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# Matrix product eigenstates for one-dimensional stochastic models and quantum spin chains

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**Abstract.** We show that all zero-energy eigenstates of an arbitrary m-state quantum spin chain Hamiltonian with nearest-neighbour interaction in the bulk and single site boundary terms, which can also describe the dynamics of stochastic models, can be written as matrix product states. This means that the weights in these states can be expressed as expectation values in a Fock representation of an algebra generated by 2m operators fulfilling  $m^2$  quadratic relations which are defined by the Hamiltonian.

#### 1. Introduction

A number of problems in many-particle systems have been studied with the help of so-called matrix product states. The idea of this technique is to express physical quantities such as ground-state wavefunctions 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 [1] the technique has been used to find ground states of various quantum spin chains [2–4].

As was shown by Derrida *et al* [5], the steady state of the one-species asymmetric exclusion process with open boundaries can be written as a matrix product state. Later works study this process in more detail [6–8]. Examples for asymmetric exclusion processes with two species were investigated in [9, 10] 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 generalized by enclosing additional operators. This was first done in the study of the dynamics of the asymmetric exclusion processes [11, 12]. Another example is the algebra for the reaction-diffusion model studied in [13] which is generated by twice as many operators as the one from [5]. In this Fock algebra the recursion property is lost. The same is true for the algebra used in [14–17] for stochastic models with parallel updating.

One natural question that arises is the following: To which kind of problems can the matrix technique 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 matrix product eigenstates? In this paper we will prove the following proposition. Any zero energy eigenstate of a Hamiltonian with nearest-neighbour interaction in the bulk and single-site boundary terms can be written as a matrix product state with respect to the

Fock algebra (3.2) and (3.3) (see later), which is that of [13]. The technique of matrix product states was called the matrix product ansatz in the literature. What we will see is that this technique, in the form of (3.2) and (3.3), is not an ansatz but rather an identical reformulation of the eigenvector equation for the zero-energy eigenstate.

The bulk of the paper is organized as follows. In section 2 we define the class of Hamiltonians and in section 3 we give the proof of the proposition. We conclude with some remarks on matrix product techniques in section 4.

# 2. Definition of a class of models

The Hamiltonian we are going to consider in this paper is of the form

$$H = h^{(L)} + \sum_{j=1}^{N-1} h_{j,j+1} + h^{(R)}$$
(2.1)

with

$$h^{(L)} = h^{(l)} \otimes I^{\otimes (N-1)} \qquad h^{(R)} = I^{\otimes (N-1)} \otimes h^{(r)}$$
 (2.2)

and

$$h_{j,j+1} = I^{\otimes (j-1)} \otimes h \otimes I^{\otimes (N-j-1)}$$
(2.3)

where I is the  $(m \times m)$  identity matrix, h is an  $(m^2 \times m^2)$  matrix describing a two-site interaction in the bulk, and  $h^{(l)}$ ,  $h^{(r)}$  are  $(m \times m)$  matrices defining single-site boundary terms. This kind of Hamiltonian appears in the study of one-dimensional stochastic systems as well 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 N sites, each of which can be in either of m states. A configuration on the lattice is completely defined by the set of occupation numbers  $\{s_i\} = s_1, s_2, \ldots, s_N$  with  $s_i = 1, \ldots, m \ \forall i = 1, \ldots, N$ . The system evolves stochastically. During an infinitesimal time step dt its configuration  $\{s_i\}$  can change to a configuration  $\{s_i'\}$  with a probability  $r(\{s_i\}, \{s_i'\})$  dt where the  $r(\{s_i\}, \{s_i'\})$  are referred to as rates. This process can be described in terms of a rate equation which reads

$$\partial_t P(\{s_i\}, t) = \sum_{\{s_i' \neq s_i\}} [r(\{s_i'\}, \{s_i\}) P(\{s_i'\}, t) - r(\{s_i\}, \{s_i'\}) P(\{s_i\}, t)]$$
 (2.4)

where  $P(\{s_i\}, t) = P(s_1, s_2, \dots, s_N, t)$  is the probability of finding the configuration  $s_1, s_2, \dots, s_N$  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. at sites 1 and N, we assume additional processes to take place.

It is convenient to introduce a vector notation [13] by writing

$$|P(t)| = \sum_{\{s_i\}} P(s_1, s_2, \dots, s_N, t)|s_1| \otimes |s_2| \otimes \dots \otimes |s_N|$$
(2.5)

with

In terms of these vectors the rate equation reads

$$\partial_t | P(t) \rangle = -H | P(t) \rangle \tag{2.7}$$

where H is an  $(m^N \times m^N)$  matrix which is defined in terms of the rates. We call H the Hamiltonian here. For the processes we are studying it has the structure of (2.1)–(2.3). 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 N which is just the steady state of the system. It is denoted by  $|P_N\rangle$  and obeys the relation

$$H|P_N) = 0. (2.8)$$

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

Quantum spin chain. Consider a chain of length N 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 N. Then the system dynamics is described by a Schrödinger equation with a Hamiltonian of type (2.1)–(2.3) if we chose a spin s-representation and m = 2s + 1. The Hamiltonian generally does not have vanishing column sums as in the stochastic case, although 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 (2.7) it has the same mathematical structure; just as for the stochastic model we are often interested in the ground state of the Hamiltonian H.

# 3. Matrix product states

Let us now turn to the matrix product states [5–13]. We introduce an auxiliary vector space  $V_a$  and we define 2m operators  $D_s$  and  $X_s$  with  $s=1,2,\ldots,m$  acting on  $V_a$  as well as two vectors  $|W\rangle$  and  $\langle V|$  in  $V_a$ . (Vectors in the auxiliary space are denoted by  $|\ldots\rangle$ , in contrast to the vectors in the configuration space which are denoted by  $|\ldots\rangle$ .) Next we define a vector  $|\tilde{P}_N\rangle$  as

$$|\tilde{P}_{N}\rangle = \langle W| \begin{pmatrix} D_{1} \\ D_{2} \\ \vdots \\ D_{m} \end{pmatrix}^{\otimes N} |V\rangle \tag{3.1}$$

where  $\otimes$  stands for the direct product in the configuration space, so that the above equation reads in terms of its components:  $\tilde{P}_N(s_1, s_2, \dots, s_N) = \langle W | D_{s_1} D_{s_2} \dots D_{s_{N-1}} D_{s_N} | V \rangle$ . We call states of type  $|\tilde{P}_N|$  matrix product states.

Let H be a Hamiltonian of type (2.1)–(2.3) which has a zero-energy eigenstate for all lattice lengths N (a Hamiltonian describing a stochastic model always has this property). Then we can state the following proposition:

(i) If  $D_s$ ,  $X_s$  and  $|W\rangle$ ,  $\langle V|$  fulfil the following relations

$$\langle W|h^{(l)}\begin{pmatrix} D_1\\ D_2\\ \vdots\\ D_m \end{pmatrix} = -\langle W|\begin{pmatrix} X_1\\ X_2\\ \vdots\\ X_m \end{pmatrix} \qquad and \qquad h^{(r)}\begin{pmatrix} D_1\\ D_2\\ \vdots\\ D_m \end{pmatrix}|V\rangle = \begin{pmatrix} X_1\\ X_2\\ \vdots\\ X_m \end{pmatrix}|V\rangle \qquad (3.3)$$

then the vector  $|\tilde{P}_N|$  defined by equation (3.1) solves the equation for the zero-energy eigenstate, i.e.

$$H|\tilde{P}_N) = 0. (3.4)$$

(ii) For any vector  $|P_N|$  solving  $H|P_N| = 0$  one can find operators  $D_s, X_s$  (s = 1, 2, ..., m) and vectors  $\langle W|, |V\rangle$  in some space  $V_a$ , such that  $|P_N|$  can be represented as a matrix product state  $|\tilde{P}_N|$  defined by equation (3.1) and relations (3.2) and (3.3) are fulfilled in  $V_a$ .

Before we come to the proof of the statement we stress again that, in contrast to the algebra defined in [5–7], the relations (3.2) and (3.3) do not lead to recurrence relations for expectation values of products of different length in the operators  $D_s$  and  $X_s$ .

The proof of (i) is based on a site-by-site cancellation of terms when H is applied on  $|\tilde{P}_N|$ . The mechanism is basically the same as the one worked out in [5]. In the appendix we explain it in detail.

In order to prove (ii) we construct a representation of operators and vectors fulfilling the Fock algebra (3.2) and (3.3) using the eigenvectors  $|P_N|$  of systems with lengths  $N=1,2,\ldots$ . Let us define for any number  $M=1,2,\ldots$  an  $m^M$ -dimensional space  $V_M$  with a set of orthogonal basis vectors  $|s_1,s_2,\ldots,s_M\rangle(s_i=1,2,\ldots,m)$  as well as the one-dimensional space  $V_0$  with the basis vector  $|\cdot\rangle$ . We define the space  $V_a$  as the direct sum of all  $V_M$  with  $M=0,1,2,\ldots$ . The above basis vectors may be written as infinite column vectors with a 1 at position  $1+s_1+ms_2+m^2s_3+\cdots+m^{M-1}s_M$  and a 0 at all other positions, and their transposed  $\langle s_1,s_2,\ldots|$  can be written as the corresponding row vectors. Next we define operators  $D_s$  and  $X_s$  as well as vectors  $\langle W|$  and  $|V\rangle$  by means of their action on all the  $|s_1,s_2,\ldots\rangle$  which provides a matrix representation if we write the  $|s_1,s_2,\ldots\rangle$  as columns. The  $D_s$  we define by

$$D_{s_1}|s_2, s_3, \dots, s_N\rangle = |s_1, s_2, s_3, \dots, s_N\rangle$$
 (3.5)

for  $N=1,2,\ldots$  and  $s_i=1,2,\ldots,m$ . The  $X_s$  act on the basis vectors of  $V_{N-1}$ , i.e. on the

 $|s_1, s_2, \ldots, s_{N-1}\rangle$ , as

for  $N=1,2,\ldots$ , where  $h_{i,i+1}$  and  $h^{(R)}$  act on the N-fold tensor product in equation (3.6) according to their definitions (2.2) and (2.3). Note that each choice of N gives a different set of basis vectors in the column on the left-hand side, and taking successively  $N=1,2,\ldots$  all basis vectors will occur in this column exactly once. Hence, the above equation defines the action of each  $X_s$  on each basis vector in a consistent way. The vectors  $|V\rangle$  and  $\langle W|$  we define by

$$|V\rangle = |\rangle \tag{3.7}$$

$$\langle W|s_1, s_2, \dots, s_N \rangle = P_N(s_1, s_2, \dots, s_N)$$
 (3.8)

for  $N=1,2,\ldots$  and  $s_i=1,2,\ldots,m$ , where  $P_N(s_1,s_2,\ldots,s_N)$  are the components of  $|P_N|$ . The above definitions fix the  $D_s$ ,  $X_s$  and the  $\langle W|,|V\rangle$  completely up to a constant  $\langle W|$ . 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  $|P_N|$  by means of equation (3.1), i.e. that  $|\tilde{P}_N|$  is equal to  $|P_N|$  and that they obey the Fock algebra (3.2) and (3.3). Let us begin the first proof by rewriting (3.5) as

$$D_{s_1}D_{s_2}\dots D_{s_N}|\ \rangle = |s_1, s_2, \dots, s_N\rangle$$
 (3.9)

for  $N=1,2,\ldots$  and  $s_i=1,2,\ldots,m$ . (The above relation gives a more intuitive meaning of the representation we have chosen: a basis vector  $|s_1,s_2,\ldots,s_M\rangle$  is created by applying the sequence  $D_{s_1}D_{s_2}\ldots D_{s_M}$  on  $|\cdot\rangle$ .) Furthermore, using (3.8) we get

$$\langle W|D_{s_1}D_{s_2}\dots D_{s_N}| \rangle = P_N(s_1, s_2, \dots, s_N)$$
 (3.10)

for N = 1, 2, ... and  $s_i = 1, 2, ..., m$ .

Rewriting (3.10) as a direct product of vectors in the configuration space and using  $| \rangle = | V \rangle$  yields

$$\langle W | \begin{pmatrix} D_1 \\ D_2 \\ \vdots \\ D_m \end{pmatrix}^{\otimes N} |V\rangle = |P_N\rangle \tag{3.11}$$

for N = 1, 2, ..., which is what we were trying to prove.

In order to show that the above representation fulfils the algebra (3.2) and (3.3) we rewrite the definition (3.6) using (3.9) and multiply the column vector

$$\begin{pmatrix} D_1 \\ D_2 \\ \cdot \\ \cdot \\ \cdot \\ D_m \end{pmatrix}^{\otimes n}$$

from the left:

$$\begin{pmatrix}
D_{1} \\
D_{2} \\
\vdots \\
D_{m}
\end{pmatrix}^{\otimes n} \otimes \begin{pmatrix}
X_{1} \\
X_{2} \\
\vdots \\
X_{m}
\end{pmatrix} \otimes \begin{pmatrix}
D_{1} \\
D_{2} \\
\vdots \\
D_{m}
\end{pmatrix}^{\otimes (N-1-n)} | \rangle$$

$$= [h_{n+1,n+2} + h_{n+2,n+3} + \dots + h_{N-1,N} + h^{(R)}] \begin{pmatrix}
D_{1} \\
D_{2} \\
\vdots \\
D_{m}
\end{pmatrix}^{\otimes N} | \rangle$$

$$(3.12)$$

for n = 0, 1, ..., N - 1 and N = 1, 2, ...

The right-hand equation of (3.3) is nothing but the case n = 0, N = 1 of the above relation. Consequently it holds. Next we use (3.12) to compute

i.e.

for N = 2, 3, ....

Since the products of the  $D_s$  span the whole space  $V_a$ , (3.2) must hold in  $V_a$ . What remains to be proven is the left-hand equation of (3.3). We multiply (3.12) for n = 0 by  $\langle W |$  from the left and use (3.11):

$$\langle W | \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_N \end{pmatrix} \otimes \begin{pmatrix} D_1 \\ D_2 \\ \vdots \\ D_N \end{pmatrix}^{\otimes (N-1)} | \rangle = [h_{1,2} + h_{2,3} + \dots + h_{N-1,N} + h^{(R)}] | P_N \rangle.$$
 (3.15)

Now writing the Hamiltonian of an *N*-site system as  $H = h^{(L)} + h_{1,2} + h_{2,3} + \cdots + h_{N-1,N} + h^{(R)}$  and using  $H|P_N = 0$ , the above relation can be written as

$$\langle W | \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ \vdots \\ X_m \end{pmatrix} \otimes \begin{pmatrix} D_1 \\ D_2 \\ \vdots \\ \vdots \\ D_m \end{pmatrix}^{\otimes (N-1)} | \rangle = -h^{(L)} | P_N \rangle. \tag{3.16}$$

Using again (3.11) yields

$$\langle W | \begin{cases} h^{(l)} \begin{pmatrix} D_1 \\ D_2 \\ \vdots \\ D_n \end{pmatrix} + \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_N \end{pmatrix} \end{cases} \otimes \begin{pmatrix} D_1 \\ D_2 \\ \vdots \\ D_n \end{pmatrix}^{\otimes (N-1)} | \rangle = 0$$

$$(3.17)$$

for N = 1, 2, ...

Consequently the left-hand equation of (3.3) holds in  $V_a$ . This completes the proof that the matrices defined by (3.5)–(3.8) represent the algebra (3.2) and (3.3) and hence the proof of proposition (ii).

Let us add some remarks on the proof. We proved that the Fock algebra (3.2) and (3.3) has a non-trivial representation if an eigenstate with zero energy exists for all lattice lengths. The construction of the matrices obeying (3.2) can be performed 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  $|P_N(s_1, s_2, \ldots, s_N)\rangle$ , was only needed for the construction of a non-trivial scalar product involving the vectors  $\langle W|$  and  $|V\rangle$ . More precisely, the vectors  $|P_N(s_1, s_2, \ldots, s_N)\rangle$  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 (3.2) and (3.3) is not completely fixed and can be chosen independently in each vector space  $V_M$ . For that reason

it would be sufficient to require that at least for one lattice length N the Hamiltonian has a zero-energy eigenstate. In that case  $\langle W|$  is non-trivial only on the subspace  $V_N$ .

One may define a finite-dimensional  $V_a$  as the direct sum over all  $V_M$  with  $M \le N_{\text{max}}$  for some number  $N_{\text{max}}$ . A matrix representation of the algebra (3.2) and (3.3) can then be found to be assuming (3.5)–(3.8) for  $N=1,2,\ldots,N_{\text{max}}$  as well as  $D_s|s_1,s_2,\ldots,s_{N_{\text{max}}}\rangle=0$  and  $X_s|s_1,s_2,\ldots,s_{N_{\text{max}}}\rangle=0$ . Then equation (3.1) provides a matrix product representation for all eigenvectors  $|P_N\rangle$  with  $N \le N_{\text{max}}$ .

It is of course also possible to express the eigenstate of a non-zero eigenvalue as a matrix product state by adding an appropriate shift to the Hamiltonian. This is done by replacing h,  $h^{(l)}$  and  $h^{(r)}$  in equations (3.2) and (3.3) by  $h - \epsilon$ ,  $h^{(l)} - \epsilon^{(l)}$  and  $h^{(r)} - \epsilon^{(r)}$ , respectively. In this case the Hamiltonian H in (3.4) has to be replaced by H - E(N) with  $E(N) = \epsilon^{(l)} + \epsilon^{(r)} + (N-1)\epsilon$ , if N is the lattice length. The vector  $|P_N|$  is then an eigenstate with energy E(N). However, if  $\epsilon^{(l)}$ ,  $\epsilon^{(r)}$  and  $\epsilon$  are independent of N, equation (3.4) will have a non-trivial solution only for a finite number of lattice lengths N and  $\epsilon^{(l)}$  will therefore be non-trivial only on the corresponding subspaces  $V_N$  of  $V_a$ .

# 4. Concluding remarks

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 (3.2) and (3.3). 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 (3.2) and (3.3), one cannot 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 algebra (3.2) and (3.3) 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 was done in [5-10] where the operators  $X_s$  are replaced by numbers.

We have checked that our proposition is also true for the Fock algebra describing stochastic models with parallel updating [14].

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# Appendix. Proof of the eigenvalue equation for the matrix product state

Following the line of [5] we prove proposition (i), i.e. we show that the states (3.1) solve the eigenvalue equation (3.4) if (3.2) and (3.3) are fulfilled. Using definition (2.1) we write

$$H = h^{(l)} \otimes I^{\otimes (N-1)} + \sum_{j=1}^{(N-1)} I^{\otimes (j-1)} \otimes h \otimes I^{\otimes (N-j-1)} + I^{\otimes (N-1)} \otimes h^{(r)}.$$
(A.1)

Next we define a state  $|\overline{P}_N(k)|$  as

$$|\overline{P}_{N}(k)\rangle = \langle W| \begin{pmatrix} D_{1} \\ D_{2} \\ \vdots \\ D_{m} \end{pmatrix}^{\otimes(k-1)} \otimes \begin{pmatrix} X_{1} \\ X_{2} \\ \vdots \\ X_{m} \end{pmatrix} \otimes \begin{pmatrix} D_{1} \\ D_{2} \\ \vdots \\ D_{m} \end{pmatrix}^{\otimes(N-k)} |V\rangle. \tag{A.2}$$

Applying now the terms occurring in (A.1) on the state

$$|\tilde{P}_{N}\rangle = \langle W| \begin{pmatrix} D_{1} \\ D_{2} \\ \vdots \\ D_{m} \end{pmatrix}^{\otimes N} |V\rangle \tag{A.3}$$

yields

$$h^{(l)} \otimes I^{\otimes (N-1)} | \tilde{P}_N) = -| \overline{P}_N(1)) \tag{A.4}$$

$$I^{\otimes (j-1)} \otimes h \otimes I^{\otimes (N-j-1)} | \tilde{P}_N ) = | \overline{P}_N (j) \rangle - | \overline{P}_N (j+1) \rangle$$
(A.5)

$$I^{\otimes (N-1)} \otimes h^{(r)} | \tilde{P}_N) = | \overline{P}_N(N)$$
(A.6)

where the algebra (3.2) and (3.3) was used. Applying now the full operator H (see equation (A.1)) on the state  $|\tilde{P}_N|$  we get

$$H|\tilde{P}_{N}) = -|\overline{P}_{N}(1)| + \sum_{i=1}^{N} (|\overline{P}_{N}(j)| - |\overline{P}_{N}(j+1)|) + |\overline{P}_{N}(N)| = 0$$
(A.7)

which is what we were trying to show.

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