Characterizing Entanglement in Matrix Product Density Operators

M. Eckholt, J. J. García-Ripoll, M. Wolf and J. I. Cirac

Max-Planck-Institut für Quantenoptik
Garching bei München, Germany

Matrix Product States

Any pure state of a one-dimensional configuration of N d-dimensional system **can be represented** in terms of a matrix product state (MPS):

$$|\psi\rangle = \sum_{s_1,\ldots s_N=1}^{d} Tr\left(A[1]^{s_1} A[2]^{s_2} \ldots A[N]^{s_N}\right) |s_1,\ldots s_N\rangle$$

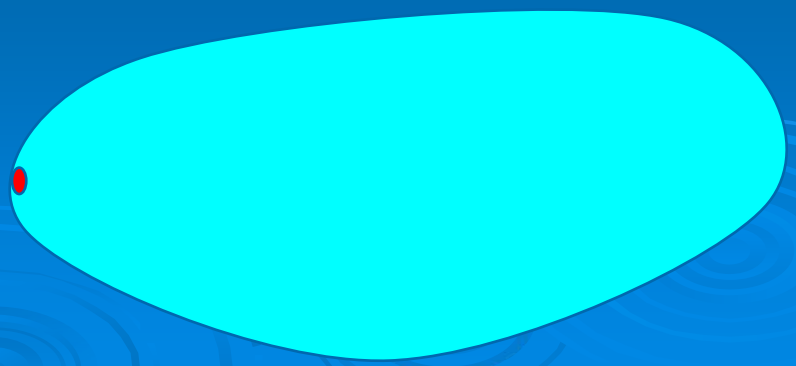
as long as the dimension D of the matrices can be chosen sufficiently large.

Thus, these states appear to be well suited to describe systems with short interactions, since a small dimension D may give a good approximation to the real state of the whole system.

MPS were firstly introduced as the ground state of the AKLT model, although an alternative derivation has been recently introduced independently by Guifré Vidal. This formalism has played a very important roll in the Density Matrix Renormalization Group (DMRG) method, providing it a coherent theoretical picture which underlies Quantum Information concepts.

Spin systems: basic properties

- The dimension of the Hilbert space scales exponentially with number of spins in the system.
- Universal ground state properties:
  - The entropy of a block of spins is proportional to the surface of the block (**holographic principle**).
  - Correlation functions typically decay with the distance between the spins (**correlation length**).
- The N-particle states with these properties form a tiny subspace of the exponentially large Hilbert space.



DMRG in brief

DMRG is a numerical technique for finding **accurate approximations of the ground state and low-lying excited states of strongly interacting quantum lattice systems.** Its accuracy, with a modest amount of computational effort, is remarkable for 1D systems and it is limited by the dimensionality or range of the interaction.

This method is based on the truncation of the Hilbert space used to represent the Hamiltonian **in a controlled way**, keeping the most probable eigenstates.

Formulated in terms of MPS, DMRG can be viewed as an **iterative method** that for a fixed D determines the matrices whose state $|\psi\rangle$ **minimizes the energy in a variational sense.**

$$E = \frac{\vec{A}[i]^\dagger H[i] \vec{A}[i]}{\vec{A}[i]^\dagger \vec{A}[i]} \quad \Longrightarrow \quad H[i]\vec{A}[i] = E\vec{A}[i]$$

MPS and Entanglement

The physical understanding of quantum many-body systems is hindered by the fact that the **number of parameters describing the physical states grows exponentially with the number of particles**. Thus, even for a relatively small number of particles, most of the problems become intractable.

In an MPS we reexpress the 2^N coefficients of $|\psi\rangle$ in terms of about $2D^2 \cdot N$ parameters

$$N \text{ qubit state} \quad \leftrightarrow \quad N \exp(E_D) \text{ parameters}$$

where $E_D := log_2(D)$ is a natural measure of entanglement.

Therefore, this leads to an efficient description of $|\psi\rangle$ if E_D scales as $\mathcal{O}(log(N))$ because in that case only $poly(N)$ parameters are required.

Matrix Product Density Operators

After the success of the MPS representation, a similar representation for mixed states has been brought forth: the class of **matrix product density operators** (MPDO)

$$\rho = \sum_{\substack{s_1 \ldots, s_N \\ s'_1 \ldots, s'_N = 1}}^{d} Tr\left(M[1]^{s_1, s'_1} M[2]^{s_2, s'_2} \ldots M[N]^{s_N, s'_N}\right) |s_1 \ldots s_N\rangle\langle s'_1 \ldots s'_N|$$

This can be done **mathematically** using the concept of purification. Through this procedure we obtain matrices with the following structure:

$$M[i]^{s_i, s'_i} = \sum_{a=1}^{d_i} A[i]^{s_i, a} \otimes \bar{A}[i]^{s'_i, a}$$

where d_i is the dimension of the reference system.

Characterization of the matrices

Any state written in the matrix-product formalism is **only** determined by a **set of N matrices**. Indeed, there is not only one set but an infinite number of them, leading to the same state.

Therefore, we can choose gauge conditions at each site to fix any mathematical freedoms we have. For **pure states** they are:

$$\sum_{s_i} A[i]^{s_i} \left(A[i]^{s_i}\right)^\dagger = \mathbb{I}$$

$$\sum_{s_i} \left(A[i]^{s_i}\right)^\dagger \Lambda[i-1] A[i]^{s_i} = \Lambda[i]$$

This constitutes the normal form for MPS. For **mixed states** we generalize these conditions to:

$$\sum_{s_i,\beta} M[i]^{s_i,s_i}_{\alpha\alpha',\beta\beta} = \delta_{\alpha\alpha'}$$

$$\sum_{s_i,\alpha,\alpha'} \bar{M}[i]^{s_i,s_i}_{\alpha\alpha',\beta\beta'} \Lambda[i-1]_{\alpha\alpha'} = \Lambda[i]_{\beta\beta'}$$

These conditions are a must for MPDO, because they do converge to the MPS normal form in the case that we deal with a **pure state** and they also imply that the matrices that appear in a **purification** of the state fulfil the MPS conditions. But they are not enough to characterize these matrices.

Considering the conditions a **density matrix** has to obey and that our state must have a **unique representation**, we find that:

$$M[i] = M[i]^\dagger$$

our matrices have to be **Hermitian**.

We would also like to find a condition for M[i] being, moreover, **positive matrices**, as appears when we work with purifications of the state.

Partial-Transpose criterion

An *easily* computable criterion for entanglement in mixed states was introduced in 1997 by Asher Peres:

If ρ is separable, then

$$\rho^{\top_A} \geq 0 \ \textit{and} \ \rho^{\top_B} = (\rho^{\top_A})^{\top} \geq 0$$

where the symbol $\top_i$ stands for the partial transpose (PT) of subsystem i.

This comes from the fact that the **transposition is a positive, but not completely positive, map**. A drawback of PT is that, in general, it is not a sufficient condition.

Entanglement in MPDO

As we have just seen, PT is an *easily* computable criteria for detecting entanglement in mixed states. It is considered *easy* because it consists of only two operations: **transposition** of one "part" of the system and **diagonalization** of the resultant matrix. But certainly, as the size of **our system grows** this becomes a *difficult* task.

On the other hand, this criterion might be applied to MPDO in an efficient way. In this representation, we only have to make the following change

$$M[i]^{s_i,s_i'} \longrightarrow M[i]^{s_i',s_i}$$

over all sites affected by the transposition.

If M[i] are positive matrices, we have that automatically **ρ is positive**, but the opposite does not have to be necessarily true. We expect that the matrices we obtain from our normal form do fulfil this, i.e.

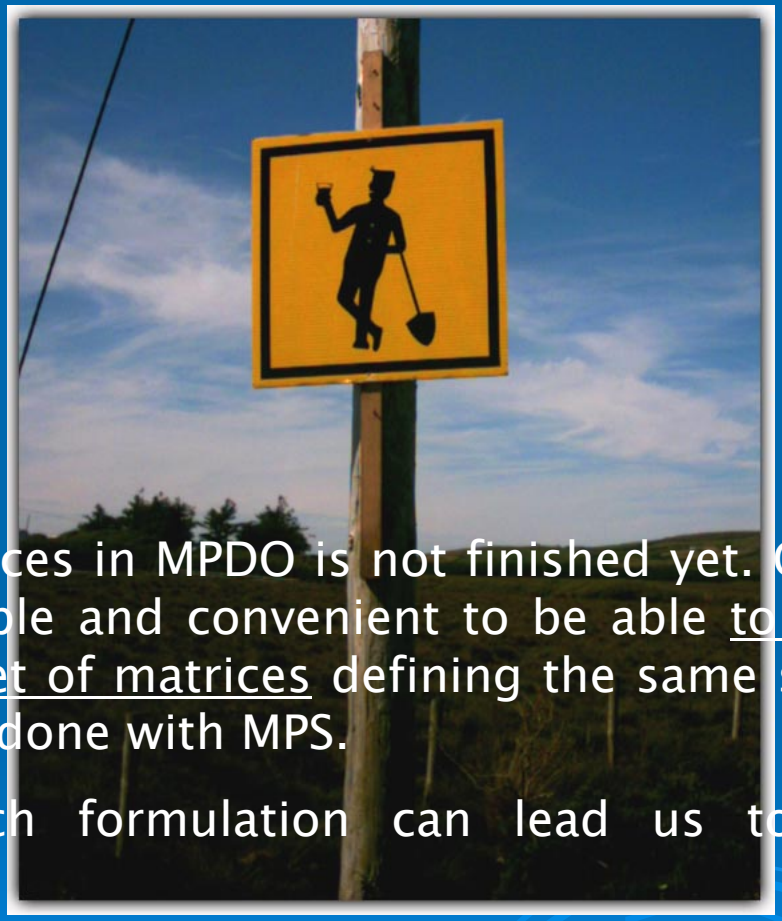
$$M[i] \geq 0 \Leftrightarrow \rho \geq 0$$

Altogether this would mean that, to apply the PT criterion to an MPDO, we would only have to check the positivity of the M[i] affected by the transposition.

If D is fixed, the **cost of this operation** for every matrix is fixed and for ρ it would only mean a linear growth with the size of the system.

Conclusions

This work is still in progress…



Our characterization of the matrices in MPDO is not finished yet. Once that is done, it would be desirable and convenient to be able to find these matrices from any other set of matrices defining the same state we are interested in, as it can be done with MPS.

It remains to be seen if such formulation can lead us to an entanglement-detection scheme.

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