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Partial multipartite entanglement in the matrix product state formalism

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We present a method to apply the well-known matrix product state formalism to partially separable states in solid-state systems. The computational effort of our method is equal to the effort of the standard density matrix renormalization group (DMRG) algorithm. Consequently, it is applicable to all the usually considered condensed-matter systems where the DMRG algorithm is successful. We also show in exemplary cases that polymerization properties of ground states are closely connected to properties of partial separability, even if the ground state itself is not partially separable.

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I. INTRODUCTION

Academically speaking, entanglement is one of the most fundamentally nonclassical features of quantum mechanics and as such is highly important to the foundations of modern physics, e.g., in high-energy physics [1,2]. In a more practical view, entanglement is most relevant in two distinct respects: technological applications (such as quantum cryptography [3,4] or future quantum computers [5–7]), and its (still widely unknown) role in nature. The latter has attracted a high degree of attention in recent years: it has, e.g., been speculated that entanglement might be involved in the extraordinary efficiency of photosynthetic light-harvesting complexes [8] or geographical orientation of birds [9]. It has even been suggested that entanglement might play a significant role in processes as macroscopic as evolution as a whole [10].

While these examples are still more speculation than scientific reality, it has been conclusively shown that entanglement is indeed closely related to macroscopic properties of more simple systems in solid-state physics, such as spin chains or crystal lattices [11]. For example, frustration [12] of or certain phase transitions [13] in such systems are known to be connected to their entanglement properties.

While generic entanglement has been studied quite extensively in the context of condensed matter since the turn of the century (see, e.g., [14–22]), only a very few works address questions concerning partial (in)separability or genuine multipartite entanglement [23–27]. In Ref. [23] partial (in)separability was first mentioned but not elaborated. The authors of Ref. [24] introduced macroscopic observables (such as energy) that are capable of detecting genuine multipartite entanglement (GME) or partial inseparability via comparing the minimal energy of the ground state to the minimal energy when optimized over the set of partial separable states. The obtained GME-gap or partial-entanglement-gap energy works well in a wide variety of systems, the only requirement being that the ground states are not separable. However, for large numbers of particles this approach becomes computationally highly demanding. In Ref. [25] the authors investigated the XY model in an external magnetic field where analytical solutions of the ground states are known, allowing direct application of criteria detecting genuine multipartite entanglement. In another recent publication [26] the genuine tripartite entanglement of the anisotropic XXZ spin model was analyzed by applying properly constructed entanglement witnesses. In Ref. [27] the behavior of genuine multipartite entanglement of paradigmatic frustrated quantum spin systems was investigated by using a geometric measure.

The aim of this work is to contribute to this field by adapting existing methods for investigating solid-state systems, namely, the matrix product state (MPS) formalism, to problems of partial separability in these systems. In particular we provide a tool that allows us to investigate the relation between typical properties, such as polymerization, and properties of states, i.e., partial separability. The article is organized as follows: in the upcoming section, basic definitions of entanglement, the MPS formalism, and solid-state systems will be reviewed. After that, we can present our main result, which is a method to use the MPS formalism to investigate partial separability in solid-state systems. We then present and discuss illustrative examples before the paper is concluded.

II. DEFINITIONS

One of the most common problems in many-body physics is finding the ground-state energy for a given Hamiltonian $\mathcal{H}$. This task can be approached by means of the MPS formalism, in which a general state $|\Psi\rangle$ is given in the MPS basis

$$|\Psi\rangle = \sum_{s_1,s_2,\ldots,s_n} |s_1,s_2,\ldots,s_n\rangle \mathrm{Tr}\big(A^1_{s_1} A^2_{s_2} \cdots A^n_{s_n}\big), \qquad (1)$$

where each sum runs over the respective subsystem (i.e., from 0 to $d-1$ for a d-dimensional subsystem) and $A^i_{s_i}$ are $D \times D$ dimensional matrices. Here, D is the bond dimension, i.e., the virtual dimension of the subsystems (for more details on the MPS formalism basics, see, e.g., Ref. [28]).

Using this representation of $|\Psi\rangle$, the expectation value $\langle\Psi|\mathcal{H}|\Psi\rangle$ can be computed in a very efficient manner using the density matrix renormalization group (DMRG) algorithm [29]. In particular, the computational complexity of such optimizations is linear in the number n of subsystems, as each $A^i_{s_i}$ can be optimized essentially individually.

Despite its simplicity the concept of partial separability turned out to be a meaningful one in respect to a classification scheme for multipartite entanglement [30]. Moreover, most complications only arise for mixed states, which are of no concern to the issues addressed in this work. Consequently, we

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will only discuss the much simpler and illustrative pure-state case.

An n-partite quantum state $|\Psi\rangle$ is called k-separable iff it can be written as a nontrivial k-fold product,

$$|\Psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_k\rangle, \tag{2}$$

with $1 \leqslant k \leqslant n$, where each of the factors $|\psi_i\rangle$ is a state of one or several subsystems. If a state is separable under a given k partition (as opposed to an unknown partition) $\gamma = \{\gamma_1,\gamma_2,\ldots,\gamma_k\}$ (with $\bigcup_i \gamma_i = \{1,2,\ldots,n\}$ and $\gamma_i \cap \gamma_j = \{\}$ for $i \neq j$), it is called γ_k-separable. A state which does not factorize at all (i.e., which is not two-separable) is called genuinely multipartite entangled.

For example, the four-partite state

$$|\Psi\rangle = \tfrac{1}{2}(|0000\rangle + |1001\rangle + |0010\rangle + |1011\rangle) \tag{3}$$

is three-separable, as it can be written as $|\Psi\rangle = |\Phi^+\rangle_{1,4} \otimes |0\rangle_2 \otimes |+\rangle_3$. Consequently, it is also biseparable (as any two of the three factors can be formally combined into one). It is, however, not four-separable since there is no basis in which the first and fourth subsystems factorize. Note that any form of partial separability that is not full separability (i.e., n-separability) is equivalent to partial entanglement.

III. USING THE MPS FORMALISM FOR PARTIAL SEPARABILITY

Since the MPS formalism relies on the state in question being given in the MPS basis, a straightforward implementation of partial separability is impossible (as k-separability is defined via the freedom of choice of local bases for state vectors). However, the problem of minimizing the energy $\langle\Psi|\mathcal{H}|\Psi\rangle$ over only states with given separability properties (instead of all states) can be approached by imposing these separability constraints on the MPS structure before optimizing.

For example, an n-partite state separable under the bipartition $\{1,2,\ldots,x|x+1,x+2,\ldots,n\}$ (for some $1 \leqslant x < n$) can be realized by setting the bond dimension D between sites x and $x+1$ to 1, thus forcing the state into two mutually separable and independent blocks (note that in the case of periodic boundary conditions, the bond dimension between sites 1 and n also has to be reduced to 1 in this case). In order to also be able to implement noncompact partitions (i.e., partitions where the parts do not form blocks but overlap, such as $\{1,3,5,\ldots|2,4,6,\ldots\}$), the enumeration of sites can be permuted accordingly in the Hamiltonian (as illustrated in Fig. 1).

Using this approach, the set of states accessible to a MPS can be effectively limited to all states separable under an arbitrary partition. The computational complexity is reduced, in contrast to the case with additional constraints.

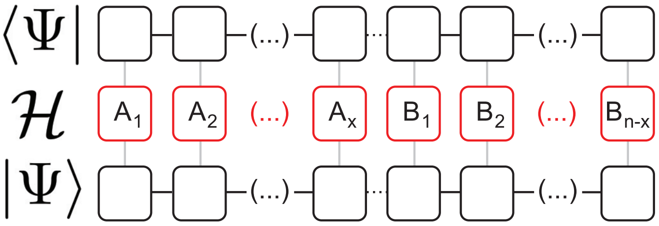

FIG. 1. (Color online) Illustration of the scalar product $\langle\Psi|\mathcal{H}|\Psi\rangle$ corresponding to the energy expectation value for a two-separable state $|\Psi\rangle$. Here, $|\Psi\rangle$ is separable with respect to the partition $\gamma = \{A_1,A_2,\ldots,A_x|B_1,B_2,\ldots,B_{n-x}\}$. The red (gray) squares correspond to the Hamiltonian's sites (reordered according to the partition γ), and the black squares correspond to the MPS's sites. The horizontal black lines connecting the MPS sites correspond to the virtual bonds of dimension D, the two dotted lines depict one-dimensional bonds which provide the desired separability properties, and the vertical gray lines correspond to the physical d-dimensional indices.

IV. EXAMPLES

In order to investigate the connection between polymerization and partial separability, let us introduce the partition step parameter p, which uniquely defines the partitions we want to investigate. Specifically, these partitions consist of blocks of p sites, alternatingly allocated to two parts of a bipartition. In other words the spin chain is split into $\frac{n}{p}$ blocks of p subsystems each, where the first, third, and all other odd-numbered blocks are separable from all even-numbered blocks. In order to better simulate the thermodynamical limit (i.e., many particles), there should always be equally many even- and odd-numbered blocks, which implies that n should always be an even multiple of p.

A. Dimerized Heisenberg model

As a first example, we consider the dimerized Heisenberg model Hamiltonian

$$\mathcal{H} = \sum_i [1 - (-1)^i \delta]\vec{s}_i \cdot \vec{s}_{i+1} \tag{4}$$

of a chain of n spin-$\frac{1}{2}$ particles. For $\delta \neq 0$, the ground state of this Hamiltonian is known to exhibit dimerization properties [31,32]. The different minimal energies for partitions corresponding to different values of p are plotted in Fig. 2. As

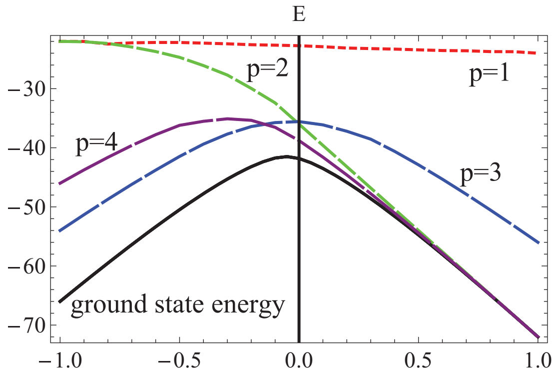

FIG. 2. (Color online) Minimal energies E for states with different separability properties in the dimerized Heisenberg model of $n = 24$ particles varied over δ. The black line depicts the ground-state energy, while the colored dashed lines correspond to minimal energies for biseparable states with different $p \in \{1,2,3,4\}$. The slight shift in the peak of the ground-state energy curve and the slight change of the $p = 1$ curve with δ are due to the open boundary conditions used in these calculations.

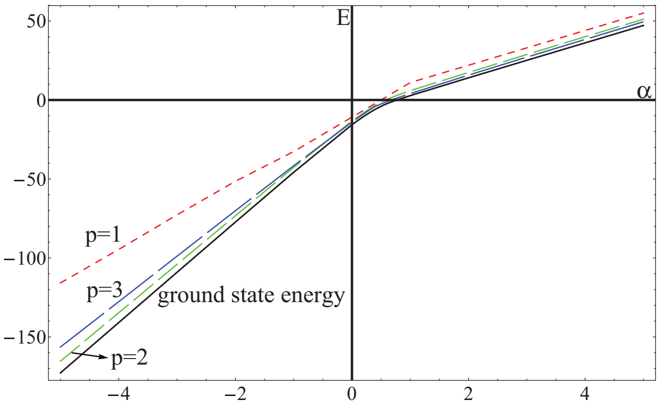

FIG. 3. (Color online) Minimal energies of biseparable states for the BLBQ Hamiltonian for $n = 12$ spin-1 particles. The black line depicts the ground-state energy, while the colored dashed lines correspond to minimal energies for biseparable states with different values $p = 1,2,3$.

expected, for $\delta \rightarrow 1$ (i.e., complete dimerization) the energies for $p = 2$ and $p = 4$ coincide with the ground-state energy. Moreover, in the entire range $0 < \delta \leqslant 1$ these energies are very close to the ground-state energy, as each block of two or four sites contains one or two pairs of dimerized particles, respectively, and is thus optimally chosen (while, e.g., for $p = 3$ there is one "unallocated" site in each block). Since for $\delta < 0$ the favored partitions are different (all site numbers are shifted by one), these energies do not indicate polymerization in this area. Whether such behavior of energies can be used as a sufficient criterion for polymerization is not entirely clear; however, it does appear to be a necessary condition.

B. Bilinear biquadratic model

An example with particularly interesting dimerization properties is the bilinear biquadratic (BLBQ) model Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j\rangle}[\vec{S}_i \cdot \vec{S}_j + \alpha(\vec{S}_i \cdot \vec{S}_j)^2] \tag{5}$$

of a chain of spin-1 particles, where the sum runs over all nearest-neighbor pairs. Such quantum magnetic systems can be realized, e.g., by spinor atoms in an optical lattice, such as ^{23}Na with a total moment $S = 1$. By confining the atoms to an optical lattice, there are two scattering channels for identical atoms with total spin $S = 0,2$ which can be mapped to an effective BLBQ spin interaction [33]. The Hamiltonian's ground state is known to possess a rich structure: it shows a dimer structure for $\alpha < -1$, a trimer structure for $\alpha > 1$, and a Haldane phase in between [34]. The model is Bethe ansatz [35] solvable at the points $\alpha = \pm 1$ and simplifies to the Affleck-Kennedy-Lieb-Tasaki-(AKLT) Model [36] for $\alpha = 1/3$.

The structure of the ground state is reflected in the minimal energies for biseparable energies under the respective partitions, as shown in Fig. 3. As expected, for $\alpha < -1$ the partition $p = 2$ approaches the ground-state energy more closely than the other partitions. For $\alpha > 1$ the partition $p = 3$ is closest to the ground-state energy. The biggest deviation from the ground-state energy is obtained for $p = 1$, where all sites are separated from their nearest neighbors (the biggest relative difference is achieved for negative values of α). The behavior of the minimal energy function in the interval $\alpha \in [0,1]$ is quite similar for all partitions into blocks and thus does not conclusively reveal any deeper structures.

C. Higher separability

Our method can straightforwardly be applied to k-separable states with $k > 2$ as well. Interesting examples arise, e.g., from considering the same block structure as in the above figures, characterized by the parameter p, and introducing additional partitions such that each block of p sites is separable from the rest of the chain (i.e., $\{1|2|\cdots|n\}$ for $p = 1$, $\{1,2|3,4|\cdots|n-1,n\}$ for $p = 2$ and so on). The resulting states are thus $\frac{n}{p}$-separable.

Interestingly, in both examples above (Figs. 2 and 3), these additional separability constraints do not alter the results at all. While qualitatively similar curves are to be expected, their being entirely identical to the results for biseparable states is somewhat astonishing.

V. CONCLUSION

We presented a simple way to use the DMRG algorithm of MPSs for partially separable states. This is done by imposing a structure of mutually separable blocks on the MPS and reordering the subsystems in the Hamiltonian according to the desired partition. Compared to usual applications of the DMRG algorithm, our method does not increase the computational effort since no external constraints are necessary (in fact, the computational effort is even slightly reduced due to the imposed one-dimensional bonds). As the convergence of the DMRG algorithm is based on local Hamiltonians, it is worth emphasizing that our method (based on essentially nonlocal Hamiltonians) still converges in most cases. In particular, having local blocks of a few sites each in the (otherwise nonlocal) Hamiltonian appears to be more than sufficient for fast convergence.

Applying our method to systems with known polymerization features, we could find a direct connection between the minimal energies attainable for states partially separable under different partitions and these polymerization properties, even in cases where the ground state itself is not separable at all.

In future applications, this method can also directly be applied to multidimensional spin lattices using projected entangled pair states [28] instead of MPS, thus allowing for a deeper investigation of partial entanglement in more complex and realistic systems. Our method has the potential to reveal yet unknown connections between k-separability and other properties, such as various phase transitions (since, in particular, quantum phase transitions are connected to change of properties of the states).

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APPENDIX: THE ALGORITHM

For completeness, we review the variational calculus with MPS as it is used in our paper. The goal is to determine the MPS

$$|\Psi\rangle = \sum_{s_1,s_2,\ldots,s_n} |s_1,s_2,\ldots,s_n\rangle \mathrm{Tr}\big(A^1_{s_1}A^2_{s_2}\cdots A^n_{s_n}\big),$$

with given dimensions $D_i \times D_{i+1}$ of the matrices A^i_s, which minimizes the energy

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\,\Psi\,\rangle}. \tag{A1}$$

D_i is set equal to 1 or D, depending on the chosen partition. If the sites in one partition are not numbered consecutively, the site indices in the Hamiltonian are permuted accordingly, thus making the Hamiltonian nonlocal. Following Ref. [37], the idea is to iteratively optimize the tensors A^i one by one while fixing all the other ones until convergence is reached. The crucial observation is the fact that the exact energy of $|\Psi\rangle$ (and also its normalization) is a quadratic function of the components of the tensor A_i associated with *one* lattice site i. Because of this, the optimal parameters A_i can simply be found by solving a generalized eigenvalue problem.

The challenge that remains is to calculate the matrix pair for which the generalized eigenvalues and eigenvectors will be obtained. In principle, this is done by contracting all indices in the expressions $\langle\Psi|H|\Psi\rangle$ and $\langle\Psi|\,\Psi\,\rangle$ except those connecting to A^i. By interpreting the tensor A^i as a dD_iD_{i+1}-dimensional vector $\boldsymbol{A}^i$, these expressions can be written as

$$\langle\Psi|H|\Psi\rangle = (\boldsymbol{A}^i)^\dagger \mathcal{H}^i \boldsymbol{A}^i, \tag{A2}$$

$$\langle\Psi|\,\Psi\,\rangle = (\boldsymbol{A}^i)^\dagger \mathcal{N}^i \boldsymbol{A}^i. \tag{A3}$$

Thus, the minimum of the energy is attained for the generalized eigenvector $\boldsymbol{A}^i$ of the matrix pair $(\mathcal{H}^i,\mathcal{N}^i)$ to the minimal eigenvalue μ:

$$\mathcal{H}^i \boldsymbol{A}^i = \mu \mathcal{N}^i \boldsymbol{A}^i.$$

The matrix $\mathcal{H}^i$ can be efficiently evaluated and $\mathcal{N}^i$ can be set equal to the identity by meeting the orthonormalization conditions $\sum_s (A^j_s)^\dagger A^j_s = \mathbb{1}$ for $j < i$ and $\sum_s A^j_s (A^j_s)^\dagger = \mathbb{1}$ for $j > i$ [28]. In this way, the optimal A^i can be determined, and one can proceed with the next site, iterating the procedure until convergence.

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