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LETTER TO THE EDITOR

On matrix product states for periodic boundary conditions

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Abstract. The possibility of a matrix product representation for eigenstates with energy and momentum zero of a general m-state quantum spin Hamiltonian with nearest-neighbour interaction and periodic boundary condition is considered. For this representation we use the quadratic algebra defined in Krebs and Sandow (Krebs K and Sandow S 1997 *J. Phys. A: Math. Gen.* **30** 3165), which is generated by $2m$ operators which fulfil m^2 quadratic relations, endowed with a trace-like function reflecting periodic boundary conditions. It is shown that *not* every eigenstate with energy and momentum zero can be written in this way. An explicit counter-example is given. This is in contrast to the case of open boundary conditions where every zero-energy eigenstate can be written as a matrix product state using a Fock-like representation of the same quadratic algebra.

In a previous paper [1] 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 letter we search 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. Let us start with a summary of the previous paper [1]. Consider a Hamiltonian of the following form:

$$H_{\mathrm{op}} = h_1 + \sum_{j=1}^{L-1} h_{j,j+1} + h_L. \tag{1}$$

The bulk interaction term $h_{j,j+1}$ acts locally on the sites j and $j+1$ and is defined by

$$h_{j,j+1} = \sum_{\mu,\nu,\sigma,\tau=1}^{m} \gamma_{\sigma\tau}^{\mu\nu} E_j^{\sigma\mu} E_{j+1}^{\tau\nu} \tag{2}$$

where the $E^{\sigma\tau}$ are $m \times m$-matrices with entries $(E^{\sigma\tau})_{\mu,\nu} = \delta_{\sigma,\mu}\delta_{\tau,\nu}$. The boundary terms h_1 and h_L act on the sites 1 and L, respectively, and have the form

$$h_1 = \sum_{\mu,\sigma=1}^{m} \alpha_\sigma^\mu E_1^{\sigma\mu} \qquad h_L = \sum_{\mu,\sigma=1}^{m} \beta_\sigma^\mu E_L^{\sigma\mu}. \tag{3}$$

Following the suggestion of [2], for each Hamiltonian of this type we introduce a quadratic algebra generated by $2m$ generators $D_1, \dots, D_m$, $X_1, \dots, X_m$ fulfilling the following m^2 quadratic relations determined by the coefficients of the bulk interaction term (2):

$$\sum_{\mu,\nu=1}^{m} \gamma_{\sigma\tau}^{\mu\nu} D_\mu D_\nu = X_\sigma D_\tau - D_\sigma X_\tau \qquad \sigma, \tau = 1, \dots, m. \tag{4}$$

By giving a representation it was shown in [1] that this algebra exits for every choice of the coefficients $\gamma_{\sigma\tau}^{\mu\nu}$ in (4). Furthermore, we introduce a Fock-representation of this algebra. We assume that there is an auxiliary vector space $\mathcal{V}$, where the generators $D_1, \ldots, D_m, X_1, \ldots, X_m$ act on, and states $|V\rangle$ and $\langle W|$ in $\mathcal{V}$ and its dual, respectively, such that the following relations hold:

$$\sum_{\mu=1}^{m} \alpha_\sigma^\mu \langle W|D_\mu = -\langle W|X_\sigma \qquad \sum_{\mu=1}^{m} \beta_\sigma^\mu D_\mu |V\rangle = X_\sigma |V\rangle \qquad \sigma = 1, \ldots, m. \tag{5}$$

The theorem proved in [1] makes two statements. The first one says that the state P defined by

$$P = \sum_{\tau_1,\tau_2,\ldots,\tau_L=1}^{m} \langle W|D_{\tau_1} D_{\tau_2} \ldots D_{\tau_L}|V\rangle u_{\tau_1}^{(1)} \otimes u_{\tau_2}^{(2)} \otimes \cdots \otimes u_{\tau_L}^{(L)} \tag{6}$$

where $u_\tau^{(k)}$ ($\tau = 1, \ldots, m$ and $k = 1, \ldots, L$) denotes the basis of the vector space of the kth site, is an eigenstate of H_{op} (1) with energy zero, i.e. $H_{\mathrm{op}} P = 0$. This can be shown using only the relations (4) and (5). A state of the form (6) is called a matrix product state. The second statement says that for *every* zero-energy eigenstate P' of H_{op} one can find a representation of the operators D_τ, X_τ and vectors $\langle W|, |V\rangle$ such that P' can be written in the form (6). We would like to stress that the bulk algebra (4) exists for every choice of the coefficients $\gamma_{\sigma\tau}^{\mu\nu}$ whereas the existence of the Fock representation (5), more precisely of the vectors $\langle W|$ and $|V\rangle$, depends on the existence of a zero-energy eigenstate of H_{op}.

Now we turn to periodic boundary conditions and ask for statements analogous to that described above. We consider a Hamiltonian of the form

$$H_{\mathrm{per}} = \sum_{j=1}^{L} h_{j,j+1} \tag{7}$$

with periodic boundary conditions where the bulk interaction term $h_{j,j+1}$ is again given by (2). As in the open boundary case, to each Hamiltonian of the form (7) we may again associate the quadratic algebra (4) which is determined just by the coefficients of $h_{j,j+1}$. 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 (4). Thus, for a trace-like function tr and for any two elements A and B of the algebra the relations

$$\mathrm{tr}(AB) = \mathrm{tr}(BA) \tag{8}$$

$$\sum_{\mu,\nu=1}^{m} \gamma_{\sigma\tau}^{\mu\nu}\, \mathrm{tr}(AD_\mu D_\nu B) = \mathrm{tr}(AX_\sigma D_\tau B) - \mathrm{tr}(AD_\sigma X_\tau B) \tag{9}$$

hold. If a non-trivial trace-like function tr exists on the quadratic algebra (4), the state P_0 defined by

$$P_0 = \sum_{\tau_1,\ldots,\tau_L=0}^{m-1} \mathrm{tr}(D_{\tau_1} \ldots D_{\tau_L}) u_{\tau_1}^{(1)} \otimes u_{\tau_2}^{(2)} \otimes \cdots \otimes u_{\tau_L}^{(L)} \tag{10}$$

is an eigenstate of H_{per} with energy and momentum zero (cf [3]). This corresponds to the first statement of the theorem of [1]. 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 $\mathrm{tr}_{P_0'}$ such that P_0' is obtained by (10). 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 (10).

Before we come to this counter-example we would like to add some remarks on the relations between trace-like functions on the algebra (4) and traces of representations of (4). If one has a representation of (4) 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 [3, section 3.2]. This algebra can be decomposed into two sectors. For each sector a representation with a well-defined and non-trivial trace is given in [3]. 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 [4] 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 of 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 (4), which is obtained by taking $X_\tau = 0$ for $\tau = 1, \dots, m$, without any additional structure. If this coset algebra exists, the coefficients of the independent monomials are the weights of zero-energy eigenstates of the corresponding Hamiltonian with closed boundary conditions (i.e. the Hamiltonian (1) with $h_1 = h_L = 0$) [5]. 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 [5] 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 [6]. (It is interesting to note that only the sector with an equal number of particles for all species was treated in [6]. 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 (10) has momentum zero if and only if tr is invariant under cyclic permutations. Functions 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 [7]. A useful observation is that the relations (4) 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 (10) since for this state an appropriate trace-like function on the algebra (4) does not exist. Originally, my aim was to prove the analogue of the theorem of [1] 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 (4) needs more detailed conditions as the proof of the existence of a Fock-representation in the open boundary case [1]. Such conditions are still missing.

We consider the Hamiltonian H_3 which is defined as the Hamiltonian (7) on a three-site lattice with three states per site and the following coefficients of the bulk interaction term (2):

$$\gamma_{21}^{12} = \gamma_{12}^{21} = -\gamma_{13}^{31} = -\gamma_{23}^{32} = -\gamma_{12}^{12} = -\gamma_{21}^{21} = \gamma_{31}^{31} = \gamma_{32}^{32} = \alpha. \tag{11}$$

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

$$N_\tau = \sum_{j=1}^{3} E_j^{\tau\tau} \qquad \tau = 1, 2. \tag{12}$$

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 (4). Therefore we have to look for the conditions which the relations (8) and (9) put onto the values of any trace-like functions. If tr is such a trace-like function these conditions have the form

$$\mathrm{tr}(X_{\tau_1} D_{\tau_2} D_{\tau_3}) - \mathrm{tr}(X_{\tau_2} D_{\tau_3} D_{\tau_1}) = \sum_{\mu,\nu} \gamma^{\mu\nu}_{\tau_1\tau_2}\, \mathrm{tr}(D_\mu D_\nu D_{\tau_3}) \tag{13}$$

$$\mathrm{tr}(X_{\tau_1} X_{\tau_2} D_{\tau_3}) - \mathrm{tr}(X_{\tau_3} X_{\tau_1} D_{\tau_2}) = \sum_{\mu,\nu} \gamma^{\mu\nu}_{\tau_2\tau_3}\, \mathrm{tr}(X_{\tau_1} D_\mu D_\nu) \tag{14}$$

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 (13) and (14). We consider (13) and (14) 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 (10), there is a class of solutions of (13) and (14). (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 (13) and (14) can be found? It turns out that only ten independent classes of solutions exist corresponding to ten states of the form (10). Thus, one state out of 11 remains which cannot be written in this form. Let us now study the 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 ten. All symmetric states can be written with the help of a trace-like function on the algebra (4). 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 (4) with the coefficients of (11) reduce to the equations

$$\begin{aligned} 0 &= d_1 x_2 - d_2 x_1 \\ \alpha d_1 d_3 &= d_1 x_3 - d_3 x_1 \\ \alpha d_2 d_3 &= d_2 x_3 - d_3 x_2 \end{aligned} \tag{15}$$

where we have replaced the capital letters in (4) 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 (15) 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 (10) are just the independent monomials of degree three in the three variables d_1, d_2 and d_3. There are ten such monomials allowing as many independent states of the form (10). 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 (10). The orthogonal complement of the symmetric sector is generated by the single state φ defined by

$$\varphi = \sum_{\sigma\in S_3} \mathrm{sign}(\sigma) u^{(1)}_{\sigma(1)} \otimes u^{(2)}_{\sigma(2)} \otimes u^{(3)}_{\sigma(3)} \tag{16}$$

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 (4) with the coefficients (11) and allows us to write the state φ in the form (10). (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 (10), i.e.

$$\mathrm{tr}^*_\varphi(D_{\sigma(1)}D_{\sigma(2)}D_{\sigma(3)}) = \mathrm{sign}(\sigma) \qquad \sigma \in S_3. \tag{17}$$

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 (13) and (14) which immediately result from the quadratic relations (4) and the invariance of the trace-like function under cyclic permutations (8) and thus hold for any trace-like function tr. We claim that tr^*_φ is a trace-like function and use the necessary condition (13) to determine the values of tr^*_φ for monomials with one X-generator. Note that on the left-hand side of (13) only differences of traces-like functions of monomials appear whose indices differ through a cyclic permutation. Hence, if $\mathrm{tr}^*_\varphi(X_{\tau_1}D_{\tau_2}D_{\tau_3}) = t_{\tau_1\tau_2\tau_3}$ is a solution of (13) for given values of $\mathrm{tr}^*_\varphi(D_{\tau_1}D_{\tau_2}D_{\tau_3})$ then $\mathrm{tr}^*_\varphi(X_{\tau_1}D_{\tau_2}D_{\tau_3}) = t_{\tau_1\tau_2\tau_3} + w_{\tau_1\tau_2\tau_3}$, 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 (13). Making use of this ambiguity, the values $\mathrm{tr}^*_\varphi(X_{\tau_1}D_{\tau_2}D_{\tau_3})$ determined by (13) can be written in the form

$$\begin{aligned} &\mathrm{tr}^*_\varphi(X_1D_2D_3) = w_{123} + \alpha \qquad && \mathrm{tr}^*_\varphi(X_1D_3D_2) = w_{132} - \alpha \\ &\mathrm{tr}^*_\varphi(X_2D_3D_1) = w_{123} + \alpha && \mathrm{tr}^*_\varphi(X_2D_1D_3) = w_{132} - \alpha \\ &\mathrm{tr}^*_\varphi(X_3D_1D_2) = w_{123} && \mathrm{tr}^*_\varphi(X_3D_2D_1) = w_{132} \end{aligned} \tag{18}$$

where w_{123} and w_{132} are arbitrary constants. Up to these constants, the values of tr^*_φ in (18) are uniquely determined by (13). 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 (14) can be fulfilled by the function tr^*_φ defined so far. Therefore we define the following function:

$$Z_{\tau_1\tau_2\tau_3}[\mathrm{tr}] = \sum_{\mu\nu}[\gamma^{\mu\nu}_{\tau_1\tau_2}\,\mathrm{tr}(X_{\tau_3}D_\mu D_\nu) + \gamma^{\mu\nu}_{\tau_2\tau_3}\,\mathrm{tr}(X_{\tau_1}D_\mu D_\nu) + \gamma^{\mu\nu}_{\tau_3\tau_1}\,\mathrm{tr}(X_{\tau_2}D_\mu D_\nu)]. \tag{19}$$

From (14) we find $Z_{\tau_1\tau_2\tau_3}[\mathrm{tr}] = 0$ as a necessary condition for tr being a trace-like function. Taking the values of tr^*_φ defined in (18) we find

$$Z_{012}[\mathrm{tr}^*_\varphi] = 2\alpha^2 \neq 0. \tag{20}$$

Hence, the function tr^*_φ defined above is *not* a trace-like function on the algebra (4). 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 (20). Therefore a trace-like function on the quadratic algebra (4) whose values on the monomials without X-generators are determined by (17) does not exist at all. Hence, the state φ cannot be written in the form (10) with the help of an appropriate trace-like function on the quadratic algebra (4). This is what we wanted to show.

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