Note on a canonical form of matrix product states

2006 J. Phys. A: Math. Gen. 39 L357

(http://iopscience.iop.org/0305-4470/39/22/L02)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) L357–L360 doi:10.1088/0305-4470/39/22/L02

LETTER TO THE EDITOR

Note on a canonical form of matrix product states

Tomaž Prosen

Physics Department, Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia
and
Centre Emile Borel, Institut Henri Poincaré, 11 Rue P. et M. Curie, 75231 Paris Cedex 05, France

Received 6 February 2006
Published 16 May 2006
Online at stacks.iop.org/JPhysA/39/L357

Abstract

A canonical form for a matrix product state representation of a general finitely correlated quantum state on a one-dimensional (finite or infinite) lattice is proposed by exploring the gauge symmetry of the matrix product. This representation is unique in the sense that it is the only one which generates canonical forms for all reduced density matrices of the state.

PACS numbers: 03.67.Mn, 05.10.Cc

Finitely correlated states of one-dimensional interacting many-body quantum systems [1–3] admit a very useful *matrix product state* (MPS) representation which has recently been extensively explored for developing efficient renormalization group based numerical methods (e.g. [4–6]). However, the MPS representation suffers from ambiguity which makes numerical approximations potentially difficult to control. For example, when computing time evolution in terms of MPS representation, e.g. by the *time-evolved-block-decimation* scheme of Vidal [4], one has to truncate the MPS representation after each time step to a suitable small and finite dimension, but this truncation may in general depend on the representation of MPS as will be discussed below.

In this letter a unique canonical form of the MPS representation is proposed. This particular representation is distinguished by the fact that it generates canonical forms[1] of all possible reduced density matrices of the state, with all possible divisions of the lattice. For example, truncation of the auxiliary space in the proposed canonical representation will produce minimal distortion of the spectra of reduced density matrices.

Let us consider a finitely correlated state Ψ of a lattice of Nd-level quantum systems, $\Psi \in \mathbb{C}^{d^N}$, which is distinguished by the fact that its components in any *local* basis can be written in terms of matrix products

$$\Psi_{\alpha_1,\alpha_2,\ldots,\alpha_N} = \langle L|A_1^{\alpha_1} A_2^{\alpha_2} \cdots A_N^{\alpha_N}|R\rangle, \tag{1}$$

[1] This means that matrix products over a part of the lattice are orthogonal eigenvectors of the reduced density matrix corresponding to the complementary part of the lattice.

with a pair of vectors $|L\rangle, |R\rangle \in \mathbb{C}^D$ and a set of $N \times d$ matrices $A_n^\alpha \in \mathbb{C}^{D\times D}, n = 1, \ldots, N, \alpha = 1, \ldots, d$, acting in an auxiliary space of finite (and typically quite small) dimensionality D. [2] The smallest dimension D for which such MPS representation of the state Ψ can be achieved is related to the largest possible rank of the reduced density matrix

$$\rho^{(n)}_{(\alpha_1,\ldots,\alpha_n),(\beta_1,\ldots,\beta_n)} = \sum_{\gamma_{n+1},\ldots,\gamma_N} \Psi_{(\alpha_1,\ldots,\alpha_n,\gamma_{n+1},\ldots,\gamma_N)} \Psi^*_{(\beta_1,\ldots,\beta_n,\gamma_{n+1},\ldots,\gamma_N)}, \tag{2}$$

for all possible divisions $n = 1, 2, \ldots, N-1$, and consequently $\ln D$ is the upper bound on their Von Neuman entropies. Let us first assume that the system length N is *finite*, whereas we shall comment on the $N = \infty$ case at the end of the letter.

However, we note a great redundancy in parametrization (1), namely one should observe that the same state Ψ is generated,

$$\Psi_{\alpha_1,\alpha_2,\ldots,\alpha_N} = \langle \tilde{L}|\tilde{A}_1^{\alpha_1}\tilde{A}_2^{\alpha_2}\cdots\tilde{A}_N^{\alpha_N}|\tilde{R}\rangle, \tag{3}$$

by applying an arbitrary *local gauge transformation* of MPS data,

$$\tilde{A}_n^\alpha = G_{n-1}A_n^\alpha G_n^{-1}, \tag{4}$$

$$\langle\tilde{L}| = \langle L|G_0^{-1}, |\tilde{R}\rangle = G_N|R\rangle, \tag{5}$$

where $G_n, n = 0, 1, \ldots, N$, is an arbitrary set of *invertible* $D \times D$ matrices. In this letter we propose to explore the gauge symmetry (4) and define a unique canonical MPS which directly connects the data $\tilde{A}_n^\alpha, |\tilde{R}\rangle, |\tilde{L}\rangle$ to the spectra of the reduced density matrices $\rho^{(n)}$.

It is important to observe that MPS representation (1) does not in general explicitly generate canonical forms for the reduced density matrices $\rho^{(n)}$. We explain this fact below. Let us choose some ortho-normal basis $\{|j\rangle, j = 1, 2, \ldots, D\}$ of $\mathbb{C}^D$, and plugging the identity $1 = \sum_{j=1}^D |j\rangle\langle j|$ somewhere into (1) expresses our state Ψ as

$$\Psi_{\alpha_1,\ldots,\alpha_N} = \sum_{j=1}^D \Phi^{(L,n,j)}_{\alpha_1,\ldots,\alpha_n}\Phi^{(R,n,j)\,*}_{\alpha_{n+1},\ldots,\alpha_N}, \tag{6}$$

where $\Phi^{(L,n,j)}_{\alpha_1,\ldots,\alpha_n} := \langle L|A_1^{\alpha_1}\cdots A_n^{\alpha_n}|j\rangle$, $\Phi^{(R,n,j)}_{\alpha_{n+1},\ldots,\alpha_N} := \langle R|A_N^{\alpha_N\,\dagger}\cdots A_{n+1}^{\alpha_{n+1}\,\dagger}|j\rangle$. Again, this is in general *not* the Schmidt decomposition of the pure state Ψ (1) with respect to division n, the reason being that the D-tuple of states $\{\Phi^{(\mathtt{a},n,j)}, j = 1, \ldots, D\}$, where $\mathtt{a} = L, R$, are not orthogonal in general. A simple question which we pose here is whether there exists a gauge transformation (4) such that (6) would indeed become Schmidt decompositions for all partitions n, simultaneously. Indeed, as we show below the answer is positive and the solution is unique, modulo spectral degeneracies; thus it may be justified to call it *the canonical form of an MPS*.

Let us define, for each cut $1 \leqslant n \leqslant N-1$, $D \times D$ Hermitian and *non-negative* covariance matrices of the states $\Phi^{(\mathtt{a},n,j)}$,

$$\langle j'|V_n^L|j\rangle := \sum_{\alpha_1,\ldots,\alpha_n} \Phi^{(L,n,j')\,*}_{\alpha_1,\ldots,\alpha_n}\Phi^{(L,n,j)}_{\alpha_1,\ldots,\alpha_n}, \tag{7}$$

$$\langle j'|V_n^R|j\rangle := \sum_{\alpha_1,\ldots,\alpha_n} \Phi^{(R,n,j')\,*}_{\alpha_{n+1},\ldots,\alpha_N}\Phi^{(R,n,j)}_{\alpha_{n+1},\ldots,\alpha_N}, \tag{8}$$

which can be efficiently recursively generated in terms of *transfer operators*

$$\mathcal{A}_n(X) := \sum_{\alpha=1}^d A_n^\alpha X A_n^{\alpha\,\dagger}, \qquad \mathcal{A}_n^\dagger(X) := \sum_{\alpha=1}^d A_n^{\alpha\,\dagger} X A_n^\alpha, \tag{9}$$

[2] Note that superscript α is an index and not a matrix power.

namely

$$V_n^L = \mathcal{A}_n^\dagger\big(V_{n-1}^L\big), \qquad V_1^L = \mathcal{A}_1^\dagger(|L\rangle\langle L|), \tag{10}$$

$$V_n^R = \mathcal{A}_{n+1}\big(V_{n+1}^R\big), \qquad V_{N-1}^R = \mathcal{A}_N(|R\rangle\langle R|). \tag{11}$$

The reduced density matrix (2) can now be expressed as

$$\rho^{(n)}_{(\alpha_1,\ldots,\alpha_n),(\beta_1,\ldots,\beta_n)} = \sum_{j,j'=1}^{D} \Phi^{(L,n,j')}_{\alpha_1,\ldots,\alpha_n} \langle j'|V_n^R|j\rangle \Phi^{(L,n,j)*}_{\beta_1,\ldots,\beta_n} \tag{12}$$

and, similarly, by interchanging the indices L and R, for the complementary reduced density matrix where we trace over the left part.

Our main proposition will be based on the following observation. The non-vanishing part of the spectrum of $\rho^{(n)}$ agrees with the non-vanishing part of the spectrum of the matrix $V_n^L V_n^R$, or in other words, for any positive integer p, the spectral moments are the same

$$\mathrm{tr}(\rho^{(n)})^p = \mathrm{tr}\left(V_n^L V_n^R\right)^p. \tag{13}$$

This can be proven by recursive applications of equation (12) and using definitions (10),(11). For example, the normalization of the state can be expressed as $\|\Psi\|^2 = \mathrm{tr}\, V_n^L V_n^R$, for any n.

The question is whether the products $V_n^L V_n^R$ can be put in a simple, e.g. diagonal, form by a suitable gauge transformation (4). The transformation of covariance matrices can be derived straightforwardly

$$\tilde{V}_n^L = G_n^{-\dagger} V_n^L G_n^{-1}, \tag{14}$$

$$\tilde{V}_n^R = G_n V_n^R G_n^\dagger, \tag{15}$$

where we write $G_n^{-\dagger} := \big(G_n^{-1}\big)^\dagger$. Even though each covariance matrix separately does not transform according to a similarity transformation, their products do,

$$\tilde{V}_n^L \tilde{V}_n^R = G_n^{-\dagger} V_n^L V_n^R G_n^\dagger, \tag{16}$$

$$\tilde{V}_n^R \tilde{V}_n^L = G_n V_n^R V_n^L G_n^{-1}. \tag{17}$$

It is straightforward to prove that the product of non-negative Hermitian matrices is always diagonalizable[3], so we choose G_n, $n = 1, \ldots, N-1$, to be the matrix which transforms the product (17) into the diagonal form. Then, automatically, the other product (16) is diagonalized by $G_n^{-\dagger}$, so it follows that both $\tilde{V}_n^L$ and $\tilde{R}_n^L$ should be diagonal, $\tilde{V}_n^{\mathtt{a}} = \mathrm{diag}\big\{v_{n,j}^{\mathtt{a}};\, j = 1, 2 \ldots, D\big\}$. But in fact, only the product of eigenvalues $v_{n,j}^L v_{n,j}^R$ has a physical meaning, namely it is precisely the *eigenvalue of the reduced density matrix* $\rho^{(n)}$.

Note that with equation (17) the matrix G_n remains unspecified up to a left multiplication with an arbitrary non-degenerate diagonal transformation. This freedom we can use to make the diagonal covariance matrices strictly equal $\tilde{V}_n^L = \tilde{V}_n^R$ provided the matrices V_n^L, V_n^R were strictly positive (non-degenerate).[4] For example, for a practical numerical computation, one would first diagonalize the following positive Hermitian matrix,

$$\big(V_n^L\big)^{1/2} V_n^R \big(V_n^L\big)^{1/2} = U_n K_n U_n^\dagger, \tag{18}$$

[3] For strictly positive covariance matrices this is trivial, since $V_n^L V_n^R \sim (V_n^L)^{1/2} V_n^R (V_n^L)^{1/2}$, but in the case of non-trivial null spaces one can show explicitly that non-trivial Jordan blocks for eigenvalue 0 are prohibited.

[4] This is expected to be a typical situation for minimal dimension D allowed for a given state and sufficiently far from the edges, namely when $d^n, d^{N-n+1} > D$.

where U_n is unitary, and K_n is diagonal. Then we set

$$G_n = K_n^{-1/4} U^\dagger \left(V_n^L\right)^{1/2} \tag{19}$$

and we have, using (14),(15),

$$\tilde{V}_n^L = \tilde{V}_n^R = K_n^{1/2}. \tag{20}$$

The boundary gauge matrices, G_0 and G_n, which are still free, may always be chosen (5) to simplify the boundary states $|\tilde{L}\rangle = |\tilde{R}\rangle = |1\rangle$.

At the end, let us briefly comment on the case of *translationally invariant* states in infinite systems, $N = \infty$, $A_n^\alpha \equiv A^\alpha$. Then one has to consider the canonization described above just for one pair of covariance matrices which are given as maximal eigenvalue (1, if the state is normalized) eigenvectors of the transfer operators $\mathcal{A}$, $\mathcal{A}^\dagger$, or in practical calculations, as limits

$$V^L = \lim_{n\to\infty} \frac{1}{n^{r-1}} \mathcal{A}^{\dagger n}(|L\rangle\langle L|), \qquad V^R = \lim_{n\to\infty} \frac{1}{n^{r-1}} \mathcal{A}^n(|R\rangle\langle R|), \tag{21}$$

where r is the size of the Jordan block of the maximal eigenvalue, since in general a supermatrix of the transfer operator $\mathcal{A}$ may be *defective*. For example, $r = 1$ for the GHZ state $\Psi = 2^{-1/2}(|00\ldots\rangle + |11\ldots\rangle)$, $r = 2$ for W-state $\Psi = \lim_{N\to\infty} N^{-1/2}(|100\ldots\rangle + |010\ldots\rangle + \cdots)$, etc. Since now the canonizing gauge transformation is global, $G_n = G$, one has no freedom in selection of the boundary states $|\tilde{L}\rangle$, $|\tilde{R}\rangle$.

Acknowledgments

The author acknowledges the hospitality of the Institut Henri Poincaré (Paris) where this work has been performed, and support by Slovenian Research Agency, in particular by the grant J1-7347 and the programme P1-0044, and CNRS (France).

References

[1] Fannes M, Nachtargaele B and Werner R F 1992 *Commun. Math. Phys* **144** 443
[2] Klümper A, Schadschneider A and Zittartz J 1991 *J. Phys. A: Math. Gen.* **24** L955
[3] Ostlund S and Rommer S 1995 *Phys. Rev. Lett.* **75** 3537
[4] Vidal G 2003 *Phys. Rev. Lett.* **91** 147902
Vidal G 2004 *Phys. Rev. Lett.* **93** 040502
Zwolak M and Vidal G 2004 *Phys. Rev. Lett.* **93** 207205
[5] White S R and Feiguin A E 2004 *Phys. Rev. Lett.* **93** 076401 (see also *Preprint* cond-mat/0510124)
[6] Verstraete F, Garcia-Ripoll J J and Cirac J I 2004 *Phys. Rev. Lett.* **93** 227205