Algebraic Methods in Non-Equilibrium Statistical Mechanics

Dissertation

zur

Erlangung des Doktorgrades (Dr. rer. nat.)

der

Mathematisch–Naturwissenschaftlichen Fakultät

der

Rheinischen Friedrich–Wilhelms–Universität Bonn

vorgelegt von

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aus

Oberwesel/Rhein

Bonn 2000

Angefertigt mit Genehmigung der Mathematisch–Naturwissenschaftlichen Fakultät der Rheinischen Friedrich–Wilhelms–Universität Bonn

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Tag der Promotion: 10. 1. 2001

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Chapter 1

Introduction

This thesis is concerned with non-equilibrium statistical mechanics. There is a large variety of non-equilibrium phenomena not only in nature but also in economy and society. Prominent examples are relaxation processes to thermal equilibrium [1], chemical reaction [2], interface growth [3], super-ionic conductors [4], but also traffic flow [5] to name only a few.

Statistical mechanics tries to capture the main features of collective phenomena using models which consist of a large number of interacting particles. As an example one may take the Ising model of ferromagnetism [6]. The simplest class of models for non-equilibrium systems are reaction-diffusion models on a lattice which evolve stochastically in time. In this models particles sit on lattice sites and are allowed to move and to undergo reactions. One may think of molecules which diffuse and make chemical reactions. Examples for reaction-diffusion models are the exclusion process [7, 8], and binary reaction models such as the annihilation model or the coagulation model [9, 10]. However, the range of applications of reaction-diffusion models is not restricted to chemical reaction at all.

Reaction-diffusion models on a lattice are described by a master equation [11] This equation is essentially a book keeping of gain and loss of the probability to find the system in a certain states. It establishes a mapping of reaction-diffusion models to quantum spin Hamiltonians [12] which, in some cases, are known from equilibrium theory. There several techniques for solving these Hamiltonians have been developed, especially in one dimension [13]. Through the mapping described above these techniques can be applied to one-dimensional reaction diffusion models as well and vice versa.

The models in non-equilibrium statistical mechanics turn out to be more complicated than those in equilibrium statistical mechanics. Analytical solutions are only known in one dimension [14]. Therefor the study of tools for solving such models is of special interest. Two of such method are the subject of the present work.

The present thesis consists of two parts. The first part (chapter 2) studies the application of quadratic algebras to the calculation of zero energy eigenstates of one-dimensional m-state quantum spin Hamiltonians with nearest neighbour interaction. This method has already been applied to a number of problems in statistical mechanics, for example to directed lattice animals [15], valence bond ground states [16], and asymmetric exclusion processes with various number of species [8, 17, 18, 19, 20].

Instead of considering the eigenvalue problem one defines an algebra which is generated by $2m$ generators fulfilling m^2 quadratic relations [21, 22] whose coefficients are matrix elements of the Hamiltonian. Physical quantities, i. e. wave functions of the zero energy eigenstate, are then obtained as products of generators of the algebra. The method can be applied to both kinds of boundary conditions: open boundaries (with single-site interaction terms at both boundary sites) and periodic boundaries. A detailed discussion of boundary conditions can be found in [19]. In the case of open boundaries one considers a Fock–like representation of the algebra. For periodic boundary conditions a trace on the algebra is used to represent eigenstates with energy and momentum zero.

In this context a number of questions are studied in chapter 2. The first question addresses the existence of the quadratic algebra given in [21, 22]. Here we find that for a given quantum spin Hamiltonian such a quadratic algebra exists. The second question is which special properties an eigenstate should have in order to be representable by a quadratic algebra. The answer depends on the boundary conditions. In the case of open boundary conditions we find a positive answer[23]: Every zero energy eigenstate can be written using a Fock–representation of the quadratic algebra given in [21, 22]. In the case of periodic boundary conditions we find that the answer is in general negative: We give an example of a state which cannot be written in terms of a trace on the quadratic algebra [24]. If the positivity of the stationary state wave function is not required (as it is for reaction-diffusion models) an additional operation on the quadratic algebra, i. e. the super-trace can be used in some cases to obtain zero energy eigenstates with momentum π [25].

In the second part of this thesis we study the asymmetric coagulation–decoagulation model with a spatial asymmetry. In this model one considers a one dimensional lattice where each site is either empty or occupied by exactly one particle. Particles are allowed to hop to neighbouring sites if these are empty. If there are two particles on adjacent sites they may melt together (coagulation) and a single particle may split into two particles if at least one of its neighbouring sites is empty (decoagulation). These processes occur independently of each other with certain rates i. e. probabilities per time unit.

This model has been studied for over several decades [26, 27, 28] and is one of the classical examples of reaction-diffusion models. It has a number of interesting features: In the case of vanishing decoagulation the corresponding field theory of the model has the critical dimension $d_c = 2$ [29]. For a special tuning of the reaction rates (i. e. equal rates for coagulation and diffusion) the spatially symmetric version of the model has been solved by means of the so called *interparticle distribution functions*. These functions are defined as the probabilities to find empty intervals, i. e. an holes, in the system and will be called *hole*-functions further on. They were introduced in the symmetric coagulation–decoagulation model in [10, 27, 30]. The time evolution for the hole-functions forms a hierarchy of differential equations which decouples similarly to that obtained in the Glauber model [1]: The time evolution of the n-hole functions knows about the m-hole function only if $m < n$. Therefore the 1-hole functions evolve independently of the rest of the system. In [31] the most general conditions for the decoupling of the hierarchy are given together with the spectrum of eigenvalues for the lowest sector, i. e. the 1-hole sector, for periodic boundary conditions. In general the reaction rates are not necessarily symmetric. In [31] it was also found that the Hamiltonian of this model can be written in terms of free fermions for equal asymmetry of coagulation and decoagulation rates. Therefore the model can be solved completely in that case.

In chapter 3 the method of hole-functions is used to study the asymmetric coagulation–decoagulation with closed boundary conditions (i. e. a non-periodic chain where no input or output of particles is allowed). The decoupling condition found in [31] are still valid in this case. However, due to the missing symmetry the solution of the equation turns out to be more difficult for closed boundary conditions than for periodic ones: Even for the 1-hole-sector an analytical solution is obtained only in the case of equal asymmetry of coagulation and decoagulation rates. For a complete solution a total decoupling of the hierarchy of hole-functions is necessary. This can be done by extending a method given in [32] for a similar problem in the hierarchy of the Glauber model but, again, only for equal asymmetry of coagulation and decoagulation rates. It is interesting to note that this condition is just the free fermion condition known from [31].

So far for the more technical aspects of the model. The model also has interesting physical phenomena. If one considers the stationary state one finds that the model has two phases: A high-density phase and a low density phase. In the high-density phase the bulk density approaches a finite value which depends on the ratio of total coagulation and decoagulation rates. In the low density phase the bulk lattice is empty. In both cases the boundary corrections decay exponentially. On the transition line of both phases the density profile shows a linear behaviour interpolating between both densities. The parameter triggering the transition between both phases is just the ratio between the decoagulation and the asymmetry. This phenomenon is shown to be related to boundary induced phase transitions [33]. The spectrum of eigenvalues of the corresponding Hamiltonian is massive in the high- and the low-density phase but is massless on the transition line. Both results, the density profile and the spectrum of eigenvalues are most elegantly obtained by means of the hole-functions. In [34] I have studied a generalisation of the coagulation-decoagulation model where injection and extraction of particles at the boundaries are allowed. In this case one can again find a decoupling subsystem which allows an analytical treatment. This work is not included in the present thesis.

In chapter 4 we give a summary of our results. The bulk of this thesis is published in [23], [24] and [35].

Chapter 2

Quadratic Algebras and Quantum Spin Chains

1 Introduction

A number of problems in many particle systems have been studied with the help of quadratic algebras. The idea of this technique is to express physical quantities such as ground state wave functions or correlation functions as products of operators acting on an auxiliary space and fulfilling algebraic relations defined by the Hamiltonian of the system. Introduced in the context of lattice animals [15] the technique has been used to find ground states of various quantum spin chains [16, 36, 37, 38].

As it has been shown by Derrida, Evans, Hakim, and Pasquier [17] the steady state of the one species asymmetric exclusion process with open boundaries can be written using quadratic algebras. Later works study this process in more detail [18, 39, 40]. Examples for asymmetric exclusion processes with two species were investigated in [41, 42] with the help of the same technique. The algebra used in these studies is generated by as many operators as states a single site can take. It has the important property that it leads to recurrence relations for the steady state of systems of different lattice lengths. For other problems this algebra had to be generalised by enclosing additional operators. This was first done in the study of the dynamics of the asymmetric exclusion process [22, 43, 44]. Another example is the algebra for the reaction–diffusion model studied in [21] which is generated by twice as many operators as the one from [17]. In the Fock–representation of this algebra the recursion property is lost. The same is true for the algebra used in [45, 46, 47, 48] for stochastic models with parallel updating.

One of the questions coming up naturally in this context is the following: To which kind of problems can quadratic algebras be applied? In other words: Does a Hamiltonian, which describes either a quantum spin system or a stochastic process, need to have any particular property in order to have an eigenstate which can be expressed in terms of a quadratic algebra? (States with this property are also called *matrix product states* in the literature.) We will see that the answer depends on the boundary conditions. In the case of open boundary conditions where a Fock–representation of the algebra is used, we find that the answer is positive. We will prove the following statement: *Any zero energy eigenstate of a Hamiltonian with nearest neighbour interaction in the bulk and single site boundary terms can be written in terms of expectation values in a Fock-representation of a quadratic algebra.* In the proof we use quadratic algebra (2.10)-(2.11) which was suggested in [21, 22]. We give the proof with the help of an explicit representation. Therefore as a byproduct we get the existence of the quadratic algebra itself. The technique to write states with the help of quadratic algebras has sometimes been called *matrix product ansatz* in the literature. The statement above says that it is not an ansatz but rather an identical reformulation of the eigenvector equation for the zero energy eigenstate. This fact is actually used in the proof.

In the case of periodic boundary conditions where the quadratic algebra together with a trace is considered, we show that such a general statement does not hold. We give an explicit counter-example of a 3-state Hamiltonian on a 3-site lattice which has a zero energy eigenstate which cannot be represented as a matrix product state.

The bulk of this chapter is organised as follows: In section 2 we define the class Hamiltonian we are going to consider. In section 3 we introduce the quadratic algebra and the Fock-representation for the application of the algebra to open boundary conditions. The proof of the existence theorem stated above is given here. In section 4 we introduce a trace-like function for the application of the algebra to periodic boundary conditions. We present an example of a state which cannot be written as with the help of a trace-like function on the quadratic algebra.

2 Definition of a class of models

Consider an L–site lattice where each site can be in one state out of m. The configuration space of this lattice is the m^L-dimensional complex vector space. On this configuration we consider Hamiltonians with nearest neighbour interaction in the bulk and two types of boundary conditions: open boundries, where single site acting on the boundary sites are added to the bulk term, and periodic boundary conditions.

Open Boundary Conditions In the case of open boundary conditions the Hamiltonian is of the form:

$$H_{\rm op} = h_1 + \sum_{k=1}^{L-1} h_{k,k+1} + h_L. \tag{2.1}$$

where $h_{k,k+1}$ is the bulk interaction term acting on the sites k and $k+1$ and h_1 and h_L are single site boundary terms. To write these terms down explicitly it is convenient to introduce the matrices $E_k^{\sigma\tau}$ defined by

$$E_k^{\sigma\tau} = \mathbb{I}^{\otimes(k-1)} \otimes E^{\sigma\tau} \otimes \mathbb{I}^{\otimes(L-k)} \tag{2.2}$$

where $E^{\sigma\tau}$ are $m \times m$–matrices with entries $(E^{\sigma\tau})_{\mu,\nu} = \delta_{\sigma,\mu}\delta_{\tau,\nu}$ and $\mathbb{I}$ is the $m \times m$ identity matrix. In this notation the bulk interaction term $h_{k,k+1}$ is now defined by

$$h_{k,k+1} = \sum_{\mu,\nu,\sigma,\tau=1}^{m} \gamma_{\sigma\tau}^{\mu\nu} E_k^{\sigma\mu} E_{k+1}^{\tau\nu} \tag{2.3}$$

and the boundary terms h_1 and h_L by

$$h_1 = \sum_{\mu,\sigma=1}^{m} \alpha_\sigma^\mu E_1^{\sigma\mu} \qquad h_L = \sum_{\mu,\sigma=1}^{m} \beta_\sigma^\mu E_L^{\sigma\mu}. \tag{2.4}$$

Periodic Boundary Conditions In the case of periodic boundary conditions we start with a lattice with $L+1$ site and idendify the site $L+1$ with the site 1 so that we end up again with a L-site lattice. On this lattice we consider the Hamiltonian of the form

$$H_{\text{per}} = \sum_{k=1}^{L} h_{k,k+1} \tag{2.5}$$

with the same interaction terms in the bulk as (2.1) and no additional terms. This Hamiltonian in invariant under tarnslation, i. e. cyclic permutation of the lattice sites.

Hamiltonians of the type H_{op} and H_{per} appear as well in the study of one–dimensional stochastic systems as in the study of quantum spin chains. We will now describe both applications in more detail.

Stochastic model: Let us consider a one-dimensional lattice with L sites, each of which can be in either of m states. A configuration $\underline{\tau}$ on the lattice is completely defined by the set of occupation numbers $\underline{\tau} = \{\tau_1, \tau_2, \ldots, \tau_L\}$ with $\tau_i = 1, ..., m \;\; \forall\, i = 1, ..., L$. The system evolves stochastically. During an infinitesimal time step dt its configuration $\underline{\tau}$ can change to a configuration $\underline{\tau}'$ with a probability $w(\underline{\tau} \to \underline{\tau}')dt$ where the $w(\underline{\tau} \to \underline{\tau}')$ are referred to as rates. This process can be described in terms of a rate equation which reads

$$\frac{d}{dt}P(\underline{\tau}, t) \;=\; \sum_{\{\tau_j' \neq \tau_i\}} \left[\; w(\underline{\tau}' \to \underline{\tau})\; P(\underline{\tau}', t) \;-\; w(\underline{\tau} \to \underline{\tau}')\; P(\underline{\tau}, t)\;\right] \tag{2.6}$$

where $P(\underline{\tau}, t) = P(\tau_1, \tau_2, \ldots, \tau_L, t)$ is the probability of finding the configuration $\tau_1, \tau_2, \ldots, \tau_L$ at time t . Throughout this paper we restrict ourselves to dynamics where the configuration can change only at two adjacent sites at a time and the rate for such a change depends only on these two sites. The rates are assumed to be independent of the position in the bulk of system. At the boundaries, i.e. for sites 1 and L, we assume additional processes to take place.

It is convenient to introduce a vector notation [11, 12] by writing

$$P(t) \;=\; \sum_{\underline{\tau}} P(\tau_1,\tau_2,\ldots,\tau_L,t)\; u_1^{(1)}(\tau_1)\otimes u_2^{(2)}(\tau_2)\otimes\cdots\otimes u_L^{(L)}(\tau_L) \tag{2.7}$$

with where $u_\tau^{(k)}$ ($\tau = 1,\cdots,m$ and $k = 1,\cdots,L$) denotes the basis of the vector space of the kth site. In terms of these vectors the rate equation reads

$$\frac{d}{dt}P(t) = -HP(t) \tag{2.8}$$

where H is an $m^L \times m^L$-matrix which is defined in terms of the rates. We call H the Hamiltonian here. For the processes with nearest nieghbour interaction it has the structure of (2.1) or (2.5) for open or periodic boundary conditions, respectively, with local terms given by (2.3)-(2.4). For stochastic models the matrices H have a particular property: They have to have vanishing column sums because the total probability has to be conserved. This implies that there is a zero energy eigenstate for every lattice length L which is just the steady state of the system. It is denoted by P_L and obeys the relation

$$HP_L = 0 \tag{2.9}$$

In Section 3 we will discuss a representation of these states.

Quantum spin chain: Consider a chain of length L with a spin s-particle sitting on each site. Suppose there is an interaction between adjacent particles and some surface fields acting on sites 1 and L. Then the system dynamics is described by a Schrödinger equation with a Hamiltonian of type (2.1) respective (2.5)) if we chose a spin s-representation and $m = 2s+1$. The Hamiltonian generally does not have vanishing columns sums like in the stochastic case, though it has to be hermitian. This condition does not effect the construction of matrix product states below. Although the physical meaning of the Schrödinger equation is different from the meaning of the rate equation (2.8) it has the same mathematical structure. And just as for the stochastic model we are often interested in the ground state of the Hamiltonian H.

3 Open Boundary Conditions: An Existence Theorem

Consider now a Hamiltonian with open boundary conditions as defines in (2.1) with local terms given by (2.3)-(2.4). Following the suggestion of [21, 22], for each Hamiltonian of this type we introduce a quadratic algebra generated by $2m$ generators $D_1, \cdots, D_m$, $X_1, \cdots, X_m$ fulfilling the following m^2 quadratic relations determined by the coefficients of the bulk interaction term (2.3):

$$\sum_{\mu,\nu=1}^{m} \gamma_{\sigma\tau}^{\mu\nu} D_\mu D_\nu = X_\sigma D_\tau - D_\sigma X_\tau \qquad \text{with} \quad \sigma, \tau = 1, \cdots, m. \tag{2.10}$$

By giving a non-trivial representation we will show below that this algebra indeed exists. Furthermore we introduce a Fock-representation of this algebra: We assume that there is an auxiliary vector space $\widehat{\mathcal{V}}$ where the generators $D_1, \cdots, D_m$ and $X_1, \cdots, X_m$ act on and states $|V\rangle$ and $\langle W|$ in $\widehat{\mathcal{V}}$ and its dual, respectively, such that the following relations hold:

$$\begin{aligned} \sum_{\mu=1}^{m} \alpha_\sigma^\mu \langle W| D_\mu &= -\langle W| X_\sigma \\ \sum_{\mu=1}^{m} \beta_\sigma^\mu D_\mu |V\rangle &= X_\sigma |V\rangle \qquad \text{with} \quad \sigma = 1, \cdots, m. \end{aligned} \tag{2.11}$$

Then we can state the following theorem:

(i) *If one can find an algebra generated by the $2m$ operators $D_{\tau_1}, \ldots D_{\tau_L}$ and $X_{\tau_1}, \ldots, X_{\tau_L}$ fulfil the m^2 quadratic relations (2.10) and if there is a vector space $\widehat{\mathcal{V}}$ where the operators $D_{\tau_1}, \ldots D_{\tau_L}$ and $X_{\tau_1}, \ldots, X_{\tau_L}$ act on and states $|V\rangle$ and $\langle W|$ in $\widehat{\mathcal{V}}$ and its dual, respectively such that the relations (2.11) hold then the vector $\tilde{P}_L$ defined by*

$$\tilde{P}_L = \sum_{\tau_1, \ldots, \tau_L = 1}^{m} \langle W| D_{\tau_1} \cdots D_{\tau_L} |V\rangle \; u_{\tau_1}^{(1)} \otimes u_{\tau_2}^{(2)} \otimes \cdots \otimes u_{\tau_L}^{(L)} \tag{2.12}$$

solves the equation for the zero energy eigenstate, i.e.,

$$H \tilde{P}_L = 0 \tag{2.13}$$

(ii) *For any vector P_L solving $H\ P_L = 0$ one can find operators D_τ , X_τ ($\tau = 1, 2, \ldots, m$) and vectors $\langle W|$, $|V\rangle$ in some space $\widehat{\mathcal{V}}$, such that P_L can be represented as a matrix product state $\tilde{P}_L$ defined by (2.12) and relations (2.10) and (2.11) are fulfilled in $\widehat{\mathcal{V}}$.*

Before we come to the proof of the statement we stress again that, in contrast to the algebra defined in [17, 18, 39], the relations (2.10)-(2.11) do not lead to recurrence relations for expectation values of products of different length in the operators D_τ and X_τ.

The proof of (i) is based on a site by site cancellation of terms when H is applied on $\tilde{P}_L$ and follows the line of Ref. [17] We define a states $\overline{P}_L(k)$ as

$$\overline{P}_L(k) = \sum_{\tau_1, \cdots, \tau_L = 1}^{m} \langle W| D_{\tau_1} \cdots D_{\tau_{k-1}} X_{\tau_k} D_{\tau_k + 1} \cdots D_{\tau_L} |V\rangle \; u_{\tau_1}^{(1)} \otimes u_{\tau_2}^{(2)} \otimes \cdots \otimes u_{\tau_L}^{(L)} \tag{2.14}$$

Applying the terms occurring in (2.1) on the state

$$\tilde{P}_L = \sum_{\tau_1,\cdots,\tau_L=1}^{m} \langle W|D_{\tau_1}\cdots D_{\tau_L}|V\rangle \; u^{(1)}_{\tau_1}\otimes u^{(2)}_{\tau_2}\otimes\cdots\otimes u^{(L)}_{\tau_L} \tag{2.15}$$

yields

$$h_1\tilde{P}_L \;=-\; \overline{P}_L(1) \tag{2.16}$$

$$h_{k,k+1}\tilde{P}_L \;=\; \overline{P}_L(j) \;-\; \overline{P}_L(j+1) \tag{2.17}$$

$$h_L\,\tilde{P}_L \;=\; \overline{P}_L(L) \tag{2.18}$$

where the algebra relations (2.10)-(2.11) have been used. Applying now the full operator H (see (2.1)) on the state $\tilde{P}_L$ we get

$$H\tilde{P}_L = -P_L(1) + \sum_{j=1}^{L}\left(\overline{P}_L(j) - \overline{P}_L(j+1)\right) + \overline{P}_L(L) = 0 \tag{2.19}$$

which is proofs (i)

In order to prove (ii) we construct a representation of operators and vectors fulfilling the relations (2.10)-(2.11) using the eigenvectors P_L of systems with lengths $L = 1,2,\ldots$. Let us define for any number $M = 1,2,\ldots$ an m^M-dimensional space $\widehat{\mathcal{V}}_M$, with a set of orthogonal basis vectors $|\tau_1,\tau_2,\ldots,\tau_M\rangle$ with $\tau_i = 1,2,\ldots,m$ as well as the one-dimensional space $\widehat{\mathcal{V}}_0$ with the basis vector $|\;\rangle$. We define the space $\widehat{\mathcal{V}}$ as the direct sum of all $\widehat{\mathcal{V}}_M$ with $M = 0,1,2,\ldots$. The above basis vectors may be written as infinite column vectors with a 1 at position $1+\tau_1+m\tau_2+m^2\tau_3+\ldots+m^{M-1}\tau_M$ and a 0 at all other positions, and their transposed $\langle\tau_1,\tau_2,\ldots|$ can be written as the corresponding row vectors. Next we define operators D_τ and X_τ as well as vectors $\langle W|$ and $|V\rangle$ by means of their action on all the $|\tau_1,\tau_2,\ldots\rangle$ which provides a matrix representation if we write the $|\tau_1,\tau_2,\ldots\rangle$ as columns. For each $L = 1,2,\ldots$ we define the D_τ and X_τ by

$$D_{\tau_1}|\tau_2,\tau_3,\ldots,\tau_L\rangle = |\tau_1,\tau_2,\tau_3,\ldots,\tau_L\rangle \quad \text{for} \quad L = 1,2,\ldots \tag{2.20}$$

and

$$X_{\tau_1}|\tau_2,\ldots,\tau_{L-1}\rangle = \sum_{\sigma_L}^{m}\beta^{\sigma_L}_{\tau_L}|\tau_1,\ldots,\tau_{L-1}\sigma_L\rangle \tag{2.21}$$

$$+\sum_{k=1}^{L-1}\sum_{\sigma_k,\sigma_{k+1}=1}^{m}\gamma^{\sigma_k,\sigma_{k+1}}_{\tau_k,\tau_{k+1}}|\tau_1,\ldots,\tau_{k-1},\sigma_k,\sigma_{k+1},\tau_{k+2},\ldots,\tau_L\rangle.$$

Note that each choice of L gives a different set of basis vectors in the column on the l.h.s., and taking successively $L = 1,2,\ldots$ all basis vectors will occur in this column exactly once.

Hence, the above equation defines the action of each X_τ on each basis vector in a consistent way. The vectors $|V\rangle$ and $\langle W|$ we define by

$$
\begin{aligned}
|V\rangle &= |\,\rangle & (2.22)\\
\langle W|\tau_1,\tau_2,\ldots,\tau_L\rangle &= P_L(\tau_1,\tau_2,\ldots,\tau_L) \qquad \text{for} \quad L=1,2,\ldots & (2.23)
\end{aligned}
$$

where $P_L(\tau_1,\tau_2,\ldots,\tau_L)$ are the components of P_L. The above definitions fix the D_τ , X_τ and the $\langle W|$, $|V\rangle$ completely up to a constant $\langle W|\,\rangle$. This constant can be fixed arbitrarily, since it does not enter into any result.

We have to prove now that these operators and vectors lead back to P_L by means of (2.12), i.e., that $\tilde{P}_L$ is equal to P_L, and that they obey the Fock-representation (2.10)-(2.11). Let us begin the first proof by rewriting (2.20) as

$$D_{\tau_1}D_{\tau_2}\ldots D_{\tau_n}|\tau_{n+1},\ldots,\tau_L\rangle = |\tau_1,\tau_2,\ldots,\tau_L\rangle \tag{2.24}$$

for all $L=1,2,\ldots$ and $0\le n\le L$. (The above relation gives a more intuitive meaning of the representation we have chosen: A basis vector $|\tau_1,\tau_2,\ldots,\tau_M\rangle$ is created by applying the sequence $D_{\tau_1}D_{\tau_2}\ldots D_{\tau_M}$ on $|\,\rangle$.) Furthermore, using (2.23) we get:

$$\langle W|D_{\tau_1}D_{\tau_2}\ldots D_{\tau_L}|\,\rangle = P_L(\tau_1,\tau_2,\ldots,\tau_L) \qquad \text{for} \quad L=1,2,\ldots \tag{2.25}$$

Rewriting (2.25) as a direct product of vectors in the configuration space and using $|\,\rangle = |V\rangle$ yields

$$\langle W|D_{\tau_1}D_{\tau_2}\cdots D_{\tau_L}|V\rangle = P_L(\tau_1,\ldots,\tau_L) \tag{2.26}$$

which is what we were to prove.

In order to show that above representation fulfils the algebra (2.10)-(2.11) we rewrite the definition (2.21) using (2.24) and multiply $D_{\tau_1}\cdots D_{\tau_n}$ from the left:

$$
\begin{aligned}
& D_{\tau_1}\cdots D_{\tau_n}X_{\tau_{n+1}}D_{\tau_{n+2}}\cdots D_{\tau_L}|\,\rangle = \\
& \qquad \sum_{\sigma_L}^{m}\beta_{\tau_L}^{\sigma_L}D_{\tau_1}\cdots,D_{\tau_{L-l}}D_{\sigma_L}|\,\rangle & (2.27)\\
& + \sum_{k=n+1}^{L-1}\sum_{\sigma_k,\sigma_{k+1}=1}^{m}\gamma_{\tau_k,\tau_{k+1}}^{\sigma_k,\sigma_{k+1}}D_{\tau_1}\cdots D_{\tau_{k-1}}D_{\sigma_k}D_{\sigma_{k+1}}D_{\tau_{k+2}}\cdots D_{\tau_L}|\,\rangle & (2.28)
\end{aligned}
$$

for $n=0,1,\ldots,L-1$ and $L=1,2,\ldots$. The second equation of (2.11) is nothing but the case $n=0$, $L=1$ of above relation. Consequently it holds. Next we use (2.27) to compute

$$
\begin{aligned}
& (X_{\tau_1}D_{\tau_2}-D_{\tau_1}X_{\tau_2})\,|\tau_3,\ldots,\tau_L\rangle = & (2.29)\\
& X_{\tau_1}D_{\tau_2}D_{\tau_3}\cdots D_{\tau_L}|\,\rangle - D_{\tau_1}X_{\tau_2}D_{\tau_3}\cdots D_{\tau_L}|\,\rangle =
\end{aligned}
$$

$$\sum_{\sigma_1,\sigma_2=1}^{m} \gamma_{\tau_1\tau_2}^{\sigma_1\sigma_2} D_{\sigma_1} X_{\sigma_2} D_{\tau_3} \cdots D_{\tau_L} |\ \rangle =$$

$$\sum_{\sigma_1,\sigma_2=1}^{m} \gamma_{\tau_1\tau_2}^{\sigma_1\sigma_2} D_{\sigma_1} D_{\sigma_2} |\tau_3, \ldots, \tau_L\rangle \tag{2.30}$$

Since the products of the D_τ span the whole space $\widehat{\mathcal{V}}$, (2.10) must hold in $\widehat{\mathcal{V}}$. What remains to be proven is the first equation of (2.11). We multiply (2.27) for $n = 0$ by $\langle W|$ from the left and use (2.26):

$$\langle W|X_{\tau_1}|\tau_2, \ldots, \tau_L\rangle \tag{2.31}$$

$$= \sum_{k=1}^{L-1} \sum_{\sigma_k,\sigma_{k+1}=1}^{m} \gamma_{\tau_k\tau_{k+1}}^{\sigma_k\sigma_{k+1}} \langle W|\tau_1, \ldots, \tau_{k-1}, \sigma_k, \sigma_{k+1}, \tau_{k+2}, \ldots, \tau_L\rangle$$

$$+ \sum_{\sigma_L}^{m} \beta_{\tau_L}^{\sigma_L} \langle W|\tau_1, \ldots, \tau_{L-1}, \sigma_L\rangle \tag{2.32}$$

$$= \sum_{k=1}^{L-1} \sum_{\sigma_k,\sigma_{k+1}=1}^{m} \gamma_{\tau_k\tau_{k+1}}^{\sigma_k\sigma_{k+1}} P_L(\tau_1, \ldots, \tau_{k-1}, \sigma_k, \sigma_{k+1}, \tau_{k+2}, \ldots, \tau_L)$$

$$+ \sum_{\sigma_L}^{m} \beta_{\tau_L}^{\sigma_L} P_L(\tau_1, \ldots, \tau_{L-1}, \sigma_L) \tag{2.33}$$

$$= - \sum_{\sigma_1=1}^{m} \alpha_{\tau_1}^{\sigma_1} P_L(\sigma_1, \tau_2, \ldots, \tau_L) \tag{2.34}$$

$$= - \sum_{\sigma_1=1}^{m} \alpha_{\tau_1}^{\sigma_1} \langle W|D_{\tau_1}|\tau_2, \ldots, \tau_L\rangle \tag{2.35}$$

In the step from (2.31) to (2.31) we used the definition of X_τ in (2.21) and relation (2.24). The next step we use (2.25). From (2.33) to (2.34) we make use of the fact that the sates P_L is a zero energy eigenstate of the Hamiltonian H which reads in components:

$$\sum_{\sigma_1=1}^{m} \alpha_{\tau_1}^{\sigma_1} P_L(\sigma_1, \tau_2, \ldots, \tau_L) \quad + \tag{2.36}$$

$$\sum_{k=1}^{L-1} \sum_{\sigma_k,\sigma_{k+1}=1}^{m} \gamma_{\tau_k\tau_{k+1}}^{\sigma_k\sigma_{k+1}} P_L(\tau_1, \ldots, \sigma_k, \sigma_{k+1}, \tau_{k+2} \ldots \tau_L) \quad + \quad \sum_{\sigma_L=1}^{m} \beta_{\tau_L}^{\sigma_L} P_L(\tau_1, \ldots, \tau_{L-1}\sigma_1) = 0$$

Comparing (2.31 with (2.35)) gives the first equation of (2.11). Hence, the proof of proposition (ii) is complete.

Let us add some remarks on the proof. We proved that the Fock–representation of the algebra (2.10)-(2.11) has a nontrivial representation if an eigenstate with zero energy exists for all lattice lengths. The construction of the matrices obeying (2.10) can be done without any demand for special properties of H. (An associative algebra generated by $2m$ generators with m^2 quadratic relations is always a well defined mathematical object.) The special property of H, i.e. the existence of zero energy eigenstates $|P_L\rangle$, was only needed for the construction of a non trivial scalar product involving the vectors $\langle W|$ and $|V\rangle$. More precisely, the vectors P_L only enter the definition of the vector $\langle W|$ and the equation which determines $\langle W|$ is just the equation for the zero energy eigenstate.

Due to the lack of recurrence relations the scalar product in (2.10)-(2.11) is not completely fixed and can be chosen independently in each vector space $\widehat{\mathcal{V}}_M$. For that reason it would be sufficient to require that at least for one lattice length L the Hamiltonian has a zero energy eigenstate. In that case $\langle W|$ is nontrivial only on the subspace $\widehat{\mathcal{V}}_L$.

One may define a finite dimensional $\widehat{\mathcal{V}}$ as the direct sum over all $\widehat{\mathcal{V}}_M$ with $M \leq L_{\max}$ for some number $L_{\max}$. A matrix representation of the algebra (2.10)-(2.11) can then be found be assuming E q. (2.20)-(2.23) for $L = 1, 2, \ldots, L_{\max}$ as well as $D_\tau|\tau_1, \tau_2, \ldots, \tau_{L_{\max}}\rangle = 0$ and $X_\tau|\tau_1, \tau_2, \ldots, \tau_{L_{\max}}\rangle = 0$. Then (2.12) provides a matrix product representation for all eigenvectors $|P_L\rangle$ with $L \leq L_{\max}$.

It is of course also possible to express eigenstate of non zero eigenvalues as matrix product state by adding an appropriate shift to the Hamiltonian. This is done by adding a shift, i. e. by replacing $\gamma^{\mu\nu}_{\sigma\tau}$, α^μ_σ and β^μ_σ in (2.10)-(2.11) by $\gamma^{\mu\nu}_{\sigma\tau} - \epsilon\delta^\mu_\sigma\delta^\nu_\tau$, $\alpha^\mu_\sigma - \epsilon_1\delta^\mu_\sigma$ and $\beta^\mu_\sigma - \epsilon_L\delta^\mu_\sigma$, respectively. In this case the Hamiltonian H in (2.13) has to be replaced by $H - E(L)$ with $E(L) = \epsilon_1 + \epsilon_L + (L-1)\epsilon$ if L is the lattice length. The vector P_L is then an eigenstate with energy $E(L)$. However, if ϵ_1, ϵ_L and ϵ are independent of L, (2.13) will have a non trivial solution only for a finite number of lattice lengths L and $\langle W|$ will therefore be non trivial only on the corresponding subspaces $\widehat{\mathcal{V}}_L$ of $\widehat{\mathcal{V}}$.

We proved that any zero energy eigenstate of a Hamiltonian of the form (2.1) can be written as a matrix product state with respect to the Fock representation of the algebra (2.10)-(2.11). The proof has been done by showing that the operators as well as the scalar product can be defined in a non trivial way. The equations defining the scalar product are exactly the equations for the zero energy eigenstate. This shows that by application of the algebra on an abstract level, i.e. by using only the relations (2.10)-(2.11), one can not gain any insight into the form of the eigenstates. One ends up with nothing but a reformulation of the equation for the zero energy eigenstate. Therefore the so called *matrix product ansatz*, i.e. the application of the Fock-representation of the quadrtatic algebra (2.10-(2.11)) to an eigenvector problem, is not really an ansatz, it is an identity. The eigenvector problem is not transformed into another problem, it remains unchanged. However, the situation becomes different if one considers a more special form of the algebra as done in [17, 18, 39, 40, 41, 42] where the operators X_s are replaced by numbers.

We checked that our proposition is also true for the Fock–representation of the quadratic algebra describing stochastic models with parallel updating [45].

4 Periodic Boundaries: A Counter-Example

In the previous section it was shown that every zero energy eigenstate of a general m-state quantum spin Hamiltonian with nearest neighbour interaction in the bulk and open boundary conditions (i. e. with single site terms at each boundary) can be written with the help of a quadratic algebra. In this section we ask for an analogous statement for periodic boundary conditions. By giving a counter–example we show that such a statement does not hold for periodic boundary conditions.

We consider a Hamiltonian of the form (2.5) with periodic boundary conditions where the bulk interaction term $h_{k,k+1}$ is again given by (2.3). As in the open boundary case, to each Hamiltonian of the form (2.5) we may again associate the quadratic algebra (2.10) which is determined just by the coefficients $\gamma_{\tau\sigma}^{\mu\nu}$ of $h_{k,k+1}$. On this algebra we introduce a *trace–like* function. By this we mean a linear number–valued function which is invariant under cyclic permutations and compatible with the quadratic relations (2.10). Thus, for a trace–like function tr and for any two elements A and B of the algebra the relations

$$tr(AB) = tr(BA) \tag{2.37}$$

$$\sum_{\mu,\nu=1}^{m} \gamma_{\sigma\tau}^{\mu\nu} tr(AD_\mu D_\nu B) = tr(AX_\sigma D_\tau B) - tr(AD_\sigma X_\tau B) \tag{2.38}$$

hold. If a non–trivial trace–like function tr exists on the quadratic algebra (2.10), the state P_0 defined by

$$P_0 = \sum_{\tau_1 \cdots \tau_L = 0}^{m-1} tr(D_{\tau_1} \cdots D_{\tau_L}) u_{\tau_1}^{(1)} \otimes u_{\tau_2}^{(2)} \otimes \cdots \otimes u_{\tau_L}^{(L)} \tag{2.39}$$

is an eigenstate of H_{per} with energy and momentum zero (cf. [49]). This corresponds to the first statement of the theorem of [23]. To get the analogue of the second statement we ask the following question: Given an eigenstate P_0' of H_{per} with energy and momentum zero, we ask for the corresponding trace–like function $tr_{P_0'}$ such that P_0' is obtained by (2.39). As we will see below, such a trace–like function does not exist in every case. We will present an example of a Hamiltonian which has an eigenstate with energy and momentum zero which cannot be written in the form (2.39).

Before we come to this counter–example we would like to add some remarks on the relations between trace–like functions on the algebra (2.10) and traces of representations of (2.10). If one has a representation of (2.10) which admits a trace on the whole algebra or only on some sectors, it is obvious that the values of this trace define a trace–like function. Therefore the existence of a trace–like function is a necessary condition for the existence of a representation with a trace. On the other hand it is not clear that any trace–like function can be obtained as the trace of an appropriate representation. Consider for example the algebra discussed in [49] (section 3.2 in this paper). This algebra can be decomposed into two sectors. For each sector a representation with a well–defined and non–trivial trace is given in [49]. However, a representation which has a trace on both sectors at the same time is not known to exist whereas a trace–like function with this property can easily be defined. In [50] an infinite dimensional representation is used for which the trace is not well–defined. Nonetheless, finite values which fulfil the relation for a trace–like function can be obtained with the help on an ordering procedure. Next we would like to mention that a trace–like function can be defined without using an appropriate representation with a trace on it at all. For example consider the coset algebra of (2.10), which is obtained by taking $X_\tau = 0$ for $\tau = 1, \cdots, m$, without any additional structure. If this coset algebra exists, the coefficients of the independent monomial are the weights of zero energy eigenstates of the corresponding Hamiltonian with closed boundary conditions (i. e. the Hamiltonian (2.1) with $h_1 = h_L = 0$) [19]. In some cases there are sectors of this algebra where the coefficients of the independent monomials are invariant under cyclic permutations. In these cases the approach of [19] also works for the corresponding models with periodic boundary conditions (but only in the corresponding sectors) and the mapping which assigns to each monomial its coefficients of the independent monomials defines a trace–like function. This happens in the case of the three state diffusion model considered in [51]. (It is interesting to note that only the sector with equal number of particles for all species was treated in [51]. One can show that on all other sectors of this algebra a trace–like function does not exist). We would like to stress that a state of the form (2.39) has momentum zero if and only if tr is invariant under cyclic permutations. Function which are not invariant under cyclic permutations can be useful for the solution of inhomogeneous equations. This is the case in the calculation of the diffusion constant on the ring [52]. A useful observation is that the relations (2.10) are homogeneously quadratic. Therefore they do not lead to relations of monomials or trace–like functions of monomials of different lengths. Hence, on each sector generated by all monomials of a given length L, a trace–like function can by defined separately. We will make use of this fact later.

In the following we give an example for a Hamiltonian which has an eigenstate with energy and momentum zero which cannot be written in the form (2.39) since for this state an appropriate trace–like function on the algebra (2.10) does not exist. Originally, my aim was to prove the analogue of the theorem of [23] for periodic boundary conditions. Therefore I studied simple Hamiltonians with a large number of zero energy eigenstates. Among those I found the subsequent counter–example. It has no physical significance. However, from this study it is clear that a general positive statement for the existence of a trace–like function on the algebra (2.10) needs more detailed conditions as the proof of the existence of a Fock–representation in the open boundary case [23]. Such conditions are still missing.

We consider the Hamiltonian H_3 which is defined as the Hamiltonian (2.5) on a 3–site lattice with 3 states per site and the following coefficients of the bulk interaction term (2.3):

$$\gamma_{21}^{12} = \gamma_{12}^{21} = -\gamma_{13}^{31} = -\gamma_{23}^{32} = -\gamma_{12}^{12} = -\gamma_{21}^{21} = \gamma_{31}^{31} = \gamma_{32}^{32} = \alpha \tag{2.40}$$

All other coefficients are zero. This Hamiltonian has the following conserved quantities:

$$N_\tau = \sum_{j=1}^{3} E_j^{\tau\tau} \qquad \tau = 1, 2 \tag{2.41}$$

A straightforward but lengthy calculation shows that on the zero momentum sector all matrix elements of H_3 vanish. Hence, every translational invariant state has energy zero. We call this sector $\mathcal{U}_0$. Its dimension is 11. We ask which of the states of $\mathcal{U}_0$ can be obtained with the help of a trace–like function on the algebra (2.10). Therefore we have to look for the conditions which the relations (2.37) and (2.38) put onto the values of any trace–like functions. If tr is such a trace–like function these conditions have the form

$$\begin{aligned} tr(X_{\tau_1} D_{\tau_2} D_{\tau_3}) - tr(X_{\tau_2} D_{\tau_3} D_{\tau_1}) &= \sum_{\mu,\nu} \gamma_{\tau_1\tau_2}^{\mu\nu} tr(D_\mu D_\nu D_{\tau_3}) &(2.42)\\ tr(X_{\tau_1} X_{\tau_2} D_{\tau_3}) - tr(X_{\tau_3} X_{\tau_1} D_{\tau_2}) &= \sum_{\mu,\nu} \gamma_{\tau_2\tau_3}^{\mu\nu} tr(X_{\tau_1} D_\mu D_\nu) &(2.43)\end{aligned}$$

where $\tau_1, \tau_2, \tau_3 = 1, 2, 3$. To simplify the notation for the following calculations we use the invariance under cyclic permutations to push the X–generators in the argument of tr to the first positions as done in (2.42),(2.43). We consider (2.42) and (2.43) as a system of equations whose solutions are trace–like functions. For each state in $\mathcal{U}_0$, which can be written in the form (2.39), there is a class of solutions of (2.42) and (2.43). (A class of solutions consists of all trace–like functions whose values differ only on the monomials with one or more X–generators.) Our question is now, how many independent classes of solutions of (2.42) and (2.43) can be found. It turns out that only 10 independent classes of solutions exist corresponding to 10 states of the form (2.39). Thus, one state out of 11 remains which cannot be written in this form. Let us now study solutions in detail.

The sector $\mathcal{U}_0$ can be divided up into the sub–sector of symmetric states (states which are invariant not only under cyclic permutation but under arbitrary permutations) and its orthogonal complement. The symmetric sector has dimension 10. All symmetric states can be written with the help of a trace–like function on the algebra (2.10). To see this we consider one–dimensional representations, i. e. we choose the generators to be numbers and the trace–like function to be the ordinary product of numbers. In this case the quadratic relations

(2.10) with the coefficients of (2.40) reduce to the equations

$$\begin{aligned} 0 &= d_1x_2 - d_2x_1 \\ \alpha d_1 d_3 &= d_1x_3 - d_3x_1 \\ \alpha d_2 d_3 &= d_2x_3 - d_3x_2 \end{aligned} \tag{2.44}$$

where we have replaced the capital letters in (2.10) by small ones. It is easy to check that for each choice of d_1, d_2 and d_3 one can find numbers x_1, x_2 and x_3 such that the relations (2.44) are fulfilled. Therefore the values of d_1, d_2 and d_3 can be chosen arbitrarily. For one–dimensional representations the coefficients of the state (2.39) are just the independent monomials of degree 3 in the 3 variables d_1, d_2 and d_3. There are 10 of such monomials allowing as many independent states of the form (2.39). Taking into account that a linear combination of trace–like functions is again a trace–like function every symmetric state can be written in the form (2.39). The orthogonal complement of the symmetric sector is generated by the single state φ defined by

$$\varphi = \sum_{\sigma\in S_3} \mathrm{sign}(\sigma)\; u^{(1)}_{\sigma(1)} \otimes u^{(2)}_{\sigma(2)} \otimes u^{(3)}_{\sigma(3)} \tag{2.45}$$

where S_3 is the group of permutations of three objects. This state *cannot* be written with the help of a trace–like function. To show this we attempt to construct a function tr^*_φ which fulfils all properties of a trace–like function on the algebra (2.10) with the coefficients (2.40) and allows us to write the state φ in the form (2.39). (The star indicates that it is not yet clear whether tr^*_φ can be extended to a trace–like function on all monomials of length 3.) As pointed out above it is sufficient to define tr^*_φ only for monomials of length 3. For all further calculations the function tr^*_φ is assumed to be invariant under cyclic permutations. The values of tr^*_φ for monomials of length 3 containing only D–generators are uniquely determined by the requirement that tr^*_φ allows a representation of φ in the form (2.39), i. e.

$$tr^*_\varphi(D_{\sigma(1)}D_{\sigma(2)}D_{\sigma(3)}) = \mathrm{sign}(\sigma) \qquad \sigma \in S_3. \tag{2.46}$$

The values of tr^*_φ on all other monomials containing only D–generators have to be zero. The next step is to determine the values of tr^*_φ on the monomials with one X–generator. These values are constrained by the necessary conditions (2.42) and (2.43) which immediately result from the quadratic relations (2.10) and the invariance of the trace–like function under cyclic permutations (2.37) and thus hold for any trace–like function tr. We claim that tr^*_φ is a trace–like function and use the necessary condition (2.42) to determine the values of tr^*_φ for monomials with one X–generator. Note that on the left hand side of (2.42) only differences of traces–like functions of monomials appear whose indices differ through a cyclic permutation. Hence, if $tr^*_\varphi(X_{\tau_1}D_{\tau_2}D_{\tau_3}) = t_{\tau_1\tau_2\tau_3}$ is a solution of (2.42) for given values of

$tr^*_\varphi(D_{\tau_1}D_{\tau_2}D_{\tau_3})$ then $tr^*_\varphi(X_{\tau_1}D_{\tau_2}D_{\tau_3}) = t_{\tau_1\tau_2\tau_3} + w_{\tau_1\tau_2\tau_3}$, where the $w_{\tau_1\tau_2\tau_3}$ are arbitrary numbers with $w_{\tau_1\tau_2\tau_3} = w_{\tau_2\tau_3\tau_1}$, is again a solution of (2.42). Making use of this ambiguity, the values $tr^*_\varphi(X_{\tau_1}D_{\tau_2}D_{\tau_3})$ determined by (2.42) can be written in the form

$$\begin{array}{llll} tr^*_\varphi(X_1D_2D_3) & = w_{123}+\alpha & \quad tr^*_\varphi(X_1D_3D_2) = w_{132}-\alpha \\ tr^*_\varphi(X_2D_3D_1) & = w_{123}+\alpha & \quad tr^*_\varphi(X_2D_1D_3) = w_{132}-\alpha \\ tr^*_\varphi(X_3D_1D_2) & = w_{123} & \quad tr^*_\varphi(X_3D_2D_1) = w_{132} \end{array} \tag{2.47}$$

where w_{123} and w_{132} are arbitrary constants. Up to these constants, the values of tr^*_φ in (2.47) are uniquely determined by (2.42). The values of tr^*_φ on all other monomials with one X–generator do not appear in further calculations. It remains to check whether condition (2.43) can be fulfilled by the function tr^*_φ defined so far. Therefore we define the following function:

$$Z_{\tau_1\tau_2\tau_3}[tr] = \sum_{\mu\nu}\left[\gamma^{\mu\nu}_{\tau_1\tau_2}tr(X_{\tau_3}D_\mu D_\nu) + \gamma^{\mu\nu}_{\tau_2\tau_3}tr(X_{\tau_1}D_\mu D_\nu) + \gamma^{\mu\nu}_{\tau_3\tau_1}tr(X_{\tau_2}D_\mu D_\nu)\right]. \tag{2.48}$$

From (2.43) we find $Z_{\tau_1\tau_2\tau_3}[tr] = 0$ as a necessary condition for tr being a trace–like function. Taking the values of tr^*_φ defined in (2.47) we find

$$Z_{012}[tr^*_\varphi] = 2\alpha^2 \neq 0. \tag{2.49}$$

Hence, the function tr^*_φ defined above is *not* a trace–like function on the algebra (2.10). We would like to stress that there was no ambiguity in the definition of tr^*_φ so far up to the constants w_{123} and w_{132} which in turn do not appear in (2.49). Therefore a trace–like function on the quadratic algebra (2.10) whose values on the monomials without X–generators are determined by (2.46) does not exist at all. Hence, the state φ cannot be written in the form (2.39) with the help of an appropriate trace–like function on the quadratic algebra (2.10). This is what we wanted to show.

Chapter 3

The Asymmetric Coagulation-Decoagulation Model

The study of exactly solvable models has been an important activity in equilibrium statistical physics and it is equally desirable to find such models in the field of non-equilibrium phenomena. In this context it has proved very useful to exploit the formal analogy between the master equation for classical stochastic systems and the quantum-mechanical Schrödinger equation. For example, by relating the one-dimensional kinetic Ising model to a quantum spin chain [53, 54, 55, 56] it becomes obvious why the system is solvable with Glauber's [1] choice of the rates. Similarly, the hopping of classical particles with hard-core repulsion on a lattice can be formulated as a spin problem, namely the ferromagnetic Heisenberg model [4, 57], and in one dimension this is again a solvable model.

In recent work, this approach has been extended to more general situations. They include diffusion with a preferred direction as well as reactions between particles or coupling to external reservoirs [9, 12, 58, 59, 60, 61, 43]. The spin of the resulting quantum models is $s+1$ if s types of particles are involved. Fermionic or bosonic representations have also been used, for example for models of self-organized criticality [62, 63]. In general, the inclusion of more processes makes the time evolution operator more complicated. On the other hand, by tuning the various rates one may also achieve simplifications which make the problem integrable in some cases.

One of the systems where this happens is the coagulation model in which particles hop on a one-dimensional lattice and, in addition, can merge and separate again with certain probabilities. This model was introduced and treated in a continuum approximation by Doering et.al. [27, 28, 64, 10]. It was found later that it is exactly solvable on a lattice if the rates for hopping and for coagulation are equal [65]. The time evolution operator can then be brought into the form of the Hamiltonian for a spin one-half XY chain with a Z field. It is the dual of the operator for the Glauber model mentioned above and can be diagonalized in terms of fermions. The spectrum has a gap determined by the decoagulation rate. If this rate vanishes, one finds an algebraic decay of the concentration with exponent minus one-half. The model can then be mapped onto a pair annihilation model [65] and there is also an interesting physical realization in terms of excitons in the quasi one-dimensional substance TMMC [66].

In treating this model, it turned out that physical quantities like the density are most easily calculated from the probabilities to find empty intervals of arbitrary length ("holes"). Their equations of motion form closed sets and can be solved for a ring as well as for a chain. They have been used also in related models [67]. An intriguing aspect is that these closed sets even exist if the creation of particles is allowed [31]. The relaxational spectrum of the hole functions then has the form of the Wannier-Stark ladder found for lattice electrons in a homogeneous electric field [68, 69]. However, no fermionic solution is possible in this case and the question of complete integrability has remained open so far.

In the present chapter we study the properties of the coagulation model for the case of a preferred direction. The geometry will be the open chain where an interplay between the boundaries and the spatial asymmetry occurs. Our aim is to pursue the question of integrability further, and also to find the basic physical features of the model. We focus on the case where all processes have the same asymmetry and the rates for hopping and coagulation are chosen equal. Then the model contains two free parameters. We show that, as for symmetric rates, the spin operator describing the time evolution can be brought into a form where it is quadratic in fermions. Thus one finds complete integrability also in this case. However, in contrast to simple hopping or symmetric coagulation the problem has no quantum group symmetry. This can be related to particular boundary terms which correspond to fields in the magnetic language and lead to special selection rules. There is, however, a discrete S_3-symmetry which shows up in the multiplicity of the relaxational modes.

We also consider the hole equations, both in the one-hole sector and in general. Following an approach by Bedeaux et.al. [32] the different levels in the hierarchy can be decoupled and a complete solution achieved. By considering more general rates and processes, it is seen that this procedure only works in the free fermion case. This is also what the Reshetikhin criterion for integrability [70] gives. Thus the other cases where the one-hole equations can be solved, correspond to partially integrable systems. Such a situation occurs also in kinetic spin models [55, 71] and in reaction-diffusion models where for particular rates the equations for the density correlations form closed sets [72].

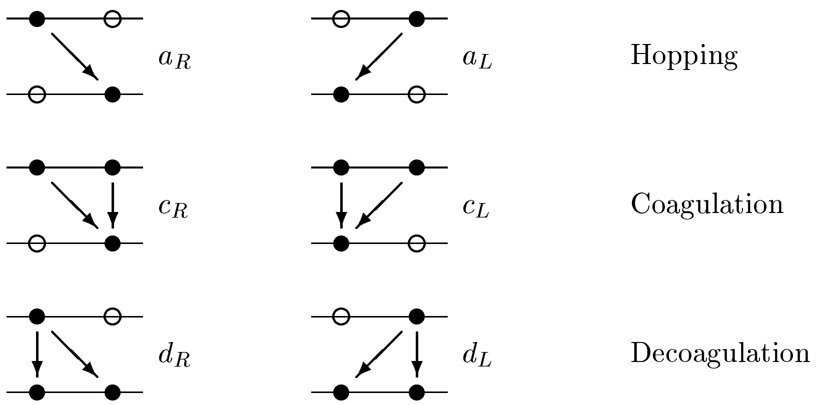
The physical properties of the model are also interesting. In the stationary state the density is inhomogeneous and determined by a competition between asymmetry and decoagulation. If the latter is small, the density is finite only near one boundary. In the opposite case, it is constant in the bulk of the system with some additional boundary effects. In between, a transition takes place, where the profile becomes linear over the major part of the system. These different regimes are also reflected in the form of the relaxation spectrum. In general, one finds a gap but at the transition it vanishes and one has slow modes as in symmetric diffusion. The phenomenon may be viewed as another example of a boundary-induced transition [33, 61, 73, 74].

We shall present the material as follows. In section 2 we introduce the model and the spin formalism used in its treatment. The time evolution operator is derived and brought into convenient forms in section 3. In section 4 its spectrum is found by diagonalization via fermions. Section 5 deals with the equations of motion in the one-hole sector and in section 6 the n-hole problem is treated via cumulant-like functions. From these results, density profile and correlation functions in the steady state are obtained as special cases and discussed in section 7. Finally, section 8 contains a summary and concluding remarks.

1 The Model

We consider classical particles on a chain of L sites, each of which can either be empty or occupied with at most one particle. The dynamics of the system consists of transitions which involve only the configurations of neighbouring sites. As discussed previously [31], one can then distinguish altogether 12 different processes, namely hopping, coagulation and decoagulation as well as birth and death of single particles and of pairs. Each process is described by a rate constant and, in the absence of detailed balance, all these constants are independent.

In the bulk of the chapter we will only consider the first three processes which are shown below together with their rates:



The left-right asymmetry which we assume could result from external fields. We will use a spin language to describe the system. The state of site n is specified by a variable $\sigma_n = \pm 1$ such that $\sigma_n = +1(-1)$ if the site is occupied (empty). A configuration of the total system is denoted by $\underline{\sigma} = \{\sigma_1, \sigma_2, \ldots \sigma_L\}$. The probability $P(\underline{\sigma}, t)$ to find configuration $\underline{\sigma}$ at time t then obeys the master equation

$$\frac{\partial}{\partial t} P(\underline{\sigma}, t) \;=\; -\sum_{\underline{\sigma}'} P(\underline{\sigma}, t)\, w(\underline{\sigma} \to \underline{\sigma}') + \sum_{\underline{\sigma}'} P(\underline{\sigma}', t)\, w(\underline{\sigma}' \to \underline{\sigma}) \tag{3.1}$$

where the two terms on the right represent the loss and the gain processes, respectively. The transition probabilities $w(\underline{\sigma} \to \underline{\sigma}')$ are sums of contributions from the various nearest neighbour processes.

To formulate the problem in quantum-mechanical terms [53, 11] one uses a ket vector notation in the 2^L-dimensional state space, writing

$$|P(t)\rangle \;=\; \sum_{\underline{\sigma}} P(\underline{\sigma}, t)\, |\underline{\sigma}\rangle\,. \tag{3.2}$$

The master equation then takes the form

$$\frac{\partial}{\partial t} |P(t)\rangle \;=\; -H|P(t)\rangle \tag{3.3}$$

from which the analogy with the Schrödinger equation is obvious. The time evolution operator H will therefore be called Hamiltonian in the following. However, since $|P(t)\rangle$ is already the probability, expectation values differ from the quantum-mechanical ones. For a quantity $A(\underline{\sigma})$ one has

$$\langle A(t)\rangle \;=\; \sum_{\underline{\sigma}} A(\underline{\sigma})\, P(\underline{\sigma}, t) \;=\; \langle 0|A|P(t)\rangle \tag{3.4}$$

with the bra vector

$$\langle 0| \;=\; \sum_{\underline{\sigma}} \langle \underline{\sigma}|\,. \tag{3.5}$$

The operator H is the sum of nearest-neighbour terms

$$H \;=\; \sum_{n=1}^{L-1} H_{n,n+1} \tag{3.6}$$

and the (4×4) matrix $H_{n,n+1}$ can be written down easily [31]. In a basis of states $(\,|--\rangle, |-+\rangle, |+-\rangle, |++\rangle)$ the result is, including birth processes (rates b_R, b_L) and pair creation (rate c) for further reference

$$H_{n,n+1} \;=\; \begin{pmatrix} c+b_L+b_R & 0 & 0 & 0 \\ -b_R & a_L+d_L & -a_R & -c_R \\ -b_L & -a_L & a_R+d_R & -c_L \\ -c & -d_L & -d_R & c_L+c_R \end{pmatrix}. \tag{3.7}$$

Due to probability conservation, the elements in the columns sum to zero. $H_{n,n+1}$ and therefore the total operator H is non-hermitean.

In the next sections we will consider the case of no birth and pair creation ($b_R = b_L = c = 0$), equal rates for hopping and coagulation ($c_R = a_R, c_L = a_L$) and equal asymmetry for all processes. Up to a common constant which we set equal one, the rates can then be written

$$a_R = \frac{1}{q}\,, \qquad a_L = q\,, \qquad d_R = \frac{\Delta}{q}\,, \qquad d_L = \Delta q\,. \tag{3.8}$$

Thus the parameter q as usual describes the asymmetry, while Δ gives the ratio of decoagulation to coagulation rates and therefore governs the (average) density.

2 The time evolution operator

Starting e.g. from Eq. (3.7), the Hamiltonian H can be expressed in terms of Pauli-matrices σ_i^α ($\alpha{=}x, y, z$). It is the sum of diffusion and coagulation contributions

$$H \;=\; H_D + H_C\,, \tag{3.9}$$

where H_D is given by

$$\begin{aligned} H_D \;=\; -\frac{1}{4}\sum_{i=1}^{L-1}\Big\{ & q^{-1}\sigma_i^-\sigma_{i+1}^+ + q\,\sigma_i^+\sigma_{i+1}^- + (q+q^{-1})\,\sigma_i^z\sigma_{i+1}^z \\ & +(q-q^{-1})(\sigma_i^z - \sigma_{i+1}^z) - (q+q^{-1})\Big\}\,. \end{aligned} \tag{3.10}$$

The standard $U_q[SU(2)]$-symmetric form of H_D is then obtained by a position-dependent rescaling of σ^+ and σ^- [12, 59, 61]. Physically, this corresponds to factorizing out of $P(\underline{\sigma}, t)$ the quantity $P_0^{1/2}(\underline{\sigma})$, where $P_0(\underline{\sigma})$ is the stationary distribution in the case of simple hopping. The coagulation part reads

$$\begin{aligned} H_C \;=\; -\frac{1}{4}\sum_{i=1}^{L-1}\Big\{ & (q^{-1}\sigma_i^- + \Delta\, q\,\sigma_i^+)(1+\sigma_{i+1}^z) \;+\; (1+\sigma_i^z)(q\sigma_{i+1}^- + \Delta q^{-1}\sigma_{i+1}^+) \\ & -(q+q^{-1})(1-\Delta)\,\sigma_i^z\sigma_{i+1}^z \;-\; (q+q^{-1})(\sigma_i^z + \sigma_{i+1}^z) \\ & +\Delta\,(q-q^{-1})(\sigma_i^z - \sigma_{i+1}^z) \;-\; (q+q^{-1})(1+\Delta)\Big\}\,. \end{aligned} \tag{3.11}$$

It is more complicated than H_D because of the single spin terms σ_i^+, σ_i^-, σ_i^z which appear in it. One should note, however, that the contribution $(\sigma_i^z - \sigma_{i+1}^z)$ is effectively only a boundary term. For $q = 1$ it vanishes altogether and H reduces to the expression found previously [12, 65]. In that case, H was brought into a simpler form by two local transformations in spin space: A hyperbolic rotation around the z-axis with generator

$$V_1 = \prod_n e^{\lambda\sigma_n^z}\,; \qquad\qquad e^{-2\lambda} = \sqrt{\Delta} \tag{3.12}$$

which rescales the $\sigma^{\pm}$ operators, and a real rotation around the y-axis with generator

$$V_2 = \prod_n e^{-i\frac{\Theta}{2}\sigma_n^y}\,; \qquad cos(\Theta) = \frac{1}{\sqrt{1+\Delta}} \tag{3.13}$$

which forms linear contributions of σ^x and σ^z.

It turns out that the same transformation can be used also for $q \neq 1$. The result for the new operator $H' = V_2 V_1 H V_1^{-1} V_2^{-1}$ then is

$$\begin{aligned} H' \;=\; -\frac{D}{2}\sum_{i=1}^{L-1}\Bigg\{ & \gamma\,\sigma_i^x\sigma_{i+1}^x \;+\; \gamma^{-1}\sigma_i^y\sigma_{i+1}^y \;+\; i\,\frac{1-q^2}{1+q^2}\,(\sigma_i^x\sigma_{i+1}^y - \sigma_i^y\sigma_{i+1}^x) \\ & -\frac{2}{q+q^{-1}}\,(q^{-1}\sigma_i^z + q\sigma_{i+1}^z) \;-\; (\gamma+\gamma^{-1}) \\ & -\frac{1-q^2}{1+q^2}\,\sqrt{\gamma-\gamma^{-1}}\left[\sqrt{\gamma}\,(\sigma_i^x - \sigma_{i+1}^x) \;+\; i\,\frac{1}{\sqrt{\gamma}}\,(\sigma_i^y - \sigma_{i+1}^y)\right]\Bigg\} \end{aligned} \tag{3.14}$$

where $\gamma = \sqrt{1+\Delta}$. and $D = \frac{1}{2}(q+q^{-1})\gamma$.

This operator has two non-hermitean parts: the third term, which is a kind of chiral contribution from the bulk, and the last term which again acts only at the two boundaries. Both vanish in the symmetric case ($q = 1$) and H' then reduces to the dual of the Glauber model operator.

The bulk terms in H' are all quadratic in fermion operators after a Jordan-Wigner transformation. There are, however, also boundary terms in σ^x, σ^y and σ^z. The last one is unproblematic, but σ^x and σ^y are linear in the fermions. There is, however, a well-known way around this difficulty: One extends the chain by one site at each end and uses the additional spin operators, which are constants of the motion, to make boundary terms quadratic. Thus the operator H' is solvable via fermions.

Actually, one can bring it into a slightly simpler form by performing a rotation by 180°

$$V_3 = \prod_n e^{i\frac{\pi}{2}\sigma_n^y} \tag{3.15}$$

and a further transformation with the generator

$$V_4 = \prod_n e^{\rho\sigma_n^z}\,; \qquad e^{-2\rho} = \sqrt{\frac{\gamma-1}{\gamma+1}} \tag{3.16}$$

to obtain

$$\begin{aligned} H'' \;=\; -\frac{1}{2}\gamma\sum_{i=1}^{L-1}\Bigg\{ & (\eta+\eta^{-1})\sigma_i^x\sigma_{i+1}^x + i\,(q\sigma_i^x\sigma_{i+1}^y + q^{-1}\sigma_i^y\sigma_{i+1}^x) \\ & +(q^{-1}\sigma_i^z + q\sigma_{i+1}^z) - \frac{1}{2}(q-q^{-1})(\gamma-\gamma^{-1})(\sigma_i^x - \sigma_{i+1}^x) - (\eta+\eta^{-1})\Bigg\} \end{aligned} \tag{3.17}$$

where $(\eta + \eta^{-1}) = \frac{1}{2}(q + q^{-1})(\gamma + \gamma^{-1})$.

There is no σ^y boundary term in this expression so that the only non-hermitean part is the chiral bulk term. This operator will be diagonalized in the next section.

We mention that H' and H'' have a simple symmetry, namely they are invariant under the transformation $q \leftrightarrow 1/q$ combined with spatial reflection $i \to L - i + 1$.

3 Analysis of the spectrum

In order to diagonalize the Hamiltonian (3.17) in terms of fermions, we write $H'' = H_0'' + H_1''$ where

$$H_1'' \;=\; \frac{\kappa}{2}(\sigma_1^x - \sigma_L^x) \tag{3.18}$$

is the linear boundary term and

$$\kappa \;=\; \frac{\gamma}{2}(q - q^{-1})(\gamma - \gamma^{-1})\,. \tag{3.19}$$

As outlined in the last section, one appends one site at each end of the chain and extends H_1'' by two Pauli matrices σ_0^x and σ_{L+1}^x. Then

$$\tilde{H}_1'' \;=\; \frac{\kappa}{2}(\sigma_0^x\sigma_1^x - \sigma_L^x\sigma_{L+1}^x) \tag{3.20}$$

is bilinear in fermions so that standard diagonalization methods [75] can be applied[1]. The eigenvectors of the extended Hamiltonian $\tilde{H}'' = H_0'' + \tilde{H}_1''$ include those of the original chain H'' as follows: Since the appended matrices are constants of the motion, the spectrum of $\tilde{H}''$ decomposes into four sectors $(++,+-,-+,--)$ corresponding to the eigenvalues of σ_0^x and σ_{L+1}^x. This implies that all eigenvectors of $\tilde{H}''$ have the form

$$|\tilde{\psi}\rangle \;=\; \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \otimes |\psi\rangle \otimes \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}, \tag{3.21}$$

where $|\psi\rangle$ is a vector with 2^L components. Since in each sector the appended matrices can be replaced by their eigenvalues, the spectrum of the original chain appears in the $(++)$ sector and the vectors $|\psi\rangle$ are just the eigenvectors of H''. Therefore we can determine the eigenvectors of the original problem by projection onto the $(++)$ sector. One should mention that a very similar situation occurs in calculations using the corner transfer matrix of the two-dimensional Ising model [13, 76]. In that case the sectors arise from the fixed inner and outer spins in the corner geometry.

Defining anticommuting Clifford operators $\tau_j^{x,y} = (\prod_{i=0}^{j-1}\sigma_i^z)\sigma_j^{x,y}$ one can rewrite $\tilde{H}''$ as a

[1]In the same way one could also add σ^y-matrices or any linear combination of σ^x and σ^y.

bilinear expression in τ_j^x and τ_j^y. Then a second linear transformation $a_k^\pm = \frac{1}{2}\sum_{j=1}^{L}(\phi_{k,j}^x \tau_j^x \pm i\phi_{k,j}^y \tau_j^y)$ yields

$$\tilde{H}'' = \Big(\sum_k \lambda_k \, a_k^+ a_k^-\Big) - \kappa \tag{3.22}$$

which is a diagonal expression in fermionic creation and annihilation operators a_k^+ and a_k^-. The one-particle energies λ_k and the eigenvectors $\vec{\phi}_k^\pm = (\phi_{k,1}^x, \pm i\phi_{k,1}^y, \ldots, \phi_{k,L}^x, \pm i\phi_{k,L}^y)$ can be derived from the eigenvalue problem $M\vec{\phi}_k^\pm = \mp\lambda_k \vec{\phi}_k^\pm$ with

$$M = i\gamma \begin{pmatrix} 0 & D & & & & & \\ -D^T & B & A & & & & \\ & -A^T & B+C & A & & & \\ & & \cdots & \cdots & \cdots & & \\ & & & -A^T & B+C & A & \\ & & & & -A^T & C & -D \\ & & & & & D^T & 0 \end{pmatrix} \tag{3.23}$$

where A, B, C and D denote the 2×2 block matrices

$$A = \begin{pmatrix} -i/q & 0 \\ \eta+\eta^{-1} & iq \end{pmatrix}, \quad B = \begin{pmatrix} 0 & q^{-1} \\ -q^{-1} & 0 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & q \\ -q & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 \\ \kappa/\gamma & 0 \end{pmatrix}.$$

The eigenvalues of M are real and occur in pairs with different signs. It should be emphasized at this point that although a_k^+ and a_k^- obey the usual fermionic commutation relations $\{a_k^+, a_l^-\} = \delta_{kl}$, we have $a_k^+ \neq (a_k^-)^\dagger$ because of the nonhermiticity of $\tilde{H}''$.

Assuming that the wave function $\phi_{k,j}^\pm$ consists of exponential contributions $e^{-\zeta j}$, the bulk equations (3.23) yield the dispersion relation

$$\lambda = \gamma\,(\eta + \eta^{-1} - qe^{-\zeta} - q^{-1}e^{\zeta}). \tag{3.24}$$

Including the boundary conditions which determine ζ, we obtain three types of fermionic one-particle states:

- One trivial zero mode ($\lambda_0 = 0$) which is localized at the ends of the extended chain. This zero mode represents conserved quantities σ_0^x and σ_{L+1}^x and causes two-fold degeneracies of all levels.

- Two exponential modes with excitation energies $\lambda_I = \lambda_{II} = \kappa$. Their wave functions $\phi_I^\pm$ and $\phi_{II}^\pm$ decay exponentially with three different length scales corresponding to the values $\ln(\gamma)$, $\ln(q^2\gamma)$ and $\ln(q^2\gamma^{-1})$ for ζ. These modes reflect the influence of the boundary term H_1''.

- $L-1$ oscillatory modes with $\lambda_k = \gamma(\eta+\eta^{-1}) - 2\gamma\cos\frac{\pi k}{L}$ where $k=1,\ldots,L-1$. The corresponding wave functions show damped oscillations of the form $\phi_{k,j} \sim q^{\pm j} e^{\pm i\pi k/L}$. This implies the presence of a fourth length scale with $\zeta = \ln q$. The damping is a consequence of the nonhermiticity of the Hamiltonian for $q \neq 1$.

One can show that the lowest level of $\tilde{H}''$ is a two-fold degenerate state in the sectors $(+-)$ and $(-+)$ with a negative eigenvalue $\Lambda = -\kappa$. The lowest level in the $(++)$ sector with eigenvalue zero is already an excited state. The total number of excited modes in this sector has to be odd and one can distinguish:

- States with an even number of excited oscillatory modes. The levels are two-fold degenerate because either mode I or mode II can be occupied. This class contains the ground state with $\Lambda = 0$ and the lowest gap is

$$\Delta\Lambda \;=\; \gamma(\eta + \frac{1}{\eta} - 2)\,. \tag{3.25}$$

- States with an odd number of excited oscillatory modes. Here the modes I and II are either both occupied, which gives a contribution $(+\kappa)$ to Λ, or both empty, which gives $(-\kappa)$, i.e. we have two bands of excitations which are shifted symmetrically by $\pm\kappa$. Their lowest gaps are

$$\Delta\Lambda(\kappa) = \gamma(\gamma q + \frac{1}{\gamma q} - 2)\,, \qquad \Delta\Lambda(-\kappa) = \gamma(\frac{\gamma}{q} + \frac{q}{\gamma} - 2)\,. \tag{3.26}$$

The nature of these three branches (singlets and doublets) suggests a symmetry in the problem. This is indeed the case: From the operators for the two exponential modes one can construct the quantities

$$\begin{aligned} \sigma &= 1 - (a_I^+ a_I^- + a_{II}^+ a_{II}^-) + (a_I^+ a_{II}^- + a_{II}^+ a_I^-) \\ \tau &= 1 - \frac{3}{2}(a_I^+ a_I^- - a_{II}^+ a_{II}^-)^2 - \frac{\sqrt{3}}{2}(a_I^+ a_{II}^- - a_{II}^+ a_I^-). \end{aligned} \tag{3.27}$$

They satisfy the relations

$$\sigma^2 = 1, \quad \tau^3 = 1, \quad \sigma\tau\sigma = \tau^2 \tag{3.28}$$

which characterize the generators of the permutation group S_3 and commute with both $\tilde{H}''$ and H''. Thus the levels can be chosen as irreducible representations of S_3 which, according to group theory [77], consist of two types of singlets and one doublet. The operator σ has a simple meaning, it interchanges the two degenerate fermion modes.

The smallest gap is obtained from one of the expressions (3.26) which differ by a reflection $q \to q^{-1}$. It vanishes if $\gamma = q$ $(q > 1)$ or $\gamma = q^{-1}$ $(q < 1)$. One band of excitations is then massless and algebraic long-time behaviour is expected. At this point a transition takes place between a low-density phase (for $\gamma < q$) and a high-density phase (for $\gamma > q$). This will be seen in section 7 from the steady-state properties of the system. One should note, however, that the situation is different from a Pokrovskii-Talapov type of transition [78] since here the spectrum has a gap on both sides ($\gamma \lesseqgtr q$) and always varies quadratically with the momentum k.

4 The hole formalism

Although the diagonalization in terms of fermions solves the model in principle, another complementary approach is simpler for practical purposes and gives additional insight. In this approach the states of the system are described in terms of strings of empty sites (holes) instead of spin configurations [27]. In this way one can distinguish different sectors characterized by the number of holes. The equations for the probabilities couple a sector only to the one with lower order. For the one-hole sector of the coagulation model (3.7) with free ends they were already derived in Ref. [31]. Denoting by $\Omega(x, y, t)$ the probability to find the sites $x+1, \ldots, y$ empty and using the abbreviations

$$\begin{aligned} \alpha_{L,R} &= a_{L,R} + d_{L,R} - b_{L,R} - c \\ \gamma_{L,R} &= a_L + a_R + d_{L,R} \\ \delta &= b_L + b_R + c \end{aligned} \tag{3.29}$$

they read

- for holes which do not touch the boundaries ($0 < x < y < L$):

$$\begin{aligned} \frac{d}{dt}\Omega(x,y,t) &= \alpha_R\,\Omega(x-1,y,t) + a_L\,\Omega(x+1,y,t) \\ &\quad + a_R\,\Omega(x,y-1,t) + \alpha_L\,\Omega(x,y+1,t) \\ &\quad - (\gamma_L + \gamma_R + (y-x-1)\delta)\,\Omega(x,y,t) \end{aligned} \tag{3.30}$$

- for holes touching the left boundary ($0 = x < y < L$):

$$\begin{aligned} \frac{d}{dt}\Omega(0,y,t) &= a_R\,\Omega(0,y-1,t) + \alpha_L\,\Omega(0,y+1,t) \\ &\quad - (\gamma_L + (y-1)\delta)\,\Omega(0,y,t) \end{aligned} \tag{3.31}$$

- for holes touching the right boundary ($0 < x < y = L$):

$$\begin{aligned} \frac{d}{dt}\Omega(x,L,t) &= \alpha_R\Omega(x-1,L,t) + a_L\Omega(x+1,L,t) \\ &\quad - (\gamma_R + (L-x-1)\delta)\,\Omega(x,L,t) \end{aligned} \tag{3.32}$$

- for the hole extending over the whole chain ($x = 0, y = L$):

$$\frac{d}{dt}\Omega(0,L,t) \;=\; -(L-1)\delta\,\Omega(0,L,t)\,, \tag{3.33}$$

where we formally define $\Omega(x,x,t) = 1$ according to [31]. This is the coupling to the lower sector (no holes), which here leads to an *inhomogeneous* system. The integrable case discussed in the preceeding sections corresponds to

$$\alpha_{L,R} = \gamma^2 q^{\pm 1}, \quad a_{L,R} = q^{\pm 1}, \quad \gamma_{L,R} = q^{\mp 1} + \gamma^2 q^{\pm 1}, \quad \delta = 0\,. \tag{3.34}$$

Introducing rescaled probabilities $\tilde{\Omega}(x,y,t)$ via

$$\tilde{\Omega}(x,y,t) \;=\; \gamma^{y-x} q^{y+x}\,\Omega(x,y,t) \tag{3.35}$$

and separating the time dependence $exp(-\Lambda t)$, Eqs. (3.30)–(3.33) reduce to:

$$\begin{aligned}
\Big(\gamma(q+q^{-1})(\gamma+\gamma^{-1}) - \Lambda\Big)\tilde{\Omega}(x,y) \;&=\; \gamma\Big(\tilde{\Omega}(x-1,y) + \tilde{\Omega}(x+1,y) \qquad (3.36)\\
&\qquad + \tilde{\Omega}(x,y-1) + \tilde{\Omega}(x,y+1)\Big)\\
\Big(q^{-1} + \gamma^2 q - \Lambda\Big)\,\tilde{\Omega}(0,y) \;&=\; \gamma\Big(\tilde{\Omega}(0,y-1) + \tilde{\Omega}(0,y+1)\Big) \qquad (3.37)\\
\Big(q + \gamma^2 q^{-1} - \Lambda\Big)\,\tilde{\Omega}(x,L) \;&=\; \gamma\Big(\tilde{\Omega}(x+1,L) + \tilde{\Omega}(x-1,L)\Big) \qquad (3.38)\\
\Lambda\,\tilde{\Omega}(0,L) \;&=\; 0 \qquad (3.39)
\end{aligned}$$

with the inhomogeneous boundary condition $\tilde{\Omega}(x,x) = q^{2x}$. These equations can be solved using similar techniques as in Ref. [65] which rely mainly on the invariance of the bulk equation (3.36) under reflections $x \leftrightarrow y$ and $x \leftrightarrow L-y$. A trivial *inhomogeneous* solution is the empty lattice, for which $\tilde{\Omega}(x,y) = \gamma^{y-x} q^{y+x}$. The *homogeneous* set of solutions satisfies the condition $\tilde{\Omega}(x,x) = 0$ and reads

$$\begin{aligned}
\Phi_0(x,y) \;&=\; h(L-x)g(y) - h(L-y)g(x) \qquad (3.40)\\
\Lambda_0 \;&=\; 0
\end{aligned}$$

$$\begin{aligned}
\Phi_k^{(L)}(x,y) \;&=\; \sin\frac{\pi k x}{L}\,h(L-y) - \sin\frac{\pi k y}{L}\,h(L-x) \qquad (3.41)\\
\Lambda_k^{(L)} \;&=\; \gamma\left(\gamma q + \gamma^{-1} q^{-1} - 2\cos\frac{\pi k}{L}\right)
\end{aligned}$$

$$\begin{aligned}
\Phi_k^{(R)}(x,y) \;&=\; \sin\frac{\pi k x}{L}\,g(y) - \sin\frac{\pi k y}{L}\,g(x) \qquad (3.42)\\
\Lambda_k^{(R)} \;&=\; \gamma\left(\gamma q^{-1} + \gamma^{-1} q - 2\cos\frac{\pi k}{L}\right)
\end{aligned}$$

$$\Phi_{k,l}(x,y) = \sin\frac{\pi kx}{L}\sin\frac{\pi ly}{L} - \sin\frac{\pi ky}{L}\sin\frac{\pi lx}{L} \tag{3.43}$$
$$\Lambda_{k,l} = \gamma\left((q+q^{-1})(\gamma+\gamma^{-1}) - 2(\cos\frac{\pi k}{L} + \cos\frac{\pi l}{L})\right)$$

where $1 \leq k < l \leq L-1$ and the functions g and h are

$$g(x) = \frac{(\gamma q)^x - (\gamma q)^{-x}}{(\gamma q)^L - (\gamma q)^{-L}}\,, \qquad h(x) = \frac{(\gamma/q)^x - (\gamma/q)^{-x}}{(\gamma/q)^L - (\gamma/q)^{-L}}\,. \tag{3.44}$$

We can now compare the eigenvalues $\Lambda_0, \Lambda_k^{L,R}$ and $\Lambda_{k,l}$ with the spectrum computed in the last section. As in the symmetric case [65], Λ_0 gives a two-fold degenerate ground state while $\Lambda_k^{L,R}$ and $\Lambda_{k,l}$ are seen to be one- and two-particle excitations. However, in contrast to the symmetric case we have $\Lambda_k^L \neq \Lambda_k^R$ since these levels are shifted by $\pm\kappa$. Therefore the boundary effects of $\tilde{H}_2''$ do not change the selection rules, they only modify the mass gaps of the one-particle modes.

5 Probabilities for n holes

For a complete treatment of the system one has to study configurations with an arbitrary number of holes. This was already discussed in Ref. [31] and we will now carry out such a study. The probability to find the strings of sites $(x_1+1,\cdots,y_1),(x_2+1,\cdots,y_2),\cdots,(x_n+1,\cdots,y_n)$ with $0 \leq x_1 < \cdots < y_n \leq L$ empty at time t is denoted by $\Omega_n(x_1,y_1,\cdots,x_n,y_n,t)$ and will also be called n–hole function. If no hole extends up to the boundaries, the time evolution of Ω_n takes the form :

$$\begin{aligned}\frac{d}{dt}\Omega_n(x_1,y_1,\cdots,x_n,y_n,t) &= \sum_{i=1}^{n}\Big[-\Big(\gamma_L+\gamma_R+(y_i-x_i-1)\delta\Big)\Omega_n(x_1,y_1,\cdots,x_n,y_n,t)\\ &\quad +\alpha_R\Omega_n(\cdots,x_i-1,y_i,\cdots,t) + a_L\Omega_n(\cdots,x_i+1,y_i,\cdots,t)\\ &\quad +a_R\Omega_n(\cdots,y_i-1,x_{i+1},\cdots,t) + \alpha_L\Omega_n(\cdots,y_i+1,x_{i+1},\cdots,t)\Big]\end{aligned} \tag{3.45}$$

with the parameters defined in (3.29). The $i^{\rm th}$ term in the sum on the right hand side can be identified as time evolution of a one–hole function (3.30). In the following we choose the reaction rates according to (3.8) and rescale the Ω_n as in the previous section:

$$\tilde{\Omega}_n(x_1,y_1,\cdots,x_n,y_n,t) = \gamma^{\sum_{i=1}^n(y_i-x_i)}\,q^{\sum_{i=1}^n(x_i+y_i)}\,\Omega_n(x_1,y_1,\cdots,x_n,y_n,t)\;. \tag{3.46}$$

Then the rescaled time evolution equation turns out to be invariant under an arbitrary permutation of the variables $(x_1,\cdots,y_n)$. This symmetry can be taken into account by introducing new coordinates $(z_1,z_2,\cdots,z_{2n-1},z_{2n}) := (x_1,y_1,\cdots,x_n,y_n)$. The complete system of equations then reads:

- if no holes touch the boundaries ($0 < z_1, z_{2n} < L$):

$$\begin{aligned}\frac{d}{dt}\tilde{\Omega}_n(z_1,\cdots,z_{2n},t) &= -n\gamma(\gamma+\gamma^{-1})(q+q^{-1})\tilde{\Omega}_n(z_1,\cdots,z_{2n},t) \\ &\quad +\gamma\sum_{i=1}^{2n}\Big[\tilde{\Omega}_n(\cdots,z_i-1,z_{i+1},\cdots,t)+\tilde{\Omega}_n(\cdots,z_i+1,z_{i+1},\cdots,t)\Big]\end{aligned} \tag{3.47}$$

- if the leftmost hole touches the boundary ($0 = z_1, z_{2n} < L$):

$$\begin{aligned}\frac{d}{dt}\tilde{\Omega}_n(0,z_2,\cdots,z_{2n},t) &= -((n-1)\gamma(\gamma+\gamma^{-1})(q+q^{-1})+\gamma^2 q+q^{-1})\tilde{\Omega}_n(z_1,\cdots,z_{2n},t) \\ &\quad +\gamma\sum_{i=2}^{2n}\Big[\tilde{\Omega}_n(\cdots,z_i-1,z_{i+1},\cdots,t)+\tilde{\Omega}_n(\cdots,z_i+1,z_{i+1},\cdots,t)\Big]\end{aligned} \tag{3.48}$$

- if the rightmost hole touches the boundary ($0 < z_1, z_{2n} = L$):

$$\begin{aligned}\frac{d}{dt}\tilde{\Omega}_n(z_1,\cdots,z_{2n-1},L,t) &= -((n-1)\gamma(\gamma+\gamma^{-1})(q+q^{-1})+\gamma^2 q+q^{-1})\tilde{\Omega}_n(z_1,\cdots,z_{2n},t) \\ &\quad +\gamma\sum_{i=1}^{2n-1}\Big[\tilde{\Omega}_n(\cdots,z_i-1,z_{i+1},\cdots,t)+\tilde{\Omega}_n(\cdots,z_i+1,z_{i+1},\cdots,t)\Big]\end{aligned} \tag{3.49}$$

- if the leftmost and the rightmost holes touch the boundaries ($0 = z_1, z_{2n} = L$):

$$\begin{aligned}\frac{d}{dt}\tilde{\Omega}_n(0,z_2,\cdots,z_{2n-1},L,t) &= -(n-1)\gamma(\gamma+\gamma^{-1})(q+q^{-1})\tilde{\Omega}_n(z_1,\cdots,z_{2n},t) \\ &\quad +\gamma\sum_{i=2}^{2n-1}\Big[\tilde{\Omega}_n(\cdots,z_i-1,z_{i+1},\cdots,t)+\tilde{\Omega}_n(\cdots,z_i+1,z_{i+1},\cdots,t)\Big]\end{aligned} \tag{3.50}$$

However, this set of linear equations for the n–hole functions is not closed since on the right hand side terms with $z_i = z_{i+1}$ appear. These terms have to be identified with $(n-1)$–hole functions according to

$$\tilde{\Omega}_n(z_1,\cdots,z_{2n}) = q^{2z_i}\,\tilde{\Omega}_{n-1}(z_1,\cdots,z_{i-1},z_{i+2},\cdots,z_{2n}) \text{ if } z_i = z_{i+1} \tag{3.51}$$

and therefore cause a coupling to the lower sectors as mentioned before. This coupling constitutes the main difficulty in solving the equations. A similar situation occurs for the spin correlation functions of the Glauber model, and in that case a method to solve the problem was developed by Bedeaux, Schuler and Oppenheim [32]. It can be applied in the present case, too. For that purpose we introduce new cumulant-like functions C_n with the property that

(1) C_n obeys the differential equations (3.47)-(3.50)

(2) $C_n(z_1,\cdots,z_{2n},t) = 0$ if $z_i = z_{i+1}$

Following Ref. [32], these functions are defined by

$$C_n(z_1,\cdots,z_{2n},t) = \sum_{\xi}(-1)^{|P|}\,(-1)^{(k-1)}\,(k-1)!\,\tilde\Omega_{n_1}(z_1^\xi,\cdots,z_{2n_1}^\xi,t) \times\tilde\Omega_{n_2}(z_{2n_1+1}^\xi,\cdots,z_{2n_1+2n_2}^\xi,t)\cdots\tilde\Omega_{n_k}(z_{2n-2n_k+1}^\xi,\cdots,z_{2n}^\xi,t)\ . \tag{3.52}$$

The sum on the right hand side of (3.52) runs over partitions ξ of the numbers $z_1,\cdots,z_{2n}$ into k subsets $(z_1^\xi,\cdots,z_{2n_1}^\xi),(z_{2n_1+1}^\xi,\cdots,z_{2n_1+2n_2}^\xi),\cdots,(z_{2n-2n_k+1}^\xi,\cdots,z_{2n}^\xi)$, with sizes n_j where $j=1,\cdots,k$. Within these subsets the z_i^ξ are ordered according to their magnitude. P is the permutation which transforms $(z_1,\cdots,z_{2n})$ into $(z_1^\xi,\cdots,z_{2n}^\xi)$ and $|P|$ denotes its (uniquely defined) sign. The first two functions C_1 and C_2 read explicitly:

$$C_1(z_1,z_2,t) = \tilde\Omega_1(z_1,z_2,t) \tag{3.53}$$

$$C_2(z_1,z_2,z_3,z_4,t) = \tilde\Omega_2(z_1,z_2,z_3,z_4,t)-\tilde\Omega_1(z_1,z_2,t)\tilde\Omega_1(z_3,z_4,t) -\tilde\Omega_1(z_1,z_4,t)\tilde\Omega_1(z_2,z_3,t)+\tilde\Omega_1(z_1,z_3,t)\tilde\Omega_1(z_2,z_4,t) \tag{3.54}$$

The proof that the C_n have the property (2) by which the sectors are decoupled, is completely analogous to the one given in [32]. Property (1) holds since each term on the right hand side of equation (3.52) solves the differential equation (3.47)-(3.50).

However, this is only true if the conditions $\delta=0$ and $\alpha_R a_L=\alpha_L a_R$ are satisfied so that the rescaled equations (3.47)-(3.50) are symmetric in the starting points x and end points y of the holes. In the general case, i.e. for arbitrary values of the parameters $\delta,\alpha_L,\alpha_R,a_L$ and a_R, this symmetry is lost and arbitrary products of $\tilde\Omega$–functions are no longer solutions of the generalisation of (3.47)-(3.50). Then the given construction of the C–functions fails. It may not be so surprising that the method of Bedeaux et.al., which was developed for the Glauber model, works also here only in the free fermion case. To get an idea whether the general case is integrable or not, one can apply Reshetikhin's criterion for integrability [70]:

$$\Big[\,H_n+H_{n+1},\Big[\,H_n,\ H_{n+1}\Big]\Big] = X_n - X_{n+1} \tag{3.55}$$

to the Hamiltonian (3.7), where X_n is an arbitrary 4×4 matrix. We found that it leads to the same restriction on the reaction rates, namely $\delta=0$ and $\alpha_R a_L=\alpha_L a_R$. It is known, however, that this criterion is not a necessary condition.

Turning to the solution of the equations, one first observes that they are inhomogeneous only for $n=1$. A particular solution C^P is again the empty lattice:

$$C_1^P(z_1,z_2)=\gamma^{(z_2-z_1)}q^{(z_2+z_1)}\,,\qquad C_n^P=0\quad\text{for}\quad n\geq 2\ . \tag{3.56}$$

For the solutions of the homogeneous system we write

$$C_n^H(z_1,\cdots,z_{2n},t)=e^{-\Lambda t}\Phi^{(n)}(z_1,\cdots,z_{2n}) \tag{3.57}$$

and are left with an eigenvalue problem as in the previous section. As there, one finds four types of solutions (c.f. Eqs. (3.40)-(3.43)):

$$\Phi^{(n)}_{k_1,k_2,\cdots,k_{2n}} = \sum_{\tau\epsilon S_{2n}} (-1)^{|\tau|} \prod_{i=1}^{2n} \sin\frac{\pi k_i}{L} z_{\tau(i)} \tag{3.58}$$

$$\Lambda = n\gamma(\gamma+\gamma^{-1})(q+q^{-1}) - 2\gamma\sum_{i=1}^{2n}\cos\frac{\pi k_i}{L}$$

$$\Phi^{(n,L)}_{k_2,k_3,\cdots,k_{2n}} = \sum_{\tau\epsilon S_{2n}} (-1)^{|\tau|} \left(h(L-z_{\tau(1)}) \prod_{i=2}^{2n} \sin\frac{\pi k_i}{L} z_{\tau(i)} \right) \tag{3.59}$$

$$\Lambda = ((n-1)\gamma(\gamma+\gamma^{-1})(q+q^{-1}) + \gamma^2 q + q^{-1}) - 2\gamma\sum_{i=2}^{2n}\cos\frac{\pi k_i}{L}$$

$$\Phi^{(n,R)}_{k_1,k_2,\cdots,k_{2n-1}} = \sum_{\tau\epsilon S_{2n}} (-1)^{|\tau|} \left(\prod_{i=1}^{2n-1} \sin\frac{\pi k_i}{L} z_{\tau(i)} g(z_{\tau(2n)}) \right) \tag{3.60}$$

$$\Lambda = ((n-1)\gamma(\gamma+\gamma^{-1})(q+q^{-1}) + \gamma^2 q + q^{-1}) - 2\gamma\sum_{i=1}^{2n-1}\cos\frac{\pi k_i}{L}$$

$$\Phi^{(n,L,R)}_{k_2,k_3,\cdots,k_{2n-1}} = \sum_{\tau\epsilon S_{2n}} (-1)^{|\tau|} \left(h(L-z_{\tau(1)}) \prod_{i=1}^{2n-1} \sin\frac{\pi k_i}{L} z_{\tau(i)} g(z_{\tau(2n)}) \right) \tag{3.61}$$

$$\Lambda = (n-1)\gamma(\gamma+\gamma^{-1})(q+q^{-1}) - 2\gamma\sum_{i=2}^{2n-1}\cos\frac{\pi k_i}{L}$$

In these equations the k_i are integers with $1 \leq k_1 < \cdots < k_{2n} \leq L-1$. The sum runs over all elements of the permutation group S_{2n}. To understand these solutions we remark that each term in the sum of (3.58-3.61) solves equations (3.47-3.50) up to boundary conditions. These are satified by taking the totaly antisymmetric combination. In the case $n=1$ one recovers the results of section 5.

Comparing the eigenvalues Λ with the spectrum given in section 4 we find that they correspond to the excitation of $2n$, $2n-1$ and $2(n-1)$ fermions for the cases (3.58), (3.59)-(3.60) and (3.61), respectively. Furthermore, one has as many solutions as n–hole functions. Therefore the system of eigenfunctions found above is complete and the problem is thereby fully solved.

6 Properties of the steady state

The simplest application of the previous results is the investigation of stationary properties. The system has two steady states, namely a trivial one (the empty lattice) and a nontrivial one where particles are present. Considering the situation where at least one particle is present (i.e. $\Omega_{stat}(0,L)=0$) we have:

$$\Omega_{stat}(x,y) \;=\; 1-\gamma^{(L-y+x)}q^{(L-y-x)}\Phi_0(x,y) \tag{3.62}$$

Inserting Φ_0 from Eq. (3.40) then gives the following exact expression for the concentration $c(j)=1-\Omega_{stat}(j-1,j)$ at site j:

$$c(j)=\frac{1}{K}\Big\{\gamma^{2L}\Big((\gamma^2-1)+(q^2-1)\gamma^2(q\gamma)^{-2j}\Big)-q^{2L}\Big((\gamma^2-1)q^{2-4j}+(q^2-1)(q/\gamma)^{-2j}\Big)\Big\} \tag{3.63}$$

where

$$K=\gamma^2\left(\gamma^{2L}+\gamma^{-2L}-q^{2L}-q^{-2L}\right) \tag{3.64}$$

The density profile $c(j)$ is shown in Fig. 1 for 100 sites, a fixed asymmetry $q=1.2$ towards the left and various decoagulation rates Δ. As can be seen, there are three types of curves: If Δ is small, particles are found only near the preferred (left) boundary, while for large Δ a plateau exists together with some additional boundary effects. At the border between these two cases, the concentration decays linearly in the bulk. Computing the leading order of $c(j)$ for $L\to\infty$ gives the following explicit forms for the profile

$$c(j) \;=\; \begin{cases} \frac{\Delta}{1+\Delta}q^{2-4j}+\frac{q^2-1}{1+\Delta}(\frac{q}{\gamma})^{-2j} & \text{if} \quad \Delta<q^2-1 \\ \frac{\Delta}{1+\Delta}(q^{2-4j}+1-\frac{j}{L}) & \text{if} \quad \Delta=q^2-1 \\ \frac{\Delta}{1+\Delta}+(q^2-1)((q\gamma)^{-2j}-(\frac{q}{\gamma})^{2L-2j}) & \text{if} \quad \Delta>q^2-1 \end{cases} \tag{3.65}$$

From these expressions one sees that three different inverse length scales given by $4\ln(q)$, $2\ln(q/\gamma)$ and $2\ln(q\gamma)$ appear which are related to those found in the fermion eigenfunctions of section 4. The mean concentration per site $\overline{c}$ in leading order for $L\to\infty$ is

$$\overline{c} \;=\; \begin{cases} \frac{A}{L} & \text{if} \quad \Delta<q^2-1 \\ \frac{1}{2}\frac{\Delta}{1+\Delta} & \text{if} \quad \Delta=q^2-1 \\ \frac{\Delta}{1+\Delta} & \text{if} \quad \Delta>q^2-1 \end{cases} \tag{3.66}$$

where

$$A \;=\; \frac{(1+\Delta-q^4)(1+\Delta-q^{-2})}{(1+\Delta-q^2)(1+\Delta)(q^2-q^{-2})} \;\geq\; 1\,. \tag{3.67}$$

Thus we have to distinguish two different phases. In the *low-density phase* $\Delta<q^2-1$ the asymmetric diffusion is strong enough to move the bulk particles to the boundaries where

they can coagulate. Here one has a stationary state with a finite number of particles $A \geq 1$ and therefore the mean concentration $\overline{c}$ is of order $1/L$. In the *high-density phase* $\Delta > q^2 - 1$, the bulk concentration $\frac{\Delta}{1+\Delta}$ is finite and independent of the asymmetry q so that $\overline{c}$ is of order one. At the transition $\Delta = q^2 - 1$ (i.e. $q = \gamma$ or $q = \gamma^{-1}$), one of the lengths diverges and one has a linear decay of the concentration in the bulk. This is also the point where the gap in the spectrum vanishes (c.f. section 4).

This phase structure also shows up in the stationary two-point correlation function. Denoting by n_i and n_j the occupation numbers at the positions $i < j$, its connected part is given by

$$\begin{aligned} g(i,j) &= \langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle \qquad (3.68) \\ &= \langle (1-n_i)(1-n_j) \rangle - \langle (1-n_i) \rangle \langle (1-n_j) \rangle \\ &= \Omega_2^{stat}(i-1,i,j-1,j) - \Omega_1^{stat}(i-1,i)\Omega_1^{stat}(j-1,j) \\ &= \gamma^{2(j-i-1)} \Big(\Omega_1^{stat}(i-1,j)\Omega_1^{stat}(i,j-1) - \Omega_1^{stat}(i-1,j-1)\Omega_1^{stat}(i,j) \Big) \end{aligned}$$

To derive the last formula one uses Eqs. (3.53), (3.54) and the f act that for stationary states all functions C_n for $n \geq 2$ vanish because their relaxational spectrum has no zero eigenvalues. Inserting the expression for the funtion $\Omega_1^{stat}(i,j)$ one has:

$$\begin{aligned} g(i,j) \;&= \gamma^{L+j-i-3}\, q^{L-j-i+1} \quad \Big[\Big(h(L-i+1) - (\gamma q^{-1})\, h(L-i) \Big) \Big((\gamma q)\, g(j-1) - g(j) \Big) \\ &\qquad - \Big((\gamma q)\, h(L-j+1) - h(L-j) \Big) \Big(g(i-1) - (\gamma q^{-1})\, g(i) \Big) \Big] \\ &\qquad - c(i)c(j) \qquad (3.69) \end{aligned}$$

In the symmetric case ($q = 1$) the system has a ground state of product form. Therefore the particle concentration $\Delta/(1+\Delta)$ equals the mean field value and the connected correlation function is zero. If there is an asymmetry to the left ($q > 1$), one finds the following properties

- In the low-density phase $\Delta < q^2 - 1$ the only region where correlations are present is the left boundary. Here the correlation function is negative since the dominating coagulation process reduces the probability that particles meet each other.

- In the high-density phase $\Delta > q^2 - 1$ there are correlations at both boundaries. As in the previous case they are negative at the left boundary and vanish in the bulk. At the right boundary where the particle concentration is reduced, decoagulation is the dominating process which increases the probability of neighbouring particles.

- At the phase transition $\Delta = q^2 - 1$ there is a linear decay of the correlation function for large distances. For large L and i/L, j/L fixed one has

$$g(i/L, j/L) = (\frac{\Delta}{1+\Delta})^2 \; (i/L)(1 - j/L) \qquad (3.70)$$

For short distances the correlations are nontrivial only near the left boundary where they have exponential form. For large L and i, j fixed

$$g(i,j) = -(\frac{\Delta}{1+\Delta})^2 \ (1 \ + \ \gamma^{-4i+2}) \ \gamma^{-4j+2} \tag{3.71}$$

In this case the remaining length scale $1/4\ln(\gamma)$ enters and describes the boundary effect.

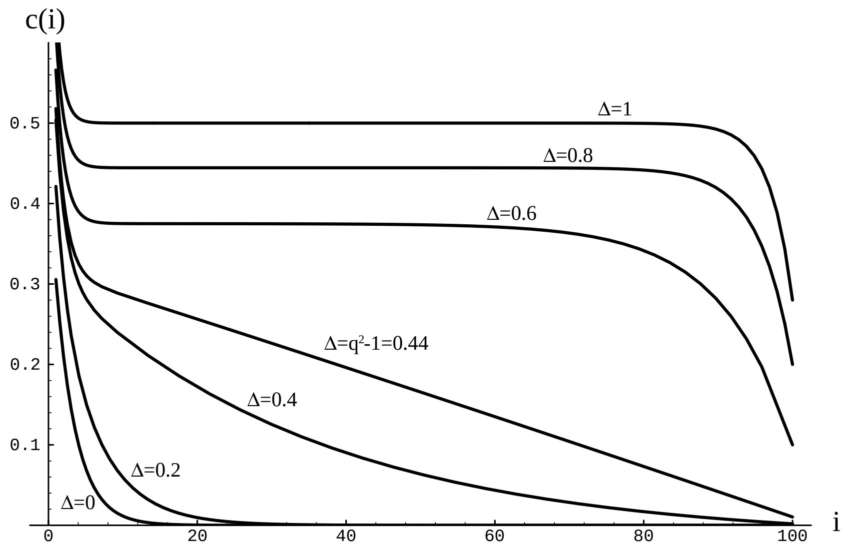


Figure 1: Particle concentration $c(i)$ for $q = 1.2$ and various values of Δ on a chain of 100 sites

7 Concluding remarks

We have studied the combined effect of a preferred direction and of open boundaries in a one-dimensional coagulation model. By formulating it as a quantum spin chain, the complete integrability was shown. The relaxation spectrum, although obtained from a non-hermitean operator, turned out to be real, with a gap determined by the asymmetry as well as by the decoagulation. An underlying S_3-symmetry of the Hamiltonian was found and the relaxational modes seen in the hole functions could be understood from the general result.

The hierarchy of equations for these functions was considered and decoupled by a method introduced previously for the kinetic Ising model. In this way a complete solution was achieved. The decoupling approach lead to the same restrictions on the rates as Reshetikhin's integrability criterion. There are other solvable cases where a relation to the XXZ Hamiltonian is used [72]. Whether further integrable situations exist, remains open.

As to the physical properties, it was found that the model has two phases with low and high average particle density, respectively. The corresponding density profiles and correlations were calculated. They contain the various lengths which arise from the interplay of decoagulation and asymmetry. The approach to the steady state also turns out to be interesting. Calculations show that at the transition point an initially full system first develops a plateau at the mean field value of the density before a slow relaxation to the linear density profile sets in. Only at the boundary one finds a simple algebraic decay with a $t^{-1/2}$ law.

A system with simple open ends, as considered here, is not the only possible case. More generally, one can supply and withdraw particles at the ends. The studies on this model will be published in [34]. Another possible direction would be to describe the coagulation process in more detail. This, however, would lead to models with more than two states per site which are more difficult to solve.

Chapter 4

Conclusion

In the present thesis we have investigated two algebraic methods for studying one-dimensional non-equilibrium systems.

The first method applies quadratic algebras to the eigenvector problem of one-dimensional quantum spin chains. It has been shown in chapter 2 that for any given m-state quantum spin Hamiltonian the quadratic algebra proposed in [21, 22] has at least one non-trivial representation. Furthermore every zero energy eigenstate of a m-state quantum spin Hamiltonian with open boundaries and single site boundary terms can be written in terms of a Fock–representation of the algebra. This was done in section 3 of chapter 2 by explicitely constructing the corresponding vacuum–like states of the Fock–representation. For periodic boundary conditions a trace on the quadratic algebra is used instead of the Fock–representation. In this case a general positive answer like in the open boundary case is not possible: There are eigenstates with energy and momentum zero which cannot be written in terms of a trace–like function on the algebra. An explicite example is given in the text (cf. section 4).

The second method applies so-called *hole*-functions (sometimes called interparticle distribution functions in the literature) to the asymmetric coagulation-decoagulation model with closed boundary conditions (cf. chapter 3). We found that the decoupling of the hierarchy of the hole-function requires the same conditions as in the case of periodic boundary conditions [31] whereas the solution of the lowest sector requires as additional condition equal asymmetry for coagulation and decoagulation rates. With these conditions a complete solution of the hierarchy was achieved by extending a method used by Bedeuax et. al. [32] in the context of the Glauber model. It was verified that the Hamiltonian corresponding to this model can be diagonalized in terms of free fermions if and only if the hierarchy of hole functions can by solved completely. The physical properties of the models have been studied using the hole-functions in the case where a total solution is possible. It was found that the stationary state of the model has two phases, a high-density and a low-density phase where the transition is triggered by the ratio between decoagulation and asymmetry rates. It has been shown that the application of hole-functions to the one-species coagulation-decoagulation model yields a complete solution of the model for an appropriate tunig of the reaction rates.

A generalization of this method to reaction-diffusion models with more than one species of particles has not been tried yet. This would be an interesting task for further studies, in particular because for these models a tool like “free fermions” is not available.

Acknowledgements

First of all I would like to thank V. Rittenberg for many discussions, helpful hints and for asking a numerous 'good questions'. I thank Haye Hinrichsen, Ingo Peschel for fruitful and friendly collaboration. Next I thank our group for the wonderful atmosphere. Especially, my thank goes to Thomas Heinzel, Ulrich Bilstein, Peter Arndt and Horatiu Simon for many discussions on life in general and physics in particular. Furthermore I would like to mention the fruitful discussions with Fabian Eßler and Gunter Schütz. Last, but not least, my thank goes to Thomas Sonntag for many discussions on physics, music, art and all that, and for correcting the proofs of this thesis.

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