for a recent review, see [14]). According to this formalism the steady state of some one-dimensional driven diffusive systems can be written in terms of products of noncommuting operators which satisfy a quadratic algebra.

However, little is known about the microscopic dynamics of multiple shocks in these systems. The only example is given in [3], where multiple shocks are studied for a partially asymmetric simple exclusion process with open boundaries. In this paper, we investigate the dynamics of a double-shock structure in a branching coalescing system with nonconserving dynamics and reflecting boundaries. The steady state properties of this system have already been studied in [15] and [16]. It turns out that, depending on the microscopic reaction rates of the system, it can be in two different phases: a high- and a low-density phase. Since the dynamics of the system is nonconserving, the mean density of the particles in the system in the high-density phase is greater than that in the low-density phase. However, it has been shown that, if one considers a canonical ensemble in which the total number of particles is conserved, then the system has two phases: a high-density and a shock phase. In this case the shock does not have any dynamics [17]. In [4] the authors have shown that a single shock with biased random walk dynamics can evolve in this system provided that the boundaries are open so that the particles can enter and leave the system from there. Later, in [12] and [13], it was shown that in an infinite system double-shock structures with random walk dynamics can also evolve in the system. However, nothing is known about the dynamics of these double-shock structures in a system with boundaries. Our main attempt in this paper is to study the microscopic dynamics of such structures on a lattice with finite length and reflecting boundaries.

In what follows we first define the model and then using the Hamiltonian formalism show how a double-shock product measure evolves in time under the Hamiltonian of the system. From there we construct the steady state probability distribution function of the system as a linear combination of such double-shock product measures. The mean distance between the shock positions is also calculated in the thermodynamic limit.

The system in question consists of identical classical particles on a one-dimensional lattice of length L. There is no injection or extraction of particles at the boundaries. The reaction rules between two consecutive sites k and $k+1$ on the lattice are as follows:

$$
\begin{aligned}
\emptyset + A &\rightarrow A + \emptyset \quad \text{with rate } q,\\
A + \emptyset &\rightarrow \emptyset + A \quad \text{with rate } q^{-1},\\
A + A &\rightarrow A + \emptyset \quad \text{with rate } q,\\
A + A &\rightarrow \emptyset + A \quad \text{with rate } q^{-1},\\
\emptyset + A &\rightarrow A + A \quad \text{with rate } \Delta q,\\
A + \emptyset &\rightarrow A + A \quad \text{with rate } \Delta q^{-1},
\end{aligned} \tag{1}
$$

in which A and $\emptyset$ stand for the presence of a particle and a hole, respectively. As can be seen, the parameter q determines the asymmetry of the system. For $q>1$ ($q<1$) the

*farhad@ipm.ir

particles have a tendency to move in the leftward (rightward) direction. For any q the model is also invariant under the following transformations:

$$q \to q^{-1}, \quad k \to L-k+1, \tag{2}$$

in which k is a given site on the lattice. Throughout this paper we will consider only the case $q>1$. The results for the case $q<1$ can easily be obtained using (2). By formulating the stochastic Hamiltonian of the system as a quantum spin chain, it has been shown that it is completely integrable [15,16]. As we mentioned, the system has two different phases depending on the values of q and Δ. For $q>1$ it has a high-density phase for $q^2<1+\Delta$ and a low-density phase for $q^2>1+\Delta$. In the high-density phase the density profile of particles has its maximum value near the left boundary while it is a constant $\rho=\frac{\Delta}{1+\Delta}$ in the bulk of the lattice. It also drops exponentially to zero near the right boundary. The particle correlations exist at both boundaries. In the low-density phase the density profile of particles again has its maximum value near the left boundary but it quickly drops exponentially to zero in the bulk and remains zero throughout the lattice. In this phase the particle correlations exist only near the left boundary. The mean density of particles is of order $\frac{1}{L}$ in this phase. On the transition line $q^2=1+\Delta$, the density profile of particles drops exponentially near the left boundary while it changes linearly in the bulk of the system. The mean density of particles in the bulk of the lattice is equal to $\frac{\Delta}{2(1+\Delta)}$ in the thermodynamic limit.

Recently, it has been shown that the steady state probability distribution function of some one-dimensional driven diffusive systems can be written in terms of interactions of single-shock structures [6]. In the following we will show that the steady state of our coalescence system defined by Eq. (1) can also be written in terms of superposition of double-shock structures. These shocks repel each other while performing biased random walks on the lattice.

Any state of the system is defined through a probability measure P_η on the set of all configurations $\eta=(\eta_1,\eta_2,\ldots,\eta_L)$, $\eta_k\in\{\emptyset,A\}$. For our purposes it is convenient to use the Hamiltonian formalism where one assigns a basis vector $|\eta\rangle$ of the vector space $(\mathbb{C}^2)^{\otimes L}$ to each configuration and the probability vector is defined by $|P\rangle=\Sigma_\eta P_\eta|\eta\rangle$, which is normalized such that $\langle s|P\rangle=1$ where $\langle s|=\Sigma_\eta\langle\eta|$. The time evolution is now described by the master equation

$$\frac{d}{dt}|P(t)\rangle = H|P(t)\rangle, \tag{3}$$

in which H is called the Hamiltonian and its matrix elements are the hopping rates between any two configurations. For a system defined on a lattice of length L with reflecting boundaries the Hamiltonian can be written as

$$H=\sum_{k=1}^{L-1} h_{k,k+1}, \tag{4}$$

where $h_{k,k+1}$ acts nontrivially only on sites k and $k+1$. In a basis defined as

$$|\emptyset\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |A\rangle = \begin{pmatrix}0\\1\end{pmatrix}, \tag{5}$$

the local Hamiltonian of our system in Eq. (4) has the following form:

$$h_{k,k+1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -q(1+\Delta) & q^{-1} & q^{-1} \\ 0 & q & -q^{-1}(1+\Delta) & q \\ 0 & q\Delta & q^{-1}\Delta & -(q+q^{-1}) \end{pmatrix}. \tag{6}$$

We define a double-Bernoulli-shock measure, which is a product measure with two jumps in the local particle density associated with two random walkers (the shock fronts) at sites m and n, as

$$|P_{m,n}\rangle = \begin{pmatrix}1\\0\end{pmatrix}^{\otimes m} \otimes \begin{pmatrix}1-\rho\\ \rho\end{pmatrix}^{\otimes n-m-1} \otimes \begin{pmatrix}1\\0\end{pmatrix}^{\otimes L-n+1}, \tag{7}$$

in which $0\le m\le n-1$ and $1\le n\le L+1$. Here we have introduced two auxiliary sites 0 and $L+1$. A simple sketch of this shock measure is given in Fig. 1. It is easy to verify that this family of shock measures generates a subspace of the vector space of states that is invariant under the time evolution generated by H, and thus the many-particle problem is reduced to a two-particle one. As we mentioned earlier, the time evolution of such a product shock measure has already been studied for an infinite system with no boundaries [12,13]; nevertheless, in this paper, we aim to study a finite system with reflecting boundaries. The time evolution equations for $|P_{m,n}\rangle$ are given by

$$\begin{aligned} H|P_{m,n}\rangle &= q^{-1}|P_{m+1,n}\rangle + q(1+\Delta)|P_{m-1,n}\rangle + q^{-1}(1+\Delta)|P_{m,n+1}\rangle \\ &\quad + q|P_{m,n-1}\rangle - (q+q^{-1})(2+\Delta)|P_{m,n}\rangle \\ &\quad \text{for } m=1,\ldots,L-2 \text{ and } n=m+2,\ldots,L, \end{aligned}$$

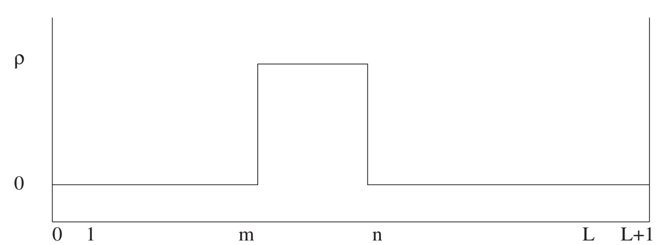

FIG. 1. Sketch of a double-shock structure. The shock positions are defined at the sites m and n.

$$H|P_{0,n}\rangle = (q^{-1}-q)|P_{1,n}\rangle + q^{-1}(1+\Delta)|P_{0,n+1}\rangle + q|P_{0,n-1}\rangle - q^{-1}(2+\Delta)|P_{0,n}\rangle \quad \text{for } n=2,\ldots,L,$$

$$H|P_{m,L+1}\rangle = q^{-1}|P_{m+1,L+1}\rangle + q(1+\Delta)|P_{m-1,L+1}\rangle + (q-q^{-1}) \times|P_{m,L}\rangle - q(2+\Delta)|P_{m,L+1}\rangle \quad \text{for } m=1,\ldots,L-1,$$

$$H|P_{0,L+1}\rangle = (q^{-1}-q)|P_{1,L+1}\rangle + (q-q^{-1})|P_{0,L}\rangle,$$

$$H|P_{m,m+1}\rangle = 0 \quad \text{for} \quad m=0,\ldots,L. \tag{8}$$

As can be seen, for $q>1$ the left random walker performs a biased random walk and preferentially hops to the left regardless of the values of q and Δ. In contrast, the right random walker preferentially hops to the left for $q^2>1+\Delta$ and to the right for $q^2<1+\Delta$. On the coexistence line where $q^2=1+\Delta$, the right random walker performs an unbiased random walk. The left (right) random walker can also leave the lattice only from the left (right) boundary. The diffusion coefficients and also the velocities of the random walkers can now be easily calculated from Eq. (8).

Let us now explain why the random walkers repel each other. It can easily be seen from Eq. (8) that, as long as the shock positions are more than a single site apart, they never meet each other during the time evolution. However, it seems from there that the random walkers can meet each other when they are a single site apart. In what follows we show that this is not the case. For instance we consider the first equation in Eq. (8) for $n=m+2$ where the shock positions are a single site apart. Rewriting this equation in terms of a new definition for the shock measure as

$$|\widetilde{P}_{m,n}\rangle = \begin{pmatrix}1\\0\end{pmatrix}^{\otimes m} \otimes \begin{pmatrix}0\\1\end{pmatrix}^{\otimes n-m-1} \otimes \begin{pmatrix}1\\0\end{pmatrix}^{\otimes L-n+1}, \tag{9}$$

one finds

$$H|\widetilde{P}_{m,m+2}\rangle = q\Delta|\widetilde{P}_{m-1,m+2}\rangle + q|\widetilde{P}_{m-1,m+1}\rangle + q^{-1}|\widetilde{P}_{m+1,m+3}\rangle + q^{-1}\Delta|\widetilde{P}_{m,m+3}\rangle - (q+q^{-1})(1+\Delta)|\widetilde{P}_{m,m+2}\rangle.$$

As can be seen the shock positions never get closer than a single site apart. In fact, the dynamical rules (1) do not allow the shock fronts to get closer together than a single site since this results in an empty lattice. This is why we say that the random walkers repel each other. One can easily check this for other equations in Eq. (8) in which the shock positions are a single site apart to see that in terms of the $|\widetilde{P}_{m,n}\rangle$ the shock positions never meet and the minimum distance between them is at least a single site.

In this paper, we are especially interested in the steady state of the system. One should note that an empty lattice is a trivial steady state for the system. It can be seen from Eq. (1) that an empty lattice never evolves in time. There is actually a nontrivial steady state for the system in which the lattice contains some particles. The nontrivial steady state of the system can now be constructed as a superposition of double-shock measures as follows:

$$|P^*\rangle = \frac{1}{Z_L}\sum_{m=0}^{L}\sum_{n=m+1}^{L+1}\psi_{m,n}|P_{m,n}\rangle, \tag{10}$$

provided that we exclude the empty lattice from $|P^*\rangle$ by requiring

$$\langle 0|P^*\rangle = 0, \tag{11}$$

in which

$$|0\rangle = |\emptyset\rangle^{\otimes L} = \begin{pmatrix}1\\0\\ \vdots \\0\end{pmatrix} \tag{12}$$

is associated with a configuration with no particles in the system. The normalization factor Z_L in Eq. (10) can easily be obtained from $Z_L=\sum_{m=0}^{L}\sum_{n=m+1}^{L+1}\psi_{m,n}$. By requiring $H|P^*\rangle=0$ we find a system of equations for the $\psi_{m,n}$'s. It turns out that this system of equations has the following solution:

$$\psi_{m,n} = \frac{(q^2-1)}{(1-q^2)^{\delta_{m,0}}\left(\frac{q^2-1}{q^2}\right)^{\delta_{n,L+1}}} q^{-2(m+n)}[1-(1+\Delta)^{n-m-1}] \quad \text{for } 0\le m\le L-1 \text{ and } m+2\le n\le L+1. \tag{13}$$

Note that the $\psi_{m,n}$'s in Eq. (13) are also valid for $q^2=1+\Delta$, and at the coexistence line one should only replace Δ with q^2-1 in Eq. (13). One can see from Eq. (7) that there are $L+1$ states in which the shock positions are at two consecutive sites. The states $|P_{m,m+1}\rangle$ point to an empty lattice. Since the empty lattice is a trivial steady state of the system, the coefficients of these states in Eq. (10), i.e., the $\psi_{m,m+1}$'s, are taken to be equal to ψ'. The condition (11) for $q^2\neq 1+\Delta$ can now be calculated and it is equal to

$$\psi' = \frac{1}{L+1}\left[\frac{q^2\Delta}{(q^4-1)[1-q^2(1+\Delta)]} + \frac{q^2\Delta^2}{(q^2-1)(q^2-1-\Delta)[1-q^2(1+\Delta)]}\left(\frac{1}{q^2(1+\Delta)}\right)^L + \frac{q^2\Delta}{(q^4-1)(q^2-1-\Delta)}q^{-4L}\right]. \tag{14}$$

It turns out that, on the transition line $q^2=1+\Delta$, ψ' becomes

$$\psi' = -\frac{[(q^4-1)L-q^2]q^{-4L}+q^2}{(L+1)(q^4-1)(q^2+1)}. \tag{15}$$

The normalization factor Z_L, which is called the grand-canonical partition function of the system, can now be calculated and after substituting ψ' from Eqs. (14) and (15) one finds

$$Z_L = \begin{cases} \frac{q^2\Delta^2(q^2-1)^{-1}}{[1-q^2(1+\Delta)](1+\Delta-q^2)}\left[1-\left(\frac{1+\Delta}{q^2}\right)^L-\left(\frac{1}{q^2(1+\Delta)}\right)^L+q^{-4L}\right] & \text{for } q^2 \neq 1+\Delta, \\ \frac{1-q^{-4L}}{1+q^2}L & \text{for } q^2 = 1+\Delta. \end{cases} \tag{16}$$

As one can see our results obtained here are exactly those obtained in [15] and [16] using different approaches. Using the steady state probability distribution function (10), one can easily calculate the density profile of the particles and also any correlations in the steady state. However, since the results are exactly those obtained in the above mentioned papers, the results are not given here.

Having the probability of finding the random walkers at sites m and n in the steady state, one can calculate the mean distance of the shock fronts in the steady state, defined as,

$$\langle d\rangle = \frac{1}{Z_L}\sum_{m=0}^{L}\sum_{n=m+1}^{L+1}(n-m-1)\psi_{m,n}. \tag{17}$$

It turns out that in the thermodynamic limit $L\to\infty$ it is given by

$$\langle d\rangle \sim \begin{cases} L & \text{for } q^2 < 1+\Delta, \\ \frac{1}{2}L & \text{for } q^2 = 1+\Delta, \\ O(1) & \text{for } q^2 > 1+\Delta. \end{cases} \tag{18}$$

In the high-density phase $q^2 < 1+\Delta$ the shock fronts have their maximum distance while in the low-density phase they have the minimum distance, which is of the order of a single site. One should note that the mean distance between the two shock fronts changes abruptly from one phase to the other phase, which can be a sign of a phase transition in the system.

It is also interesting to study the probability of finding each shock front at a given site in the steady state. The probability of finding the left shock front at the site m is defined as

$$P_m = \sum_{n=m+1}^{L+1}\psi_{m,n} \quad \text{for } 0 \le m \le L. \tag{19}$$

In the thermodynamic limit $L\to\infty$ and in the high-density phase, P_m is an exponential function with the inverse length scale $\ln(q^4)$, while in the low-density phase it is an exponential function with the inverse length scale equal to $\ln[q^2(1+\Delta)]$. On the other hand, the probability of finding the right shock front at site n is given by

$$P_n = \sum_{m=0}^{n-1}\psi_{m,n} \quad \text{for } 1 \le n \le L+1. \tag{20}$$

In the thermodynamic limit $L\to\infty$ and in both the high- and the low-density phases, this probability distribution function has an exponential behavior with the inverse length scale $\ln[q^2(1+\Delta)^{-1}]$. This explains why the system has three different length scales.

In this paper we have studied a coalescence system with reflecting boundaries and showed that its steady state can be explained in terms of superposition of the probability distribution of two interacting random walkers which perform biased random walks while repelling each other. The random walkers can also leave or enter from the boundaries. One should note that the random walk picture actually fails at the left boundary for $q>1$ (and at the right boundary for $q<1$). In fact, as can be seen from Eq. (8), the left random walker should enter the system with a negative rate. This has already been observed in the branching-coalescing model with open boundaries studied in [4]. Apart from this, we have found that the steady state probability distribution function of the system is exactly the one obtained in [15,16] which obviously generates the same density profile of particles in the system in each phase as was calculated by the same authors. It is interesting to consider more general reaction rates in Eq. (1) and see under what constraints the random walk picture exists in a system with reflecting boundaries. This is under investigation and will be presented elsewhere.

[1] P. A. Ferrari, in *Probability and Phase Transition*, edited by G. Grimmett (Kluwer, Dordrecht, 1994).
[2] B. Derrida, L. Lebowitz, and E. R. Speer, J. Stat. Phys. **89**, 135 (1997).
[3] V. Belitsky and G. M. Schütz, Electron. J. Probab. **7**, 1 (2002).
[4] K. Krebs, F. H. Jafarpour, and G. M. Schütz, New J. Phys. **5** 145 (2003).
[5] F. H. Jafarpour and S. R. Masharian, J. Stat. Mech.: Theory Exp. (2007) P03009.
[6] F. H. Jafarpour and S. R. Masharian, J. Stat. Mech.: Theory Exp. (2007) P10013.
[7] A. Rákos and G. M. Schütz, J. Stat. Phys. **117**, 55 (2004).
[8] F. H. Jafarpour, Physica A **358**, 413 (2005).
[9] F. Tabatabaei and G. M. Schütz, Diffus. Fundam. **4**, 1 (2006).
[10] F. Tabatabaei and G. M. Schütz, Phys. Rev. E **74**, 051108 (2006).

[11] F. H. Jafarpour, Physica A **339**, 369 (2004).
[12] M. Arabsalmani and A. Aghamohammadi, Eur. Phys. J. B **55**, 439 (2007).
[13] M. Arabsalmani and A. Aghamohammadi, Phys. Rev. E **74**, 011107 (2006).
[14] R. A. Blythe and M. R. Evans, J. Phys. A **40**, R333 (2007).
[15] H. Hinrichsen, K. Krebs, and I. Peschel, Z. Phys. B: Condens. Matter **100**, 105 (1996).
[16] H. Hinrichsen, S. Sandow, and I. Peschel, J. Phys. A **29**, 2643 (1996).
[17] F. H. Jafarpour, Physica A **322**, 270 (2004); F. H. Jafarpour and S. R. Masharian, Phys. Rev. E **70**, 056121 (2004).