Resenhas IME-USP 1999, Vol. 4, No. 1, 17 - 43.

Stochastic many-body systems and quantum spin chains [1]

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Abstract: We present a brief tutorial introduction into the quantum Hamiltonian formalism for stochastic many-body systems which are defined in terms of a master equation. These models describe interacting classical particle systems where particles hop on a lattice and may undergo reactions. In the quantum Hamiltonian formalism the generator of the stochastic process is reformulated as the Hamiltonian of some generalized quantum spin system. This correspondance is particularly useful if the quantum Hamiltonian associated to the process has continuous global symmetries or if it is integrable, i.e. has an infinite set of conservation laws. This is demonstrated in the case of the one-dimensional exclusion process for which we derive various duality relations and some explicit results on the dynamics of shocks.

Key words: Exclusion process, duality relations, quantum Hamiltonian formalism.

1 Classical stochastic many-body dynamics in the quantum Hamiltonian formalism

The time evolution of many systems encountered in nature is most appropriately described by *stochastic laws* rather than by deterministic equations as in Newtonian mechanics for classical physics. The randomness of the time evolution leads to the description of the process in terms of *random variables* and to the connection of the theory with measurements in terms of *expectation values*. Rather than predicting the actual value of some observable in a given measurement, one calculates e.g. the mean value of the observable as obtained by repeating the same measurement many times, starting from the same initial state. Despite the randomness of the motion, complex systems of *many interacting particles* [1, 2, 3, 4] may exhibit very interesting patterns of collective behaviour, including various types of phase transitions, development of spatially stable shocks, or coarsening phenomena. The purpose of these lecture notes is to review a framework for the study of such systems which uses ideas and techniques borrowed from many-body quantum mechanics.

There are various approaches to a stochastic description [5] such as the Langevin or Fokker-Plank equations. Here we adopt the strategy of describing the system by a probability distribution, the time evolution of which is governed by a *master equation*. Solving the master equation, which is a first-order linear differential equation in the time variable, yields the probability of finding any given state the system may take given that it started from some initial state. One can

[1] Research partially supported by Capes / Probal 047/97 and Fapesp 98 / 04422-5.

then calculate expectation values and hence make contact with actual measurements. This program may appear rather ambitious at first sight. Indeed, as shown below, it is technically of the same difficulty as many-body quantum mechanics, an analogy which becomes understandable through a simple relationship between the generator of the Markovian time evolution of the master equation and the generator of the time evolution of a quantum-mechanical wave function. The point of using this analogy is to make use of the special-purpose tools developed so successfully in the past for the treatment of quantum mechanical problems (particularly in one dimension) and to exploit these techniques for problems arising in the study of classical interacting particle systems. Below we shall illustrate this strategy by solving some specific problems arising in the investigation of diffusive hard-core particles.

The idea of formulating the master equation in terms of a many-body quantum Hamiltonian is not new. Systematic treatments of various aspects of the quantum Hamiltonian formalism go back to [6], [7] and [8]. Particularly for the "bosonic" description of the process in these works the renormalization group has proved to be a powerful tool [9]. More recent expositions, with particular emphasis on the relationship to quantum spin systems which we shall use here, can be found in Refs. [10, 11, 12, 13] and in the references therein. To make clear the ideas we shall consider mostly systems with finite state space X, i.e. systems which can be found only in a finite number of different states $\eta \in X$. The extension to infinite systems can be made on the level of expectation values by taking appropriate limits.

1.1 The master equation

1.1.1 Discrete-time dynamics

Before discussing many-particle systems we illustrate the master equation approach to stochastic processes in a simple example. The simplest stochastic model system that can be described in this way is a two-state system such as a coin which can show either heads or tails, or a spin which can either point up or down. We imagine some random mechanism (such as tossing the coin or a thermally activated spin-flip process) which may alter the state of the system after a time lapse Δt and we assume that the random updating is independent of the previous history of the system. Such processes are Markov processes. The probability $P_\eta(t + \Delta t)$ of finding the system at time $t + \Delta t$ after one updating event in the state η depends only on the state of the system at time t. The dynamical evolution can be represented by a set of rules which state the respective probabilities of moving from some state η to a state η' in one update. If spin up ($\uparrow$) flips to spin down ($\downarrow$) with probability p and spin down flips to spin up with probability q, then the probabilities $P_{\uparrow,\downarrow}(t + \Delta t)$ of finding the system in either of the two states evidently satisfy the *master equation*

$$P_\uparrow(t + \Delta t) \quad = \quad (1 - p)P_\uparrow(t) + qP_\downarrow(t) \tag{1}$$

$$P_\downarrow(t+\Delta t) \;=\; pP_\uparrow(t) + (1-q)P_\downarrow(t). \tag{2}$$

From this description it becomes also obvious that $P_\eta(t+\Delta t)$ is related to $P_\eta(t)$ by a linear map. Thus it is convenient to write the master equation as a vector equation for the probability vector

$$|\,P(t)\,\rangle = \begin{pmatrix} P_\uparrow(t) \\ P_\downarrow(t) \end{pmatrix}. \tag{3}$$

The master equation then reads

$$|\,P(t+\Delta t)\,\rangle = T|\,P(t)\,\rangle \tag{4}$$

with the *transfer matrix* or transition matrix T. For the two-state spin model defined above T reads

$$T = \begin{pmatrix} 1-p & q \\ p & 1-q \end{pmatrix}. \tag{5}$$

One may choose as basis vectors of this two-dimensional vector space the canonical unit vectors

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{6}$$

With this notation one may write $|\,P(t)\,\rangle = P_\uparrow(t)|\uparrow\rangle + P_\downarrow(t)|\downarrow\rangle$.

Generally, the strategy of writing the master equation in vector form can be summarized as follows: To each state $\eta \in X$ one assigns a basis vector $|\,\eta\,\rangle$ of the vectorspace $\mathbf{X} = \mathbb{C}^m$. Here m is the cardinality of X, i.e. the number of distinct states of the system. Together with their transposed vectors $\langle\,\eta\,|$ (row vectors forming a basis of the dual space) they form an orthonormal basis with scalar product $\langle\,\eta\,|\,\eta'\,\rangle = \delta_{\eta,\eta'}$. The probability vector is $|\,P(t)\,\rangle = \sum_\eta P_\eta(t)|\,\eta\,\rangle$ and the matrix elements $T_{\eta,\eta'} \equiv \langle\,\eta\,|T|\,\eta'\,\rangle = p_{\eta'\to\eta}$ of the transfer matrix T are the transition probabilities from state η' to state η.

Expectation values of an observable F are by definition the quantities $\langle\,F\,\rangle = \sum_\eta F(\eta)P_\eta(t)$. Here $F(\eta)$ is some function of the random variables η, e.g. the spin $F(\uparrow) = 1$, $F(\downarrow) = -1$. In a series of measurements the system may be found in states η of the system with probabilities $P_\eta(t)$. Hence the expression $\langle\,F\,\rangle$ is the average value of what one measures in a series of many identical experiments, using the same initial state. If the initial states are not always the same fixed state, but some collection of different states, given by an initial distribution $P_\eta(0)$, then the expression $\langle\,F\,\rangle$ involves not only averaging over many realizations of the same process, but also averaging over the initial states. To calculate expectation values in vector notation it is useful to introduce the row vector $\langle\,s\,| = \sum_\eta \langle\,\eta\,|$ all components of which are equal to one. Furthermore we define the diagonal matrix $F = \sum_\eta F(\eta)|\,\eta\,\rangle\langle\,\eta\,|$ which has the values of the function $F(\eta)$ as diagonal entries. Then one may the write the expectation value in the form

$$\langle\,F\,\rangle = \langle\,s\,|F|\,P(t)\,\rangle. \tag{7}$$

If we want to specify time and initial condition, we write $\langle F(t) \rangle_{P_0}$. Notice that the mathematical operation of taking the expectation value corresponds to taking the scalar product of the summation vector with the (column) vector $F|P(t)\rangle$ which has as components the weighted quantities $F(\eta)P_\eta(t)$. This is equivalent to taking the scalar product of the probability vector $|P(t)\rangle$ with the vector $\langle s|F$ which is the (row) vector with $F(\eta)$ as its components. The probability vector is the analog of a measure in usual probability theory and taking the scalar product corresponds to an integration over the measure. The time evolution of the measure is operationally performed by the action of the transfer matrix on the probability vector.

Conservation of probability, i.e. $1 = \sum_\eta P_\eta(t) = \langle s|P(t)\rangle$ implies

$$\langle s|T = \langle s|. \tag{8}$$

This means that in each column η of T all matrix elements, i.e., transition probabilities $p_{\eta\to\eta'}$ add up to 1 (see (5) for illustration). This is nothing but a technical way of expressing completeness of the set X: the system always moves to some state $\eta \in X$.[2] A matrix with the property (8) and in which all matrix elements are real and satisfy $0 \le T_{\eta,\eta'} \le 1$ is called a stochastic transfer matrix.

For time-homogeneous Markov chains (which we consider throughout this paper), the solution to the master equation (4) with a given initial distribution $|P(0)\rangle$ can formally be written

$$|P(t)\rangle = T^n|P(0)\rangle \tag{9}$$

where $t = n\Delta t$. The action of the transfer matrix has a simple interpretation in terms of the history of a given realization of the random process: In any given realization the system starts at some initial state η_0 and proceeds through a series of n states to a final state η_n at time $t = n\Delta t$. This particular realization of the stochastic time evolution happens with probability $p_{\eta_0\to\eta_1}p_{\eta_1\to\eta_2}\cdots p_{\eta_{n-1}\to\eta_n}$. The matrix element $\langle \eta'|T^n|\eta_0\rangle$ is just the sum of all probabilities of histories which lead from η_0 to some $\eta' = \eta_n$ in n steps.

1.1.2 Continuous-time dynamics

The dynamics in the previous subsection was defined in terms of discrete-time updates as performed e.g. on a computer or as seen in a real system by taking snapshots at time intervals of length Δt. Now we pass on to the continuous-time formulation of Markov processes. This will eventually lead to the quantum Hamitonian formalism for interacting particle systems.

One obtains a continuous-time representation of the processes described above by defining the off-diagonal transition probabilities in terms of rates $w_{\eta\to\eta'} =$

[2] One may restrict the description of a stochastic process to its motion on a subset of X. In this case (which we shall not consider here) the system has a finite probability of being outside this subset and hence (8) is violated for such a transfer matrix T'.

$p_{\eta\to\eta'}/\Delta t$ which are the transition probabilities per time unit. This allows one to write the transfer matrix in the form $T = 1 - H\Delta t$. The off-diagonal matrix elements of H are the (negative) transition rates, $H_{\eta,\eta'} = -w_{\eta'\to\eta}$. The diagonal elements $H_{\eta,\eta}$ are the (positive) sum of all the rates in each column η, i.e. the sum of all outgoing rates $w_{\eta\to\eta'}$. Taking the limits $\Delta t \to 0$, $n \to \infty$ in such a way that $t = n\Delta t$ remains fixed, the time evolution may be written $T^n = T^{t/(\Delta t)} \to e^{-Ht}$ with a '*quantum Hamiltonian*' H. The term 'quantum Hamiltonian' originates from the observation that by expanding the master equation (4) up to first order in Δt one finds

$$\frac{d}{dt}|\,P(t)\,\rangle = -H|\,P(t)\,\rangle. \tag{10}$$

This equation has the form of a quantum mechanical Schrödinger equation in imaginary time. The formal solution $|\,P(t)\,\rangle = e^{-Ht}|\,P(0)\,\rangle$ reflects the exponential waiting time distribution for events in the corresponding Markov process. The standard notation $d/dtP_\eta(t) = \sum_{\eta'}[w_{\eta'\to\eta}P_{\eta'}(t) - w_{\eta\to\eta'}P_\eta(t)]$ of the master equation can be recovered from (10) by inserting the definition of $|\,P(t)\,\rangle$ and taking the scalar product with $\langle\,\eta\,|$.

For the two-state spin model with $p = \alpha\Delta t$, $q = \beta\Delta t$ the corresponding quantum Hamiltonian reads

$$H = \begin{pmatrix} \alpha & -\beta \\ -\alpha & \beta \end{pmatrix}. \tag{11}$$

It is useful to introduce the three Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{12}$$

where i is the imaginary unit. Introducing also the spin ladder operators $s^\pm = (\sigma^x \pm i\sigma^y)/2$ and the diagonal projectors $n = (1-\sigma^z)/2$ and $v = (1+\sigma^z)/2$ one may write $H = \alpha(v - s^-) + \beta(n - s^+)$. The off-diagonal part of H represents the flip events with their respective rates, while the diagonal elements ensure conservation of probability: In each column all matrix elements add up to zero, as required by probability conservation $\langle\,s\,|e^{-Ht} = \langle\,s\,|$, or, equivalently,

$$\langle\,s\,|H = 0. \tag{13}$$

Introducing the (non-diagonal) time-dependent operator in the Heisenberg representation $F(t) = e^{Ht}Fe^{-Ht}$ one can write expectation values, using (13),

$$\langle\,F\,\rangle = \langle\,s\,|F(t)|\,P(0)\,\rangle = \langle\,s\,|Fe^{-Ht}|\,P(0)\,\rangle. \tag{14}$$

1.1.3 Stationary states

One of the most basic questions to ask is the behaviour of the system at late times of the stochastic evolution. If the system is ergodic the probability distribution

in the limit $t \to \infty$ is independent of the initial state and one would like to know quantities like the mean density, density fluctuations, or the spatial structure of the density distribution and its correlations. For transition rates that are constant in time this asymptotic distribution is invariant under time translations and hence called stationary. We shall denote such a distribution by $|\, P^* \,\rangle$. From the considerations of the previous subsections it is clear that $|\, P^* \,\rangle$ is a right eigenvector of H with eigenvalue zero,

$$H|\, P^* \,\rangle = 0. \tag{15}$$

This is, by construction, the eigenvalue of H with the lowest real part This follows from a theorem by Gershgorin [14]. Therefore in quantum mechanical language the stationary vector corresponds to the ground state of H. However, if H is not hermitian this vector is *not* the transposed vector $\langle\, s \,|$, but a more complicated object.

The expression 'quantum Hamiltonian' is perhaps somewhat misleading in three respects: Firstly, a stochastic quantum Hamiltonian need not be Hermitian, instead its off-diagonal elements have to be negative and real, and in each column the sum of all matrix elements has to vanish. Secondly, expectation values $\langle\, F \,\rangle$ are not of the usual quantum mechanical form $\langle\, \Psi \,|F|\, \Psi \,\rangle$. In fact, the probability vector $|\, P(t) \,\rangle$ represents the probability itself, rather than a complex probability amplitude. Finally, time is euclidean. However, the name quantum Hamiltonian formalism has become fairly standard and is justified not only by the form of the master equation (10), but also by the fact that for numerous interacting particle systems of interest H is indeed the Hamiltonian of some quantum many-body system known from other fields in physics. The following table summarizes the formal correspondence between some "quantum mechanical" concepts and probabilistic notions.

state space X, cardinality m	$\to$	vector space $\mathbb{C}^m$
configuration η	$\to$	orthogonal basis vectors $|\, \eta \,\rangle, \langle\, \eta \,|, \langle\, \eta \,|\, \eta \,\rangle = \delta_{\eta,\eta'}$
probability $P(\eta;t)$	$\to$	probability vector $|\, P(t) \,\rangle = \sum_{\eta \in X} P(\eta;t)|\, \eta \,\rangle$
master equation	$\to$	"Schrödinger equation" $\frac{d}{dt}|\, P(t) \,\rangle = -H|\, P(t) \,\rangle$
time evolution	$\to$	time translation operator e^{-Ht}
function $F(\eta)$	$\to$	diagonal matrix $F = \sum_{\eta \in X} F(\eta)|\, \eta \,\rangle\langle\, \eta \,|$
expectation value	$\to$	scalar product $\langle\, F(t) \,\rangle_{P_0} = \langle\, s \,|F|\, P(t) \,\rangle$
conservation of probability	$\to$	left "ground state" eigenvector $\langle\, s \,|H = 0$
invariant measure	$\to$	right "ground state" eigenvector $H|\, P^* \,\rangle = 0$

1.1.4 Relations between different processes

The definition of a stochastic matrix introduced above is manifestly basis dependent. A change of basis, i.e. a similarity transformation of the stochastic time evolution operator, will generically not lead to a stochastic quantum Hamiltonian. However, in special cases either such a transformed Hamiltonian or its transposed

does define a new stochastic process and thus one can relate results obtained for one process to quantities of the transformed process. If two processes are related by a similarity transformation, $\tilde{H} = \mathcal{B}H\mathcal{B}^{-1}$ with some invertible matrix $\mathcal{B}$, we call these two processes *equivalent*. On the other hand, if the transposed and transformed matrix $\hat{H}^T = \mathcal{B}H\mathcal{B}^{-1}$ describes some stochastic process, then these two processes are called *enantiodromic*.[3]

For both kinds of relations knowledge of properties of one process implies certain knowledge of properties of the related process. In some instances the related process may be simpler than the original process and progress may be achieved. Also transformations to non-stochastic matrices may provide useful insight if properties of such a non-stochastic matrix is known within a different context.

1.2 Many-body systems

1.2.1 The tensor basis

In the two-state spin model discussed above we had just a single spin flipping up and down. In many-body physics and in the study of interacting particle systems one is interested in the behaviour of many coupled spins sitting on some lattice. By identifying a spin up with a vacancy and a spin down with the presence of a particle on the lattice site, spin models can be seen as particle systems where each lattice site may be occupied by at most one particle. This correspondence can be generalized: Allowing for different species of particles, or site occupation by more than one particle, one obtains models where each lattice site can be in one of n distinct states. Such a model can be viewed as spin-$(n-1)/2$ system.[4]

We shall from now on use mainly particle language rather than spin language. States η are defined by a set of occupation numbers $\eta = \{\eta(1), \ldots, \eta(L)\}$ for a lattice of L sites. For two-states models one has $\eta(i) = 0, 1$. The natural extension of the vector description of a single spin to many spins on a lattice is by taking a tensor basis as basis of the state space. Using the convention of considering spin down as a particle, a many particle configuration η is represented by the basis vector $|\,\eta\,\rangle = |\,\eta(1)\,\rangle \otimes \ldots \otimes |\,\eta(L)\,\rangle$. These vectors form a basis of the tensor space $(\mathbb{C}^n)^{\otimes L}$. In this basis each lattice site corresponds to some position in the tensor product. The basis of the dual space is constructed analogously.

The choice of a tensor basis for the state space leads a description of local operators (either diagonal or offdiagonal) in terms of tensor products A_i of local matrices. Here $A_i = \mathbb{1} \otimes \ldots \otimes A \otimes \ldots \mathbb{1}$ is the tensor product of the $n \times n$ unit matrices $\mathbb{1}$ with the matrix A at the position in the tensor product which corresponds to lattice site i. E.g. the matrix s_i^+ annihilates a particle at site i and

[3] One may weaken the definitions by using $\tilde{H}\mathcal{B} = \mathcal{B}H$ and $\hat{H}^T\mathcal{B} = \mathcal{B}H$ as defining relations. The matrix $\mathcal{B}$ is then not required to be a square matrix, i.e. the state spaces of the related processes need not be isomorphic.

[4] For unrestricted occupancy, i.e. allowing for infinitely many states on each lattice site, see [6, 7, 8, 9]. Here we restrict ourselves to 2-states systems.

s_i^- represents a creation event. The diagonal matrix n_i is a projector on states which have a particle at site i, i.e. its eigenvalues are the occupation numbers $\eta(i)$.

1.2.2 Expectation values

The expectation values one is usually interested in are m-point correlation functions $\langle\, n_{i_1}(t_1)\ldots n_{i_m}(t_m)\,\rangle$ with $t_i \geq t_{i+1}$. These are the joint probabilities of finding particles at sites i_l at times t_l which are given by the expression

$$\langle\, n_{i_1}(t_1)\ldots n_{i_m}(t_m)\,\rangle = \langle\, s\,|n_{i_1}e^{-H(t_1-t_2)}n_{i_2}\ldots n_{i_m}e^{-Ht_m}|\,P(0)\,\rangle. \qquad (16)$$

The summation vector for a many-particle system is a tensor product of the single-site summation vectors. It is always the constant row vector $(1,1,\ldots,1)$ and is denoted by $\langle\, s\,|$, irrespective of the system.

A (homogeneous) product measure $|\,\rho\,\rangle$ with density ρ is a tensor product of single-site states with density ρ, i.e. a state where one finds a particle at any given site with probability ρ. An inhomogeneous product measure with site-densities ρ_i is then a tensor product of single-site vectors with densities ρ_i. Since the scalar product of two tensor states factorizes into the product of single-site scalar products it is obvious that there are indeed no correlations in a tensor state.

The empty lattice is represented by the vector $|\,0\,\rangle$. When we are dealing with finite many-body systems we shall sometimes denote a vector $|\,\eta\,\rangle$ which represents a state with particles on sites $k_1,\ldots,k_N$ by $|\,k_1,\ldots,k_N\,\rangle$.

1.2.3 Construction of the quantum Hamiltonian

To construct H for a given process we note that as in the single-site two-states model above, the flip events are represented by offdiagonal matrices. To be precise, they represent attempts rather than actual events: Acting on a state with an already occupied site with s^- yields zero, i.e. no change in the probability vector. This reflects the rejection of any attempt at creating a second particle on a given site. Thus the exclusion of double occupancy is encoded in the properties of the Pauli matrices.

Simultaneous events are represented by products of Pauli matrices acting on different sites. E.g. hopping of a particle from site i to site j is equivalent to annihilating a particle at site i and at the same time creating one at site j. Thus it is given by the matrix $s_i^+ s_j^-$. The hopping attempt is successful only if site i is occupied and site j is empty. Otherwise acting with $s_i^+ s_j^-$ on the state gives zero and hence no change. The rate of hopping (or of any other possible stochastic event) is the numerical prefactor of each hopping matrix (or other attempt matrix). Of course, in principle the rate may depend on the configuration of the complete system. Suppose the hopping rate is given by a function $w(\eta)$ where η is the configuration prior to hopping. In this case the hopping matrix is given by $s_i^+ s_j^- w(\eta)$ where in $w(\eta)$ one replaces any $\eta(i)$ by the projector n_i. If e.g. for some

reason hopping from site i to site j should occur only if a third site site k is empty, then the hopping matrix would be given by $s_i^+ s_j^- (1 - n_k)$. For a hopping rate which is proportional to the number of particles on neighboring sites one finds the matrix $s_i^+ s_j^- (1 + w \sum_k n_k)$. The construction of the attempt matrices for other processes or for n-states model is analogous.

For two-states models one notes the useful identities

$$\langle s | s_i^+ = \langle s | n_i \ , \quad \langle s | s_i^- = \langle s | (1 - n_i) \tag{17}$$

which follow immediately from the tensor structure of the summation vector and the definition of the local Pauli matrices. With these relations it is easy to construct the diagonal part of the quantum Hamiltonian in order ensure conservation of probability. To each off-diagonal attempt matrix one constructs a diagonal matrix by replacing all s_i^+ by n_i and by replacing all s_i^- by $1 - n_i$. E.g. to hopping from i to j with rate w represented by $-w s_i^+ s_j^-$ one adds $w n_i (1 - n_j)$. The (negative) sum of all attempt matrices minus their diagonal counterparts is then the full quantum Hamiltonian. In the same way one constructs the diagonal parts of n-states models by using the analogues of Eqs. (17). Conservation of probability (13) is then automatically satisfied.

The formulation of the master equation in terms of a many-body quantum operator does not only allow for a very convenient derivation of the equations of motion for expectation values (see e.g. [15, 16]), but suggests also analysis of the process by specifically quantum mechanical methods.

2 Integrability

In the previous chapter we have encountered a relationship between classical interacting particle systems and quantum spin systems. The stochastic time evolution is generated by a matrix involving quantum mechanical spin operators. To utilize this equivalence we recall some of the basic notions that appear in the study of exactly solvable spin models, in particular, the notion of integrability. This is a remarkable and important property as it allows, at least in principle, for the derivation of non-trivial exact results.

To understand the origin of integrability one has to go back to the description of (equilibrium) statistical mechanics models in terms of a transfer matrix.[5] A statistical mechanics model (as e.g. the two-dimensional Ising model or the six vertex model) is considered exactly solvable (or integrable) if there exists an infinite set of independent conserved charges.[6] Integrability manifests itself in the concept of *commuting transfer matrices*

$$[T(u), T(u')] = 0 \tag{18}$$

[5] See e.g. [17] or any other textbook on statistical mechanics.

[6] In an integrable quantum system of finitely many degrees of freedom, such as a spin system on a finite lattice, the number of conserved charges is, of course, finite.

where the system parameter u is a suitably chosen function of temperature, field strengths and other parameters of the model and where we have used the commutator symbol $[A, B] \equiv AB - BA$. The importance of this commutation relation for different values of u becomes explicit by expanding $T(u) = \sum_n (u-u_0)^n T_n(u_0)$ around some value u_0. This expansion yields a set of matrices $T_n(u_0)$ and (18) implies $[T_n\,,\,T_m] = 0\ \forall\ m,n$. In particular, $[T_n\,,\,T(u)] = 0$. This commutation relation states that if some vector $|\,v\,\rangle$ is an eigenvector of T_n, then also $T^p|\,v\,\rangle$ is an eigenstate of T_n, i.e. this property is conserved under the action of T. If all the T_n are independent, i.e. not polynomial functions of each other, then the commutator (18) proves the existence of an infinite set of (independent) conservation laws which can be constructed by expanding the transfer matrix in powers of u. As a result, the eigenstates of the transfer matrix can be classified by a set of conserved charges which are the "quantum numbers" related to the eigenvalues of the T_n.

This work is not the place to review the mathematical framework underlying integrability as such. We are only concerned with the *consequences* of integrability in the theory of stochastic interacting particle systems. One obtains an integrable stochastic process if either the transfer matrix T [18, 19, 20, 21, 22] or some linear combination of the matrices T_n can be turned into a stochastic transfer matrix or stochastic Hamiltonian by some similarity transformation. It turns out that for a certain choice of parameters one of the conserved charges T_n of the transfer matrix of the six-vertex model is the quantum Hamiltonian of the isotropic Heisenberg ferromagnet

$$H = -J \sum_i \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z - 1\right). \tag{19}$$

in one dimension. As shown below this is the stochastic generator of the symmetric exclusion process.

One of the most basic properties of the isotropic Heisenberg quantum spin system in the absence of the magnetic field ($h = 0$) is the $SU(2)$ symmetry which generates continuous rotations in spin-space. It is easy to verify by direct calculation that each interaction matrix $\vec{\sigma}_i \cdot \vec{\sigma}_{i+1} \equiv \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z$ commutes with $S^{\pm} = \sum_k s_k^{\pm}$, $S^3 = \sum_k \sigma_k^z/2 = \sum_k (1/2 - n_k)$. These matrices form a spin-1/2 tensor representation of the Lie algebra $SU(2)$ defined by the relations

$$[S^+\,,\,S^-] = 2S^3, [S^{\pm}\,,\,S^3] = \pm S^{\pm}. \tag{20}$$

Hence H is symmetric under the action of $SU(2)$, i.e.

$$[H\,,\,S^{\pm,3}] = 0. \tag{21}$$

This is easy to verify by observing that in a tensor product local operators acting non-trivially at different sites commute, i.e., $[a_i\,,\,b_j] = 0$ for $i \neq j$. In the presence of the magnetic field the symmetry reduces to $U(1)$, generated by S^3. This symmetry corresponds to invariance under continuous rotations around the z-axis

in spin-space. This spin symmetry is not related to the integrability of the model which implies the existence of other matrices which commute with H. It is a very long way to go from the notion of commuting transfer matrices to practical applications of integrability. We merely point out that the Bethe ansatz used below for the calculation of conditional probabilities has its origin in integrability.

An important integrable generalization of the isotropic Heisenberg ferromagnet (19) is the anisotropic Heisenberg Hamiltonian

$$H^{XXZ} = -J \sum_i \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z + h \sigma_i^z \right) \tag{22}$$

where the coupling in the z-direction of the spin variable is different from the couplings in the $x-y$ plane. This model has the same $U(1)$ symmetry as the isotropic Heisenberg chain with non-vanishing field. The associated two-dimensional classical statistical mechanics model is also the integrable six-vertex model, but for different values of parameters [17, 23, 24].

3 Diffusion of hard-core particles

3.1 The symmetric exclusion process

A classical example where the quantum Hamiltonian formalism has turned out to be fruitful is the exclusion process [1, 2, 13]. In its simplest form this is a one-species process where each particle hops with exponential waiting time distribution between nearest neighbour sites with constant rate D [25]. The particles have a hard-core exclusion interaction: hopping attempts which would lead to a double occupancy of a site are rejected. This process can be visualized by representing particles by the symbol A and vacancies by the symbol $\emptyset$ and writing

$$\emptyset\, A \rightleftharpoons A\, \emptyset \qquad \text{with rate} \qquad D$$

for the hopping events between sites i, j. According to the construction described above the stochastic Hamiltonian for hopping between any pair of sites is given by the matrix $D(n_i(1-n_j) + (1-n_i)n_j - s_i^+ s_j^- - s_i^- s_j^+)$. In terms of the usual Pauli matrices this matrix reads $D(1 - \sigma_i^x \sigma_j^x - \sigma_i^y \sigma_j^y - \sigma_i^z \sigma_j^z)/2$ and hence the Hamiltonian for the full symmetric exclusion process is given by the $SU(2)$-symmetric Heisenberg quantum ferromagnet [26]

$$H = -\frac{D}{2} \sum_{<i,j>} \left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z - 1 \right). \tag{23}$$

This is an instance where the stochastic time evolution operator is indeed identical to the quantum Hamiltonian of a non-trivial many-body system which has a long history in condensed matter physics. In one dimension with nearest neighbour hopping one recovers the integrable model (19).

3.1.1 Self-duality

The symmetric exclusion process was studied in detail by Spitzer [25], the main result being duality relations which express time-dependent m-point correlation functions $\langle\, n_{k_1}(t) \ldots n_{k_m}(t) \,\rangle$ for an arbitrary many-particle initial state in terms of correlators of the same system, but containing only m particles. Generally, duality between two Markov processes η_t and ζ_t with state spaces X and Y respectively, means

$$E^{\eta} F(\eta_t, \zeta) = E^{\zeta} F(\eta, \zeta_t) \tag{24}$$

for a bounded, measurable function F on $X \times Y$. Thus it is a relation between expectation values which is defined with respect to F. To formulate the duality relations for the symmetric exclusion process we note that a configuration η which is defined by a set of L occupation numbers $\eta(k) = 0, 1$ may alternatively be represented by the set C of occupied sites, $C = \{k_1, \ldots, k_N\}$ with cardinality $|C| = N$. So instead of defining the exclusion process on the state space $X = \{0,1\}^S$ where $S = \{1, \ldots, L\}$ are the sites on the lattice, one may define the process on the collection Y of subsets of S. For the symmetric exclusion process one defines for $\eta \in X$ and $C \in Y$ the indicator function

$$F(\eta, C) = \begin{cases} 1 & \text{if } \eta(k) = 1 \ \ \forall \ \ k \in C \\ 0 & \text{else} \end{cases} \tag{25}$$

Let us now assume that initially N particles are located on a set of sites $A_N = \{l_1, \ldots, l_N\}$ and we want to compute the probability $\langle\, n_{k_1}(t) \cdots n_{k_m}(t) \,\rangle_{A_N}$ of finding (any) m particles on sites $B_m = \{k_1, \ldots, k_m\}$, at time t. The duality relations (24) with the function (25) state that the probability that $\eta(k) = 1$ at time t on all sites B_m with initial condition A_N is equal to the probability that (the original) configuration has $\eta(l) = 1$ on the sites occupied by a m-particle system at time t which started at sites B_m [25]. Thus the problem of calculating an m-point correlation function of an interacting particle system of N particles has been reduced to the calculation of a correlation function of an m-particle system. In particular, the density expectation value $\langle\, n_k(t) \,\rangle$ is completely given in terms of the dynamics of just a single particle. For finite systems this result was later rederived and extended using the global $SU(2)$ symmetry of H [27]. Here we present a shortened and improved proof of duality using the $SU(2)$ symmetry.

In the quantum Hamiltonian formulation duality is a result of enantiodromy. For two dual processes $H, \hat{H}$ the general duality relation (24) may be written $\langle\, s\,|F_\zeta e^{-Ht}|\,\eta\,\rangle = \langle\, s\,|F_\eta e^{-\hat{H}t}|\,\zeta\,\rangle$. For $C = \{k_1, \ldots, k_m\}$ one may write the function $F(\eta, C) = n_{k_1} \cdots n_{k_m}$ which in operator form becomes the diagonal matrix $F_C = n_{k_1} \cdots n_{k_m}$. Therefore the statement to be proved takes the form

$$\langle\, n_{k_1}(t) \cdots n_{k_m}(t) \,\rangle_{A_N} = \sum_{B'_m \subset A_N} \langle\, n_{l_1}(t) \cdots n_{l_m}(t) \,\rangle_{B_m}. \tag{26}$$

In this expression the sum runs over all sets $B'_m = \{l_1, \ldots, l_m\}$ which are contained in the set A_N, i.e., the m-point correlation function $\langle\, n_{k_1}(t) \cdots n_{k_m}(t) \rangle_{A_N}$ of the

N-particle system is given by sums of m-particle correlation functions (we assume $m \leq N$) which are the conditional probabilities

$$\langle n_{l_1}(t) \cdots n_{l_m}(t) \rangle_{B_m} = \langle l_1, \ldots, l_m | \mathrm{e}^{-Ht} | k_1, \ldots, k_m \rangle \tag{27}$$

of finding the m particles on the set of sites B'_m at time t if at time $t = 0$ they had been on sites B_m.

To prove (26) notice that s_k^+ creates a particle when acting to the *left* on the vacuum, i.e., $\langle 0 | s_{k_1}^+ \ldots s_{k_1}^+ = \langle k_1 \ldots k_n |$. Furthermore, because of the tensor structure of $\langle 0 |$ and of e^{S^+} (where $S^\pm = \sum_k s_k^\pm$) one may write the summation vector as $\langle s | = \langle 0 | e^{S^+} = \langle 0 | \prod_k (1 + s_k^+)$. With the commutation relations (20) one then finds

$$\langle s | n_{k_1} \ldots n_{k_m} = \langle k_1, \ldots, k_m | e^{S^+} \tag{28}$$

The crucial idea is then to use the $SU(2)$-symmetry (20) to commute e^{S^+} with e^{-Ht}. Since moreover H is a symmetric matrix, i.e. $H = H^T$ we find the self-enantiodromy relation

$$H = e^{S^+} H^T e^{-S^+} \tag{29}$$

and hence $\langle s | n_{k_1} \ldots n_{k_m} e^{-Ht} | A_N \rangle = \langle k_1, \ldots, k_m | e^{-H^T t} e^{S^+} | A_N \rangle$. In the next step of the proof one uses conservation of the z-component of the angular momentum of the Heisenberg chain (equivalent to particle number conservation of the process) to insert an unit operator

$$\mathbf{1} = \sum_{l_1, \ldots, l_m \in S} | l_1, \ldots, l_m \rangle \langle l_1, \ldots, l_m | \tag{30}$$

restricted to the m-particle sector between $e^{-H^T t}$ and e^{S^+}.[7] Finally, one applies again (28) and takes the transposition of the time-dependent conditional probability. This concludes the proof of (26).

The duality relations may be understood as a consequence of the selection rules of $SU(2)$: The projector n_k is a spin-1/2 operator. On the other hand, the summation vector $\langle s |$ in the chain with L sites has total angular momentum $S = L/2$. Therefore $\langle s | n_{k_1} \cdots n_{k_m}$ may be decomposed into states with $L/2 \geq S' \geq L/2 - m$ which have non-vanishing scalar product with states with up to m particles. Thus only m-particle amplitudes enter into the r.h.s. of Eq. (26) (see also [28]). The $SU(2)$ symmetry allows for the derivation of similarly strong results for multi-time correlation functions $\langle n_{i_1}(t_1) \ldots n_{i_k}(t_k) \rangle$ and also for their extension to the partial exclusion process [27]. The partial exclusion process is the spin-s version of this model where each lattice site i can be occupied by at most $2s_i$ particles and where single-particle hopping from site i to site j occurs with rate $n_i(2s_j - n_j)$.

[7] Here we use the expression $\sum_{l_1, \ldots, l_m \in S}$ as a sum over all distinct sets of m lattice sites on the lattice S.

3.1.2 Bethe ansatz solution of the one-dimensional process

It is interesting to analyze the relaxational behaviour of the one-dimensional model with nearest-neighbour hopping for which the m-particle conditional probabilities can be calculated explicitly using the Bethe ansatz originally developed for the study of the eigenfunctions of H [29].

The calculation of the density expectation value $\langle n_k(t) \rangle$ is reduced by self-duality to the calculation of the one-particle conditional probability $P(l;t|k;0) = \langle l | e^{-Ht} | k \rangle$ of finding the particle on site k at time t given that it was on site l at time $t = 0$. On an infinite one-dimensional lattice with nearest neighbour hopping rate D, $P(l;t|k;0)$ satisfies the differential-difference equation $d/dt P(l;t|k;0) = D[P(l+1;t|k;0)+P(l-1;t|k;0)-2P(l;t|k;0)]$ with initial value $P(l;0|k;0) = \delta_{k,l}$. This equation is readily solved by Fourier transformation in the space coordinate l and one finds

$$P(l;t|k;0) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dp e^{-2D(1-\cos p)t} e^{ip(k-l)} = e^{-2Dt} I_{k-l}(2Dt) \tag{31}$$

with the modified Bessel function $I_n(2Dt)$.

Now we consider the two-point correlator $\langle n_i(t) n_j(t) \rangle$. Self-duality yields

$$\langle n_i(t) n_j(t) \rangle = \sum_{m,l} \langle n_l(0) n_m(0) \rangle \langle l, m | e^{-Ht} | i, j \rangle. \tag{32}$$

Since the particles have no long-range interaction, but only on-site repulsion one might wonder to which extent these conditional probabilities deviate from those obtained for completely non-interacting particles. We address this question by using the Bethe ansatz. The idea behind the Bethe ansatz is first to turn the master equation for the N-particle conditional probability $P(x_1, \ldots, x_N; t) = \langle x_1, \ldots, x_N | e^{-Ht} | y_1, \ldots, y_N \rangle$ into an eigenvalue equation by the ansatz $P(x_1, \ldots, x_N; t) = e^{-\epsilon t} P_\epsilon(x_1, \ldots, x_N)$ and then to write $P_\epsilon(x_1, \ldots, x_N)$ as a superposition of plane waves with pseudo momenta p_i conjugate to the particle positions x_l. Since all particles are identical this superposition is a sum over permutations of the momenta in the plane waves $e^{i\sum_l p_{j(l)} x_l}$. The magic of the ansatz (which originates in the underlying integrability of the system) consists in the fact that the amplitude of each permutation in the sum factorizes into a product of corresponding permutations of two-particle amplitudes. We do not go here into any detail, but merely demonstrate how the Bethe ansatz works for the two-particle problem. Adapted to the problem at hand, the Bethe ansatz for the conditional probability reads

$$P(x_1, x_2; t | y_1, y_2; 0) = \frac{1}{(2\pi)^2} \int dp_1 \int dp_2 e^{-(\epsilon_1+\epsilon_2)t - ip_1 y_1 - ip_2 y_2} \Psi_{p_1,p_2}(x_1, x_2) \tag{33}$$

with the Bethe wave function

$$\Psi_{p_1,p_2}(x_1, x_2) = e^{ip_1 x_1 + ip_2 x_2} + S(p_1, p_2) e^{ip_2 x_1 + ip_1 x_2}. \tag{34}$$

The free parameters, determined by the master equation for two particles, are the "energies"

$$\epsilon_i = 2D(1 - \cos p_i) \tag{35}$$

and the two-particle scattering amplitude

$$S(p_1, p_2) = -\frac{1 + e^{ip_1+ip_2} - 2e^{ip_2}}{1 + e^{ip_1+ip_2} - 2e^{ip_1}}. \tag{36}$$

The energy expression arises from the diffusive motion of the particles: The time evolution operator acts on the conditional probability like a lattice Laplacian if the difference between the coordinates is larger than 1, i.e. if the two particles do not "feel" the presence of the other. The scattering amplitude arises from the need to satisfy the master equation with this energy term also if the difference in coordinates is equal to one. This requires to define $\Psi_{p_1,p_2}(x_1, x_2)$ in the unphysical domain $x_1 = x_2$ by $\Psi_{p_1,p_2}(x, x) + \Psi_{p_1,p_2}(x + 1, x + 1) = 2\Psi_{p_1,p_2}(x, x + 1)$. This condition fixes the relative amplitude S of the two plane waves. The contour of integration is determined by the initial condition $P(x_1, x_2; 0|y_1, y_2; 0) = \delta_{x_1,y_1}\delta_{x_2,y_2}$ and we consider the coordinates to be ordered, $x_1 < x_2$ and $y_1 < y_2$.[8]

To analyze (33) we note that at late times the main contribution to the integral arises from small values of p_1, p_2. So we can expand the cosine in the energy term to first non-vanishing order and make a substitution of variables $p_i \to \tilde{p}_i = p_i\sqrt{t}$, $x_i, y_i \to \tilde{x}_i, \tilde{y}_i = x_i/\sqrt{t}, y_i/\sqrt{t}$. Expanding S for small arguments $\tilde{p}_i/\sqrt{t}$ leads to $S = 1 + O(t^{-1/2})$. Thus we arrive at the somewhat surprising conclusion that the leading contribution to the conditional probability comes simply from $S = 1$, corresponding to non-interacting particles. Furthermore, because of the factorization of the plane wave amplitudes for n-particle conditional probabilities, the same result holds true in this case. Thus, *all n-point correlation functions of the symmetric exlusion process are, to leading order in time, identical to the same n-point correlators of non-interacting particles.* Corrections are of order $1/\sqrt{t}$ [32].

3.2 The asymmetric simple exclusion process

The asymmetric exclusion process is a generalization of the symmetric process in which hopping across a bond is biased in one direction. We shall consider only the one-dimensional process with nearest-neighour hopping with rates $D_{R,L}$ to the right and left respectively.

Unfortunately there are no simple self-enantiodromy relations (and resulting self-duality relations) for density correlation functions for this model as one has for the undriven case. However, we shall show that the one-dimensional system with constant spatial asymmetry in left- and right-hopping rates and with reflecting boundary conditions, where particles cannot enter or leave the system, has an unusual non-abelian symmetry which we explore in a similar way as the $SU(2)$

[8] See [30] where the general case of biased hopping is treated. For an earlier full solution of the symmetric two-particle case see [31].

symmetry of the unbiased exclusion process. This will lead us to enantiodromy relations analogous to those known for the symmetric model. However, these relations for the asymmetric case do not involve density correlators, but exponentials of integrated densities (see below).

First we consider closed (reflecting) boundaries which particles cannot cross. Defining the time scale factor $w = \sqrt{D_R D_L}$ and the hopping asymmetry $q = \sqrt{D_R/D_L}$, the Hamiltonian is given by

$$H = w \sum_{k=1}^{L-1} h_k \tag{37}$$

with the two-site hopping matrix $h_k = q(n_k v_{k+1} - s_k^+ s_{k+1}^-) + q^{-1}(v_k n_{k+1} - s_k^- s_{k+1}^+)$. This model is related to the anisotropic Heisenberg chain (22) $H^{XXZ} = V^{-1} H V$ by the the diagonal similarity transformation

$$V = q^{\sum_{k=1}^{L} k n_k}. \tag{38}$$

The parameter $q = e^{\beta \delta E}$ represents the energy gain δE incurred by a particle drifting in the direction of the driving field.

It is obvious that H (37) is not $SU(2)$-symmetric. There is, however, a symmetry of H under the action of the quantum deformation $\mathrm{U}_q[\mathrm{SU}(2)]$ of the universal enveloping algebra of $SU(2)$. The generators $S^{\pm,z}$ of the quantum algebra $\mathrm{U}_q[\mathrm{SU}(2)]$ satisfy, by definition, the following relations [33, 34]:

$$[S^+, S^-] = [2S^z]_q, \quad [S^z, S^\pm] = \pm S^\pm \tag{39}$$

where the expression $[x]_q$ is defined by

$$[x]_q = \frac{q^x - q^{-x}}{q - q^{-1}}. \tag{40}$$

In the limit $q \to 1$ (symmetric hopping) one has $[x]_q = x$ and the quantum algebra relations (39) reduce to the usual commutation relations (20) for $SU(2)$.

A representation of the generators of the quantum algebra in terms of Pauli matrices is given by[9]

$$S^+ = \sum_{k=1}^{L} s_k^+(q) \ , \ S^- = \sum_{k=1}^{L} s_k^-(q) \ , \ S^z = \sum_{k=1}^{L} (1/2 - n_k) \tag{41}$$

with

$$s_k^-(q) = \left(q^{\sum_{j=1}^{k-1} v_j}\right) s_k^- \left(q^{-\sum_{j=k+1}^{L} v_j}\right), \tag{42}$$

$$s_k^+(q) = \left(q^{-\sum_{j=1}^{k-1} n_j}\right) s_k^+ \left(q^{\sum_{j=k+1}^{L} n_j}\right). \tag{43}$$

[9] Our representation is related to the representation given in [34] by the similarity transformation V (38). In [33] the same representation as in [34] is used, but with the replacement $q \to q^{1/2}$.

The commutation relations (39) can be verified using $q^{n_k} s_k^+ = s_k^+$, $s_k^+ q^{n_k} = q s_k^+$ and $q^{n_k} s_k^- = q s_k^-$, $s_k^- q^{n_k} = s_k^-$. Unlike the usual local spin operators $s_k^\pm$ the q-spin operators do *not* commute at different sites:

$$s_k^\pm(q) s_l^\pm(q) = q^{\mp 2} s_l^\pm(q) s_k^\pm(q) \text{ for } l > k. \tag{44}$$

Each term h_k in the Hamiltonian H commutes with $S^\pm$ and $S^z = L/2 - N$. Hence

$$[H, S^\pm] = [H, S^z] = 0. \tag{45}$$

This can be derived on a purely algebraic level by expressing h_k in terms of quantities related to the generators of the algebra [33]. However, these commutation relations are straightforward to verify by using the explicit representation (42), (43) in terms of Pauli matrices.

3.2.1 Equilibrium properties

Because of the reflecting boundaries there can be no stationary current. By using the explicit representation of the hopping matrices h_k one verifies the detailed balance condition

$$H^T = V^{-2} H V^2. \tag{46}$$

Hence the model with reflecting boundaries is an equilibrium system which satisfies detailed balance with respect to a one-parameter family of stationary product measures $P_\eta^* \propto q^{2\sum_k (k+\mu)\eta(k)}$ where the "chemical potential" μ fixes the particle density. In particular, the stationary density profile ρ_k takes the form

$$\rho_k = \langle s | n_k | P^* \rangle = \frac{1}{2}\left(1 + \tanh\left[\beta(k-\alpha)\delta E\right]\right) \tag{47}$$

with a constant α determined by the space-averaged density. This density profile has the form of a step extending over a finite region of length $\propto 1/(\delta E)$ (Fig. 1). There are no correlations in this stationary grand-canonical distribution which is also defined for the infinite system [1].

The canonical N-particle stationary distributions with fixed N can be obtained using the symmetries of the system. Following [35] one obtains the unnormalized zero-energy eigenstates and N-particle summation vectors by applying the q-deformed ladder operators on the vacuum state

$$|\tilde{N}\rangle = \frac{1}{[N]_q!}(S^-)^N |0\rangle \text{ and } \langle N| = \frac{1}{[N]_q!}\langle 0|(S^+)^N. \tag{48}$$

Here the q-factorial is defined by $[m]_q! = [1]_q[2]_q \ldots [m]_q$. The proof that these are stationary eigenvectors of H is trivial: Noting that the empty lattice is stationary one uses the commutation relations (45) to see also the vectors (48) are eigenvectors of H with vanishing eigenvalue.

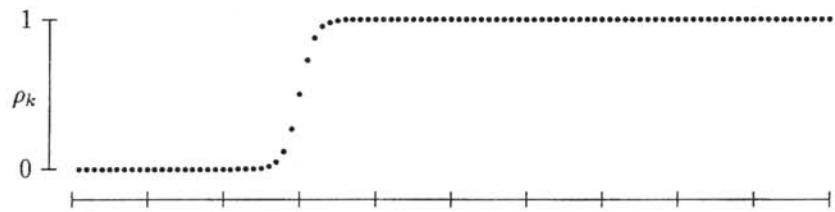

Figure 1: Stationary density profile of the ASEP with reflecting boundaries with 100 sites. The position of the step is determined by the particle number, its width depends on the driving field. Here we have chosen $\beta\delta E = 1/2$, corresponding to $q = \sqrt{e}$.

The normalized N-particle stationary states may be written

$$|\, N^* \,\rangle \equiv |\, \tilde{N} \,\rangle / Z_{L,N} = q^{-N(L+1)} q^{2\sum_{k=1}^{L} k n_k} |\, N \,\rangle / Z_{L,N}, \tag{49}$$

where the partition function is given by the q-binomial coefficient

$$Z_{L,N} = \frac{[L]_q!}{[L-N]_q![N]_q!}. \tag{50}$$

Using the commutation relation for Pauli matrices one then finds from (49) the relation $s_k^+ |\, N \,\rangle = q^{-L-1+2k}(1-n_k)|\, N-1 \,\rangle$ therefore the recursion relation $\rho_k^*(N) = \langle\, s\,|n_k|\, N^* \,\rangle = [N]_q q^{-L-1+2k}[1-\rho_k^*(N-1)]/[L-N+1]_q$ for the stationary density profile. Iterating this recursion yields an exact expression for the density ρ_k in a finite system. The step-function form of the grand-canonical density profile suggests for fixed N a step centered around $k = L - N$. Therefore we investigate the vicinity of this point by setting $r = L + 1 - N + k$. In the thermodynamic limit $L, N \to \infty$ the recursion reduces to $\rho_r = q^{2r}(1 - \rho_{r-1})$ which is solved by

$$\rho_r = \sum_{n=0}^{\infty} (-1)^n q^{-n(n+1)+2r(n+1)}. \tag{51}$$

A simple analysis shows that the stationary distribution has a step-function-like density profile with a step of finite width $\propto 1/(\delta E)$, very similar to that of the uncorrelated distribution (Fig. 1).

The difference between the canonical step distribution and the uncorrelated grand-canonical distribution appears more clearly on the level of correlation functions. One can derive exact expressions for all density correlation functions in the steady state in terms of the density itself by using the commutation rules of the $s_k^+(q)$ for different k [35]. For the two-point function one finds

$$\langle\, n_k n_l \,\rangle_N = \frac{q^{2k}\langle\, n_k \,\rangle_N - q^{2l}\langle\, n_l \,\rangle_N}{q^{2k} - q^{2l}}. \tag{52}$$

Setting $r_1 = L+1-N+k$, $r_2 = L+1-N+l$ and subtracting $\rho_{r_1}\rho_{r_2}$ one realizes that unlike in the grandcanonical stationary distribution (47) the system has non-vanishing correlations in the domain-wall region even in the thermodynamic limit. To understand the relationship between these distributions we note that in an infinite system the reference point $r = 0$ is arbitrary. Hence any normalized superposition of shifted canonical stationary distributions with density profile (51) is stationary. The uncorrelated grand-canonical distribution (47) is a special case of such a superposition of canonical distributions.

3.2.2 Self-enantiodromy

Having understood the stationary properties of the system we can proceed to derive self-enantiodromy relations for the asymmetric exclusion process from the $U_q[SU(2)]$-symmetry. Algebraically speaking the essential feature in the derivation of the enantiodromy-relations for density correlators in the symmetric exclusion was the fact that n_k is a spin-1/2 operator. Unfortunately this is not the case in the $U_q[SU(2)]$-symmetric case of driven diffusion. Instead one has to consider another complete set of observables build by products of the operators

$$Q_k = q^{2N_k} \tag{53}$$

or their discrete lattice derivatives

$$\tilde{Q}_k \;=\; (Q_k - Q_{k-1})/(q^2-1) \;=\; q^{2N_{k-1}} n_k \tag{54}$$

where $N_k = \sum_{j=1}^{k} n_j$ is the space-averaged density up to site k. Some further non-trivial ingredients are necessary for the derivation of self-enantiodromy relations. Since $\langle\, s \,|$ is not a factorized state w.r.t. the q-deformed local spin-lowering operators $s_j^+(q)$, the similarity transformation $\mathcal{B} = e^{S^+}$ is not very useful for the asymmetric exclusion process. Instead, we first note that for an N-particle initial state any expectation value $\langle\, F \,\rangle$ is given by the summation $\langle\, F \,\rangle = \langle\, N \,|F|\, P(t) \,\rangle$ restricted to the N-particle sector (because of particle number conservation). We recall the symmetry relation (48) for $\langle\, N \,|$ and calculate the commutator

$$\left[\, \frac{(S^+)^N}{[N]_q!}\,,\, Q_k \right] = q^{N-1}(q^2-1) Q_k S_k^+ \frac{(S^+)^{N-1}}{[N-1]_q!} \tag{55}$$

where $S_k^+ = \sum_{j=1}^{k} s_j^+(q)$. Then, with $\langle\, 0 \,|\tilde{Q}_k = 0$ and (48), (55), one finds

$$\begin{aligned} \langle\, N \,|\, \tilde{Q}_k \;&=\; \langle\, 0 \,|\, [\, \tfrac{(S^+)^N}{[N]_q!}\,,\, \tilde{Q}_k \,] \\ &=\; q^{N-1} \langle\, k \,|\, \frac{(S^+)^{N-1}}{[N-1]_q!}, \end{aligned} \tag{56}$$

and, by repeated application of (56),

$$\langle\, N \,|\, \tilde{Q}_{k_1} \cdots \tilde{Q}_{k_m} = q^{m(N-1)} \langle\, k_1, \ldots, k_m \,|\, \frac{(S^+)^{N-m}}{[N-m]_q!} \;. \tag{57}$$

The $k_i \in B_m \equiv \{k_1, \ldots, k_m\}$ are assumed to be pairwise different.

With (57) the last steps in the derivation are straightforward. Multiplying (57) by $\exp(-Ht)|\,P_0\,\rangle$, using the $U_q[SU(2)]$ symmetry (45) of the time evolution operator and inserting a unit operator (30) gives the self-enantiodromy relations for the asymmetric exclusion process [36]

$$\begin{aligned}
\langle\, \tilde{Q}_{k_1} \cdots \tilde{Q}_{k_m} \,\rangle_{P_0} &= \langle\, N\,|\tilde{Q}_{k_1} \cdots \tilde{Q}_{k_m}\, \mathrm{e}^{-Ht}|\, P_0\,\rangle \\
&= \sum_{\eta} \langle\, k_1, \ldots, k_m|\mathrm{e}^{-Ht}|\,\eta\,\rangle\langle\,\eta\,|q^{-m(N-1)}\frac{(S^+)^{N-m}}{[N-m]_q!}|\,P_0\,\rangle \\
&= \sum_{1\le k_1'<\ldots<k_m'\le L} \langle\, N\,|\tilde{Q}_{k_1'} \cdots \tilde{Q}_{k_m'}|\,P_0\,\rangle \times \\
&\qquad \langle\, k_1, \ldots, k_m\,|\,\mathrm{e}^{-Ht}\,|\,k_1', \ldots, k_m'\,\rangle \\
&= \sum_{1\le k_1'<\ldots<k_m'\le L} q^{2\sum_{i=1}^m (k_i - k_i')} \langle\, N\,|\tilde{Q}_{k_1'} \cdots \tilde{Q}_{k_m'}|\,P_0\,\rangle \times \\
&\qquad \langle\, k_1', \ldots, k_m'\,|\,\mathrm{e}^{-Ht}\,|\,k_1, \ldots, k_m\,\rangle \ .
\end{aligned} \tag{58}$$

In the last step we have invoked detailed balance (46), giving the factor $q^{2\sum_{i=1}^m (k_i - k_i')}$ inside the sum. This factor can be absorbed in a redefinition $\tilde{Q}_k \mapsto q^{-k}\tilde{Q}_k$. Relations involving correlators of $\tilde{Q}_k$ where some of the k_i are identical, i.e., involving integer powers $(\tilde{Q}_k)^n$ of $\tilde{Q}_k$, can be obtained in the same way. Using the commutation relations (57) one may also derive relations for correlation functions involving different times.

3.2.3 Motion of a single shock

The $U_q[SU(2)]$ symmetry has another remarkable consequence for the relaxational behaviour of the system. For the expectation value of the lattice operator Q_k we derive from (58) the biased diffusion equation

$$\frac{d}{dt}\langle\, Q_k(t)\,\rangle = q^{-1}\langle\, Q_{k+1}(t)\,\rangle + q\langle\, Q_{k-1}(t)\,\rangle - (q+q^{-1})\langle\, Q_k(t)\,\rangle. \tag{59}$$

Because of particle number conservation, also the expectation value of the quantity $z^N Q_k$ with z arbitrary satisfies this equation. Notice that

$$PH^TP^{-1} = H + (D_R - D_L)(n_1 - n_L) \tag{60}$$

where P is the reflection operator mapping sites $k \to L+1-k$. In the absence of the boundary term this would constitute a self-enantiodromy relation. It therefore of interest to study the consequences of this relation in the thermodynamic limit where the boundaries are sent to $\pm\infty$ respectively.

By transposition the left vector $\langle\, s\,|z^N Q_k$ turns into an unnormalized initial distribution parametrized by real-valued parameter z. Normalizing by $\langle\, s\,|z^N Q_k|\,s\,\rangle$

and taking the thermodynamic limit leads to an uncorrelated initial distribution $|\rho_L, \rho_R; k\rangle$ with density $\rho_L = zq^2/(1+zq^2)$ up to site k and density $\rho_R = z/(1+z)$ for all sites larger than k. The two shock densities are related by $D_L\rho_R(1-\rho_L) = D_R\rho_L(1-\rho_R)$. The linear form of the diffusion equation for the expectation value Q_k which results from the quantum algebra symmetry then implies a linear equation for shock distributions $|\rho_L, \rho_R; k\rangle$ indexed by the shock position k. Furthermore, one can show that the boundary terms become diagonal pieces in the thermodynamic limit. Hence the shock distribution satisfies the evolution equation

$$\frac{d}{dt}|\rho_L, \rho_R; k\rangle = c_R|\rho_L, \rho_R; k+1\rangle + c_L|\rho_L, \rho_R; k-1\rangle - (c_R+c_L)|\rho_L, \rho_R; k\rangle \quad (61)$$

with shock hopping rates $c_{R,L} = (D_R - D_L)\rho_{R,L}(1-\rho_{R,L})/(\rho_R - \rho_L)$. This result implies that the initial shock profile retains its structure and shape at all times, but the position k of the shock, i.e. the sudden increase in density, performs a biased lattice random walk with rates $c_{R,L}$ resp. For this non-generic special situation the quantum algebra symmetry allows us to obtain detailed information on the time evolution of the initial shock measure at all times. In the generic case of arbitrary shock densities the position and structure of the shock can be probed using a second class particle technique. One obtains results on the structure of the shock as seen from this second class particle in the limit of infinite time [37] and about its location and (spatially) asymptotic form for large times [38].

3.2.4 Bethe ansatz

Also the ASEP is integrable and one may use the Bethe ansatz [39] to obtain further results on the dynamics. Rigorous analysis of the Bethe ansatz equations for the spectrum of H on a finite lattice with periodic boundaries yields low-lying eigenvalues which vanish with system size L in a power-law fashion as $L^{-3/2}$ [40, 41]. This gives the exact dynamical exponent $z = 3/2$ which relates temporal and spatial scaling behaviour on large scales. The Bethe ansatz solution for an infinite system with finitely many particles [30] may be used to obtain the time evolution of a family of initial distributions with finitely many shocks [42].

3.3 Kinetics of Biopolymerization

Back in 1968 MacDonald et al. [43, 44] studied the kinetics of biopolymerization on nucleic acid templates. The mechanism they try to describe is (in a very simplified manner) the following: Ribosomes attach to one end of a messenger-RNA chain and "read" the genetic information which is encoded in triplets of base pairs by moving along the m-RNA.[10] At the same time the ribosome adds monomers to a biopolymer attached to it: Each time a unit of information is being read a monomer is added to a biopolymer attached to the ribosom and which is

[10] The m-RNA is a long molecule made up of such consecutive triplets.

in this way synthesized by the ribosom. After having added the monomer the ribosom moves one triplet further and reads again. So in each reading step the biopolymer grows in length by one monomer. Which monomer is added depends on the genetic information read by the ribosom. The ribosoms are much bigger than the triplets on the m-RNA, they cover 20-30 of such triplets. Therefore different ribosomes hopping stochastically on the m-RNA cannot overtake each other. When a ribosome has reached the other end of the m-RNA the biopolymer is fully synthesized and the ribosome is released.

In order to describe the kinetics of this process MacDonald et al. introduced the following simple model. The m-RNA is represented by a one-dimensional lattice of L sites where each lattice site represents one triplet of base pairs. The ribosom is a hard-core particle covering r neighbouring sites (for real systems $r = 20 \ldots 30$) but moving forward by only one lattice site with constant rate p. At the beginning of the chain particles are added with rate αp and at the end of the chain they are removed with rate βp. One can also allow for back-hopping with rate q. In the idealized case $r = 1$ this model became later known as the asymmetric exclusion process with open boundary conditions. Its steady state was first studied using a mean-field approach [43]. In a second paper [44] the generalized case $r > 1$ was studied numerically and compared to experimental data on the stationary density distribution of ribosomes along the chain. These were found to be consistent with the results obtained from the model with $q = 0$ and $\alpha = \beta < p/2$. Furthermore it turned out that the phase diagram for general r is similar to the much simpler case $r = 1$ in the sense that there are three distinct phases, a low density phase, a high density phase and a maximal current phase.

These observations allow for a physical understanding of certain dynamcial aspects of this biological system. The experimentally relevant case is the phase transition line from the low-density phase to the high-density phase. Both mean field and numerical calculations predict a region of low density of ribosomes from the beginning of the chain up to some point where the density suddenly jumps (over a few lattice sites) to a high density value, comparable to a jam in traffic flow.[11] These predictions make an exact solution of at least the simple case $r = 1$ desirable. The stochastic dynamics of this model are given by the integrable Hamiltonian of the anisotropic spin-1/2 Heisenberg chain (37) with non-diagonal boundary fields [45, 46]

$$H = H^{ASEP} + \alpha p(v_1 - s_1^-) + \beta p(n_L - s_L^+) \tag{62}$$

For $\alpha = \beta = 0$ the model can be solved by the coordinate or algebraic Bethe ansatz. However, the boundary fields break the $U(1)$ symmetry of the model and other approaches are necessary to find at least the steady state of the system, i.e.

[11] This description of the stationary mean-field density profile describes correctly the situation for $r = 1$, but disregards a more complicated sublattice structure for $r > 1$. However the figures provided in [44] suggest that the description remains qualitatively correct if one averages over this sublattice structure.

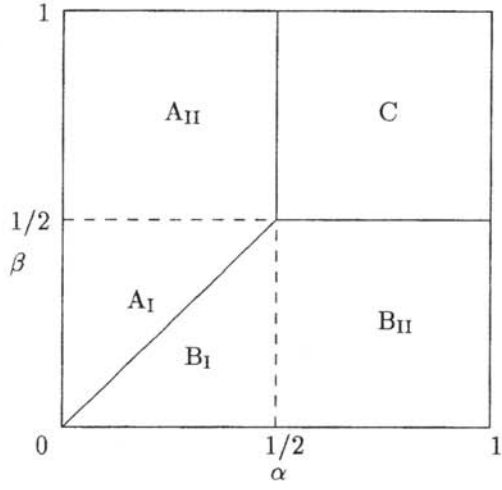

Figure 2: Phase diagram of the model in the $\alpha - \beta$ plane ($p = 1$). Region A is the low density phase, region B the high density phase and region C is the maximal current phase. The phases are separated by the curves $\alpha = \beta < 1/2$ and $\alpha = 1/2$, $\beta > 1/2$ and $\beta = 1/2$, $\alpha > 1/2$ respectively. The low (high) density phase is divided into two phases A_I and A_{II} (B_I and B_{II}) along the curve $\beta = 1/2$ ($\alpha = 1/2$). The mean-field phase diagram shows the exact phase transition lines between phases A,B,C, but not the non-analytical behaviour along the dashed lines within the phases A and B respectively.

the ground state of H. In what follows we will consider only $q = 0$. We set $p = 1$ which fixes the time scale of the process.

It turns out that the stationary distribution of a system of L sites can be expressed recursively in terms of the solution for $L - 1$ sites [47]. The exact solution of the bulk density [47] and the density profile obtained from the solution of these recursion relations [48, 49] reproduces the three phases predicted by mean field, but also reveals an intricate interplay between two correlation lengths which determine the phase diagram and the nature of the phase transitions [48, 50]. In particular, it turns out that the correlation length on the phase transition line between the low-density phase and the high-density phase is infinite, which is incompatible with the mean field result. The exact solution gives a linearly increasing density profile rather than the sharp shock predicted by mean field. This can be explained by assuming that a sharp shock exists, but, due to current fluctuations, performs a random walk along the lattice [47, 51]. Therefore, if one waits long enough, the shock will have been at each lattice site with equal probability. This picture which is discussed in [48] for a finite lattice yields a linearly increasing density and is confirmed by an exact solution of dynamical properties

of a related exclusion process with deterministic bulk dynamics [19]. What one therefore expects for an experimental sample is indeed a region of low density of ribosoms followed by a sharp transition to a region of high density of ribosoms as found experimentally. This rapid increase can be anywhere on the m-RNA, but with a probability distribution given by the effective initialization and release rates α, β. If $\alpha = \beta$ the distribution of shock position would be constant over the lattice, otherwise exponential on a length scale $\xi = 1/(\ln[\alpha(1-\alpha)/\beta(1-\beta)])$.

4 Conclusions

It has been realized in recent years that the stochastic time evolution of many one-dimensional reaction-diffusion processes can be mapped to quantum spin systems, and in special cases to integrable quantum chains. This insight has made available the tool box of quantum mechanics and particularly of integrable models for these interacting particle systems far from equilibrium. With these methods many new exact results for their dynamical and stationary properties have been derived. It is also amusing to note that the Hamiltonians for such systems are mostly not hermitian and therefore from a quantum mechanical point of view not interesting. The interpretation as time evolution operators for stochastic dynamics thus extends the physical relevance of integrable systems to non-hermitian models. Reaction-diffusion mechanisms which can be described in this way are not only actual chemical systems, but comprise a large variety of phenomena in physics and beyond.

Acknowledgments

It is a pleasure to acknowledge fruitful collaborations and numerous useful discussions with many active workers in the various fields of non-equilibrium physics covered in these lecture notes.

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