

Reaction-Diffusion Processes of Hard-Core Particles

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We study a 12-parameter stochastic process involving particles with two-site interaction and hard-core repulsion on a d -dimensional lattice. In this model, which includes the asymmetric exclusion process, contact processes, and other processes, the stochastic variables are particle occupation numbers taking values $n_x = 0, 1$. We show that on a ten-parameter submanifold the k -point equal-time correlation functions $\langle n_{x_1} \cdots n_{x_k} \rangle$ satisfy linear differential-difference equations involving no higher correlators. In particular, the average density $\langle n_x \rangle$ satisfies an integrable diffusion-type equation. These properties are explained in terms of dual processes and various duality relations are derived. By defining the time evolution of the stochastic process in terms of a quantum Hamiltonian H , the model becomes equivalent to a lattice model in thermal equilibrium in $d+1$ dimensions. We show that the spectrum of H is identical to the spectrum of the quantum Hamiltonian of a d -dimensional, anisotropic, spin-1/2 Heisenberg model. In one dimension our results hint at some new algebraic structure behind the integrability of the system.

KEY WORDS: Reaction-diffusion processes; correlation functions; integrable models.

1. INTRODUCTION

An interesting class of nonequilibrium problems with a rich dynamical behavior is made up of stochastic reaction-diffusion systems.^(1,2) These processes may involve one or several species of particles A, B, C, \dots and an inert state \emptyset equivalent to the absence of any of the interacting particles. Examples of such processes are, to name but a few, coagulation $A + A \rightarrow A$,⁽³⁾ pair annihilation $A + A \rightarrow \emptyset$,⁽⁴⁻⁶⁾ or two-species annihilation $A + B \rightarrow \emptyset$.^(7,8) Formulated as a lattice model, \emptyset corresponds to a

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vacancy on a site of the lattice and particles, represented by particle occupation numbers, may hop in the lattice ($A\emptyset \rightarrow \emptyset A$) and take part in the reactions. Such lattice systems are, in general, difficult to treat by rigorous means and, correspondingly, considering the vast number of such models, relatively few exact results are known.

Over the past few years the formulation of stochastic processes in terms of quantum spin systems has turned out to be a convenient tool in the study of nonequilibrium lattice problems (see, e.g., refs. 5, 6, and 9–14 and references therein). A paradigmatic example is the representation of symmetric diffusion of hard-core particles (known as the symmetric exclusion process^(15,16) by the spin-1/2 Heisenberg model (see ref. 9 for a detailed discussion). But also asymmetric hopping,^(6,10–12) multimer processes,⁽⁵⁾ and reaction-diffusion processes^(6,13,14) have been similarly represented. By these means, standard techniques for quantum spin systems such as spin-wave theory,^(5,17) Bethe ansatz and related algebraic techniques,^(6,10,11,13,14,18) global symmetries,^(9,12) and Goldstone broken symmetry arguments⁽⁵⁾ have given many new results for stochastic systems.

An intriguing feature of these models is that even though these are interacting many-particle systems, some of them are known to give rise to closed systems of differential-difference equations for time-dependent correlation functions and exact results have been obtained. In one possible scenario the time derivative of a k -point correlation function does not involve higher-order correlators, or, in other words, one obtains a closed set of not more than k coupled, linear, differential-difference equations. Some well-known examples of single-species processes where this happens are the symmetric exclusion process and symmetric partial exclusion process describing diffusion of particles on a lattice in any dimension,^(9,15,16) the asymmetric exclusion process describing driven diffusion in one dimension,⁽¹²⁾ or the voter model describing annihilation (death) processes and decoagulation⁽¹⁶⁾ (for details see below). In another scenario, certain subsets of correlation function decouple from each other. This happens, e.g., in the Glauber model,⁽¹⁹⁾ in random sequential dimer deposition,⁽²⁰⁾ or in the generalized models studied in ref. 21.

This observation raises a number of questions, the most obvious one being whether there is a classification of these processes, i.e., a general criterion on the reaction and diffusion rates such that the resulting equations for the correlation functions decouple. Clearly, the answer depends on which correlation functions one wishes to study. Here we consider density correlation functions, which are the ones in which one is usually interested. Other correlation functions, e.g., exponentials of integrated densities⁽¹²⁾ or particle-string correlation functions,^(12,20,21) give rise to other necessary and sufficient equations for the rates leading to decoupled equations. As

we shall show below, the quantum Hamiltonian formalism that we use throughout this paper is a convenient tool for the derivation of these equations [see (3.8)] for the rates and it opens the way to a (partial) physical and mathematical understanding of this phenomenon. This is because by expressing the process in terms of a quantum Hamiltonian one relates a d -dimensional nonequilibrium problem to a $(d+1)$ -dimensional equilibrium problem into which one may have (and in the cases discussed here actually *has*) some insight. Here we study only stochastic processes of hard-core particles with a two-site interaction. The corresponding quantum Hamiltonian turns out to be that of a generalized spin-1/2 Heisenberg model. However, our strategy is easily generalized to many-species models or to models with interactions involving more than only two sites.

In some of the known cases which are contained in our more general model the observed decoupling of the correlation functions can be understood in terms of a dual stochastic process.^(15,16) In the case of the (self-dual) symmetric exclusion process, duality relates the time-dependent k -point density correlation function to the process with a k -particle initial state. Because of particle number conservation this is a great simplification and many exact results have been obtained in this way. Also for other processes duality may be used to derive new results⁽¹⁶⁾ and so one other question we discuss is the existence of dual processes to those which satisfy the constraints (3.8) on the rates discussed above. The dual processes that we shall obtain involve additional restriction on the rates arising from the positivity of the dual rates and conservation of probability in the dual process. In any case, the dual process contains only hopping and various annihilation terms, but no nonzero particle creation rates. This is another way of understanding the decoupling of the correlation functions from higher-order correlators.

One more problem that we shall address, albeit only briefly, is that of the integrability of the system. From the structure of the equations derived in Section 3 and from the solution of these equations for the one-point function (i.e., the density profile) obtained in Section 6 it becomes apparent that the system is partially integrable in any space dimension. This means that some of the equations for the k -point functions are integrable and therefore yield the spectrum of a subspace of the Hamiltonian. In Section 5 we show that the spectrum of H is identical to that of a spin-1/2 Heisenberg Hamiltonian, which, in one dimension, is completely integrable by the Bethe ansatz. However, the generalized Hamiltonian H is not related to the Heisenberg Hamiltonian by a similarity transformation. The integrability of H cannot be derived from the usual Baxterization procedure⁽²²⁾ and the algebraic structure underlying the generalized model remains an open problem.

The paper is organized as follows. In Section 2 we give for the benefit of the reader not familiar with the quantum Hamiltonian formalism a full discussion of its relation to the usual description of the stochastic process in terms of a master equation. We also introduce various definitions and relations used later. We define the problem on a hypercubic lattice in d dimensions with periodic boundary conditions even though many of the results derived later are also valid for other lattices or boundary conditions. When appropriate, this is indicated by an additional explicit remark. Otherwise one should always think of the periodic hypercubic lattice. In Section 3 we derive the equations for the rates such that one obtains linear, inhomogeneous differential-difference equations, i.e., equations for the k -point correlation functions which are decoupled from higher-order correlators. In Section 4 we discuss duality and derive the criteria on the existence of a dual process. This leads also to a number of duality relations for the correlation functions. In Section 5 we discuss the mapping of the stochastic problem to the Heisenberg quantum Hamiltonian and in Section 6 we calculate the time-dependent density profile with an arbitrary initial state. In Section 7 we summarize the main results and present some open questions.

2. STOCHASTIC PROCESSES IN THE QUANTUM HAMILTONIAN FORMALISM

We study one-species exclusion processes in d dimensions, i.e., a system of particles on a hypercubic lattice with M sites where each site is either empty or occupied by at most one particle. The state space of the system is therefore $X = \{0, 1\}^M$ and a given state of the system may be represented by a configuration $\underline{n} = \{n_1, n_2, \dots, n_M\}$, where $n_i = 0, 1$ and $1 \leq i \leq M$ labels the sites of the lattice. An alternative possibility is to give the set $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$ of occupied lattice sites. In this notation, the empty set represents the empty lattice and $1 \leq N \leq M$ is the total number of particles in the configuration. Here $\mathbf{x}_i = (x_i^{(1)}, x_i^{(2)}, \dots, x_i^{(d)})$ is a d -component object defining the (integer) coordinates of the particle in the lattice. When working on finite lattices, we shall label each space coordinate by an integer $1 \leq x^{(a)} \leq L^{(a)}$, while for an infinite lattice $x^{(a)} \in \mathbf{Z}$. For later convenience, it is useful to introduce also the unit vector in the a direction, $\mathbf{e}^{(a)} = (0^{(1)}, \dots, 1^{(a)}, \dots, 0^{(d)})$.

The stochastic dynamics of the system may be defined in terms of a master equation for the probability $f(\underline{n}; t)$ of finding the configuration $\{n_1, n_2, \dots, n_M\}$ at time t . We shall use quantum Hamiltonian language, which has proven to be a useful formalism for stochastic processes on lattices. Each state $\underline{n} \in X$ is represented by a vector $|\underline{n}\rangle$ (or $|\mathbf{x}_1, \dots, \mathbf{x}_N\rangle$,

with $|0\rangle \equiv | \rangle$ being the empty state) and the probability distribution is mapped to a state vector

$$|f(t)\rangle = \sum_{\underline{n} \in X} f(\underline{n}; t) |\underline{n}\rangle \tag{2.1}$$

The vectors $|\underline{n}\rangle$ together with the transposed vectors $\langle \underline{n}|$ form an orthonormal basis of $(C^2)^{\otimes M}$ and the time evolution is defined in terms of a linear ‘‘Hamilton’’ operator H acting on this space of dimension 2^M ,

$$\frac{\partial}{\partial t} |f(t)\rangle = -H |f(t)\rangle \tag{2.2}$$

A state at time $t = t_0 + \tau$ is therefore given in terms of an initial state at time t_0 by

$$|f(t_0 + \tau)\rangle = e^{-H\tau} |f(t_0)\rangle \tag{2.3}$$

From (2.1) and (2.2) and using $f(\underline{n}; t) = \langle \underline{n} | f(t)\rangle$, we find that the master equation takes the form

$$\frac{\partial}{\partial t} f(\underline{n}; t) = -\langle \underline{n} | H |f(t)\rangle \tag{2.4}$$

Note that

$$\langle s | f(t)\rangle = \sum_{\underline{n} \in X} f(\underline{n}; t) = 1 \tag{2.5}$$

where

$$\langle s | = \sum_{\underline{n} \in X} \langle \underline{n} | \tag{2.6}$$

which expresses conservation of probability. This implies $\langle s | H = 0$ for any stochastic process. The right eigenvector(s) of H with eigenvalue $E_0 = 0$ and normalized according to (2.5) is (are) the steady state(s) of the stochastic process. In general H is not symmetric, which means that the rate $w(\underline{n}; \underline{n}') = -\langle \underline{n} | H | \underline{n}'\rangle$ with which a configuration \underline{n}' switches to a configuration \underline{n} is not, in general, equal to its reverse rate $w(\underline{n}'; \underline{n})$. As a result the stationary distribution(s) $S(\underline{n})$ may be highly nontrivial. The real part of all eigenvalues of H is larger than or equal to zero.

Average values $\langle Q \rangle$ are calculated as matrix elements of suitably chosen operators Q which may be expressed in terms of the usual Pauli matrices $\sigma_j^{x,y,z}$ acting on site j . A complete set of observables are the

occupation numbers $n_j = 0, 1$. Defining projection operators on states with a particle on site j of the chain as

$$n_j = \frac{1}{2} (1 - \sigma_j^z) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}_j \tag{2.7}$$

one finds that the average density of particles at site j is given by $\langle n_j \rangle = \langle s | n_j | f(t) \rangle$. Correlation functions $\langle n_{x_1} \cdots n_{x_k} \rangle$, i.e., the probabilities of finding particles on the set of sites $\{x_1, \dots, x_k\}$, are computed analogously. Note that in ordinary quantum mechanics average values would be taken as matrix elements between normalized eigenstates of H , i.e., $\langle Q \rangle = \langle k | Q | k \rangle$, whereas here an average value is the quantity $\langle s | Q | f \rangle$ where $|f\rangle$ is (in general) not an eigenstate, but a state with real coefficients $0 \leq f(n; t) \leq 1$, (2.1), in the basis spanned by the set $\{|n\rangle\}$ and normalized such that $\langle s | f \rangle = 1$.

For later convenience we also introduce the operators $s_j^\pm = (\sigma_j^x \pm i\sigma_j^y)/2$. In our convention

$$s_j^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_j \tag{2.8}$$

creates a particle at site j when acting to the right, while

$$s_j^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_j \tag{2.9}$$

annihilates a particle at site j . Note that

$$\langle s | s_j^+ = \langle s | n_j \quad \text{and} \quad \langle s | s_j^- = \langle s | (1 - n_j) \tag{2.10}$$

Introducing the ladder operator $S^\pm = \sum_j s_j^\pm$, one may write

$$\langle s | = \langle 0 | e^{S^+} \tag{2.11}$$

Using the commutation relations for the Pauli matrices then yields (2.10).

Now we are in a position to define the stochastic processes we intend to study by a quantum Hamiltonian H . We define

$$H = \xi \sum_j \sum_{a=1}^d u_j^{(a)} \tag{2.12}$$

with the nearest neighbor reaction matrices

$$u_j^{(a)} = - \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix}_{(j;a)} \tag{2.13}$$

acting on nearest neighbor sites \mathbf{j} and $\mathbf{j} + \mathbf{e}^{(a)}$. The sum runs over the whole lattice and we take periodic boundary conditions in all space directions, i.e., $u_{(j^{(1)}, \dots, L^{(a)}, \dots, j^{(d)})}^{(a)}$ acts on sites $(j^{(1)}, \dots, L^{(a)}, \dots, j^{(d)})$ and $(j^{(1)}, \dots, 1^{(a)}, \dots, j^{(d)})$. The normalization ξ sets the time scale and is for the purposes of this paper of no particular interest. The diagonal elements a_{kk} of $u_{\mathbf{j}}^{(a)}$ satisfy

$$a_{kk} = - \sum_{\substack{k'=1 \\ k' \neq k}}^4 a_{k'k} \tag{2.14}$$

which is imposed by conservation of probability. This implies

$$\langle s | u_{\mathbf{j}}^{(a)} = 0 \quad \forall \mathbf{j}, a \tag{2.15}$$

In order to keep the interpretation of H as defining a stochastic process, (2.14) has to be supplemented by the condition $a_{kk'} \geq 0$ for the off-diagonal matrix elements $k \neq k'$.

The processes described by H are reactions changing the configurations on two nearest neighbor sites. A configuration $\{n_{\mathbf{j}}, n_{\mathbf{j} + \mathbf{e}^{(a)}}\}$ changes into configurations $\{n'_{\mathbf{j}}, n'_{\mathbf{j} + \mathbf{e}^{(a)}}\}$ with rates $a_{kk'}$ as follows:

$$\begin{aligned} \{0, 0\} &\rightarrow a_{21}\{0, 1\} + a_{31}\{1, 0\} + a_{41}\{1, 1\} \\ &\quad \text{(birth/pair creation)} \\ \{0, 1\} &\rightarrow a_{12}\{0, 0\} + a_{32}\{1, 0\} + a_{42}\{1, 1\} \\ &\quad \text{(death/diffusion/decoagulation)} \\ \{1, 0\} &\rightarrow a_{13}\{0, 0\} + a_{23}\{0, 1\} + a_{43}\{1, 1\} \\ &\quad \text{(death/diffusion/decoagulation)} \\ \{1, 1\} &\rightarrow a_{14}\{0, 0\} + a_{24}\{0, 1\} + a_{34}\{1, 0\} \\ &\quad \text{(pair annihilation/coagulation)} \end{aligned} \tag{2.16}$$

These processes take place with equal rates everywhere in the lattice.

This generalized nearest neighbor exclusion process includes many well-known processes, such as the asymmetric exclusion process⁽¹⁶⁾ (with hopping rates $a_{23}, a_{32} \neq 0$, all other rates 0), the voter model⁽¹⁶⁾ (with death rates and decoagulation rates $a_{12} = a_{13} = a_{42} = a_{43} \neq 0$), or Glauber dynamics⁽¹⁹⁾ ($a_{23} + a_{32} = a_{14} + a_{41} \neq 0$). Altogether there are 12 independent parameters, one of which is trivial, as one may always change the normalization ξ without changing the physical properties of the system. We shall set $\xi = 1$ throughout the paper.

3. EQUAL-TIME CORRELATION FUNCTIONS

The equal-time k -point correlation function satisfies the equation

$$\frac{\partial}{\partial t} \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_k} \rangle = - \sum_{a=1}^d \sum_{\mathbf{j} \in C^{(a)}} \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_k} u_{\mathbf{j}}^{(a)} \rangle \quad (3.1)$$

where, owing to the property (2.15) of the two-site reaction matrix $u_{\mathbf{j}}^{(a)}$, the sum over \mathbf{j} does not run over the whole lattice, but only over the union $C^{(a)}$ of the set of sites $\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$ with the set of their nearest neighbors $\{\mathbf{x}_1 - \mathbf{e}^{(a)}, \dots, \mathbf{x}_k - \mathbf{e}^{(a)}\}$. It is important to realize that since each $u_{\mathbf{j}}^{(a)}$ acts nontrivially only on two sites, the r.h.s. of (3.1) involves only $(k-2)$ -point functions, $(k-1)$ -point functions, k -point functions, and $(k+1)$ -point functions. This can be seen as follows: Suppose one of the $\mathbf{x}_i \in \{\mathbf{x}_1, \dots, \mathbf{x}_k\}$ (say \mathbf{x}_k) is equal to $\mathbf{j} + \mathbf{e}^{(a)}$. Using (2.10), one finds

$$\begin{aligned} \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-1}} (n_{\mathbf{x}_k} u_{\mathbf{x}_k - \mathbf{e}^{(a)}}^{(a)}) \rangle &= A_1 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-1}} \rangle \\ &\quad + B_1 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-1}} n_{\mathbf{x}_k - \mathbf{e}^{(a)}} \rangle \\ &\quad - C_1 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-1}} n_{\mathbf{x}_k} \rangle \\ &\quad + D_1 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-1}} n_{\mathbf{x}_k} n_{\mathbf{x}_k - \mathbf{e}^{(a)}} \rangle \end{aligned} \quad (3.2)$$

with

$$\begin{aligned} A_1 &= a_{21} + a_{41}, & B_1 &= a_{23} + a_{43} - a_{21} - a_{41} \\ C_1 &= a_{12} + a_{32} + a_{21} + a_{41}, & D_1 &= C_1 - a_{23} - a_{43} - a_{14} - a_{34} \end{aligned} \quad (3.3)$$

A similar result arises if one of the \mathbf{x}_i (again, without loss of generality \mathbf{x}_k) is equal to \mathbf{j} :

$$\begin{aligned} \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-1}} (n_{\mathbf{x}_k} u_{\mathbf{x}_k}^{(a)}) \rangle &= A_2 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-1}} \rangle \\ &\quad + B_2 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-1}} n_{\mathbf{x}_k + \mathbf{e}^{(a)}} \rangle \\ &\quad - C_2 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-1}} n_{\mathbf{x}_k} \rangle \\ &\quad + D_2 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-1}} n_{\mathbf{x}_k} n_{\mathbf{x}_k + \mathbf{e}^{(a)}} \rangle \end{aligned} \quad (3.4)$$

with

$$\begin{aligned} A_2 &= a_{31} + a_{41}, & B_2 &= a_{32} + a_{42} - a_{31} - a_{41} \\ C_2 &= a_{13} + a_{23} + a_{31} + a_{41}, & D_2 &= C_2 - a_{32} - a_{42} - a_{14} - a_{24} \end{aligned} \quad (3.5)$$

The r.h.s. of (3.2) and (3.4) consist only of $(k-1)$ -point functions, k -point functions, and $(k+1)$ -point functions.

If two of the \mathbf{x}_i are nearest neighbors in the lattice, e.g., $\mathbf{x}_{k-1} = \mathbf{x}_k - \mathbf{e}^{(a)} = \mathbf{j}$, then the action of $u_j^{(a)}$ yields

$$\begin{aligned} \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-2}} (n_{\mathbf{x}_{k-1}} n_{\mathbf{x}_{k-1} + \mathbf{e}^{(a)}} u_{\mathbf{x}_{k-1}}^{(a)}) \rangle &= A_3 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-2}} \rangle \\ &+ B_3 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-2}} n_{\mathbf{x}_{k-1} + \mathbf{e}^{(a)}} \rangle \\ &+ D_3 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-2}} n_{\mathbf{x}_{k-1}} \rangle \\ &- C_3 \langle n_{\mathbf{x}_1} \cdots n_{\mathbf{x}_{k-2}} n_{\mathbf{x}_{k-1}} n_{\mathbf{x}_{k-1} + \mathbf{e}^{(a)}} \rangle \end{aligned} \quad (3.6)$$

with

$$\begin{aligned} A_3 &= a_{41}, & B_3 &= a_{42} - a_{41} \\ D_3 &= a_{43} - a_{41}, & C_3 &= a_{14} + a_{24} + a_{34} + a_{42} + a_{43} - a_{41} \end{aligned} \quad (3.7)$$

The r.h.s. of (3.6) consists only of $(k-2)$ -point functions, $(k-1)$ -point functions, and k -point functions.

If $D_1 \neq 0$ or $D_2 \neq 0$, the time derivative (3.1) of the k -point correlation function gives rise to a set of M coupled differential-difference equations involving all k -point correlators.² Solutions to such a set of equations have been found in some special cases where subsets of these equations decouple,⁽²¹⁾ but there is no general solution. On the other hand, if $D_1 = D_2 = 0$, i.e., for

$$\begin{aligned} a_{34} &= a_{21} + a_{41} + a_{12} + a_{32} - a_{23} - a_{43} - a_{14} \\ a_{24} &= a_{31} + a_{41} + a_{13} + a_{23} - a_{32} - a_{42} - a_{14} \end{aligned} \quad (3.8)$$

the problem simplifies considerably, as one has a closed system of only k equations. In this case Eq. (3.1) may be regarded as an inhomogeneous, linear differential-difference equation for the k -point function with $(k-1)$ -point and $(k-2)$ -point correlators as inhomogeneities.

Note that one may also study correlation functions of the operators $\tilde{n} = n - \alpha$ with an arbitrary constant α . One obtains again a closed system of k equations for the k -point correlation function if $D_1 = D_2 = 0$, but with new constants

$$\tilde{A}_1 = A_1 + \alpha(B_1 - C_1), \quad \tilde{A}_2 = A_2 + \alpha(B_2 - C_2) \quad (3.9)$$

² In N -particle systems with particle number conservation the hierarchy breaks off at $k = N \leq M$.

and

$$\begin{aligned}\tilde{A}_3 &= A_3 + \alpha(B_3 + D_3) - \alpha^2 C_3 \\ \tilde{B}_3 &= B_3 - \alpha(C_3 + B_2 - C_1) \\ \tilde{D}_3 &= B_3 - \alpha(C_3 + B_1 - C_2)\end{aligned}\quad (3.10)$$

in Eqs. (3.2), (3.4), and (3.6). The $B_{1,2}$ and $C_{1,2}$ do not change. In particular, the inhomogeneity arising from $A_1, A_2 \neq 0$ in the one-point function can be removed by taking $\alpha = \rho$ with

$$\rho = \frac{2a_{41} + a_{21} + a_{31}}{2a_{41} + a_{21} + a_{31} + 2a_{14} + a_{24} + a_{34}} = \frac{A_1 + A_2}{C_1 + C_2 - B_1 - B_2} \quad (3.11)$$

With this choice one has $\tilde{A}_1 + \tilde{A}_2 = 0$. The differential-difference equation for higher-order correlation functions has then inhomogeneous terms proportional to \tilde{A}_3 [coupling to $(k-2)$ -point functions] and $\tilde{B}'_3 = \tilde{B}_3 + \tilde{A}_1$, $\tilde{D}'_3 = \tilde{D}_3 + \tilde{A}_2$ [coupling to $(k-1)$ -point functions]. We conclude:

Equation (3.1) becomes a closed, inhomogeneous linear differential-difference equation in one (continuous) time coordinate and $d \cdot k$ (discrete) space coordinates on a 10-parameter submanifold defined by Eqs. (3.8) of the 12-parameter model.

One may add the remark that this differential-difference equation becomes homogeneous [i.e., contains no $(k-1)$ -point and $(k-2)$ -point correlation functions] on a seven-parameter submanifold defined by $\tilde{A}_3 = \tilde{B}'_3 = \tilde{D}'_3 = 0$. From the derivation presented above it is obvious that this result is easy to generalize to other lattices and interactions. With $D_1 = D_2 = 0$, Eq. (3.1) is a closed set of k equations independent of the dimensionality of the system or of the kind of lattice on which the model is defined. Furthermore, the two sites on which the reaction matrix u acts nontrivially are not even required to be nearest neighbors. The result remains true for arbitrary long-range interactions with reaction matrices $u_{\mathbf{x},\mathbf{y}}$, where \mathbf{x} and \mathbf{y} are any two points on the lattice. Finally, it is also not necessary to keep the reaction rates $a_{kk'}$ space independent as long as (3.8) is satisfied for each reaction matrix $u_{\mathbf{x},\mathbf{y}}$. For the decoupling from lower-order correlators a stronger condition is necessary for this general case. Besides $D_1 = D_2 = 0$, one needs $\tilde{A}_1 = \tilde{A}_2 = \tilde{A}_3 = \tilde{B}_3 = \tilde{D}_3 = 0$, i.e., one is left with a five-parameter space only.

We demonstrate this result for the one-dimensional case. In one dimension, Eq. (3.1) for the one-point function becomes

$$\frac{\partial}{\partial t} \langle n_x \rangle = -\langle n_x (u_{x-1} + u_x) \rangle \quad (3.12)$$

where we have set $\xi = 1$ and dropped the coordinate index a in $u_j^{(a)}$. This is easy to calculate and one finds

$$\begin{aligned} \frac{\partial}{\partial t} \langle n_x \rangle &= A_1 + A_2 \\ &+ B_1 \langle n_{x-1} \rangle - (C_1 + C_2) \langle n_x \rangle + B_2 \langle n_{x+1} \rangle \\ &+ D_1 \langle n_{x-1} n_x \rangle + D_2 \langle n_x n_{x+1} \rangle \end{aligned} \quad (3.13)$$

where the constants with index 1 and index 2 arise from the action of u_{x-1} and u_x , respectively. One sees that if $D_1 = D_2 = 0$, (3.13) becomes an inhomogeneous, linear differential-difference equation. Introducing \tilde{n} with $\alpha = \rho$ as defined in (3.11) leads to the homogeneous equation

$$\frac{\partial}{\partial t} \langle \tilde{n}_x \rangle = B_1 \langle \tilde{n}_{x-1} \rangle + B_2 \langle \tilde{n}_{x+1} \rangle - (C_1 + C_2) \langle \tilde{n}_x \rangle \quad (3.14)$$

For the two-point function one obtains

$$\begin{aligned} \frac{\partial}{\partial t} \langle n_x n_y \rangle &= -\langle n_x (u_{x-1} + u_x) n_y \rangle - \langle n_x n_y (u_{y-1} + u_y) \rangle \\ &= (A_1 + A_2) (\langle n_x \rangle + \langle n_y \rangle) + B_1 (\langle n_{x-1} n_y \rangle + \langle n_x n_{y-1} \rangle) \\ &+ B_2 (\langle n_{x+1} n_y \rangle + \langle n_x n_{y+1} \rangle) - 2(C_1 + C_2) \langle n_x n_y \rangle \end{aligned} \quad (3.15)$$

if x and y are not nearest neighbors and

$$\begin{aligned} \frac{\partial}{\partial t} \langle n_x n_{x+1} \rangle &= -\langle n_x n_{x+1} (u_{x-1} + u_x + u_{x+1}) \rangle \\ &= A_3 + (A_2 + D_3) \langle n_x \rangle + (A_1 + B_3) \langle n_{x+1} \rangle \\ &+ B_1 \langle n_{x-1} n_{x+1} \rangle + B_2 \langle n_x n_{x+2} \rangle \\ &- (C_1 + C_2 + C_3) \langle n_x n_{x+1} \rangle \end{aligned} \quad (3.16)$$

for the nearest neighbor correlator. Similar equations are obtained for correlators involving \tilde{n} .

For $D_1 = D_2 = 0$ and the special choice $a_{k1} = a_{4k} = 0$ (no birth, pair creation, and decoagulation) one has $A_i = B_3 = D_3 = 0$ and (3.16) simplifies to the completely decoupled, homogeneous equation

$$\begin{aligned} \frac{\partial}{\partial t} \langle n_x n_{x+1} \rangle &= B_1 \langle n_{x-1} n_{x+1} \rangle + B_2 \langle n_x n_{x+2} \rangle \\ &- (C_1 + C_2 + C_3) \langle n_x n_{x+1} \rangle \end{aligned} \quad (3.17)$$

In this case, time derivatives of higher k -point correlation functions also decouple completely, i.e., involve only k -point correlation functions.

4. DUAL PROCESSES

The fact that the time derivative of the k -point correlation functions may give rise to a closed set of equations is reminiscent of the duality relations, e.g., for the symmetric exclusion process,^(15,16) where self-duality is indeed just an expression of this fact. One may therefore ask whether the closure of the equations for the k -point functions is equivalent to the existence of some dual process.

Before we discuss this question we would like to remind the reader of the meaning of self-duality (of the symmetric exclusion process) in the operator language used in this paper. Let us assume that initially N particles are located on a set of sites $A_N = \{y_1, \dots, y_N\}$ represented by a vector $|A_N\rangle = |y_1, \dots, y_N\rangle$. We want to compute the probability $\langle n_{x_1} \cdots n_{x_k} \rangle_{A_N}$ of finding (any) k particles on sites $B_k = \{x_1, \dots, x_k\}$, at time t . The duality relations state^(15,16,19)

$$\langle n_{x_1} \cdots n_{x_k} \rangle_{A_N} = \sum_{B'_k \subset A_N} \langle n_{x'_1} \cdots n_{x'_k} \rangle_{B_k} \quad (4.1)$$

In this expression the sum runs over all sets $B'_k = \{x'_1, \dots, x'_k\}$ which are contained in the set A_N , i.e., the k -point correlation function $\langle n_{x_1} \cdots n_{x_k} \rangle_{A_N}$ of the N -particle system is given by sums of k -particle correlation functions (we assume $k \leq N$). Using (2.10), (2.11), and the fact that H for the symmetric exclusion process is symmetric and $SU(2)$ invariant (i.e., commutes with S^+), we can derive the duality relations (4.1) as follows⁽⁹⁾:

$$\begin{aligned} \langle n_{x_1} \cdots n_{x_k} \rangle_{A_N} &= \langle s | n_{x_1} \cdots n_{x_k} e^{-Ht} | A_N \rangle \\ &= \sum_{\underline{n}} \langle 0 | s_{x_1}^+ \cdots s_{x_k}^+ e^{-Ht} | \underline{n} \rangle \langle \underline{n} | e^{S^+} | A_N \rangle \\ &= \sum_{\underline{n}} \langle A_N | e^{S^-} | \underline{n} \rangle \langle x_1, \dots, x_k | e^{-Ht} | \underline{n} \rangle \\ &= \sum_{B'_k \subset A_N} \langle x'_1, \dots, x'_k | e^{-Ht} | B_k \rangle \\ &= \sum_{B'_k \subset A_N} \langle s | n_{x'_1} \cdots n_{x'_k} e^{-Ht} | B_k \rangle \end{aligned} \quad (4.2)$$

where $|B_k\rangle = |x_1, \dots, x_k\rangle$. Because of particle number conservation we have substituted $\langle x'_1, \dots, x'_k |$ in the last line by

$$\langle s | n_{x'_1} \cdots n_{x'_k}$$

In other words, the averaging is performed over all k -particle states such that the sets B'_k of occupied sites are contained in the set A_N of initially occupied sites. These sets B'_k arise from the matrix element $\langle A_N | e^{S^-} | \underline{n} \rangle$ together with particle number conservation.

Generally we define a duality relation by

$$\langle s | Q e^{-Ht} | A \rangle = \langle s | Q' e^{-\tilde{H}t} | A' \rangle \tag{4.3}$$

where Q and Q' are some functions of the projection operators n_x and $|A\rangle$ and $|A'\rangle$ are initial states. The dual process \tilde{H} is obtained by taking the transposed matrix H^T of the time evolution operator and performing some suitably chosen similarity transformation V such that

$$\tilde{H} = V H^T V^{-1} \tag{4.4}$$

indeed defines a stochastic process. The observable Q' and the initial condition $|A'\rangle$ are then given by

$$\langle s | Q' = \langle A | V^{-1}, \quad |A'\rangle = V Q |s\rangle \tag{4.5}$$

where $|\dots\rangle = (\langle \dots |)^T$. By taking $V = \exp(-S^-)$ and $Q = n_{x_1} \dots n_{x_k}$ one recovers (4.1) with $\tilde{H} = H$.

In this kind of duality the points $\{x_1, \dots, x_k\}$ occurring in the correlator are mapped to an initial state with particles occupying sites $\{x_1, \dots, x_k\}$. The dual process may be considered as a process describing the time evolution of particles on these points. $\tilde{H} = H$ means that the symmetric exclusion process is self-dual.

After this reminder we are in a position to formulate the problem more specifically: We saw in the previous section that as in the symmetric exclusion process, the time derivative of the k -point function of the generalized model does not involve higher correlators. The transformation $V = \exp(-S^-)$ relates the k -point correlator to a k -particle initial state. We therefore ask the question whether the dual operator \tilde{H} of (4.4) with this particular V defines a stochastic process on the ten-parameter manifold $D_1 = D_2 = 0$. In order to answer this question, one has to check whether the transformed dual rates \tilde{a}_{kl} satisfy (2.14) (guaranteeing conservation of probability) and the condition of positivity $\tilde{a}_{kl} \geq 0$ for $k \neq l$.

A short calculation gives for the dual matrices

$$\tilde{a}_j^{(a)} = - \begin{pmatrix} 0 & A_1 & A_2 & A_3 \\ 0 & -C_1 & B_2 & B_3 \\ 0 & B_1 & -C_2 & D_3 \\ 0 & 0 & 0 & -C_3 \end{pmatrix}_{(j;a)} \tag{4.6}$$

with the quantities A_i, B_i, C_i defined by (3.3), (3.5), and (3.7), respectively. Using positivity and conservation of probability, we can read off the conditions for the existence of a dual process, namely $A_i, B_i, D_3 \geq 0$ and

$$A_1 + B_1 - C_1 = A_2 + B_2 - C_2 = A_3 + B_3 + D_3 - C_3 = 0$$

Note that the condition

$$\begin{aligned} C_3 &= a_{42} + a_{43} - a_{41} + a_{14} + a_{24} + a_{34} \\ &= A_3 + B_3 + D_3 = a_{42} + a_{43} - a_{41} \end{aligned}$$

implies $a_{k4} = 0, \forall k$, because of the positivity of the original rates.

The dual process \tilde{H} has only hopping terms B_1 and B_2 and various nonvanishing annihilation rates, but no particles are created. Thus the duality relations (4.3) with $Q = n_{x_1} \cdots n_{x_k}$ read

$$\begin{aligned} \langle n_{x_1} \cdots n_{x_k} \rangle_{A_N} &= N \langle 0 | e^{-\tilde{H}t} | B_k \rangle + \sum_{y \in A_N} \langle y | e^{-\tilde{H}t} | B_k \rangle \\ &+ \cdots + \sum_{y_1, \dots, y_k \in A_N} \langle y_1, \dots, y_k | e^{-\tilde{H}t} | B_k \rangle \\ &= \sum_{p=0}^k \sum_{B'_p \subset A_N} \langle s | Q'(p) | B_k \rangle \end{aligned} \quad (4.7)$$

where $Q'(p) = P_p n_{y_1} \cdots n_{y_p}$ and P_p is the projector on p -particle states arising from the matrix element $\langle A_N | e^{S^-} | \underline{n} \rangle$. The averaging extends therefore over all p -particle states with $0 \leq p \leq k$ such that the sets B'_p of occupied sites are contained in the set A_N of initially occupied sites. Note that (4.7) holds for any choice of the parameters A_i, B_i, D_3 , irrespective of whether \tilde{H} defines a stochastic process or not.

One may define other dual processes involving other operators Q . The main requirement for the kind of dual processes in which we are interested is that the set of sites B_k defined by the product of projectors n_{x_i} translates into an initial configuration of occupied sites. This feature determined the transformation V . The results of the preceding section indicate that it might be interesting to study correlation functions of the shifted density projectors $\tilde{n}_{x_i} = n_{x_i} - \alpha$. We introduce the local operator

$$w_j = \begin{pmatrix} 1 + \alpha & \alpha \\ -\alpha & 1 - \alpha \end{pmatrix}_j \quad (4.8)$$

and

$$W = \prod_j w_j \quad (4.9)$$

It is easy to check that $\langle s | w_j = \langle s |$ and $\langle s | n_j = \langle s | (n_j - \alpha) w_j$. Therefore

$$\langle s | \tilde{n}_{x_1} \cdots \tilde{n}_{x_k} = \langle s | n_{x_1} \cdots n_{x_k} W \quad (4.10)$$

and

$$\langle \tilde{n}_{x_k} \cdots \tilde{n}_{x_k} \rangle_A = \langle s | n_{x_1} \cdots n_{x_k} e^{-H't} | A' \rangle \tag{4.11}$$

with $H' = WHW^{-1}$ and the transformed initial state $|A'\rangle = W|A\rangle$. Now one may apply (4.7) to (4.11). Averaging is now performed over the weighted set of states \underline{n} with total particle number $p \leq k$ and with weights $f_A(\mathbf{y}_1, \dots, \mathbf{y}_k) = \langle A' | e^{S^-} | \mathbf{y}_1, \dots, \mathbf{y}_k \rangle$:

$$\langle \tilde{n}_{x_1} \cdots \tilde{n}_{x_k} \rangle_A = \sum_{\substack{\mathbf{y}_1, \dots, \mathbf{y}_k \\ 0 \leq p \leq k}} f_A(\mathbf{y}_1, \dots, \mathbf{y}_k) \langle \mathbf{y}_1, \dots, \mathbf{y}_k | e^{-\tilde{H}t} | B_k \rangle \tag{4.12}$$

One obtains the dual time evolution operator $\tilde{H} = V(WHW^{-1})^T V^{-1}$ with the doubly transformed dual reaction matrices

$$\tilde{u}_j^{(a)} = - \begin{pmatrix} 0 & \tilde{A}_1 & \tilde{A}_2 & \tilde{A}_3 \\ 0 & -C_1 & B_2 & \tilde{B}_3 \\ 0 & B_1 & -C_2 & \tilde{D}_3 \\ 0 & 0 & 0 & -C_3 \end{pmatrix}_{(j;a)} \tag{4.13}$$

where the quantities defined in Eqs. (3.9), (3.10) are used. Positivity and conservation of probability yield again the conditions on the existence of the dual process defined by \tilde{H} .

We conclude that:

The closure of the differential-difference equations for the k -point density (or shifted density) correlation functions does not, in general, imply the existence of a dual stochastic process as discussed here. Additional constraints on the original reaction rates arise in order to conserve probability and positivity for the dual process.

Other duality relations and dual processes may be obtained by considering other correlation functions⁽¹²⁾ or transformations to other initial states.

5. THE HEISENBERG HAMILTONIAN

In the previous section we have shown that on a 10-dimensional sub-manifold of the 12-parameter problem all equal-time correlation functions can be calculated by solving (in)homogeneous, linear differential-difference equations. From the solutions to these equations one may obtain the spectrum of H , (2.12), by looking for the poles of the Laplace transform of the

correlation function. From the one-point function (3.1) or (6.1) below one finds a series of eigenvalues

$$E(\mathbf{k}) = \sum_{a=1}^d (B_1 e^{ik_a} + B_2 e^{-ik_a} - C_1 - C_2), \quad 0 \leq k_a < 2\pi \quad (5.1)$$

which may be interpreted as nonrelativistic, free single-particle excitations. The full spectrum would be obtained from the solution to all correlation functions. From (5.1) we find that the system is partially integrable in any number of space dimensions. Note that in the discussion in the previous section the positivity of the constants $a_{k,l}$ was only necessary for the interpretation of H as generating a stochastic process. The partial integrability of H is ensured by the constraints (3.8) alone.

In order to get some insight into the physical origin of the one-particle excitations and of the structure of the equations for the higher-order correlators we study the relationship of the stochastic Hamiltonian (2.12) to the Heisenberg quantum Hamiltonian defined below. This is motivated by the symmetric exclusion process, in which case (2.12) is the Hamiltonian of the isotropic Heisenberg ferromagnet.

In this section we show that:

The spectrum of H , (2.12), with the constraint (3.8) is identical to the spectrum of the Hamiltonian of an anisotropic spin-1/2 Heisenberg quantum Hamiltonian H_{XXZ} in a magnetic field. The behavior of the k -point correlation functions is determined by the excitations of the p -magnon sector, where $0 \leq p \leq k$.

The ferromagnetic Heisenberg quantum Hamiltonian H_{XXZ} is of the same form as (2.12), but with matrices

$$\begin{aligned}
 h_j^{(a)} &= -\frac{1}{2\gamma} (\sigma_j^x \sigma_{j+e^{(a)}}^x + \sigma_j^y \sigma_{j+e^{(a)}}^y + \Delta \sigma_j^z \sigma_{j+e^{(a)}}^z + \beta_1 \sigma_j^z + \beta_2 \sigma_{j+e^{(a)}}^z + c) \\
 &= - \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & h_{22} & 1 & 0 \\ 0 & 1 & h_{33} & 0 \\ 0 & 0 & 0 & h_{44} \end{pmatrix}_{(j;a)} \quad (5.2)
 \end{aligned}$$

where we have chosen the normalization $\gamma = 1$ and the constant $c = -(b_1 + b_2 + \Delta)$ such that $h_{11} = 0$, $h_{22} = -(\beta_2 + \Delta)$, $h_{33} = -(\beta_1 + \Delta)$, $h_{44} = -\beta_1 - \beta_2$, and $h_{23} = h_{32} = 1$. This Hamiltonian has a continuous $U(1)$

symmetry generated by $S^z = \sum_j \sigma_j^z/2$. Hence H_{XXZ} splits into sectors with fixed z component of the total spin. By identifying spin up at site j with a vacancy and spin down with a particle, this $U(1)$ symmetry amounts to particle number conservation. The sector with $S^z = M/2 - N$ corresponds to the N -particle sector.

In order to make contact with the reaction matrices $u_j^{(a)}$ we study the dual matrices $\hat{u}_j^{(a)}$, (4.6), which were obtained from the original reaction matrices by the similarity transformation V and transposition (4.4). First we renormalize \tilde{H} by a factor $\xi = (B_1 B_2)^{1/2}$ and perform another similarity transformation $\hat{H} = (\Phi \tilde{H} \Phi^{-1})/\xi$, where $\Phi = \exp[\sum_j (j \cdot \eta) \sigma_j]$ and $\eta = \eta \sum_{a=1}^d e^{(a)}$ with $\eta = (B_1/B_2)^{1/2}$. For $\tilde{A}_1 = \tilde{A}_2 = \tilde{A}_3 = \tilde{B}_3 = D_3 = 0$ this manipulation yields matrices

$$\hat{u}_j^{(a)} = - \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \hat{u}_{22} & 1 & 0 \\ 0 & 1 & \hat{u}_{33} & 0 \\ 0 & 0 & 0 & \hat{u}_{44} \end{pmatrix}_{(j;a)} \tag{5.3}$$

with $\hat{u}_{11} = 0$, $\hat{u}_{22} = C_1/\xi$, $\hat{u}_{33} = C_2/\xi$, $\hat{u}_{44} = C_3/\xi$, $\hat{u}_{32} = \hat{u}_{23} = 1$. These matrices are identical to the Heisenberg matrices (5.2) for an appropriate choice of β_1 , β_2 , and Δ . Therefore on the five-parameter submanifold of the general model on which one obtains completely decoupled equations for the k -point correlation functions one finds $\hat{H} = H_{XXZ}$.³ The duality transformation turns the state $\langle s | \tilde{n}_{x_1} \dots \tilde{n}_{x_k}$, (4.10), appearing in the k -point correlation function (4.11) into a k -particle initial state. Since H_{XXZ} (and the transformed stochastic Hamiltonian \hat{H}) conserves particle number, one finds that the correlator is given by the k -magnon excitations of the Heisenberg quantum Hamiltonian.

In order to understand the more general ten-parameter manifold $D_1 = D_2 = 0$ we split the transformed dual reaction matrices into two parts $\hat{u}_j^{(a)} = h_j^{(a)} - h_j^{\prime(a)}$, with

$$h_j^{(a)} = - \begin{pmatrix} 0 & \hat{A}_1 & \hat{A}_2 & \hat{A}_3 \\ 0 & 0 & 0 & \hat{B}_3 \\ 0 & 0 & 0 & \hat{D}_3 \\ 0 & 0 & 0 & 0 \end{pmatrix}_{(j;a)} \tag{5.4}$$

³ The transformation Φ relates the symmetric model $h_{23} = h_{32}$ to the asymmetric model $h_{23} \neq h_{32}$; see refs. 6, 12, 23, and 24 for the one-dimensional case. It induces nonperiodic, twisted boundary conditions, i.e., the constants \hat{u}_{23} and \hat{u}_{32} in the boundary matrices are different from those in the bulk matrices $\hat{u}_j^{(a)}$. The H_{XXZ} and \hat{H} agree in general only up to boundary terms.

Thus one may write $\hat{H} = H_{XXZ} + H'$. The crucial point is that H_{XXZ} conserves particle number and may therefore be block diagonalized in blocks with fixed N . On the other hand, H' connects a block with particle number N with blocks with particle numbers $N-1$ and $N-2$, but not with any $N' \geq N$. The whole matrix \hat{H} has therefore a triangular structure with block matrices labeled by N arising from H_{XXZ} on the diagonal and matrix elements resulting from H' on the upper off-diagonal. The characteristic polynomial of \hat{H} does not depend on these off-diagonal entries and therefore the characteristic polynomials of the stochastic Hamiltonians H, \hat{H} [(2.13 and (4.8)] and the Heisenberg Hamiltonian H_{XXZ} [see Eq. (5.2)] are identical.⁴ The full dynamics of the k -point correlation function is determined not only by the eigenvalues of the time evolution operator, but also by the eigenstate. Since H' annihilates only, eigenvalues and eigenstates with $p \leq k$ particles contribute to the dynamics. This explains the partial integrability of the model: To the one-point function $k=1$ only the one-magnon sector contributes. This is indeed a nonrelativistic free particle. It is interesting to note that in one dimension, H_{XXZ} is completely integrable. In this case the eigenvalues may be found from the Bethe ansatz.

6. THE AVERAGE DENSITY

In this section we give an application of the results of Section 3. The simple form of Eq. (3.1) for the shifted average particle density on a hypercubic lattice,

$$\frac{\partial}{\partial t} \langle \tilde{n}_{\mathbf{x}} \rangle = \sum_{a=1}^d (B_1 \langle \tilde{n}_{\mathbf{x}-\mathbf{e}^{(a)}} \rangle + B_2 \langle \tilde{n}_{\mathbf{x}+\mathbf{e}^{(a)}} \rangle - (C_1 + C_2) \langle \tilde{n}_{\mathbf{x}} \rangle) \quad (6.1)$$

allows for an explicit integration and thus the extraction of the critical and noncritical behavior of the system. We define

$$C = C_1 + C_2, \quad D = 2(B_1 B_2)^{1/2}, \quad \mathcal{E} = \frac{1}{2d} \ln \left(\frac{B_2}{B_1} \right) \quad (6.2)$$

and the vector $\mathcal{E} = \mathcal{E} \sum_{a=1}^d \mathbf{e}^{(a)}$ and study first the infinite system. In d dimensions the solutions $\tilde{\rho}(\mathbf{x}, t) = \langle \tilde{n}_{\mathbf{x}} \rangle$ to (6.1) is given in terms of modified Bessel functions $I_n(x)$ by

$$\tilde{\rho}(\mathbf{x}, t) = \sum_{\mathbf{y}} a_{\mathbf{y}} \{ \exp[-dCt + \mathcal{E} \cdot (\mathbf{x} - \mathbf{y})] \} \prod_{a=1}^d I_{x_a - y_a}(Dt) \quad (6.3)$$

⁴ The same argument was used in ref. 13, but on another submanifold of the parameter space.

with initial condition $\tilde{\rho}(\mathbf{x}, 0) = a_x$. With $a_x = a\delta_{x,y}$ and for large times t and large separations $r^2 = (\mathbf{x} - \mathbf{y})^2$ with r^2/t fixed this may be written

$$\tilde{\rho}(\mathbf{r}, t) = ae^{-d\mu}(2\pi Dt)^{-d/2} e^{-(r - \mathcal{E} Dt)^2/2Dt} \tag{6.4}$$

and the physical interpretation of the constants becomes apparent. D plays the role of a diffusion constant, while \mathcal{E} is a driving field leading to an average drift velocity $\mathbf{v} = D\mathcal{E}$. From this we find that the system satisfies the Einstein relation

$$\left(\frac{\partial v^{(a)}}{\partial \mathcal{E}^{(a)}} \right)_{\mathcal{E}^{(a)}=0} = D \tag{6.5}$$

The constant

$$\mu = C - \left(1 + \frac{\mathcal{E}^2}{2} \right) D \tag{6.6}$$

is a decay constant. For $\mu = 0$ the system is critical with dynamical exponent $z = 2$.

For a finite-size scaling study of the density on a hypercubic lattice we consider a one-dimensional system with L sites. The solution of (6.1) with periodic boundary condition and initial condition $\tilde{\rho}(x, 0) = a\delta_{x,y}$ (with $1 \leq x, y \leq L$ and $r = x - y$) is

$$\tilde{\rho}(r, t) = \frac{1}{L} \sum_{k=0}^{L-1} \exp \left\{ \frac{2\pi ikr}{L} + \left[2C - (B_1 + B_2) \cos \frac{2\pi k}{L} - i(B_1 - B_2) \sin \frac{2\pi k}{L} \right] t \right\} \tag{6.7}$$

Introducing the scaling variables $u = \pi[r + (B_1 - B_2)t]/L$ and $\tau = 2\pi(B_1 + B_2)t/L^2$ and taking the limit $L \rightarrow \infty$, we find that this becomes

$$\tilde{\rho}(u, \tau) = \frac{1}{L} e^{-\mu'\tau} \theta_3(u | i\tau) \tag{6.8}$$

with the decay constant $\mu' = C - B_1 - B_2$ and the Jacobi theta function

$$\theta_3(u | i\tau) = \sum_{n=-\infty}^{\infty} e^{-\pi n^2 \tau + 2inu} \tag{6.9}$$

Equations (6.7) and (6.8) describe a density distribution of width $\Delta = B_1 + B_2 = D \cosh \mathcal{E}$ with its center at $x = y - vt$, where $v = B_1 - B_2 = D \sinh \mathcal{E}$. The Einstein relation (6.5) therefore holds also in the finite system. Note that when taking the scaling limit we have implicitly assumed

that $\mathcal{E} = \varepsilon/L$ vanishes proportional to L^{-1} because otherwise u would diverge. This implies $\Delta \approx D$, $v \approx D\mathcal{E}$, and $\mu' \approx \mu$. For $\mu' = 0$ and large values of τ , i.e., for times larger than L^2 , the density in the moving frame of reference decays exponentially to its constant value $\bar{\rho}_\infty = a/L$ with decay constant $2\pi^2 D$. For small values of τ the density decays with a power-law behavior, $\bar{\rho}(0, \tau) = aL^{-1}(2\pi D\tau)^{-1/2}$. This may be shown using the Poisson resummation formula, but is already clear from (6.4).

Equation (6.1) may be solved for other boundary conditions, such as open boundary conditions with injection and absorption of particles.⁽²⁵⁾ We do not discuss this here.

If $A_1, A_2 \neq 0$, the constants B_1 and B_2 can be negative. On bipartite lattices this leads to an alternating positive and negative (relative) density $\bar{\rho}(\mathbf{x}, t)$. For other lattices the situation is more complex.

7. CONCLUSIONS

We have studied a general reaction-diffusion process of hard-core particles with two-site interactions on a lattice in d dimensions. There are 12 parameters (2.16) for the various reaction and diffusion rates. On a ten-parameter submanifold defined by (3.8) of the parameter space the differential-difference equations (3.1) satisfied by the k -point density correlation functions are inhomogeneous linear equations involving no higher-order correlators. We have mainly considered a d -dimensional hypercubic lattice with nearest neighbor interaction and space-independent rates, but this result holds for arbitrary lattices with arbitrary two-site interactions as long as (3.8) is satisfied for the interaction between each pair of sites. On a d -dimensional hypercubic lattice with periodic boundary conditions Eqs. (3.1) decouple completely on a seven-parameter submanifold.

It is perhaps worthwhile pointing out that throughout Sections 3–5 we have assumed that initially N particles are located on a set of sites $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$. All calculations can be easily repeated for an arbitrary, time-dependent initial distribution. In this way one can get similar results for two-time correlation functions.

We have shown that in general the decoupling from higher-order correlators does not imply the existence of a dual process for the time evolution of a k -particle initial state as one has in the special case of the symmetric exclusion process. This remains true only under further assumptions on the reaction rates arising from conservation of probability and positivity of rates in the dual process. The dual process to the general ten-parameter model (if it exists) is a process involving only diffusion and annihilation of particles (death, decoagulation, and pair annihilation), but no creation.

The Hamiltonian (2.13) defining the stochastic process is partially integrable and has the same spectrum as a spin-1/2 Heisenberg quantum Hamiltonian H_{XXZ} in a magnetic field and with twisted boundary conditions. This explains the occurrence of the nonrelativistic one-particle excitations appearing in the time evolution of the density profile in terms of one-magnon excitations of the Heisenberg model. The dynamics of the k -point correlators are given by p -magnon states with $p \leq k$. In one dimension, H_{XXZ} is completely integrable and its spectrum can be found from the Bethe ansatz. However, it is interesting to note that even though for $D_1 = D_2 = 0$ the spectra of H and H_{XXZ} are identical, the matrices u_j do *not*, in general, satisfy the Hecke algebra relations $u_j u_{j \pm 1} u_j - u_i = u_{j \pm 1} u_j u_{j \pm 1} - u_{j \pm 1}$, $[u_i, u_j] = 0$ for $|i - j| \geq 2$ and $u_j^2 = \lambda u_j$.^(13,14) Through Baxterization,⁽²²⁾ this would imply the integrability of the model as in the case of the normal Heisenberg Hamiltonian (5.2). This observation hints at a more general algebraic structure beyond the usual conditions for integrability in one dimension.

In Section 6 we used our results for the exact calculation of the time evolution of the density from an arbitrary initial density and analyzed its finite-size scaling behavior in the scaling regime $t \approx L^2$ (L is the size of the system). An initially sharp peak in the distribution widens diffusively and moves with a constant average velocity. It turns out that the model satisfies the Einstein relation (6.5) relating the drift velocity and the diffusion constant. Depending on the various reaction rates, there is a noncritical region with an additional exponential decay of the amplitude. Thus the time evolution of the density profile on a d -dimensional hypercubic lattice with periodic boundary conditions depends only on four combinations of the ten parameters. For other boundary conditions or lattices more parameters enter and it would be interesting to study the corresponding lattice effects. The lattice diffusion constant may be zero or even negative. The latter case corresponds to the development of an alternating structure of the average density on bipartite lattices before reaching the constant stationary density. Another open question is the behavior of the density-density correlation function in the general ten-parameter model. This quantity may be nontrivial even in the steady state, as only under strong restrictions on the rates is the steady state a product measure.

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