# Sequentially generated states for the study of two-dimensional systems

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Matrix product states can be defined as the family of quantum states that can be sequentially generated in a one-dimensional system [Schön *et al.*, Phys. Rev. Lett. **95**, 110503 (2005)]. We introduce a family of states that extends this definition to two dimensions. Like in matrix product states, expectation values of few body observables can be efficiently evaluated and, for the case of translationally invariant systems, the correlation functions decay exponentially with the distance. We show that such states are a subclass of projected entangled pair states and investigate their suitability for approximating the ground states of local Hamiltonians.

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## I. INTRODUCTION

The description of quantum many-body systems is a complex problem due to the exponential growth of the dimension of the Hilbert space with the number of particles. In many cases of physical interest, however, states can be approximately described with a small number of parameters. This is the reason for the success of techniques such as the density matrix renormalization group (DMRG) [1], or those based on matrix product state (MPS) representations [2]. Those techniques take advantage of the local character of physical interactions, which favors states with a small amount of entanglement [3]. Their applicability is, however, limited to one-dimensional systems.

MPSs have a natural generalization to higher dimensional systems, namely the projected entangled pair states (PEPSs) [4]. Both representations are complete, i.e., any state of the Hilbert space can be written as a MPS or PEPS, and they have an efficient description in terms of the required number of parameters. However, they have very different properties. For example, MPSs can be efficiently created [5] and classically simulated [3], which makes them extremely useful for the study of quantum one-dimensional (1D) systems. However, creating and simulating PEPSs has been shown to be much harder [6]. Already computing local expectation values on PEPSs has an exponential cost in the general case. Nevertheless, they have proved successful for studying the ground states properties of two-dimensional (2D) systems by means of an approximate method [4,7]. In spite of having polynomial cost in all the parameters involved, the consumption of computational resources limits the application of those methods to relatively small 2D systems [7] or large ones but with moderate precision [8].

One of the goals in the research with many-body systems is to find other families of states providing an efficient description of systems in two or higher dimensions, while keeping a more benign behavior with regard to the determination of expectation values. Those studies may find immediate applications in the numerical studies of the physics of strongly correlated quantum systems. Thus, in the last years, other classes of states and corresponding variational methods have also been proposed to describe higher dimensional systems [9–14].

In this paper we present and discuss a generalization of MPSs to two dimensions. The family of states introduced here is a subfamily of PEPSs, specialized for 2D lattices: (i) which can be efficiently constructed and (ii) for which the expectation values can be efficiently determined. These properties (inherited from MPSs) make such states candidates for variational algorithms that search for ground states of local Hamiltonians.

The rest of the paper is organized as follows. In the next section we review the definitions and properties of MPSs and their PEPSs generalization. In Sec. III we introduce the family of states by presenting two alternative ways of extending the MPSs construction to 2D systems. In Sec. III B the main properties of such generalizations are discussed, whereas Sec. III C shows their performance as ansatz for a variational algorithm. We conclude with a discussion of these results in Sec. IV. The complete proof of the exponential decay of correlations in a translationally invariant state is deferred to the Appendix.

## II. EFFICIENT REPRESENTATIONS OF QUANTUM MANY-BODY STATES

As discussed above, having a representation of quantum states that captures the essential entanglement features turns out to be most desirable for the study of quantum many-body systems. A good representation should additionally satisfy some other properties. It is not only necessary that the state can be described or well-approximated in this manner, but also to be able to find such a description and to determine physical quantities in an efficient way.

Matrix product states satisfy all these requirements for one-dimensional systems. In the case of higher dimensions, the PEPSs family also provides an efficient representation of states, which by contrast results in a costly calculation of physical quantities. The following paragraphs review both families and their properties in some detail.

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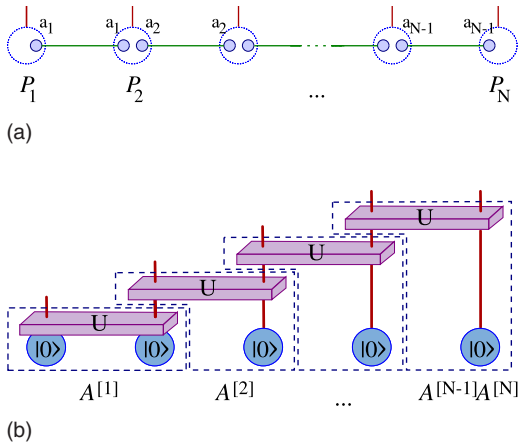


FIG. 1. (Color online) Scheme of MPS construction. In the valence bond picture (a), each entangled virtual pair is shown as a joined pair of circles, whereas the dashed circles represent the maps $P_k$ onto the physical spins, represented by vertical segments. In the sequential application of unitaries on groups of $M+1=2$ sites (b), each box represents the application of a unitary $U$ on two neighboring sites, and vertical lines correspond again to spin indices. The dashed lines show how $A$ matrices can be obtained from this sequential construction.

### A. One-dimensional systems: Matrix product states

As already discussed, MPSs constitute the paradigm of an efficient representation for one-dimensional quantum many-body systems [2]. Here we recall the various ways in which they can be defined, as well as their most significant properties.

#### 1. Definition

Let us consider a chain of $N$ $d$-dimensional systems. MPSs are defined in several equivalent ways.

(i) *Valence bond picture.* Each one of the physical spins is assigned two virtual particles of dimension $D$, each of them sharing a maximally entangled state (bond), $\Sigma_{a=1}^{D}|a,a\rangle$, with their neighbor. The state of the chain is obtained by applying at each site $k$ a map $P_k$ from the virtual pair onto the physical spin [see Fig. 1(a)]. If the mapping on site $k$ is

$$P_k = \sum_{i=1}^{d} \sum_{a,b=1}^{D} (A_k^i)_{a,b} |i\rangle\langle a,b|,$$

the states constructed by this procedure have the form

$$|\Psi\rangle = \sum_{i_1,\ldots,i_N=1}^{d} \mathrm{tr}(A_1^{i_1}\cdots A_N^{i_N})|i_1,\ldots,i_N\rangle, \qquad (1)$$

where each matrix $A_k^i$ has maximum dimension $D\times D$.

(ii) *Sequential generation.* As shown in [5], an arbitrary MPS with bond dimension $D$ can be equivalently generated by the sequential application of unitary operations between an ancilla system of dimension $D$ and the physical sites of the chain. Alternatively, the use of the ancillary system can be substituted by the application of unitary operations on sites of the chain, only, in a sequential manner [see Fig. 1(b)]. In this case, a unitary acting on $M+1$ sites can generate all MPSs with bond dimension $d^M$.

(iii) *Effective site blocks.* Another possibility to construct a MPS is to assign matrices $\tilde{A}_k^{\tilde{i}}$ to blocks of $M$ sites, instead of individual sites. The so constructed state is analogous to Eq. (1),

$$|\Psi\rangle = \sum_{\tilde{i}_1,\ldots,\tilde{i}_{N/M}=1}^{d^M} \mathrm{tr}(\tilde{A}_1^{\tilde{i}_1}\cdots\tilde{A}_{N/M}^{\tilde{i}_{N/M}})|\tilde{i}_1,\ldots,\tilde{i}_{N/M}\rangle, \qquad (2)$$

where now the sum runs over effective "spin" indices $\tilde{i}_k$ of dimension $d^M$. This gives again a way to construct the state, namely by applying unitary matrices, as described above, that act sequentially on groups of adjacent blocks.

#### 2. Properties

The most remarkable properties of MPSs are the following.

(i) Basis for DMRG. MPSs are intimately connected to DMRG and its success in the simulation of large 1D quantum systems. DMRG algorithms, in fact, optimize over MPSs of fixed bond dimension, $D$, to approximate the physical state [15]. In this sense, MPSs provide a basis for a variational DMRG procedure.

(ii) Efficiently contractable. The computation of expectation values of local operators in MPSs can be done efficiently. Given an operator $O=O_1\otimes O_2\otimes\cdots\otimes O_N$, which is a tensor product of local operators, its expectation value reduces to the trace of a matrix product

$$\langle\Psi_{MPS}|O|\Psi_{MPS}\rangle = \mathrm{tr}(E_{O_1}^{[1]}\cdots E_{O_N}^{[N]}), \qquad (3)$$

where every term $E_{O_k}^{[k]}=\Sigma_{i,i'}\langle i'|O_k|i\rangle[A_k^{i'^*}\otimes A_k^i]$ is a transfer matrix of size $D^2\times D^2$.

(iii) Exponentially decaying correlations in the translationally invariant case. If we consider an infinitely long chain, described by a translationally invariant MPS, i.e., with the same $A$ tensor for every site, generically the correlations between two sites decrease exponentially with the distance between them, $\langle O_k O_{k+\Delta}\rangle - \langle O_k\rangle\langle O_{k+\Delta}\rangle \approx e^{-\Delta/\xi}$. Here, $\xi$ is called the correlation length.

(iv) Complete family. Any state of the Hilbert space for $N$ particles can be cast in the form of a MPS with sufficiently large bond dimension [$D\approx O(d^{N/2})$ [3,16]]. Thus the MPSs classify the whole state space according to the dimension $D$. The lowest classes in this hierarchy prove to be most useful to describe the low energy sectors of quantum many-body systems with local interactions.

(v) Area law. By construction MPSs satisfy an area law, i.e., the entanglement entropy of a block of spins scales as the area of the block boundary. In the case of a MPS with bond dimension $D$, as the boundary crosses only two bonds, the entropy is upper bounded by $2\log D$.

(vi) Parent Hamiltonian. Every MPS is the ground state of a local Hamiltonian. Under some generic constraint on the MPS, this ground state is unique, and the parent Hamiltonian is gapped [2].

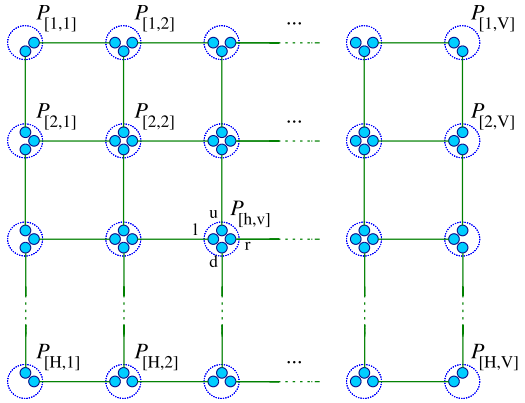


FIG. 2. (Color online) Scheme of PEPS construction. Solid lines join pairs of virtual particles that share a maximally entangled state, and dashed circles represent the mapping $P$ from the virtual particles onto the physical spin at each site.

(vii) Extensible to mixed states. The notion of a MPS is extended from pure to mixed states in the class of matrix product density operators (MPDOs) [17], which can be used to study one-dimensional many-body systems at finite temperatures.

### B. Generalization to higher dimensions: PEPS

#### 1. Definition

The valence bond construction above can be generalized in a natural way to graphs in higher dimensions by assigning to each site as many virtual particles as incoming edges. This yields the definition of PEPS. For example, a generic PEPS for a two-dimensional $H \times V$ square lattice is constructed by representing each physical site $(r,c)$ by four auxiliary systems of dimension $D$, each of them sharing a maximally entangled state with the adjacent neighbor, and then mapping all the virtual onto the physical degrees of freedom at each site (see Fig. 2). The state can be written

$$|\Psi\rangle = \sum_{i_{(1,1)}\cdots i_{(H,V)}=1}^{d} F_2(\{B^{[r,c]^{i_{(h,v)}}}\})|i_{(1,1)}\cdots i_{(H,V)}\rangle,$$

where the four-index tensors $B^i$ contain the mapping between virtual and physical systems at each site, and the function $F_2$ contracts all the virtual indices according to the bonds.

#### 2. Properties

As a generalization of the MPSs construction, PEPSs share with them some desirable characteristics. In particular they are a complete set and satisfy an area law. Nevertheless, PEPSs can support large correlations and cannot be efficiently contracted. Next we detail these and other properties.

(i) Complete basis. As MPS and PEPS form a complete set, i.e., any state can be written as a PEPS with high enough bond dimension.

(ii) No efficient contraction. Contrary to a MPS, the cost of contracting a PEPS scales in general exponentially with the number of systems. Therefore to devise a variational algorithm based on a PEPS it is necessary to use approximation methods [4,7] or to restrict the variational set to a subfamily of states (as [18] or the ones described below).

(iii) Large correlations. Different to the case of a MPS, the two-point correlation functions in a PEPS do not have to decay exponentially with the distance between sites. In [19], it was shown that there exist PEPSs with very low bond dimension $D=d$ reproducing the correlations and expectation values of classical thermal states for any classical two-body spin Hamiltonian. This is true in particular for the classical Ising model at the critical temperature, which has algebraically decaying correlations.

(iv) Area law. Like MPSs, PEPSs satisfy by construction the area law scaling of entanglement entropy, since the maximum entropy of a block is determined by the number of broken bonds, i.e., the size of the boundary [20].

(v) Parent Hamiltonian. Each PEPS is the ground state of a local Hamiltonian. If the PEPS satisfies an injectivity condition [21], the ground state is unique. Different to the case of a MPS this does not suffice to ensure the gapless character of the parent Hamiltonian.

## III. ALTERNATIVE GENERALIZATION: SEQUENTIAL FAMILIES

### A. Definition

The central idea of the generalization proposed here is to extend the sequential construction scheme of a MPS to 2D systems by allowing also the application of unitary operations along a second dimension. We can proceed in two ways.

#### 1. Sequentially generated states (SGSs)

For a $H \times V$ lattice, we may define a family of states in the following way. We consider each row $r$ to be in a pure state described by a certain MPS of bond dimension $D$, defined by tensors $A^{[r,c]}$. As already discussed, these tensors define a recipe for constructing the row states by sequentially applying unitary operations on groups of $M+1$ neighboring sites, with $M=\frac{\log D}{\log d}$. Then we apply a second layer of unitary operations as follows. Along each column, $c$, we apply unitary transformations on $M+1$ sites, starting on the $M+1$ bottommost rows and moving upwards, one row at a time [see Fig. 3(a)]. Thus the first unitary applied on column $c$ is $U^{[H,c]}$, whereas $U^{[r,c]}$ is the unitary operation acting on the physical index of $A^{[r-M,c]}$ and on the uppermost $M$ spin indices after the application of $U^{[r+1,c]}$. As in the MPS case, the bond dimension $D$ along either the vertical or the horizontal direction can be increased by applying unitary operations on a larger number of sites.

A well-known state that admits this description is the cluster state [22], which is given by the application of a single unitary to every pair of neighbors in the lattice. In such case, applications of the unitary to different sites commute among themselves and thus we can apply the unitaries in the sequential order described above.

#### 2. Block sequentially generated states (BSGSs)

Although, as described above, there is one natural way of extending the SGS construction by using larger unitaries

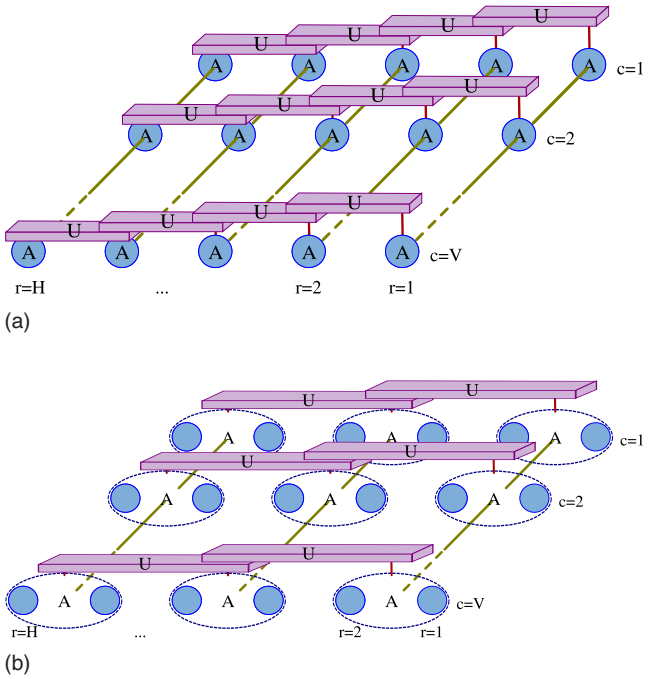


FIG. 3. (Color online) Scheme of sequential construction. In the construction of SGS, with unitaries acting on $M+1=2$ rows (a), each tilted line represents a MPS, connecting $A$ tensors in a given row, whereas boxes $U$ correspond to the action of a unitary on two neighboring rows. In (b) the construction of a BSGS is schematized, with blocks of $N=2$ rows. The dashed ellipses represent effective blocks of sites, each of them described by a single tensor $A$. The tilted lines then represent MPSs of larger dimension for a block of rows, and the unitary boxes $U$ now act on groups of effective sites.

along either direction, it turns out that this procedure does not improve the descriptive power of the SGS family. Instead, we may think of another generalization, adapting the idea of a MPS construction from effective site blocks. We must then define larger effective sites on which the two layers of unitaries are then applied. To this end, we first define a block taking together $N$ physical sites in the same column, so that we are left with a $\frac{H}{N}\times V$ lattice where sites have physical dimension $d^N$. On this system we construct a SGS by first applying unitary operations horizontally along each of the $\frac{H}{N}$ rows, to build a MPS, and then connecting the different rows by unitary operations on each column, as described above. These unitaries now connect neighboring effective sites, i.e., blocks of spins [see Fig. 3(b)].

Although the first definition (Sec. III A 1) is clearly contained in the second one, the opposite is not true. In fact, this second definition provides the systematic way to extend the family to cover the whole state space by taking larger blocks $N$, as we will discuss in the following paragraph.

### B. Properties

(i) Efficiently preparable and contractable. By construction, both families of sequentially generated states can be efficiently realized. Their implementation requires only the sequential application of local unitary operations along horizontal and vertical directions.

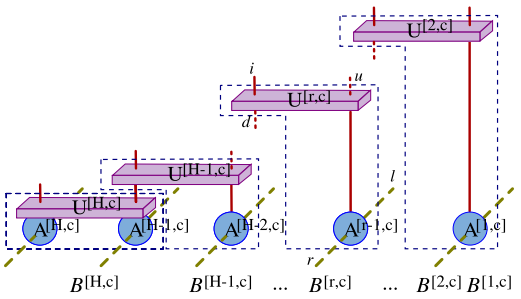


FIG. 4. (Color online) Any SGS can be written as a PEPS. The construction of the $B$ tensors for a given column, $c$, in the particular case $M=1$ (i.e., unitaries acting on two rows), is shown. For a generic site, the tensor $B^{[r,c]}$ is thus determined by the MPS matrix $A$ corresponding to the site that lies $M$ rows above and the unitary that acts on this and the $M$ sites below.

To construct a SGS with bond dimension $D$ along both directions the unitary matrices must act on $M+1$ sites, with $D=d^M$. For a $H\times V$ lattice the total number of unitary operations to be applied is then $H(V-M)+V(H-M)$.

Moreover, the contraction of a SGS can also be efficiently calculated on a classical computer. It is easy to see that computing the norm of such a state reduces to the product of norms of all the horizontal MPSs, as the product of all vertical unitaries appears contracted with exactly its adjoint. Therefore the unitarity of vertical bonding matrices reduces the normalization of the state to that of the underlying MPS.

The expectation value of the tensor product of a small number of local operators can also be efficiently calculated. Let us assume that we are interested in some tensor product of local operators acting on two sites, $(i_1,j_1)$, $(i_2,j_2)$, $\langle O\rangle = \langle O_1^{[i_1,j_1]}\otimes O_2^{[i_2,j_2]}\rangle$. The product of all the unitaries that act on a single column is itself a unitary operation that commutes with all the others, and with local operators acting on different columns. Therefore the contribution of all unitaries on columns different from $j_1$ and $j_2$ cancels in the expectation value. The same is true for unitaries on columns $j_1$ and $j_2$ that only affect rows above $i_1$ and $i_2$, respectively. The expectation value can then be written as a product of norms of the rows above times a contraction of a ladder structure. This is easily shown to scale as $d^2D^6$ [23]. These arguments also hold for the BSGS definition above, with only the appropriate effective values of $d$, $H$, and $D$.

(ii) Subfamily of PEPS. Any SGS can immediately be written as a PEPS of bond dimension upper bounded by $D$, with tensors $B^{[r,c]i}_{lurd}=\Sigma_{j=1}^{d}U^{[r,c]iu}_{dj}A^{[r-M,c]j}_{lr}$. Here $U^{[r,c]}$ is the unitary matrix that acts on rows $r-M$ to $r$ of column $c$, and $A^{[r-M,c]}$ is the MPS tensor corresponding to row $r-M$. The index $i$ is the free spin index of site $[r,c]$. So, the PEPS gets the horizontal $(l,r)$ bonds from the $r-M$ row, while the vertical bonds $u$ and $v$ are the composition of $M$ spin indices corresponding to the upper or lower rows (see Fig. 4).

The expression above is valid for rows $M<r<H$. The $B$ tensors in the last row, $r=H$, would also contain the contraction with the physical indices of all the $A$ matrices corresponding to rows below $H-M$, $B^{[H,c]}=U^{[H,c]}A^{[H-M,c]}\cdots A^{[H,c]}$. On the other hand, the corresponding term for the last unitary, $U^{[M+1,c]iu}_{dj}A^{[1,c]j}_{lr}$, will contain

the product of the $B$ tensors for rows 1 to $M+1$, which can be obtained from this term by means of singular value decompositions.

The converse is not true, as an arbitrary PEPS cannot always be expressed in this form. To express an arbitrary $B$ tensor as a SGS we could apply a singular value decomposition to split the horizontal indices, $lr$, from the rest. This may in general yield up to $D^2$ singular values. If this number is larger than the physical dimension $d$, the result will not lead to a valid $A$ matrix for a MPS with the same physical dimension. This bound on the number of singular values of $B$ constitutes a necessary condition for a state to be writable as a SGS, but it is not sufficient. One requires also that the first part of the singular value decomposition admits a reorganization of the indices to give a unitary matrix.

For the BSGS, each product $U^{[r,c]}A^{[r-M,c]}$ will render a $B$ tensor corresponding to an effective block of sites. To obtain a PEPS representation of the same state, such tensor has to be decomposed as the contraction of the vertical indices of $N$ individual $B$ tensors on the same column. This can always be achieved by an adequate singular value decomposition.

(iii) Decaying correlations. Due to their construction, which generalizes the sequential generation of a MPS, in a translationally invariant system these states show correlations that decay exponentially with the distance along both directions. In this case, the translational invariance implies that the state is described by a single $A$ tensor and a single unitary operation.

Although the complete proof of this property can be found in the Appendix, here we sketch the main ideas. To check the property, we independently analyze correlations along the horizontal and vertical directions. In the first case, we use the fact that, given the translational invariance, the underlying horizontal MPS are exponentially close to a product, so that their two-point correlations within one row decrease exponentially with the distance. Only the second layer of unitaries acting along the vertical direction can introduce corrections to this decay law. Nevertheless, we observe that such corrections can increase only linearly with the number of rows in the system, so that the exponential decay dominates as the total size and the distance tend to infinity.

On the other hand, correlations between two sites of the same column that lie on different rows are only due to the second layer of unitaries, since in the absence of the latter the state is a tensor product of MPS states for each row. In particular, for the kind of correlations under study, the only contribution comes from unitaries acting on the single column involved. It is easy to see that the situation is analogous to a translationally invariant MPS along the vertical direction with larger effective site dimension. This immediately implies that such correlations must also decay exponentially with the distance.

(iv) Area law. Being a subfamily of a PEPS, both a SGS and a BSGS satisfy the area law.

(v) Complete family. As discussed above, the family of SGSs cannot include arbitrary states, as in particular they are not always capable to describe a PEPS of given bond dimension. Nevertheless, the family of BSGSs provides a way of overcoming the limitations of the first one by increasing the size of the effective blocks. In this way, any state of a finite 2D system can be described as a BSGS by grouping together a large enough number of rows, $N$. Notice that, in the limit, $N=H$ and the BSGS description reduces to a MPS describing a chain of $V$ $d^N$-dimensional sites.

(vi) Basis for a variational algorithm. The properties above make these families a suitable ansatz for a variational algorithm that looks for the ground state of local Hamiltonians. The fact that they can be efficiently contracted grants the efficiency of such a procedure. Although the first family cannot describe arbitrary states, it is worth exploring its performance to find physically interesting states, arising as ground states of local Hamiltonians. The second family, on the other hand, grants a systematic procedure to improve the description of a system by considering larger and larger blocks of sites. The algorithm and the numerical study of its performance for both sequential families are described in the following section.

### C. Variational algorithms

We consider Hamiltonians with nearest-neighbors interactions, $H=\Sigma_{r,c}h_{[r,c]}$, where each term $h_{[r,c]}$ contains interactions of site $(r,c)$ with its adjacent neighbors in both directions, as well as possibly one-body terms. The algorithm should minimize the energy $E=\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$ with respect to the family of states in which we are interested.

The procedure can be built as in [16] by sequentially fixing all but one of the matrices ($A$ and $U$) that define the state, and then finding for the free matrix the optimal value, which minimizes the quantity above. The cost of the algorithm will be determined by the cost of contracting the lattice for local operators, which, as already discussed, can be done efficiently.

We carry out this program in two phases. First, we apply the iterative procedure over all the $A$ matrices that define the horizontal MPSs by sweeping over each row from left to right and back. This phase of the algorithm is almost identical to [16]. As described there, a gauge condition that ensures normalization is applied at each step, as well as techniques to improve the performance by storing partial contractions in memory as we move from one site to another. The only difference is that, in this case, different terms of the Hamiltonian contribute differently depending on the relative position of the rows on which they act with respect to the $A$ being optimized, and therefore more terms need to be calculated and stored as going from one row to the following.

The second phase of the algorithm consists in the optimization of the unitary matrices by a similar procedure. In this case, however, the quadratic character of $\langle\Psi|H|\Psi\rangle$ as a function of one particular $U$ is not enough to find the optimal matrices, because we must also impose the unitarity condition. This cannot be done by applying a gauge transformation, as is done for the $A$ matrices, therefore we employ a slightly different approach in order to find each $U$. Instead of directly optimizing the quotient above, we apply a small variation to the initial value of the unitary matrix, say $U^{[r,c]}=e^{i\delta K}U_0^{[r,c]}$, where $\delta$ is a small real value and $K$ is an unknown Hermitian matrix. To the first order in $\delta$, the energy is a linear function in $K$ (and its adjoint) that can be analytically

TABLE I. Lowest energy found for various two-body Hamiltonians by the variational algorithm using SGS states as ansatz. For each model and lattice size different bond dimensions $D$ are tested. The last column shows the relative error with respect to the best available PEPS result.

| Model | Lattice | $D$ | $E_0$ | $\varepsilon_r$ |
|---|---|---|---|---|
| Random | $8\times8$ | 2 | −169.309 | $5.7\times10^{-3}$ |
| | | 4 | −169.556 | $4.3\times10^{-3}$ |
| | | 8 | −169.613 | $4.0\times10^{-3}$ |
| Heisenberg | $8\times8$ | 2 | −153.737 | 0.0254 |
| | | 4 | −154.031 | 0.0235 |
| | | 8 | −154.142 | 0.0228 |
| | $10\times10$ | 2 | −244.830 | 0.0209 |
| | | 4 | −245.244 | 0.0193 |
| | | 8 | −245.383 | 0.0187 |
| Frustrated $XX$ | $8\times8$ | 2 | −90.598 | 0.016 |
| | | 4 | −91.242 | $9.0\times10^{-3}$ |
| | | 8 | −91.398 | $7.3\times10^{-3}$ |

optimized, with the constraints of Hermiticity $K=K^\dagger$ and normalization $\mathrm{tr}(K^\dagger K)=1$. For the so-found value of $K$, we update the unitary (with the largest possible $\delta$) and iterate the variation until convergence.

Contrary to the case of $A$ tensors, the latter perturbative procedure does not grant analytically that a minimum is found at each step. In practice, however, this approach shows a good convergence.

### *Numerical results*

To study the performance of this ansatz, we have implemented the algorithm above in MATLAB and applied it to the ground state of different two-body Hamiltonians, $H=\Sigma_{(ij)}h_{(ij)}$ on 2D lattices.

The tests have included random two-body Hamiltonians, where each $h_{(ij)}$ is a randomly chosen Hermitian operator acting on neighboring sites $(ij)$; the Heisenberg model, $h_{(ij)}=\sigma_x^i\sigma_x^j+\sigma_y^i\sigma_y^j+\sigma_z^i\sigma_z^j$; and a frustrated $XX$-model, $h_{(ij)}=J_{(ij)}(\sigma_x^i\sigma_x^j+\sigma_y^i\sigma_y^j)$, with $J_{(ij)}=-1$ on every fourth edge (in both directions). The algorithm has been run for lattices up to size $10\times10$, and the results have been compared with those obtained with PEPSs [24].

Table I shows the results for the SGS family. For the models mentioned above and the specified lattice sizes, the table contains the lowest energy found with this algorithm, $E_0$, using bond dimension $D$ [25], together with the relative error, $\varepsilon_r$, with respect to the PEPS result (obtained with bond dimension $D=4$ and time step $\delta t=0.001$).

We observe that in all cases a good precision is attained with very low bond dimension, and increasing $D$ does not significantly improve the result, contrary to what occurs with MPSs or general PEPSs. This can be readily understood from already discussed arguments. Any SGS with a fixed bond dimension can be represented as a PEPS of the same virtual dimension, but not the other way around. The rank of the singular value decomposition of the PEPS tensor should be smaller than $d$ for it to yield a valid MPS of the same physical dimension; and this restriction is independent of the bond dimension allowed for the SGS. Hence the ground state of these Hamiltonians can only be approximated to a finite precision with a SGS of physical dimension $d$.

TABLE II. Ground state energy found by the variational algorithm on the BSGS family, for various models and latice sizes, using effective sites of $N=2$ rows. Again, the last column shows the relative error with respect to the best available PEPS result.

| Model | Original lattice | $N$ | $D$ | $E_0$ | $\varepsilon_r$ |
|---|---|---|---|---|---|
| Random | $8\times8$ | 2 | 4 | −169.963 | $1.96\times10^{-3}$ |
| Heisenberg | $8\times8$ | 2 | 4 | −155.231 | 0.0159 |
| | $10\times10$ | 2 | 4 | −246.852 | 0.0128 |
| Frustrated $XX$ | $8\times8$ | 2 | 4 | −91.703 | $4.03\times10^{-3}$ |

However, constructing the sequential state from blocks instead of individual sites allows us to get closer to the true ground state by considering larger effective sites, and therefore larger effective $d$. We have applied the same algorithm using this BSGS family as an ansatz, with effective sites of $N=2$ rows. As Table II shows, this reduces the relative error in more than 30% in all the cases under study ($D$ now indicates the bond dimension for the MPS, which was chosen equal to the effective dimension, $d^2$).

## IV. DISCUSSION

The study of efficient representations of quantum many-body states has been very successful in the description of one-dimensional systems. Quantum information has provided a different perspective to understand these techniques [3,15,26–29]. The hierarchy of MPSs yields an adequate variational class of states for numerical methods in one dimension. In higher dimensions there are theoretical and practical limitations to the application of these states or their natural generalization. Therefore it is interesting to look for alternative representations that are capable of describing the low energy sector of physically relevant systems while offering better contractability.

Here we have presented extensions of the sequential construction of MPSs to two dimensions that can be introduced using two different approaches. Both families defined here represent subsets of states that can be efficiently prepared in practice, as their definition immediately provides a sequential recipe for its preparation. We have proved that those states show exponentially decaying correlations. Moreover, their contraction can also be done efficiently, which makes them a good ansatz for variational procedures. We have numerically studied the performance of both approaches as ground states for different local Hamiltonians. The results show that, although the suitability of the first approach is limited, the second one provides a systematic way of approximating the ground state of these systems. Our tests have only shown the feasibility of this second approach, which nevertheless has higher requirements from the computational point of view.

As already discussed, the different performance of both families is due to the fact that, for a PEPS to be writable as a SGS of dimension $d$, it is necessary (although not sufficient) that the singular value decomposition splitting the $lr$ PEPS horizontal indices from the rest has at most $d$ values different from zero. From a different point of view, it is sometimes possible to write a given PEPS with more than $d$ singular values in the decomposition above, as a certain local projection of a SGS of larger physical dimension onto a $d$-dimensional subspace for each site. It is the case of the toric code [30], which has a PEPS description of $D=2$ [19]. The $B$ tensor has four nonzero singular values according to the decomposition $iud$ vs $lr$. If we take the right part of this decomposition as a MPS description for a chain of dimension $d'=4$, it turns out to be possible to complete the rest of the decomposition onto a $8\times 8$ unitary matrix. This would correspond to free indices of dimension $d'$ from which we could recover the physical $d=2$ by projecting onto a local subspace.

Note that even if the rank of the singular value decomposition of $B$ is smaller than $d$, it is not always possible to find a SGS description for the state. For example, the PEPS constructed in [19] that reproduces the correlations and expectation values of thermal states for the classical Ising model has very low bond dimension $D=d$. From its explicit representation it is possible to see that the rank of the relevant singular value decomposition is only $d=2$. However, it is not possible in general to represent this state as a SGS.

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## APPENDIX: PROOF OF THE DECAY OF CORRELATIONS

We want to calculate a correlation function of the form $\langle O_1^{[h_1,v_1]}O_2^{[h_2,v_2]}\rangle - \langle O_1^{[h_1,v_1]}\rangle\langle O_2^{[h_2,v_2]}\rangle$ on an infinitely large 2D lattice with translational symmetry. The decay of correlations along both directions follows from the same property of MPS. Let us first calculate the decay in the vertical direction, i.e., that of application of the unitaries. Notice that if $v_1=v_2=v$, each of the expectation values above can be written as

$$\mathrm{tr}(OU^{[h]}\cdots U^{[H]}\rho_{MPS}^{\otimes H}U^{[H]^\dagger}\cdots U^{[h]^\dagger}),$$

where $\rho_{MPS}$ is the reduced density matrix for the single site occupying column $v$ in any of the rows, and $h$ is the first row touched by the corresponding operator $O$. Since the state of every row is described by the same MPS, all such reduced density matrices are the same. Therefore we are left with a tensor product of $H$ identical single site density matrices connected by the sequence of unitaries that act on column $v$. Such a construction, where all the degrees of freedom but the ones on column $v$ have been traced out, can be written as a MPDO [17],

$$\rho=\sum_{i_k,i_k'}\mathrm{tr}(M^{[h_1]^{i_1 i_1'}}\cdots M^{[H]^{i_H i_H'}})|i_1\cdots i_H\rangle\langle i_1'\cdots i_H'|,$$

with matrices of the form [31]

$$M^{[r]ii'}_{(\alpha\alpha'),(\beta\beta')}=\sum_{\gamma\gamma'}U^{[r]i\beta}_{\alpha\gamma}\rho_{\gamma\gamma'}U^{[r]*i'\beta'}_{\alpha'\gamma'}.$$

The correlation function for operators $O_1$ and $O_2$ acting on rows $h_1$ and $h_2$ can then be calculated using the purification of this MPDO, as a (translationally invariant) MPS of physical dimension $d^2$, for which the correlations decay exponentially with the distance $h_2-h_1$.

If the operators are placed along the horizontal direction, $h_1=h_2=h$, the expectation value $\langle O_1^{[h,v_1]}O_2^{[h,v_2]}\rangle$ takes a similar form,

$$\langle O\rangle=\mathrm{tr}[O_1\otimes O_2\tilde{U}^{[h_1]}\cdots\tilde{U}^{[H]}\tilde{\rho}_{MPS}^{\otimes(H-h_1+1)}(\tilde{U}^{[H]})^\dagger\cdots(\tilde{U}^{[h_1]})^\dagger], \tag{A1}$$

where each reduced density matrix, $\tilde{\rho}_{MPS}^{[r]}$, now corresponds to two physical sites of row $r$, those on columns $v_1$ and $v_2$. As the two-sites reduced density matrix of a translationally invariant MPS, it is exponentially close to a product of single-site density matrices. This can be seen by writing its explicit form

$$\tilde{\rho}^{[r]}=\mathrm{tr}(E_1^{[r,1]}E_1^{(v_1-2)}A\otimes A^\dagger E_1^{(v_2-v_1-1)}A\otimes A^\dagger E_1^{(V-v_2-1)}E_1^{[r,V]}).$$

Here $E_1$ are the $D^2\times D^2$ transfer matrices which, due to the translational invariance, do not depend on the column, except for the first and last sites of each row. Under some generic condition on matrix $E_1$ [2], the $v_2-v_1-1$ power of this matrix can be approximated by a product when the distance $v_2-v_1$ becomes very large, so that

$$\tilde{\rho}\approx\sigma^{[v_1]}\otimes\sigma^{[v_2]}+\varepsilon\tilde{\sigma}^{[v_1v_2]}, \tag{A2}$$

where $\sigma^{[k]}$, $\tilde{\sigma}^{[k]}$ act on a single system each, and the factor $\varepsilon=(\lambda_2/\lambda_1)^{v_2-v_1-1}$ is determined by the ratio of the second largest eigenvalue of $E_1$ to the largest one, and decays exponentially fast with the distance $v_2-v_1$. Moreover, if the edges of the lattice are infinitely far away, i.e., $v_1, V-v_2\to\infty$, then $\sigma^{[v_1]}=\sigma^{[v_2]}$ (with a global normalization factor).

Since each row density matrix is exponentially close to a product,

$$\|\tilde{\rho}-\sigma^{[v_1]}\otimes\sigma^{[v_2]}\|_1\leq O(\varepsilon), \tag{A3}$$

one can show by induction that this is also the case for the $H'$-fold tensor product appearing in Eq. (A1) ($H'=H-h_1+1$),

$$\|\tilde{\rho}^{\otimes H'}-(\sigma^{[v_1]})^{\otimes H'}\otimes(\sigma^{[v_2]})^{\otimes H'}\|_1\leq O(H'\varepsilon). \tag{A4}$$

The unitary matrices $\tilde{U}$ appearing in Eq. (A1) are the tensor products of a unitary matrix acting on the corresponding row and column $v_1$ times the one on column $v_2$, $\tilde{U}^{[r]}=U^{[r,v_1]}\otimes U^{[r,v_2]}$. Acting with them on the tensor product above does not increase the trace norm, and moreover respects the tensor product structure of the second term, so that the reduced density matrix corresponding to columns $v_1$ and $v_2$ satisfies

$$\|\tilde{\tau}^{[v_1v_2]} - \tau^{[v_1]} \otimes \tau^{[v_2]}\|_1 \leq O(H'\varepsilon). \tag{A5}$$

Therefore it is easy to show that, for any pair of operators $O_1$, $O_2$ each one acting on $\mathbb{C}^d$, and with operator norm bounded by 1,

$$|\mathrm{tr}(O_1 \otimes O_2 \tilde{\tau}^{[v_1v_2]}) - \mathrm{tr}(O_1 \otimes 1\tilde{\tau}^{[v_1v_2]})\mathrm{tr}(1 \otimes O_2\tilde{\tau}^{[v_1v_2]})| \leq 4O(H'\varepsilon). \tag{A6}$$

Thus the correlations decrease exponentially with distance [32].

Under some additional condition, it is possible to obtain a tighter bound on the correlations. To this end we can again define for a row $r$ the matrices

$$M^{[r,v]ii'}_{(\alpha\alpha'),(\beta\beta')} = \sum_{\gamma\gamma'} U^{[r,v]i\beta}_{\alpha\gamma}\sigma^{[v]}_{\gamma\gamma'}U^{[r,v]*i'\beta'}_{\alpha'\gamma'},$$

for $v=v_1, v_2$, and an analogous $\tilde{M}$ matrix using $\tilde{\sigma}$ and $\tilde{U}^{[r]}$, so that the reduced density matrix for sites $[h,v_1]$, $[h,v_2]$ can be written as

$$\rho_{\tilde{i}\tilde{j}} = \mathrm{tr}(M^{\tilde{i}\tilde{j}}_{[h]}G^{(H-h-1)}G_{[H]}), \tag{A7}$$

where

$$M_{[h]} = U^{[h,v_1]} \otimes U^{[h,v_2]}\tilde{\rho}(U^{[h,v_1]})^\dagger \otimes (U^{[h,v_2]})^\dagger \approx M^{[h,v_1]} \otimes M^{[h,v_2]} + \varepsilon\tilde{M}^{[h,v_1v_2]}, \tag{A8}$$

and $\tilde{i}$ ($\tilde{j}$) are the double indices $ii'$ ($jj'$) appearing in the $M$ matrices for each site. These indices are traced out on rows where no operator acts, yielding

$$G = \sum_{\tilde{i},\tilde{j}} \delta_{ii'}\delta_{jj'}M^{\tilde{i}\tilde{j}}_{[h]} \approxeq G^{[v_1]} \otimes G^{[v_2]} + \varepsilon\tilde{G}^{[v_1v_2]}, \tag{A9}$$

where each individual $G^{[v]}$ is obtained by tracing out the physical index in $M^{[h,v]}$.

If the matrices $G^{[v_1]}$ and $G^{[v_2]}$ have a single maximal eigenvalue, with multiplicity one, also the whole matrix $G$ will have a single maximal eigenvalue $\tilde{\mu}$, with the same multiplicity, so that

$$G^{(H-h-1)} \approxeq (\tilde{\mu})^{(H-h-1)}|\tilde{\mu}^L\rangle\langle\tilde{\mu}^R|,$$

plus terms that decrease exponentially with $H$. The leading eigenvectors, using perturbation theory [33], will be given by the product of eigenvectors of $G^{[v_1]}$ and $G^{[v_2]}$, plus some contributions of order $\varepsilon$ whose number is bounded by the dimension of the (finite) matrices $G$.

On the other hand, the last matrix in Eq. (A7), $G_{[H]}$, is the corresponding $G$ matrix for the bottom-most unitary, which therefore includes, instead of a single row, the tensor product of all the last $M+1$ rows, and then contributes at most with $\varepsilon(M+1)$ terms to the corrections.

$$\begin{aligned} G_{[H]} &= U^{[H,v_1]} \otimes U^{[H,v_2]}(\tilde{\rho})^{\otimes M+1}(U^{[H,v_1]})^\dagger \otimes (U^{[H,v_2]})^\dagger \\ &\approxeq G^{[v_1]}_{[H]} \otimes G^{[v_2]}_{[H]} + \varepsilon\sum_{k=0}^{M}(\sigma^{[v_1]})^k\tilde{\sigma}^{[v_1]}(\sigma^{[v_1]})^{M-k} \\ &\quad \otimes (\sigma^{[v_2]})^k\tilde{\sigma}^{[v_2]}(\sigma^{[v_2]})^{M-k}. \end{aligned} \tag{A10}$$

Therefore under this no-degeneracy assumption for matrices $G$ (which seems to be generic, after some numerics) the corrections to the tensor product structure of Eq. (A7) are of order $\varepsilon[1+O(D^4)+O(M)]$, which does not depend on the size of the system.


[1] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[2] D. Perez-García, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quantum Inf. Comput. **7**, 401 (2007).
[3] G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003).
[4] F. Verstraete and J. I. Cirac, e-print arXiv:cond-mat/0407066.
[5] C. Schön, E. Solano, F. Verstraete, J. I. Cirac, and M. M. Wolf, Phys. Rev. Lett. **95**, 110503 (2005).
[6] N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **98**, 140506 (2007).
[7] V. Murg, F. Verstraete, and J. I. Cirac, Phys. Rev. A **75**, 033605 (2007).
[8] J. Jordan, R. Orús, G. Vidal, F. Verstraete, and J. I. Cirac, e-print arXiv:cond-mat/0703788v3.
[9] G. Vidal, Phys. Rev. Lett. **99**, 220405 (2007).
[10] S. Anders, M. B. Plenio, W. Dür, F. Verstraete, and H.-J. Briegel, Phys. Rev. Lett. **97**, 107206 (2006).
[11] S. Moukouri, Phys. Rev. B **70**, 014403 (2004).
[12] N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **100**, 040501 (2008).
[13] C. M. Dawson, J. Eisert, and T. J. Osborne, Phys. Rev. Lett. **100**, 130501 (2008).
[14] M. B. Hastings, Phys. Rev. B **76**, 201102(R) (2007).
[15] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).
[16] F. Verstraete, D. Porras, and J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004).
[17] F. Verstraete, J. J. García-Ripoll, and J. I. Cirac, Phys. Rev. Lett. **93**, 207204 (2004).
[18] S. Bravyi, e-print arXiv:0801.2989v1.
[19] F. Verstraete, M. M. Wolf, D. Perez-García, and J. I. Cirac, Phys. Rev. Lett. **96**, 220601 (2006).
[20] F. Verstraete and J. I. Cirac, Phys. Rev. A **70**, 060302(R) (2004).
[21] D. Pérez-García, F. Verstraete, J. I. Cirac, and M. M. Wolf, e-print arXiv:0707.2260v1.
[22] H. J. Briegel and R. Raussendorf, Phys. Rev. Lett. **86**, 910 (2001).
[23] The scaling depends exponentially on the number of local operators applied, so that the calculation is feasible as long as this number is small.
[24] V. Murg (private communication).
[25] MPSs have bond dimension $D$, and unitaries act on $M+1$ sites, so that $d^M=D$.
[26] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).
[27] M. B. Hastings, Phys. Rev. B **73**, 085115 (2006).
[28] M. B. Hastings, Phys. Rev. B **76**, 035114 (2007).

[29] J. Eisert, Phys. Rev. Lett. **97**, 260501 (2006).
[30] A. Y. Kitaev, Ann. Phys. **303**, 2 (2003).
[31] For the bottom-most and uppermost sites, the matrices are built in slightly different form to, respectively, include the lowest MPSs and split the $M$ uppermost physical indices. These considerations do not affect the following argument.
[32] In other words, in order to get a contribution from the multiple rows, $H$, that compensates the exponential decay of MPS correlations, the size of the system should increase exponentially fast; but given a fixed large size, the correlations will suffer an exponential decay.
[33] T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, Berlin, 1995).