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1996 J. Phys. A: Math. Gen. 29 2643

(http://iopscience.iop.org/0305-4470/29/11/005)

J. Phys. A: Math. Gen. **29** (1996) 2643–2649. Printed in the UK

On matrix product ground states for reaction–diffusion models

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Received 24 October 1995

Abstract. We discuss a new mechanism leading to a matrix product form for the stationary state of one-dimensional stochastic models. The corresponding algebra is quadratic and involves four different matrices. For the example of a coagulation–decoagulation model explicit four-dimensional representations are given and exact expressions for various physical quantities are recovered. We also find the general structure of n-point correlation functions at the phase transition.

Even for complicated one-dimensional many-particle models, the ground state can have a simple form. In spin problems it may be the tensor product of factors referring to single sites. While the correlations in this case are trivial, this is not so for a generalization where the product state is formed using matrices [1–5]. It has been found that the ground state of certain spin-one models and the stationary state for classical particles diffusing between two reservoirs have such a form. Excited states have also been described by the same ansatz [6]. So far, however, only diffusive systems have been treated successfully in this way. It is the aim of the present paper to show that the approach also works for more general situations. As an example, a particular reaction–diffusion model will be studied.

We consider a stochastic two-state model on a one-dimensional lattice with N sites. Its configurations are defined by the occupation numbers $\tau_1, \tau_2, \ldots, \tau_N$ each of which can take values 0 and 1. We say the system has a matrix product ground state if its stationary probability distribution $P_0(\tau_1, \tau_2, \ldots, \tau_N)$ can be written as

$$P_0(\tau_1, \tau_2, \ldots, \tau_N) \;=\; {Z_N}^{-1}\, \langle W| \prod_{j=1}^{N} (\tau_j D \,+\, (1-\tau_j)E\,)\, |V\rangle \tag{1}$$

where E and D are square matrices and $\langle W|$ and $|V\rangle$ are vectors acting in an auxiliary space. Z_N is a normalization constant defined as $Z_N = \langle W|(D+E)^N|V\rangle$. The matrix product in (1) can be written formally as a tensor product so that the stationary state $|P_0\rangle$ represented as a vector in configuration space is given by

$$|P_0\rangle = {Z_N}^{-1}\, \langle W| \begin{pmatrix} E \\ D \end{pmatrix}^{\otimes N} |V\rangle \;. \tag{2}$$

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0305-4470/96/112643+07$19.50

The matrix product representation is a powerful tool, since various physical quantities like the particle density

$$\langle \tau_j \rangle_N = \frac{\langle W | \, C^{j-1} D C^{N-j} \, | V \rangle}{\langle W | \, C^N \, | V \rangle} \qquad \text{with} \quad C = D + E \,. \tag{3}$$

can be computed directly. Correlation functions are given by similar expressions in which C plays the role of a transfer matrix.

The matrices used for the above ansatz may by finite or infinite dimensional [2, 4]. We are going to study an example for the first case below. The fact that the probability distribution of some system is given by a product of finite-dimensional matrices has far reaching consequences. Depending on the properties of the matrix C, correlation functions in such systems can have two forms which we want to discuss briefly at this point. Suppose first that the d-dimensional matrix C is diagonalizable and has eigenvalues $\lambda_1, \ldots, \lambda_d$ with $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_{d-1} \leqslant \lambda_d$. Then any n-point correlation function can be written as

$$\langle \tau_{j_1} \tau_{j_2} \cdots \tau_{j_n} \rangle_N = \sum_{\{\sigma_i^\mu\}} c_N(\{\sigma_i^\mu\}) \, \exp\Bigg\{ - \sum_{\mu=1}^{d-1} (\xi_\mu)^{-1} \left[(j_1 - 1)\sigma_1^\mu + (j_2 - j_1 - 1)\sigma_2^\mu \right.$$

$$\left. + (j_3 - j_2 - 1)\sigma_3^\mu + \cdots + (j_n - j_{n-1} - 1)\sigma_n^\mu + (N - j_n)\sigma_{n+1}^\mu \right] \Bigg\} \tag{4}$$

where the first sum runs over all $\sigma_i^\mu = 0, 1$ under the restriction $\sum_{\mu=1}^{d-1} \sigma_i^\mu \leqslant 1$. The quantities $\xi_\mu = \{\log(\lambda_d/\lambda_\mu)\}^{-1}$ are the correlation lengths. The $c_N(\{\sigma_i\})$ are some coefficients which depend on the system size N and approach constant values for $N \gg 1$. All correlations depend exponentially on the distances involved [4] and the number of length scales equals the number of different eigenvalues of C minus one.

The situation changes if C is not diagonalizable. In this case the matrix can be classified according to its Jordan normal form. As long as the Jordan block $J_{\max}$ of the largest eigenvalue is one-dimensional, the correlation functions again decay exponentially (the only difference to equation (4) is that algebraic prefactors to the exponentials may occur). On the other hand, if the dimension l of $J_{\max}$ is larger than one, the correlations are dominated by algebraic terms with positive powers. One can easily show that the n-point correlation functions are given by

$$\langle \tau_{j_1} \tau_{j_2} \cdots \tau_{j_n} \rangle_N = \sum_{\{\sigma_i = 0, \ldots, l-1\}} \left[c_N(\{\sigma_i\}) \; (j_1 - 1)^{\sigma_1} (j_2 - j_1 - 1)^{\sigma_2} (j_3 - j_2 - 1)^{\sigma_3} \right.$$

$$\left. \times \cdots \times (j_n - j_{n-1} - 1)^{\sigma_n} (N - j_n)^{\sigma_{n+1}} \right] + \text{exponential terms.} \tag{5}$$

Here the $c_N(\{\sigma_i\})$ are coefficients, the large-N asymptotics of which are generically proportional to $N^{-(l-1)}$. The exponential terms are of type (4) with algebraic prefactors and are generally negligible for large distances $j_1, (j_2 - j_1), \ldots, (j_n - j_{n-1}), (N - j_n) \gg 1$. The correlations (5) are completely different from those in a system with diagonalizable C. They involve the powers $0, 1, 2, \ldots, l-1$ of the distances. Only in special cases where all the $c_N(\{\sigma_i\})$ vanish are the correlations of type (4). It is worth mentioning another special case: if $l = 2$ and the element $D_{d,d-1}$ of the matrix D is zero, then all $c_N(\{\sigma_i\})$ with more than one σ_i equal to 1 vanish, i.e. the correlation functions are linear in the positions $j_1, \ldots, j_n$. If in addition $D_{d,d} = 0$, the algebraic part of the correlation function depends on the arguments $(N - j_n)$ and N only, i.e. $\langle \tau_{j_1} \tau_{j_2} \cdots \tau_{j_n} \rangle_N \approx c'(1 - j_n/N) +$ exponential terms for $N \gg 1$ and $(N - j_n) \gg 1$ where c' is some constant. Let us also note that the stationary

correlations of any system with a ground state (1) containing finite-dimensional matrices do not involve negative or non-integer powers of the distances.

Up to now, matrix product ground states have been encountered in two situations. The first is found for models with the Hamiltonian $H = \sum_j h_{j,j+1}$ in which the two-site interaction h itself already annihilates the ground state, i.e. $h_{j,j+1}|0\rangle = 0$. Here the algebra of the operators E and D is given by

$$h\left[\begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix}\right] = 0\,. \tag{6}$$

An example for this type of model is the spin-1 antiferrromagnet discussed in [1]. The second case is realized in models with open boundaries and particle input and output at the ends of the chain. These models are described by a time evolution operator $H = \sum_{j=1}^{L-1} h_{j,j+1} + h_1^{(L)} + h_L^{(R)}$ where $h^{(L)}$ and $h^{(R)}$ are 2×2 matrices for particle input and output. Here the basic mechanism of the matrix product ground state relies on the fact that application of $h_{j,j+1}$ yields a divergence-like term on the right-hand side:

$$h\left[\begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix}\right] = \begin{pmatrix} e \\ d \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix} - \begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} e \\ d \end{pmatrix} \tag{7}$$

where e and d are numbers, normally $e = -d = 1$. Summing over the two-particle interactions, all these contributions cancel in the bulk of the chain. The remaining terms at the boundaries are cancelled by a proper choice of the vectors $\langle W|$ and $|V\rangle$:

$$\langle W|\, h^{(L)} \begin{pmatrix} E \\ D \end{pmatrix} = -\langle W| \begin{pmatrix} e \\ d \end{pmatrix} \qquad h^{(R)} \begin{pmatrix} E \\ D \end{pmatrix} |V\rangle = \begin{pmatrix} e \\ d \end{pmatrix} |V\rangle \tag{8}$$

so that $H|0\rangle = 0$. The most important two-state model of this type is the asymmetric exclusion process with external particle input and output [2–4, 6]. There are also three-state models to which the matrix product ansatz has been applied [5]. But, as mentioned in the beginning, all known examples are diffusive systems.

The generalization which we are going to use, consists in replacing the numbers e and d by matrices $\bar{E}$ and $\bar{D}$. The idea goes back to [6] where the special case $\bar{E} + \bar{D} = 0$ was introduced in order to solve the time evolution of the asymmetric diffusion model in one dimension. The generalized algebra

$$h\left[\begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix}\right] = \begin{pmatrix} \bar{E} \\ \bar{D} \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix} - \begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} \bar{E} \\ \bar{D} \end{pmatrix} \tag{9}$$

$$\langle W|\, h^{(L)} \begin{pmatrix} E \\ D \end{pmatrix} = -\langle W| \begin{pmatrix} \bar{E} \\ \bar{D} \end{pmatrix} \qquad h^{(R)} \begin{pmatrix} E \\ D \end{pmatrix} |V\rangle = \begin{pmatrix} \bar{E} \\ \bar{D} \end{pmatrix} |V\rangle \tag{10}$$

is quadratic on both the left- and right-hand sides. In contrast to the usual matrix ansatz (7) the generalized ansatz (9) can be applied to systems which include particle reactions.

As an example we consider the asymmetric coagulation–decoagulation model. In this model particles diffuse on a linear chain. When two of them meet, they can merge (coagulate) to a single one. In the same way a single particle can split up (decoagulate) into two particles. Assuming no particle input and output, we therefore have six different

processes:

diffusion to the left:	$\emptyset + A \to A + \emptyset$	with rate a_L
diffusion to the right:	$A + \emptyset \to \emptyset + A$	with rate a_R
coagulation at the left:	$A + A \to A + \emptyset$	with rate c_L
coagulation at the right:	$A + A \to \emptyset + A$	with rate c_R
decoagulation to the left:	$\emptyset + A \to A + A$	with rate d_L
decoagulation to the right:	$A + \emptyset \to A + A$	with rate d_R

In what follows we consider the special choice $a_L = c_L = q$, $a_R = c_R = q^{-1}$, $d_L = \Delta q$ and $d_R = \Delta q^{-1}$ where the diffusion and coagulation rates coincide and all reactions have the same bias in one spatial direction. Since in this case the model can be mapped on a free fermion model, it is integrable and various exact results have been obtained [7–9]. The model is controlled by two parameters, namely the asymmetry parameter q and the effective decoagulation rate Δ. Its phase diagram shows two phases, a low-density phase for $\Delta < q^2 - 1$ and a high-density phase for $\Delta > q^2 - 1$. At the phase transition point $\Delta = q^2 - 1$, the gap in the relaxational spectrum vanishes and algebraic long-range correlations can be observed [9]. In a basis $(\emptyset\emptyset, \emptyset A, A\emptyset, AA)$ the two-site term in the time evolution operator $H = \sum_{j=1}^{N-1} h_{j,j+1}$ reads

$$h = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & (\Delta+1)q & -q^{-1} & -q^{-1} \\ 0 & -q & (\Delta+1)q^{-1} & -q \\ 0 & -\Delta q & -\Delta q^{-1} & q + q^{-1} \end{pmatrix}. \tag{11}$$

Therefore the bulk algebra (9) is given by

$$0 = \bar{E}E - E\bar{E} \tag{12}$$

$$(\Delta+1)q\,ED - q^{-1}DE - q^{-1}DD = \bar{E}D - E\bar{D} \tag{13}$$

$$-q\,ED + (\Delta+1)q^{-1}DE - q\,DD = \bar{D}E - D\bar{E} \tag{14}$$

$$-\Delta q\,ED - \Delta q^{-1}DE + (q + q^{-1})\,DD = \bar{D}D - D\bar{D} \tag{15}$$

and the boundary conditions (10) read

$$\langle W|\,\bar{E} = \langle W|\,\bar{D} = \bar{E}|V\rangle = \bar{D}|V\rangle = 0\,. \tag{16}$$

Writing $C = E + D$, $\bar{C} = \bar{E} + \bar{D}$ and $\gamma^2 = \Delta + 1$, the algebra (12)–(15) simplifies to

$$[C, \bar{C}] = [E, \bar{E}] = 0 \tag{17}$$

$$\bar{E}C - E\bar{C} = (\gamma^2 q + q^{-1})\,EC - \gamma^2 q\,EE - q^{-1}\,CC \tag{18}$$

$$\bar{C}E - C\bar{E} = (\gamma^2 q^{-1} + q)\,CE - \gamma^2 q^{-1}\,EE - q\,CC\,. \tag{19}$$

In contrast to algebras for diffusive systems (7)–(8), the above commutation relations do not allow the number of factors in a given product of matrices to be reduced. Therefore products of different lengths are independent. Products of the same length, which correspond to a given system size, obey linear relations as follows. For a given product, e.g. $CECEE$, we compute the difference $\bar{C}ECEE - CECE\bar{E}$ by using the commutation relations (17)–(19). Writing $\langle W|\cdots|V\rangle \equiv \langle\cdots\rangle$ and using $\langle\bar{C}ECEE\rangle = \langle CECE\bar{E}\rangle = 0$ one obtains

$$\langle CECEE\rangle = \left(\gamma^2 q^{-1} + \gamma^2(q + q^{-1}) + (q + q^{-1}) + q\right)^{-1} \Big[\gamma^2 q^{-1}\langle EECEE\rangle + \gamma^2(q + q^{-1})\,\langle CEEEE\rangle + (q + q^{-1})\,\langle CCCEE\rangle + q\langle CECCE\rangle\Big]. \tag{20}$$

In general, if $\{P_i^{(k)},\ i \in 1,\ldots,N_k\}$ is the subset of products with N factors containing k matrices C, linear relations of this type have the form

$$\langle P_i^{(k)}\rangle = \sum_{j=1}^{N_{k+1}} c_{i,j}^{k,k+1}\langle P_j^{(k+1)}\rangle + \sum_{j=1}^{N_{k-1}} c_{i,j}^{k,k-1}\langle P_j^{(k-1)}\rangle \qquad (k=1,\ldots,N-1)\,. \tag{21}$$

As can be seen from the commutation relations, the coefficients $c_{i,j}^{k,k\pm1}$ obey

$$0 \leqslant c_{i,j}^{k,k\pm1} \leqslant 1 \qquad 0 < \sum_{j=1}^{N_{k\pm1}} c_{i,j}^{k,k\pm1} < 1 \qquad \sum_{m=\pm1}\sum_{j=1}^{N_{k+m}} c_{i,j}^{k,k\pm m} = 1\,. \tag{22}$$

Therefore by iterating equation (21) one gets more and more complicated linear expressions with positive coefficients which involve all subsets $k = 0,\ldots,N$. Since there are no such relations for $k = 0$ and $k = N$, one finally ends up with only two contributions:

$$\langle P_i^{(k)}\rangle = a_i^{(k)}\langle E^N\rangle + (1-a_i^{(k)})\,\langle C^N\rangle \qquad (0 < a_i^{(k)} < 1)\,. \tag{23}$$

The expectation values $\langle E^N\rangle$ and $\langle C^N\rangle$ are independent. Therefore the vector space of words $P_i^{(k)}$ of a given length decomposes into two subspaces in which the expectation values are proportional to $\langle E^N\rangle$ or $\langle C^N\rangle$, respectively. Consequently physical observables are parametrized by the ratio $\lambda := \langle E^N\rangle/\langle C^N\rangle$. This is related to the fact that the model has two independent ground states, a trivial one which is the empty lattice ($\lambda = 1$) and a non-trivial one where particles are present ($\lambda = 0$).

A trivial representation of the above algebra (16)–(19) is $E = C = 1,\ \bar{E} = \bar{C} = 0$ which describes a system without particles. In the symmetric case $q = 1$ there also is a second one-dimensional representation $E = 1,\ C = \gamma^2,\ \bar{E} = \bar{C} = 0$ corresponding to a factorized ground state with finite particle density $\Delta/(1+\Delta)$. In the general case $q \neq 1$ the model is known to involve three different length scales, and therefore any non-trivial representation of the algebra has a dimension $d \geqslant 4$. Furthermore representations of the algebra may be different in each sector so that they may depend explicitly on N and λ. We found a four-dimensional representation which is given by

$$E_1 = \begin{pmatrix} q^{-2} & q^{-2} & 0 & 0 \\ 0 & \gamma^{-2} & \gamma^{-2} & 0 \\ 0 & 0 & 1 & q^2 \\ 0 & 0 & 0 & q^2 \end{pmatrix} \qquad C_1 = \begin{pmatrix} q^{-2} & q^{-2} & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & \gamma^2 & q^2 \\ 0 & 0 & 0 & q^2 \end{pmatrix}$$

$$\bar{E}_1 = \begin{pmatrix} 0 & 0 & q^{-1} & (q^{-1}-q)^{-1} \\ 0 & 0 & q-q^{-1} & -q \\ 0 & 0 & \Delta(q-q^{-1}) & -\Delta q \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{24}$$

$$\bar{C}_1 = \begin{pmatrix} 0 & -\Delta q^{-1} & q^{-1} & (q^{-1}-q)^{-1} \\ 0 & \Delta(q^{-1}-q) & q-q^{-1} & -q \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\langle W_1| = \begin{pmatrix} 1-q^2,\ 1,\ 0,\ a \end{pmatrix} \qquad |V_1\rangle = \begin{pmatrix} b,\ 0,\ q^2,\ q^2-1 \end{pmatrix}$$

where

$$q^{2N}a - q^{-2N}b = \frac{q^{2N}(q^2-\gamma^2) + (\gamma)^{-2N}(\gamma^2-1)(q^2+1) - q^{-2N}(q^2\gamma^2-1)}{(\gamma^2-q^2)(\gamma^2-q^{-2})(q^2-q^{-2})}$$
$$+\frac{\lambda}{\lambda-1}\,\frac{(\gamma^2-1)(q^2+1)(q^{2N}+q^{-2N}-\gamma^{2N}-\gamma^{-2N})}{(\gamma^2-q^2)(\gamma^2-q^{-2})(q^2-q^{-2})}\,. \tag{25}$$

The case $\Delta \neq q^2-1$. For practical purposes it is desirable to have a representation in which the matrix C is diagonal. For $\Delta \neq q^2-1$ an appropriate similarity transformation yields

$$E_2 = \begin{pmatrix} q^{-2} & q^2-\gamma^{-2} & q^2-1 & q^2(1-\gamma^2) \\ 0 & \gamma^{-2} & 0 & \gamma^2-q^2 \\ 0 & 0 & 1 & \gamma^2(q^2-1) \\ 0 & 0 & 0 & q^2 \end{pmatrix} \qquad C_2 = \begin{pmatrix} q^{-2} & & & \\ & 1 & & \\ & & \gamma^2 & \\ & & & q^2 \end{pmatrix}$$
$$\langle W_2| = \left(\frac{1}{1-q^2\gamma^2}\,,\ 0\,,\ \frac{q^2}{q^2\gamma^2-1}\,,\ \frac{a\,(q^2-q^{-2})(\gamma^2-q^2)\gamma^2 - q^2\gamma^2}{(\gamma^2-1)(q^2+1)}\right) \tag{26}$$
$$|V_2\rangle = \left(\frac{b\,(q^4-1)(q^2\gamma^2-1)+q^4}{q^2+1}\,,\ 0\,,\ \frac{q^2(\gamma^2-1)}{\gamma^2-q^2}\,,\ \frac{(\gamma^2-1)q^2}{\gamma^4-\gamma^2q^2}\right).$$

Using this representation, it is easy to derive the particle density (3) in the sector $\lambda = 0$:

$$\langle\tau_j\rangle_N = \frac{\gamma^{2N}\left((\gamma^2-1)+(q^2-1)\gamma^2(q\gamma)^{-2j}\right) - q^{2N}\left((\gamma^2-1)q^{2-4j}+(q^2-1)(q/\gamma)^{-2j}\right)}{\gamma^2\,(\gamma^{2N}+\gamma^{-2N}-q^{2N}-q^{-2N})} \tag{27}$$

which coincides with the result obtained in [9]. We also checked that the two-point correlation function $\langle\tau_i\tau_j\rangle_N$ is obtained correctly.

The case $\Delta = q^2-1$ ($q > 1$). Here the two largest eigenvalues of the matrix C, namely $1+\Delta$ and q^2, coincide and C is not diagonalizable. We therefore choose a representation where C has Jordan normal form

$$E_3 = \begin{pmatrix} q^{-2} & q^2-q^{-2} & q^2-1 & \dfrac{q^4+q^{-2}-2q^2}{q^4-1} \\ 0 & q^{-2} & 0 & q^{-2} \\ 0 & 0 & 1 & -\dfrac{1+2q^2}{1+q^2} \\ 0 & 0 & 0 & q^2 \end{pmatrix}$$
$$C_3 = \begin{pmatrix} q^{-2} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & q^2 & 1 \\ 0 & 0 & 0 & q^2 \end{pmatrix} \tag{28}$$
$$\langle W_3| = \left(q^{-2}-1\,,\ 0\,,\ q^2-1\,,\ 1+a(1-q^{-2})\right)$$
$$|V_3\rangle = \left(1+b(q^2-q^{-2})\,,\ 0\,,\ -1\,,\ q^2-q^{-2}\right)$$

where

$$q^{2N}a - q^{-2N}b = \frac{L\,\lambda(q^{2L} - q^{-2L})}{1-\lambda} - L\,q^{-2L} - \frac{q^{2L} - q^{-2L}}{q^2 - q^{-2}}\,. \tag{29}$$

Using this representation, the density at a site j in the sector $\lambda = 0$ is easily obtained as

$$\langle \tau_j \rangle_N = \frac{q^{4N}}{q^{4N}-1}\left\{\frac{1}{N} + \left(1-q^{-2}\right)\left(1-\frac{j}{N}\right) + q^{-4j}\left[\left(q^2-1\right)\left(1-\frac{j}{N}\right) - \frac{1}{N}\right]\right\} \tag{30}$$

which agrees with the result from [9]. There is no term proportional to $(j-1)$ or $(j-1)(N-j)$ because of $D_{4,3} = D_{4,4} = 0$ (see equation (28)). It turns out that any n-point correlation function $\langle \tau_{j_1}\tau_{j_2}\cdots\tau_{j_n}\rangle_N$ depends only on the two positions j_1 and j_n. According to our discussion at the beginning of this paper, its algebraic part is a linear function in j_n only. In fact it is given by

$$\frac{q^{4N}}{q^{4N}-1}\left(1-q^{-2}\right)^{n-1}\left\{\left(1-q^{-2}\right)\left(1-\frac{j_n}{N}\right) + \frac{1}{N}\right\}\,.$$

The exponential part of $\langle \tau_{j_1}\tau_{j_2}\cdots\tau_{j_n}\rangle_N$ decays with j_1 on length scales $(2\log q)^{-1}$, $(4\log q)^{-1}$ and with j_n on the length scale $(2\log q)^{-1}$.

While an ansatz of type (1) with an algebra (9), (10) can be made for any one-dimensional reaction–diffusion model, it is not clear under which conditions a matrix representation really exists. In particular, we do not know if the existence of representations is related to the integrability of the system. One should therefore investigate non-integrable examples. Also the extension to systems with open boundaries would be of interest. However, since some open systems are known to have correlations decaying with negative powers of the positions, the corresponding matrix representations are expected to be infinite-dimensional.

Acknowledgments

HH gratefully acknowledges financial support by the Minerva foundation. We would like to thank V Rittenberg and G M Schütz for helpful hints and interesting discussions.

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