Dynamic matrix ansatz for integrable reaction-diffusion $\mathsf{processes}^\star$

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Abstract. We show that the stochastic dynamics of a large class of one-dimensional interacting particle systems may be presented by integrable quantum spin Hamiltonians. Generalizing earlier work [1,2] we present an alternative description of these processes in terms of a time-dependent operator algebra with quadratic relations. These relations generate the Bethe ansatz equations for the spectrum and turn the calculation of time-dependent expectation values into the problem of either finding representations of this algebra or of solving functional equations for the initial values of the operators. We use both strategies for the study of two specific models: (i) We construct a two-dimensional time-dependent representation of the algebra for the symmetric exclusion process with open boundary conditions. In this way we obtain new results on the dynamics of this system and on the eigenvectors and eigenvalues of the corresponding quantum spin chain, which is the isotropic Heisenberg ferromagnet with non-diagonal, symmetry-breaking boundary fields. (ii) We consider the non-equilibrium spin relaxation of Ising spins with zero-temperature Glauber dynamics and an additional coupling to an infinite-temperature heat bath with Kawasaki dynamics. We solve the functional equations arising from the algebraic description and show non-perturbatively on the level of all finite-order correlation functions that the coupling to the infinite-temperature heat bath does not change the late-time behaviour of the zero-temperature process. The associated quantum chain is a non-hermitian anisotropic Heisenberg chain related to the seven-vertex model.

PACS. 05.40+j Fluctuation phenomena, random processes, and Brownian motion – 02.50.Ga Markov processes – 05.70.Ln Nonequilibrium thermodynamics, irreversible processes

1 Stochastic dynamics and quantum systems

One-dimensional stochastic reaction-diffusion processes are of both theoretical and experimental interest in a very wide context. They are well-known models both for reaction-diffusion mechanisms in physics and chemistry and for stochastic spin flip dynamics [3]. More recently they have appeared through various mappings also as models for traffic flow [4-8], the kinetics of biopolymerization [9,10], reptation of DNA in gels [11–16], interface growth [17,18], diffusion in zeolites [19,20] and many other phenomena. Even in relatively simple models of driven diffusion such as the asymmetric exclusion process with open boundaries one finds a very rich dynamical behaviour involving dynamical and non-equilibrium phase transitions of various kinds [21-24]. Exact solutions [3,25] allow for a detailed understanding of cooperative phenomena in these classical many-body systems and provide insight in the role of inefficient diffusive mixing in diffusion-limited chemical reactions, in the dynamics of shocks, and in other fundamental mechanisms which determine the behaviour of low-dimensional systems far from thermal equilibrium.

A convenient and much used description of stochastic processes is in terms of a master equation for the probability distribution $f(\underline{n};t)$ of the stochastic variables \underline{n} . These variables represent the states in which the system may be found at any given instant of time. The master equation encodes the transition probabilities $p(\underline{n}' \to \underline{n})$ of moving from one state \underline{n}' to another state \underline{n} in one time step: the probability distribution $f(\underline{n};t + \Delta t) = \sum_{\underline{n}'} p(\underline{n}' \to \underline{n}) f(\underline{n}';t)$ is just the sum of probabilities of finding the system in state \underline{n}' at time t times the respective transition probabilities $p(\underline{n}' \to \underline{n})$. Thus the master equation expresses the probability of finding the system at time $t + \Delta t$ in a given configuration \underline{n} in terms of the probability distribution at time t. Such processes are Markov processes which may be constructed for the description of interacting particle systems [26].

Since the master equation is linear in the probability distribution, it can be expressed as a vector equation in a "quantum Hamiltonian formalism" by mapping each state \underline{n} of the system to a basis vector $|\underline{n}\rangle$ in a suitable vector space X. Thus the probability distribution becomes a vector $|f(t)\rangle = \sum_{\underline{n}} f(\underline{n};t)|\underline{n}\rangle$ and the master equation for a continuous-time process $(\Delta t \to 0)$ takes the form

 $^{^{\}star}\,$ Dedicated to J. Zittartz on the occasion of his 60th birthday

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of a Schrödinger equation in imaginary time

$$\frac{d}{dt}|f(t)\rangle = -H|f(t)\rangle. \tag{1}$$

For various interesting many-body systems the generator H of the (classical) stochastic time evolution turns out to be identical to the quantum Hamiltonian of spin chains known from condensed matter physics [27–32] (see next section). The ground state of a stochastic Hamiltonian (which by construction has energy 0) corresponds to the stationary probability distribution of the stochastic dynamics which is reached asymptotically at the late stages of the time evolution. Through this somewhat surprising connection to quantum spin systems the stochastic dynamics become tractable with the tool box of quantum mechanics and progress may be achieved¹.

A paradigmatic example of this relationship is the symmetric exclusion process [26,37]. In this lattice model particles hop between lattice sites k, l with rates $p_{k,l} = p_{l,k}$. They interact via a hard-core repulsion which prevents the occupation of a lattice site by more than one particle. The stochastic quantum Hamiltonian obtained for this system [28] is the Hamiltonian for the isotropic spin-(1/2) Heisenberg ferromagnet

$$H = -\frac{1}{2} \sum_{k,l} p_{k,l} \left[\sigma_k^x \sigma_l^x + \sigma_k^y \sigma_l^y + \sigma_k^z \sigma_l^z - 1 \right].$$
(2)

The manifest SU(2)-symmetry of H (which is not recognizable in the original master equation) can be used for obtaining exact results [29,38]. Moreover, in one dimension, the system with nearest neighbour hopping is integrable and can be solved by the Bethe ansatz [39].

The integrability is not a special feature of the symmetric exclusion process alone. Driven diffusion in one dimension $(p_{k,k+1}/p_{k+1,k} = q \neq 1)$ is described by the XXZ quantum spin chain which differs from (2) by an anisotropy $\Delta = (q + q^{-1})/2$ in the z-z coupling of the spins [29]. Using the Bethe ansatz and related methods many new exact results particularly on the dynamical properties of the process have been obtained [29,41–46]. Moreover, it turns out that a 10-parameter class of reaction-diffusion systems of identical particles [32] and various systems of non-identical particles [31,47] are described by integrable quantum chains. Unfortunately however, the Bethe ansatz requires knowledge of some reference eigenstate of H and integrability has so far failed to provide constructive methods to calculate even the ground

state of spin chains with boundary fields that destroy the reference state. Such boundary fields are of importance in stochastic dynamics of non-equilibrium systems as they allow for a modelling of open systems which are in contact with external particle reservoirs at their boundaries and thus allow for maintaining a particle current through the system.

In a very different approach the ground states of onedimensional spin Hamiltonians are formulated in terms of *matrix product states* [48–51] where the ground state wave function is expressed in terms of a trace over a product of matrices. They may be seen as representations of an operator algebra which is determined by the requirement that by acting with the Hamiltonian on this state one obtains an eigenstate (the ground state) of H. Applied to stochastic Hamiltonians one obtains in this way the stationary distribution of a stochastic process $[52–57]^2$.

By constructing an infinite-dimensional representation of the stationary matrix algebra for the asymmetric exclusion process with open boundaries Derrida *et al.* [52] produced the same exact results that were obtained independently by Schütz and Domany [22] using a different method. In fact, with hindsight our treatment may be seen as a representation-free solution of recursion relations that one can derive from the matrix algebra. It is the aim of this work to apply both strategies, *viz.* (i) construction of a matrix representation or (ii) solution of equations resulting from the algebraic relations alone, to a matrix product treatment of the *dynamics* of reaction-diffusion systems. Specifically we consider the symmetric exclusion process with open boundaries and a reaction-diffusion mechanism which is equivalent to a spin relaxation model.

The extension of the stationary matrix approach of Derrida *et al.* to a dynamical description requires one new idea. This is the introduction of auxiliary matrices S, T[1,2] which do not appear in the calculation of expectation values, but are necessary to formulate the dynamical algebra which is determined such that the probability distribution satisfies the full time-dependent master equation. The special case of this construction where S+T=0allowed among other things for the rederivation [2] of the Bethe ansatz equations [58] for the spectrum in the symmetric case with open boundaries and for the rederivation [59] of the spectrum in the asymmetric case with periodic boundary conditions [43]. With the auxiliary matrices as additional ingredient the extension of the dynamical matrix product approach to reaction-diffusion systems becomes straightforward [60] (see below).

I will first show (Sect. 2) how reaction-diffusion systems of identical hard-core particles are related to a generalized Heisenberg chain. Its spectrum can be obtained from the Bethe ansatz. This is a simplified rederivation of some results obtained earlier [32]. Then in Section 3 I will generalize the operator approach to the general reaction-diffusion problem of identical hard-core particles with nearest neighbour interaction in one dimension. As an application I will return to the symmetric exclusion

¹ For discrete time dynamics the vector form of the master equation reads $|f(t + \Delta t)\rangle = T|f(t)\rangle$. For many interesting systems in one dimension T is the transfer matrix of a twodimensional vertex model [33–36]. The frequently-used notion "quantum Hamiltonian formalism" is somewhat misleading in so far as for many stochastic applications the transition rates result in coupling constants which make H non-Hermitian. Further, since f is a (real-valued) probability and not a (complex) probability amplitude, the expectation values of the stochastic process are not the expectation values normally calculated in a quantum mechanical problem.

 $^{^{2}}$ For non-periodic systems with boundary fields one does not take a trace, but a suitably chosen scalar product [52].

Table 1. Bulk reaction and diffusion rates for nearest neighbour exclusion processes of identical particles. The numbers a_{ij} are the rate of change of the occupation numbers $\{n_k, n_{k+1}\}$.

Process	Rate		Process	Rate	
01 ightarrow 10	a_{32}	diffusion	10 ightarrow 01	a_{23}	diffusion
11 ightarrow 01	a_{24}	coagulation	$01 \rightarrow 11$	a_{42}	decoagulation
11 ightarrow 10	a_{34}	coagulation	10 ightarrow 11	a_{43}	decoagulation
00 ightarrow 01	a_{21}	creation	01 ightarrow 00	a_{12}	annihilation
00 ightarrow 10	a_{31}	creation	10 ightarrow 00	a_{13}	annihilation
00 ightarrow 11	a_{41}	pair creation	11 ightarrow 00	a_{14}	pair annihilation

process and present a two-dimensional representation of the time-dependent operator algebra³. In Section 4, I will solve a non-equilibrium spin relaxation model introduced by Droz *et al.* [61] by solving functional equations arising from the algebraic relations of the time-dependent matrix algebra. This treatment does not require the calculation of representations of the algebra. In Section 5 the main results are summarized and some open questions are pointed out.

2 Integrable reaction-diffusion processes

We will consider stochastic reaction-diffusion processes of identical particles with hard-core repulsion moving on a ring with L sites. Even though part of our approach generalizes to arbitrary lattices [32] we will study here only one-dimensional systems with nearest neighbour interaction. The stochastic variables of the system are the occupation numbers $\underline{n} = \{n_k\}$ where $n_k = 0, 1$ indicates whether site $1 \le k \le L$ in the lattice is occupied or empty. At a given time t the state of the system is completely described by the probability distribution $f(\underline{n}; t)$. In this class of models there are ten possible reactions in addition to right and left hopping (diffusion), so altogether one has to specify 12 independent rates $a_{ij} \ge 0$ (Tab. 1).

The stochastic dynamics are defined by the master equation

$$\frac{d}{dt}f(\underline{n};t) = \sum_{\underline{n}'} \left[w(\underline{n};\underline{n}')f(\underline{n}';t) - w(\underline{n}';\underline{n})f(\underline{n};t)\right] \quad (3)$$

where the reaction-diffusion rates $w(\underline{n};\underline{n}')$ for a change from configuration $\underline{n}' \to \underline{n}$ are equal to the sum

$$\begin{split} \sum_{k=1}^{L} \left\{ \delta_{n'_{k},0} \delta_{n'_{k+1},0} \left[a_{21} \delta_{n_{k},0} \delta_{n_{k+1},1} + a_{31} \delta_{n_{k},1} \delta_{n_{k+1},0} \right. \\ \left. + a_{41} \delta_{n_{k},1} \delta_{n_{k+1},1} \right] + \delta_{n'_{k},0} \delta_{n'_{k+1},1} \left[a_{12} \delta_{n_{k},0} \delta_{n_{k+1},0} \right. \\ \left. + a_{32} \delta_{n_{k},1} \delta_{n_{k+1},0} + a_{42} \delta_{n_{k},1} \delta_{n_{k+1},1} \right] \\ \left. + \delta_{n'_{k},1} \delta_{n'_{k+1},0} \left[a_{13} \delta_{n_{k},0} \delta_{n_{k+1},0} + a_{23} \delta_{n_{k},0} \delta_{n_{k+1},1} \right. \\ \left. + a_{43} \delta_{n_{k},1} \delta_{n_{k+1},1} \right] + \delta_{n'_{k},1} \delta_{n'_{k+1},1} \left[a_{14} \delta_{n_{k},0} \delta_{n_{k+1},0} \right. \\ \left. + a_{24} \delta_{n_{k},0} \delta_{n_{k+1},1} + a_{34} \delta_{n_{k},1} \delta_{n_{k+1},0} \right] \right\}. \end{split}$$

This somewhat lengthy expression becomes more compact in the quantum Hamiltonian formalism (1): To each configuration \underline{n} one assigns a vector $|\underline{n}\rangle$ which, together with the transposed vectors $\langle \underline{n} |$, form an orthonormal basis of $(\mathbf{C}^2)^{\otimes L}$. In spin language this corresponds to a mapping to a spin 1/2 chain by identifying a vacancy (particle) at site k with spin up (down) at this site. The probability distribution is then given by the state vector $|f(t)\rangle = \sum_{\underline{n}} f(\underline{n};t)|\underline{n}\rangle$ and the formal solution of the master equation (1) in terms of the initial distribution $|f(0)\rangle$ is given by $|f(t)\rangle = \exp(-Ht)|f(0)\rangle$. The stochastic dynamics are defined by the master equation (1) with [32]

$$H = \sum_{k=1}^{L} h_k \tag{4}$$

where the matrices h_k act non-trivially only on sites k, k+1 and are given by

$$h_{k} = - \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix}_{k,k+1}$$
(5)

with $a_{jj} = -\sum_{\substack{i=1\\i\neq j}}^4 a_{ij}$.

The connection of H to the Heisenberg quantum chain becomes apparent by the similarity transformation $\tilde{H} = \Phi V H V^{-1} \Phi^{-1}$ with $V = \exp(S^+)$ where $S^+ = \sum_{k=1}^{L} s_k^+$ and $s_k^{\pm} = (\sigma_k^x \pm i \sigma_k^y)/2$ are the spin lowering

³ Sections 2 and 3 of this paper are not really new. They constitute the bulk of the paper [60] which was presented at the Satellite Meeting to Statphys 19 on Statistical Models, Yang-Baxter Equation and Related Topics, at Nankai University, Tianjin (August 1995).

and raising operators acting on site k and with $\Phi = \exp(\mathcal{E}\sum_k k\sigma_k^z)$ where \mathcal{E} is a suitably chosen constant [32]. On the ten parameter submanifold defined by

$$a_{34} = a_{21} + a_{41} + a_{12} + a_{32} - a_{23} - a_{43} - a_{14} \tag{6}$$

$$a_{24} = a_{31} + a_{41} + a_{13} + a_{23} - a_{32} - a_{42} - a_{14}.$$
(7)

the transition matrices have now the structure $\tilde{h_k} = h_k^{XXZ} + h_k^-$. Here h_k^{XXZ} commutes with $S^z = \sum_{k=1}^L \sigma_k^z/2$ and h_k^- is a sum of two parts which lower the z-component of the spin on sites k, k+1 by one and two units respectively. So one finds

$$\tilde{H} = H^{XXZ} + H^{-} \tag{8}$$

where H^{XXZ} is the Hamiltonian of the anisotropic Heisenberg ferromagnet with twisted boundary conditions in a magnetic field. The crucial observation is that H^- does not change the spectrum of H^{XXZ} , since H^{XXZ} may be block-diagonalized into blocks with fixed quantum number S^z and H^- connects only blocks of given S^z with blocks with quantum numbers⁴ $S^z - 1$ and $S^z - 2$.

Quantities of interest are expectation values (i.e. *r*-point correlation functions) $\langle n_{k_1}(t) \dots n_{k_r}(t) \rangle_{f_0} =$ $\langle s | n_{k_1} \dots n_{k_r} e^{-Ht} | f(0) \rangle$ which give the probability of finding particles on the set of sites $\{k_1, \ldots, k_r\}$ at time t, if the initial distribution at time t = 0 was f_0 . Here $\langle s | =$ $\sum_{n} \langle \underline{n} |$ and $n_k = (1 - \sigma_k^z)/2$ is the projector on states with a particle on site k. From the Bethe ansatz one finds now that the spectrum has an energy gap (i.e. inverse correlation time) $\mu' = 4a_{41} + 2(a_{21} + a_{31}) + a_{12} + a_{13} - a_{42} - a_{43} \ge 0.$ If $\mu' = 0$ the dynamical exponent turns out to be z = 2. Note also that V transforms a r-point density correlation function into a matrix element in the sector with r down spins. Since H^- only creates down spins, only transformed initial states with l < r down spins will contribute to the correlation function. This surprising simplification allows for an exact calculation of the local average density for any initial state even though we are dealing with a non-trivial interacting many particle system [32].

3 The dynamic matrix ansatz

The results of the last section involve the constraints (6, 7) and do not apply *e.g.* for the asymmetric exclusion process. Also this model is integrable, but a calculation of time-dependent correlation functions has not yet been achieved. In order to solve this problem we now formulate a dynamic matrix ansatz for the general reaction-diffusion system defined by (4) and (5), generalizing earlier work [1,2] for diffusion only. Instead of periodic boundary conditions we consider a system with open boundaries where particles are injected (absorbed) at site 1 with rate α (γ) and at site *L* with rate δ (β). Therefore $H = b_1 + b_L + \sum_{k=1}^{L-1} h_k$ with suitably chosen boundary matrices b_1, b_L [1].

The ansatz is to take $|f(t)\rangle = \langle \langle W | \{\prod_{k=1}^{L} (E(t) + D(t)\sigma_{k}^{-})\} | 0 \rangle | V \rangle \rangle / Z_{L}$ where $| 0 \rangle$ is the state with all spins up and D, E are time-dependent matrices satisfying an algebra obtained from the master equation (1). The (timeindependent) vectors $\langle \langle W | \text{ and } | V \rangle \rangle$ on which D and Eact are determined from the boundary terms in the master equation and $Z_{L} = \langle \langle W | C^{L} | V \rangle \rangle$ where C = D + Eis a normalization. In this framework the *r*-point density correlation function is given by $\langle n_{k_{1}}(t) \dots n_{k_{r}}(t) \rangle_{f_{0}} =$ $\langle \langle W | C^{k_{1}-1}DC^{k_{2}-k_{1}-1}D \dots C^{L-k_{r}} | V \rangle \rangle / Z_{L}$. Therefore, given a matrix representation of the algebra satisfied by D, E, the computation of time-dependent correlation functions is reduced to the calculation of matrix elements of a product of L matrices.

It is easy to see that (1) is solved if for each pair of sites one satisfies

$$(\frac{1}{2}\frac{d}{dt} + h_k)(E + D\sigma_k^-)(E + D\sigma_{k+1}^-)|0\rangle = [(S + T\sigma_k^-)(E + D\sigma_{k+1}^-) - (E + D\sigma_k^-)(S + T\sigma_{k+1}^-)]|0\rangle$$
(9)

where S, T are auxiliary operators satisfying

$$\langle \langle W | \left[\left(\frac{1}{2} \frac{d}{dt} + b_1 \right) (E + D\sigma_1^-) + (S + T\sigma_1^-) | 0 \rangle \right] = 0$$
(10)
$$\left[\left(\frac{1}{2} \frac{d}{dt} + b_L \right) (E + D\sigma_L^-) - (S + T\sigma_L^-) | 0 \rangle \right] | V \rangle \rangle = 0.$$
(11)

By comparing each of the four terms in (9) proportional to $|0\rangle$, $\sigma_k^-|0\rangle$, $\sigma_{k+1}^-|0\rangle$ and $\sigma_k^-\sigma_{k+1}^-|0\rangle$ resp. one obtains four quadratic relations for the operators D, E, S, T. Equations (10) and (11) give two pairs of equations which define $\langle \langle W |$ and $|V \rangle \rangle$. Introducing

$$A^{(1)} = -(a_{21} + a_{31} + a_{41})E^2 + a_{12}ED + a_{13}DE + a_{14}D^2$$
(12)
$$B^{(1)} = a_{21}E^2 - (a_{12} + a_{32} + a_{42})ED + a_{23}DE + a_{24}D^2$$
(13)

$$B^{(2)} = a_{31}E^2 + a_{32}ED - (a_{13} + a_{23} + a_{43})DE + a_{34}D^2$$
(14)

$$A^{(2)} = a_{41}E^2 + a_{42}ED + a_{43}DE - (a_{14} + a_{24} + a_{34})D^2$$
(15)

one finds

$$\frac{1}{2}\frac{d}{dt}E^2 - [S, E] = A^{(1)} \tag{16}$$

$$\frac{1}{2}\frac{d}{dt}ED - SD + ET = B^{(1)}$$
(17)

$$\frac{1}{2}\frac{d}{dt}DE - TE + DS = B^{(2)}$$
(18)

$$\frac{1}{2}\frac{d}{dt}D^2 - [T,D] = A^{(2)} \tag{19}$$

 $^{^4}$ This mechanism was first noticed in a similar context in Alcaraz *et al.* [62].

and

$$\left\langle \left\langle W \right| \left\{ \frac{1}{2} \frac{d}{dt} E - \alpha E + \gamma D + S \right\} = 0 \tag{20}$$

$$\langle \langle W | \left\{ \frac{1}{2} \frac{d}{dt} D + \alpha E - \gamma D + T \right\} = 0$$
 (21)

$$\left\{\frac{1}{2}\frac{d}{dt}E - \delta E + \beta D - S\right\} |V\rangle\rangle = 0$$
 (22)

$$\left\{\frac{1}{2}\frac{d}{dt}D + \delta E - \beta D - T\right\} |V\rangle\rangle = 0.$$
 (23)

One may reduce this algebra by assuming that Cis time-independent and has a representation where it is invertible. Equations (9) then imply [C, S + T] = 0and (10, 11) imply $\langle \langle W | (S+T) = 0 = (S+T) | V \rangle \rangle$. This can be solved by assuming S + T = 0, which, as I would like to stress, is *not* the most general choice. Now one can express S in terms of C and D and is left with only two further relations to be satisfied by D and C and two relations defining $\langle \langle W |$ and $| V \rangle \rangle$. In particular, if (7) and (8) are satisfied, there is one relation involving D which is linear in D and one relation quadratic in D. For the symmetric exclusion model $a_{23} = a_{32} = 1/2$ this dynamic algebra yields eigenvalue equations for the corresponding XXX-Hamiltonian with integrable, but non-diagonal, symmetry breaking boundary fields [1,2]. However, no matrix representation has been found yet. This raises the question whether non-trivial representations do exist at all.

As I will show here for the first time, the answer to this question is yes, at least with some restrictions on the injection and absorption rates. Choosing a basis where Cis diagonal one finds the representation

$$C = \begin{pmatrix} 1 & 0 \\ 0 & c \end{pmatrix}, D = \begin{pmatrix} d & \lambda e^{-\epsilon t} \\ 0 & cd \end{pmatrix}.$$
 (24)

with $\epsilon = (\alpha + \beta + \gamma + \delta)/2$, $c = 1 - \alpha - \gamma = (1 - \beta - \delta)^{-1}$, $d = \alpha/(\alpha + \gamma) = \delta/(\beta + \delta)$ and $\langle \langle W |, |V \rangle \rangle$ arbitrary but $\langle \langle W | V \rangle \rangle \neq 0$. In this representation λ is an arbitrary parameter specifying the initial distribution. One may also use it for the construction of (right) eigenstates of H, since the expression $\langle \langle W | E^{k_1 - 1} D E^{k_2 - k_1 - 1} \dots E^{L - k_r} | V \rangle \rangle$ is a superposition of wave functions $\Psi_{\epsilon_i}(k_1, \dots, k_r)$ of eigenstates with eigenvalues ϵ_i . The argument is the position of r down spins on sites k_1, \dots, k_r . Taking $\lambda = 0$ corresponds to taking the stationary distribution as initial state. This is an eigenstate with energy 0. The terms proportional to λ give the wave function for an eigenstate with energy ϵ . The quantity $1/(\ln |c|)$ plays the role of a spatial correlation length.

4 Non-equilibrium spin relaxation

A phenomenon of wide interest in physics and chemistry is the growth of domains in non-equilibrium two-phase systems. The best-known example is perhaps the Ising model with domains of up- and down spins, separated by domain walls. The energy of the Ising model is given by the nearest neighbour sum $E = -J \sum s_i s_j$. Since the creation of a local domain wall costs an energy J the system tries to organize itself at low temperature into large domains of uniform magnetization. Starting from a high-temperature equilibrium state with many domain walls and quenching to low temperatures leads to a coarsening process: Small domains of uniform magnetization merge to form larger domains since then the total length of the domain walls and thus the energy decreases.

Glauber [63] introduced spin-flip dynamics which ensure that the system reaches the equilibrium distribution at temperature $T = 1/\beta$ of the one-dimensional Ising model. In this model a spin within a domain of equal magnetization is flipped with a rate $\mu = 1 - \tanh \beta J$, whereas a spin in a region of opposite magnetization is flipped with a rate $\lambda = 1 + \tanh \beta J$. At domain boundaries spins are flipped with unit rate, since no change in energy is involved. This process can be visualized in the following way:

$$\begin{array}{l} \uparrow\uparrow\uparrow\to\uparrow\downarrow\uparrow \quad \text{and} \quad \downarrow\downarrow\downarrow\to\downarrow\uparrow\downarrow \quad \text{with rate } \mu \\ \uparrow\downarrow\uparrow\to\uparrow\uparrow\uparrow \quad \text{and} \quad \downarrow\uparrow\downarrow\to\downarrow\downarrow\downarrow \quad \text{with rate } \lambda \\ \uparrow\uparrow\downarrow\rightleftharpoons\to\uparrow\downarrow\downarrow \quad \text{and} \quad \downarrow\uparrow\uparrow\rightleftharpoons\downarrow\uparrow\uparrow \quad \text{with rate } 1. \end{array}$$

Glauber dynamics can also be seen as a reactiondiffusion system. One simply identifies an up-spin with a vacancy and a down-spin with a particle. In one dimension at zero temperature the process can then be described as follows:

$$\begin{array}{l} A \ \emptyset \ \text{or} \ \emptyset \ A \ \to \ A \ A \ \text{with rate} \ 1 \\ A \ \emptyset \ \text{or} \ \emptyset \ A \ \to \ \emptyset \ \emptyset \ \text{with rate} \ 1 \end{array}$$

This can obtained by a translational rearrangement of the three-site interactions in terms of two-site processes. One realizes then that Glauber dynamics can be represented by a stochastic Hamiltonian of the form (4, 5) with $a_{12} = a_{13} = a_{42} = a_{43} = 1$. Furthermore, these rates satisfy the constraints (7). We stress that this relation to a reaction-diffusion system is not really a mapping, but just a certain choice of language which we use in order to make contact with Sections 2 and 3. There are two different nontrivial mappings [64,65] to the process of diffusion-limited annihilation which has little in common with the process described here. These mappings are useful as they show that Glauber dynamics can be described and solved in terms of free fermions [27, 62, 66-69] and that the associated quantum chain is a non-hermitian anisotropic Heisenberg chain related to the seven-vertex model [62].

The Glauber relaxation rules involve single spin flips and thus do not conserve the total magnetization. Kawasaki [70] introduced spin-exchange dynamics which also lead to an equilibrium Ising distribution, but which *do* conserve the total magnetization. At infinite temperature, these dynamics reduce to simple exchange of neighbouring spins with some rate $a_{23} = a_{32} = \zeta$, *i.e.* to the symmetric exclusion process described above. Due to the lack general theorems on the dynamics of non-equilibrium systems it is now of interest to investigate a spin system the behaviour of which results from a coupling to two heat baths at different temperatures — one leading to zero-temperature Glauber dynamics, the other to infinitetemperature Kawasaki dynamics [61]. In such a situation there is a competition: The diffusion process tries to disorder the system, while the Glauber process tries to create an ordered system of uniform structure. Hence the questions arise, which process wins, and how is the stationary state reached.

In one dimension this problem was addressed by studying the dynamical spin-spin (= particle-particle) correlations for a translationally invariant initial state [61], using the fact that the equations of motion for correlation functions decouple into closed subsets. By solving the equations Droz *et al.* could show that at any (finite) value ζ of the coupling strength the system orders and that the spinspin correlation function behaves at large times like the zero-temperature Glauber correlator. Here we use the matrix product ansatz to prove non-perturbatively that this remains true for *all* correlation functions of finite order. The leading contribution to time-dependent correlation functions (for large times) is always the zero-temperature Glauber correlation function [71]. Corrections resulting from the coupling to the infinite-temperature heat bath are of subleading order $1/\sqrt{t}$ (relative to the leading con $tribution)^5$.

To prove our assertion we consider the matrix algebra describing the process. Since we are more interested in spin variables we introduce $\tilde{D} = C - 2D = E - D$. We restrict ourselves to translationally invariant initial states. Because of translational invariance time-dependent spin expectation values are given by a trace over matrices

$$\langle \sigma_{k_1}^z(t) \dots \sigma_{k_r}^z(t) \rangle_{f_0} =$$

Tr $\{ C^{k_1-1} \tilde{D} C^{k_2-k_1-1} \tilde{D} \dots C^{L-k_r} \} / Z_L$ (25)

where $Z_L = \text{Tr } C^L$. We reduce the algebra (16) - (19) as in the case of the symmetric exclusion process by setting S + T = 0. Eliminating S leads then to the algebra generated by C, \tilde{D} and C^{-1} with the relations $CC^{-1} = C^{-1}C = 1$, d/(dt)C = 0 and

$$\frac{d}{dt}\tilde{D} = (1+\zeta)\left(C\tilde{D}C^{-1} + C^{-1}\tilde{D}C - 2\tilde{D}\right)$$
(26)
$$2(1-\Delta) = \tilde{D}C^{-1}\tilde{D}C^{-1} + C^{-1}\tilde{D}C^{-1}\tilde{D} - 2\Delta C^{-1}\tilde{D}^2C^{-1}$$
(27)

with the constant $\Delta = \zeta/(1+\zeta)$ determined by coupling ratio ζ . The *r*-point spin correlation function can now be rewritten

$$\langle \sigma_{k_1}^z(t) \dots \sigma_{k_r}^z(t) \rangle = \text{Tr} \{ \tilde{D}_{k_1} \dots \tilde{D}_{k_r} C^L \} / Z_L$$
 (28)

where $\tilde{D}_k = C^{k-1} \tilde{D} C^{-k}$ and $k_{i+1} > k_i$. These relations provide an alternative, purely algebraic definition of the spin relaxation process.

Relation (26) is linear in \tilde{D} and we proceed by constructing the Fourier transforms $\mathcal{D}_p = \sum_k e^{ipk} \tilde{D}_k$ to reformulate the algebra in terms of the Fourier components. Since

$$C\mathcal{D}_p C^{-1} = e^{-ip} \mathcal{D}_p, \tag{29}$$

the time-dependence of \mathcal{D}_p is now simply obtained from (26)

$$\mathcal{D}_p(t) = e^{-\epsilon_p t} \mathcal{D}_p(0) \tag{30}$$

in terms of the initial matrix $\mathcal{D}_p(0)$ and the "energy"

$$q_p = 2(1+\zeta)(1-\cos p).$$
 (31)

From (27) follows $2(1 - \Delta)\delta(p) = \int dp' \mathcal{D}_{p'} \mathcal{D}_{p-p'}(1 + e^{-ip} - 2\Delta e^{ip'-ip})$. Since this relation holds for all times (and all p), the integral can be divided into separate time-components, each of which must vanish. If p_1 and p_2 are non-zero this leads to

$$\mathcal{D}_{p_1}\mathcal{D}_{p_2} = S(p_2, p_1)\mathcal{D}_{p_2}\mathcal{D}_{p_1} \tag{32}$$

with the two-body scattering matrix

 ϵ

$$S(p_2, p_1) = -\frac{1 + e^{ip_1 + ip_2} - 2\Delta e^{ip_2}}{1 + e^{ip_1 + ip_2} - 2\Delta e^{ip_1}}$$
(33)

known from the usual anisotropic Heisenberg chain [40].

This relation for \mathcal{D}_p is derived for the dynamic components with $p \neq 0$. Hence the static term in the l.h.s. of (27) does not reappear in (32), but in a different relation involving the static parts $\mathcal{D}_0 = \sum_n C^{n-1} D C^{-n}$ and $\mathcal{I} = \sum_n n C^{n-1} D C^{-n}$. These quantities need separate treatment in a similar way as the static components of the operators for the symmetric exclusion process with open boundaries [25,75]. However, since the stationary state (all spins up or all spins down) is not interesting we do not consider the static Fourier components.

The momentum space formulation of the algebra provides another equivalent formulation of the process. To calculate expectation values we do not search for a representation of this algebra but use a different strategy.

⁵ We mention in passing that this process is a simple toy model of growing tissue cell populations [72]. The decoagulation process $A\emptyset, \emptyset A \to AA$ with unit rate describes cell division, while the particle hopping with rate ζ corresponds to the diffusive motion of cells in their environment. In addition to that we allow for a death process $A\emptyset, \emptyset A \to \emptyset\emptyset$ with rate qwhich kills both the original cell and its offspring during the decoagulation (cell mitosis). It is intuitively clear that for q < 1the cell population will grow until all space is covered, while for q > 1 the population will eventually die out. Therefore it is of interest to study the case q = 1 when creation of offsprings and the death process balance each other. The process leads to an ordered state also in three dimensions [73,74]. This implies that either all tumor cells die, or, with equal probability, cover the whole available space.

In terms of the Fourier components the correlator (28) reads

$$\langle \sigma_{k_1}^z(t) \dots \sigma_{k_r}^z(t) \rangle = \left(\prod_{i=1}^m \int \frac{dp_i}{2\pi} e^{-p_i k_i - \epsilon_{p_i} t}\right) T(\{p_i\})$$
(34)

where the so far undetermined matrix element

$$T(\{p_i\}) = \operatorname{Tr} \{\mathcal{D}_{p_1}(0) \dots \mathcal{D}_{p_m}(0)C^L\}/Z_L \qquad (35)$$

depends only on the initial distribution.

First consider the one-point function $\langle \sigma_k^z(t) \rangle$. Because of translational invariance, this local magnetization is independent of space. This is reflected in the invariance of the trace under cyclic permutation. Thus (35) for the one-point function together with (29) imply $e^{ip} = e^{2ip} =$ $e^{3ip} = \cdots = e^{ipL} = 1$ and therefore $T(p) = 2\pi c\delta(p)$. This yields $\langle \sigma_k^z(t) \rangle = c$ for all times and restates nothing but the known result that the average magnetization remains constant under the time evolution of the spin relaxation model [61]. The initial magnetization m_0 fixes $c = m_0$.

We obtain a non-trivial result for the two-point correlator. We use (29), (33) and the cyclic property of the trace and find

$$T(p_1, p_2) = \text{Tr} \{ \mathcal{D}_{p_1}(0) \mathcal{D}_{p_2}(0) C^L \} / Z_L$$

= $S(p_2, p_1) \text{Tr} \{ \mathcal{D}_{p_2} \mathcal{D}_{p_1} C^L \} / Z_L$
= $e^{ip_1 L} S(p_2, p_1) \text{Tr} \{ \mathcal{D}_{p_2} C^L \mathcal{D}_{p_1} \} / Z_L$
= $e^{ip_1 L} S(p_2, p_1) T(p_1, p_2).$ (36)

A similar cycling procedure gives a second relation

$$T(p_1, p_2) = e^{ip_2 L} S(p_1, p_2) T(p_1, p_2).$$
(37)

Using $S(p_1, p_2) = S^{-1}(p_2, p_1)$ we conclude that $T(p_1, p_2)$ is non-zero only if the momenta $p_{1,2}$ satisfy the Betheansatz equations [40]

$$e^{ip_1L} = S(p_1, p_2) \tag{38}$$

$$e^{ip_2L} = S(p_2, p_1). (39)$$

Translational invariance requires also $p_1 + p_2 = 0$.

Moreover, the first of the equations (36) yields a functional equation for the matrix element

$$T(p_1, p_2) = S(p_2, p_1)T(p_2, p_1).$$
(40)

This functional equation for $T(p_1, p_2)$ is solved by the Bethe wave functions [39,76,77]

$$\Psi_{p_1,p_2}(l_1,l_2) = A(l_1,l_2) \left(e^{ip_1 l_1 + ip_2 l_2} + S(p_2,p_1) e^{ip_2 l_1 + ip_1 l_2} \right),$$
(41)

for $k_2 > k_1$ with some amplitude $A(l_1, l_2)$ determined by the initial value of the correlator. It can be calculated from the integral representation (34) of the full time-dependent correlator by setting t = 0.

For a finite system the integral has to be replaced by a sum over the solutions of the Bethe ansatz equations (38, 39). However, in an infinite system the set of solutions becomes dense. The only subtlety arises then from the bound states defined by the pole of the scattering amplitude S. This pole corresponds to the two-particle bound state already known from the original solution of Bethe [39] for $\Delta = 1$. One can fix the contour of integration by setting $A(l_1, l_2) = \langle n_{l_1}(0)n_{l_2}(0) \rangle$. This gives

$$T(p_1, p_2) = \sum_{l_1, l_2} \langle n_{l_1}(0) n_{l_2}(0) \rangle \left(e^{ip_1 l_1 + ip_2 l_2} + S(p_2, p_1) e^{ip_2 l_1 + ip_1 l_2} \right)$$
(42)

with the sum being restricted to the domain $l_2 > l_1$. We prescribe the appropriate contour of integration by isolating in S the constant part $S_0 = -1$ which corresponds to non-interacting fermions. One writes

$$S(p_2, p_1) = -1 + 2\Delta(1 - e^{ip_1 - ip_2}) \times \int_0^\infty du \ e^{-u(e^{ip_1} + e^{-ip_2} - 2\Delta e^{ip_1 - ip_2})}.$$
 (43)

and integrates both p_1 and p_2 from 0 to 2π along the real axis *before* integrating over u. Both this definition of the integration and the choice for the amplitude $A(l_1, l_2)$ ensure that the initial condition is indeed satisfied in the physical domain $k_2 > k_1$, $l_2 > l_1$. With the constraint $p_1 + p_2 = 0$ originating in translational invariance one recovers in this way the expression for the two-point correlator derived by Droz *et al.* [61] by direct solution of the equations of motion with generating function techniques.

Note that for the pure Glauber case $\Delta = 0$ and hence $S = S_0 = -1$. In this case the \mathcal{D}_p anticommute and can represented *e.g.* by a Jordan-Wigner transformation of the usual local spin-1/2 raising or lowering operators s_k^{\pm} . We recover in a surprising way the free fermion nature of this process. However, since Glauber dynamics are well-understood [71] we do not further pursue this matrix representation. In the present context we are more interested in the observation that for large times only small p_1, p_2 contribute to the integral (34). Making a substitution of variables $p_i \to p_i/\sqrt{t}$ and expanding for large t leads to

$$S = -1 + O(t^{-1/2}) \tag{44}$$

for the late time behaviour of the scattering amplitude S (43). This proves our assertion for the two-point function: For large times the correction to the correlator due to coupling to the infinite-temperature Kawasaki heat bath is of subleading order $O(t^{-1/2})$ for any finite coupling ζ .

Higher order correlation functions are treated analogously. The permutation of \mathcal{D}_p matrices using the matrix relations (29, 33) yields the Bethe ansatz equations and functional equations for the matrix elements $T(\{p_i\})$. For a *r*-point correlator this functional equation is solved by the *r*-particle Bethe wave function [39,40]. Because of the integrability the scattering amplitudes factorize into products of two-body amplitudes. Thus for large times the leading part comes from the free-fermion amplitude S = -1 and therefore the leading part of the correlator is independent of the Kawasaki coupling ζ and given by the pure Glauber correlation function. The leading correction which results from this coupling is of order $t^{-1/2}$. This proves our assertion.

5 Conclusions

A 10-parameter class of stochastic reaction-diffusion systems can be mapped by a similarity transformation to a generalized Heisenberg quantum chain, the spectrum of which can be obtained by the Bethe ansatz. It turns out that time-dependent r-point density correlation functions are given by the $l \leq r$ -magnon sectors. As an alternative to that approach we introduced a dynamic matrix ansatz for the general 12-parameter model. This ansatz reduces the calculation of all correlators to the calculation of certain matrix elements. These matrices satisfy an infinite-dimensional algebra which is determined by the bulk dynamics of the process. The boundary conditions determine which matrix elements one has to take.

In the cases of the symmetric exclusion process and of the non-equilibrium spin relaxation model of Droz et al. the algebra satisfied by the matrices can be used to obtain the spectrum of the corresponding quantum Hamiltonian. We constructed a two-dimensional time-dependent matrix representation of the algebra for the symmetric exclusion process from which one obtains explicitly all r-point density correlators for a one-parameter class of initial states. The corresponding eigenvectors of the Heisenberg chain are the ground state with energy 0 and a bound state with energy $\epsilon = (\alpha + \beta + \gamma + \delta)/2$. An alternative treatment of the dynamical algebra exploits directly the algebraic relations which result in functional equations for the dynamical part of the correlator. We have solved these equations for the spin relaxation model in terms of Bethe wave functions. We proved that independently of the coupling to the infinite-temperature heat bath all r-point equal-time correlation functions decay to leading order in time like the zero-temperature Glauber correlators.

From a mathematical point of view the dynamical matrix algebra and its representation theory is not yet well-understood. The stationary version of the extended algebra was considered by Hinrichsen et al. [78] who constructed a four-dimensional representation for a coagulation/decoagulation model. Krebs and Sandow [56] could prove that the stationary algebra extended with the auxiliary matrices forms an equivalent formulation of the stationary master equation. This guarantees the existence of a representation for the general case. To date there is no equivalent theorem for the dynamical algebra and no representation theory. A second important question concerns the relationship between the integrability of quantum chains and the dynamic matrix ansatz which emerged here and in other work [2, 59, 79]. The result of Krebs and Sandow for the stationary algebra shows that there is no general relationship between the possibility of an algebraic description and the integrability of a system. Yet for integrable models the algebra is powerful enough not only to recover the known Bethe ansatz equations but also to

obtain results which cannot be obtained using standard Bethe ansatz techniques. This suggests that matrix algebras describing integrable models have special, as yet undiscovered properties.

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