

Effective dimension reduction with mode transformations: Simulating two-dimensional fermionic condensed matter systems with matrix-product states

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Tensor network methods have progressed from variational techniques based on matrix-product states able to compute properties of one-dimensional condensed-matter lattice models into methods rooted in more elaborate states, such as projected entangled pair states aimed at simulating the physics of two-dimensional models. In this work, we advocate the paradigm that for two-dimensional fermionic models, matrix-product states are still applicable to significantly higher accuracy levels than direct embeddings into one-dimensional systems allow for. To do so, we exploit schemes of fermionic mode transformations and overcome the prejudice that one-dimensional embeddings need to be local. This approach takes the insight seriously that the suitable exploitation of both the manifold of matrix-product states and the unitary manifold of mode transformations can more accurately capture the natural correlation structure. By demonstrating the residual low levels of entanglement in emerging modes, we show that matrix-product states can describe ground states strikingly well. The power of the approach is exemplified by investigating a phase transition of spinless fermions for lattice sizes up to 10×10 .

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I. INTRODUCTION

Recent years have enjoyed a flourishing development of tensor network methods, entanglement-based methods that allow to describe strongly correlated quantum many-body systems [1–5]. They originate from the powerful density-matrix renormalization group (DMRG) [6–8], a variational method building on matrix-product states (MPS) [9–11] that captures the physics of one-dimensional local Hamiltonian systems provably well [2,12–14]. It has been applied to countless physical systems (see the reviews in Refs. [8,15] and the comprehensive web page in Ref. [16]) and extended to time-evolving systems [17–19], open systems [20,21], and the study of excited states [22]. Generalizing the variational set of matrix-product states to projected entangled pair states in two spatial dimensions, new avenues for the study of strongly correlated systems with tensor networks followed [1,2,23], including studies of fermionic models [24–29].

Interestingly, even if the DMRG approach has originally been devised to capture one-dimensional systems only: There are regimes in which it interestingly still performs competitively well [30,31] even in situations that at first seem alien to that type of approach and in which area laws for entanglement entropies are violated [5]. Two-dimensional strongly correlated systems can be naturally embedded in highly non-local Hamiltonian models on a line. The high degree of entanglement that renders a variational approach based on matrix-product states challenging are partially compensated

by the facts that contraction is efficient, and that very large bond dimensions are accessible. DMRG produces relevant data for strongly correlated matter even in two spatial dimensions, and for systems with fermionic degrees of freedom [32]. The significance of this insight is even strengthened by the fact that DMRG is strictly variational, so that all ground-state energies generated are precisely upper bounds. And yet, given that the entanglement structure is not fully captured by matrix-product states, there are strong limitations of direct DMRG approaches.

In this work, we bring the idea of tackling two-dimensional strongly correlated matter with one-dimensional matrix-product states to a new level. We show that the potential of using one-dimensional tensor network states for classically simulating higher dimensional quantum systems—in what we refer to as an effective dimension reduction in the description—is significantly more powerful than anticipated. We do so by systematically exploiting a degree of freedom that has not sufficiently been appreciated in the study of strongly correlated condensed-matter systems: This is the degree of freedom to adaptively define suitable modes in a strongly correlated fermionic system. Its significance is already manifest when solving problems in either real or in momentum space [33–40]. For n fermionic modes, however, there is an entire $U(n)$ freedom that can be made use of and exploited when devising variational principles. In fact, a manifold structure emerges that originates from the tensor network and mode transformation degrees of freedom. Only

the joint optimization fully exploits the potential of matrix-product state approaches in the study of strongly correlated fermionic condensed-matter system. It is this serious gap in the literature that is closed in this work: We overcome the prejudice that a one-dimensional embedding necessarily has to be an embedding in real space. We come to this conclusion not only based at hand of the evidence of substantially improved energies. We also find that the mode-optimized quantum states give rise to drastically reduces values of entanglement entropies over cuts when considering the system as an effectively one-dimensional quantum system, with an area-law like saturation in the bond dimension.

II. SETTING

The Hilbert space of interacting fermions in n modes is the fermionic Fock space \mathcal{F}_n originating from the basis constituted by all Slater determinants $\{|\alpha_1, \dots, \alpha_n\rangle\}$ with $\alpha_j \in \{0, 1\}$. We denote with c_j the fermionic annihilation operator of mode j satisfying the canonical anti-commutation relations $\{c_i, c_j\} = 0$ and $\{c_i^\dagger, c_j\} = \delta_{i,j}$. MPS vectors then take the form

$$|\psi\rangle = \sum_{\alpha_1, \dots, \alpha_n=1}^d A_{[1]}^{\alpha_1} \dots A_{[n]}^{\alpha_n} |\alpha_1 \dots \alpha_n\rangle. \quad (1)$$

We build upon ideas of adaptive fermionic mode transformations [41–43], here brought to the level of applicability to condensed-matter lattice models in two spatial dimensions. To be specific, and to exemplify the power of our approach, the example of the spinless interacting fermionic (spinless Fermi-Hubbard) model,

$$H = \sum_{\langle i,j \rangle} c_i^\dagger c_j + \sum_{\langle i,j \rangle} V n_i n_j, \quad (2)$$

will be the focus of attention, where V is the interaction strength, the hopping amplitude is set to 1, $n_j = c_j^\dagger c_j$, and $\langle i, j \rangle$ denotes nearest neighbors $i, j \in [n]$ on a two-dimensional cubic $N \times N$ lattice with $n = N^2$. Periodic boundary condition will be imposed along both spatial dimensions, which has been considered as a major bottleneck for MPS-based approaches. This example will show-cast that state-of-the-art energies can be reached. Having said that, in the mindset of this work would be any translationally invariant Hamiltonian of the form

$$H = \sum_{i,j=1}^n t_{i,j} c_i^\dagger c_j + \sum_{i,j,k,l=1}^n v_{i,j,k,l} c_i^\dagger c_j^\dagger c_l c_k, \quad (3)$$

including local spin degrees of freedom. That is to say, the Hamiltonian is treated as a long-ranged fermionic model on a one-dimensional line equipped with a given ordering.

III. METHODS

We optimize the single-particle basis in conjunction with the MPS tensors withing multiple successive mode transformation iterations. We refer to this procedure leading to a state-of-the-art variational ground-state approximation with one-dimensional tensor networks as an effective dimension reduction in the description of a higher-dimensional fermionic

system. In our implementation, a single mode transformation iteration consists of a full forward and backward DMRG sweep without basis rotations using the *dynamically extended active space (DEAS)* procedure [4,35], which is followed by some number of additional sweeps with local mode transformations that adapt the single-particle basis (compare Refs. [41,42]) that also rotate the couplings in the Hamiltonian to general couplings $t'_{i,j}$ and $v'_{i,j,k,l}$. At the end of the last sweep, for the symmetric super-block configuration, we have calculated the site entropies s_i , the two-site *mutual information*

$$I_{i,j} := s_i + s_j - s_{i,j}, \quad (4)$$

the *one-particle reduced density matrix*, $\rho^{(1)}$, and the *occupation number distribution* $\langle n_i \rangle$ with $i \in \{1, \dots, n\}$. Here,

$$s_A = -\text{Tr}(\rho_A \ln \rho_A) \quad (5)$$

for $A \subset [n]$ is the von-Neumann entropy of the reduced state obtained from a partial trace of the full quantum state. The eigenvalues of $\rho_{i,j}^{(1)} = \langle c_i^\dagger c_j \rangle$ define the *natural occupation (NO)* numbers, λ_i , and its eigenvectors the NO-basis. Based on $I_{i,j}$ we have calculated an optimized ordering using the Fiedler-vector approach [44], from $\{s_i\}$ a new complete active space vector for the DEAS procedure [35] and from $\langle n_i \rangle$ a new Hartree-Fock configuration. These together with the final rotated interaction matrices are all used as inputs for the subsequent mode transformation iteration.

The basis optimization has been carried out with fixed low bond dimension $D_{\text{opt}} \simeq 64$ and 256 or with a systematic increase of D_{opt} as will be discussed below. After convergence is reached large-scale DMRG calculations are performed with increasing bond dimension or using the *dynamic block state selection (DBSS)* approach with fixed truncation error threshold [45,46]. We denote these data as (D_{opt}, D) or $(D_{\text{opt}}, \varepsilon_{\text{tr}})$, respectively. In addition, a given quantity obtained from a calculation in the optimized basis will be indicated with a tilde. In the Appendix, further results with D_{opt} up to 1024 are also discussed.

IV. NUMERICAL RESULTS

Our systematic error and convergence analysis will be given for the 6×6 two-dimensional lattice, since highly accurate reference data with the real-space basis can also be generated. For larger system sizes, namely for 8×8 and 10×10 , only final results will be discussed (further numerical aspects, data and figures are presented in the Appendix).

In the left panel of Fig. 1, we show the ground-state energy $\tilde{E}(D_{\text{opt}})$ for $V = 1$ as a function of mode transformation iterations using fixed bond dimensions $D_{\text{opt}} = 64$ and 256. Reference energies $E(D)$ obtained in the real-space basis are indicated with dashed lines for various bond dimensions up to $D = 8192$. It is obvious indeed that exploiting mode transformations, $\tilde{E}(64)$ gets significantly below $E(512)$ even after the fourth iteration step and $\tilde{E}(256)$ is below $E(2048)$. For further numerical results emphasizing how faithfully information beyond the ground-state energy can be reproduced and predicted in the optimized basis, we refer to Fig. 3 in the Appendix. In the inset of the left panel of Fig. 1, we depict the ground-state

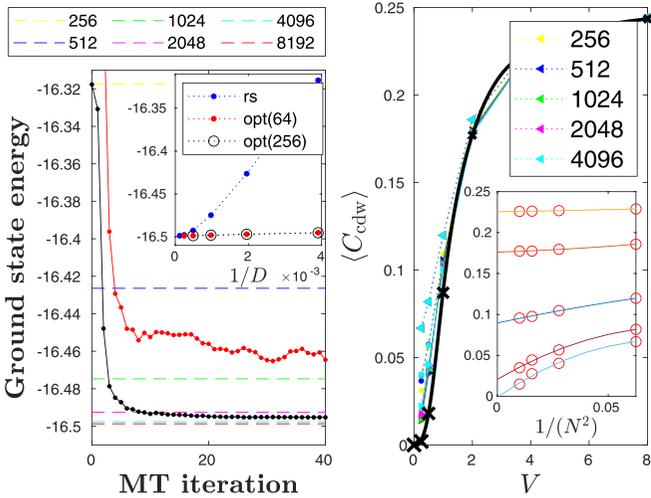


FIG. 1. (Left panel) convergence of the ground-state energy for the half-filled 6×6 spinless fermion model for $V = 1$ as a function of mode transformation iterations for fixed bond dimension of $D_{\text{opt}} = 64$ and 256 is shown by red and black curves, respectively. In the inset, the scaling of the ground-state energy with inverse bond dimension obtained in the real-space basis and in the optimized basis for $D_{\text{opt}} = 64$ and 256 are shown, respectively. (Right panel) Charge density wave order parameter for the $N \times N$ half-filled spinless fermion model as a function of V for various values of D obtained in the real-space basis. Black crosses indicate extrapolated data to the $N \rightarrow \infty$ limit obtained in the optimized basis and using finite-size scaling data shown for various interaction strengths in the inset (curves correspond from bottom to top to $V = 0.25, 0.5, 1, 2, 4, \text{ and } 8$). The solid black line is a spline fit to the extrapolated data. The error in the extrapolated data is indicated by the symbol sizes.

energy as an inverse of the bond dimension for the real-space basis and for the optimized basis with $D_{\text{opt}} = 64$ and 256 .

In the latter case, $\tilde{E}(D_{\text{opt}}, D)$ lie on the top of each other, indicating that the optimal basis has been found with $D_{\text{opt}} = 64$ already (red dots in black circles). To keep the discussion transparent and focus on the performance of the algorithm making use of mode transformations, we focus on the scaling in the bond dimension D and less so on a finite-size scaling in the system size. For larger system sizes, the improvements are even more remarkable as is shown in Fig. 4 in the Appendix for the 8×8 lattice for different values of D_{opt} and for $V = 1$ and 8 . Here, $\tilde{E}(256)$ is already lower than $E(8192)$. In addition, reliable extrapolation with $1/D$ to the $D \rightarrow \infty$ truncation free limit would require even significantly larger bond dimensions for the real-space basis. In contrast to this, in case of the optimized basis, this is no longer an issue since $\tilde{E}(256, D)$ is basically a flat curve. Our very accurate results have been obtained for a torus geometry. This reduces finite-size effects significantly and much smaller systems sizes could lead to a reliable extrapolation to the thermodynamic limit (see Table I).

The remarkable superiority of the optimized basis over the real-space basis is due to the dramatic reduction of the entanglement. As an indication of this, we depict the block entropy $s_{[l]}$, $l \in \{1, \dots, n\}$ in the left panel of Fig. 2 for various selected mode transformation iterations. Here, the maximum

TABLE I. Convergence of the bond energy, E/N^2 , with system size for various V values. DMRG results were obtained using the optimized basis and the DBSS procedure with $M_{\text{min}} = 1024$ and $\varepsilon_{\text{tr}} = 10^{-6}$.

	0.25	0.5	1	2	4	8
4×4	-0.6636	-0.5845	-0.4518	-0.2878	-0.1591	-0.0823
6×6	-0.6847	-0.5992	-0.4583	-0.2911	-0.1601	-0.0825
8×8	-0.6947	-0.6059	-0.4606	-0.2912	-0.1601	-0.0825
10×10	-0.6994	-0.6086	-0.4607	-0.2912	-0.1601	-0.0825

of $s_{[l]}$ reduced by a full order of magnitude, as can be seen by comparing the blue (real-space basis) and the black (optimized basis) curves. In addition, artifacts of the snake-like mapping of the two-dimensional lattice in real space into the one-dimensional MPS topology apparent in the blue curve are completely diminished by the basis optimization resulting in a smooth and highly symmetric profile (additional data is available in the Appendix). The iterative error norm of the block entropy measured between two subsequent mode transformation iterations, $\|s_{[l]}^{k+1} - s_{[l]}^k\|$ converges to 10^{-5} – 10^{-4} which can also be used as a criterion when to terminate the basis optimization. For larger V values, the reduction is even more pronounced, leading to a state that is close to a Slater determinant. In the right panel, the maximum of $s_{[l]}$ for $l \in \{1, \dots, n\}$ —which typically appears near the center of the chain—is laid out for various D values for the real-space basis and for the optimized one. While a strong D dependence for $V \leq 2$ is clearly visible in the real-space basis, the curves basically fall on top of each other for the optimized basis. The small peak for $0 \leq V \leq 2$ signals the residual entangle-

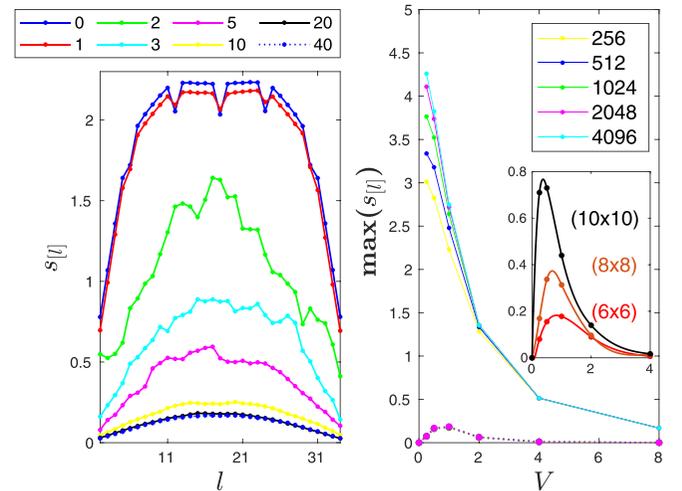


FIG. 2. (Left panel) block entropy for the 6×6 half-filled spinless fermion model for $V = 1$ for some selected mode transformation iterations with $D_{\text{opt}} = 256$, i.e., for the 0th, 1st, 2nd, 3rd, 5th, 10th, 20th, and 40th iterations. (Right panel) maximum of the block entropy as a function of V for various D values and for the real-space basis (solid lines) and for the optimized basis (dashed lines). In the inset, this is shown for various systems sizes obtained with the optimized basis and DMRG with $D_{\text{min}} = 1024$ and $\varepsilon_{\text{tr}} = 10^{-6}$. Here, a spline is fitted as guide for the eye through the data points.

ment that cannot be removed by basis optimization which also controls the required bond dimension and thus the computational complexity. As a benchmark we have performed DMRG calculations using the DBSS approach with minimum bond dimension $D_{\min} = 1024$ and a truncation error threshold $\varepsilon_{\text{tr}} = 10^{-7}$. An agreement up to four digits has been obtained compared to the real-space energy reference data calculated with $D = 8192$, but we have gained a speedup by a full order of magnitude.

Strikingly, as we discuss in great detail in the Appendix, while there are complexity theoretic obstructions against a mapping of the given Hamiltonian to a local one-dimensional gapped Hamiltonian, the mode-transformed states are numerically found to feature an entanglement entropy that is upper bounded by a constant in the bond dimension, so that larger and larger bond dimensions still lead to entanglement entropies upper bounded by constants. This provides further strong evidence for the significance of the effective dimension reduction in description (see Figs. 5 and 6 in the Appendix).

V. PHASE DIAGRAM

The power of our approach allows us to attack the physical properties such as the phase diagram of the system as well. In the limit of strong interactions, the model maps onto the antiferromagnetic Ising model in two dimensions and a *charge density wave* (CDW) phase develops. Since the hopping is restricted to nearest neighbors only, the Fermi surface takes the form of a square and perfect nesting together with Van Hove singularities providing strong arguments for an Ising transition into the CDW-ordered phase at $V_c = 0$ [47,48]. Furthermore, investigations within the Hartree-Fock approximation lead to an exponentially small order parameter in the weak coupling limit and the $1/d$ corrections starting from the $d = \infty$ limit, where Hartree-Fock theory becomes exact, provides only very small quantitative corrections in $d = 3$ and even in $d = 2$ [49]. For $d = 2$ this indicates a transition at $V_c = 0$ and that the charge density wave order parameter is an exponential function of V in the weak coupling limit. Note, however, that these simple arguments can break down as in the case of spinless fermions in one spatial dimension, $d = 1$, where the model reduces to the integrable Heisenberg model and has a transition at finite V_c [49]. Reference [50] has shown that there is a direct transition between the homogeneous and the CDW phases governed by phase separation, and a finite $V_c \simeq 0.5$ is suggested based on their obtained phase diagram. Their underlying arguments, however, have been derived for finite doping, thus an exponentially closing phase boundary between the CDW and phase separated phases together with $V_c = 0$ cannot be ruled out.

To investigate the transition, we first analyze the block entropy profiles for larger system sizes using the optimized basis and find that the peak for $V \leq 1$ remains and its height increases with system size as is shown in the inset of the right panel of Fig. 2. The center of the peak extracted from the spline fits ($V = 0.83, 0.65, 0.36$ for $N = 6, 8, 10$) tends to shift to $V = 0$ with $1/N^2$ which indicates a quantum phase transition [51] at $V_c = 0$. We also compute the CDW order

parameter [52] as expectation value of

$$C_{\text{cdw}} = \frac{1}{N^4} \sum_{i,j} \eta_{i,j} (n_i - 1/2)(n_j - 1/2) \quad (6)$$

directly, where $n_i = c_i^\dagger c_i$ in the real-space basis and $\eta_{i,j}$ is a phase matrix with elements ± 1 in a checker-board arrangement on the two-dimensional lattice. The real-space simulations show that for large values of V , $\langle C_{\text{cdw}} \rangle$ takes a finite value while for $V = 0$ it has to vanish as can be seen in the right panel of Fig. 1. The apparent finite size and D dependencies do not allow us to conclusively decide upon the behavior of $\langle C_{\text{cdw}} \rangle$ for $V \leq 1$. Alternatively, the density-density correlation function can also be taken from the elements of the one- and two-particle reduced density matrices. The latter one has entries

$$\rho_{i,j,k,l}^{(2)} = \langle c_i^\dagger c_j^\dagger c_k c_l \rangle, \quad (7)$$

which can also be calculated efficiently by the DMRG method [53]. Measuring these in the optimized basis and back-rotating to the real-space basis, we have found an agreement up to four digits between $\langle \tilde{C}_{\text{cdw}} \rangle$ and the real-space reference for $N = 4$ and 6. For $N = 8$ and $V \leq 1$ the two data sets, however, began to deviate and $\langle \tilde{C}_{\text{cdw}} \rangle$ possesses a much weaker D dependence. Finite-size scaling of the large-scale DMRG data obtained with $M_{\min} = 1024$ and $\varepsilon_{\text{tr}} = 10^{-6}$ is shown in the inset of Fig. 1 right panel for various V values. For large V the curves scale to finite values in the thermodynamic limit, while for $V \leq 1$ they show a slight downward curvature. After a rough extrapolation with $1/N$ and a spline fit on the extrapolated data (black crosses in the figure) an exponential opening of $\langle \tilde{C}_{\text{cdw}} \rangle$ at $V_c = 0$ has been obtained. This functional form agrees to the one reported in Ref. [49] after some rescaling and it is shown by a black curve in the right panel of Fig. 1. Our approach hence pushes forward the capacity of the MPS based approaches to capture two-dimensional strongly correlated systems significantly. Our results are in close agreement with analytic expectations (while some details remain open).

VI. CONCLUSION

In this work, we have demonstrated that MPS approaches, extending known DMRG methods, are surprisingly powerful for the simulation of two-dimensional quantum many body systems even imposing periodic boundary condition along both spatial dimensions. This is possible if only the key insight is acknowledged that one is not forced to do a local basis representation. Algorithmically, this is achieved by adaptively finding the optimal basis via fermionic mode transformation, optimizing over a larger manifold than that of MPS, which leads to a dramatic reduction of the correlations and entanglement in the system. A strongly interacting model in the real-space basis thus can be converted to a weakly correlated problem in the optimized basis. Due to the torus geometry, finite-size dependence is significantly reduced and intermediate system sizes make it possible to carry out more reliably extrapolations to the thermodynamic limit.

In fact, for the two-dimensional translationally invariant spinless fermion model, our results strongly suggest the presence of a quantum phase transition at $V_c \simeq 0$, but the very

small values of the charge density order parameter obtained numerically in the weak coupling limit leaves an uncertainty in our conclusion. The inclusion of a hopping between next nearest neighbors, however, would distort the square Fermi-surface and perfect nesting over an extended region of the momentum space will be destroyed. This is expected to have a have major effect, and divergencies in the susceptibilities might be removed and a finite V_c is even more likely. This behavior also shares features with the phase diagram of spinless fermions on the honeycomb lattice [54]. Then, physical properties of the transformed basis are of key importance. In general, the ground-state energy cannot be written as a sum of energies of quasiparticle states except for special cases. The $V = 0$ and large V limits belong to the latter case (the ground state is a product state), but the residual block entropy for $0 < V \leq 2$ reflects the general scenario.

Our basis optimization is very robust, it can be carried out with low bond dimension, and calculations using the optimized basis can easily lead to an order of magnitude speedup in computational time. In addition, our method is stable for weakly and strongly interacting systems, in general, while standard approaches, like basis transformation based on natural orbitals, that have been attempted earlier [55] have major limitations and drawbacks (for numerical data see Fig. 4 of the Appendix). Remarkably, the optimized basis for the spinfull Hubbard model does not resemble the characteristics of natural orbitals which reflects the existence of much stronger residual correlations in the system (as forthcoming work will explore). Conceptually most importantly, our work overcomes the deep misconception that lower-dimensional embeddings necessarily have to capture some kind of locality.

Once this prejudice is overcome, acknowledging that fermionic mode transformations are not restricted to one-dimensional embeddings, mode transformations, and effective dimension reductions in description can be brought to a new level. This is even more interesting and surprising given that a full mapping on the level of Hamiltonians and their accompanying ground states to polynomial accuracy is in general not possible (as we elaborate on in more detail in the Appendix). Due to the polynomial scaling of the non-local DMRG [56] effort as $O(D^3 n^3) + O(D^2 n^4)$, a reduction of D by one or two orders of magnitude will render DMRG competitive for simulating higher-dimensional and complex problems as well. Our approach has the potential to become a standard protocol for tensor network methods, in particular in that it can augment and strengthen existing approaches.

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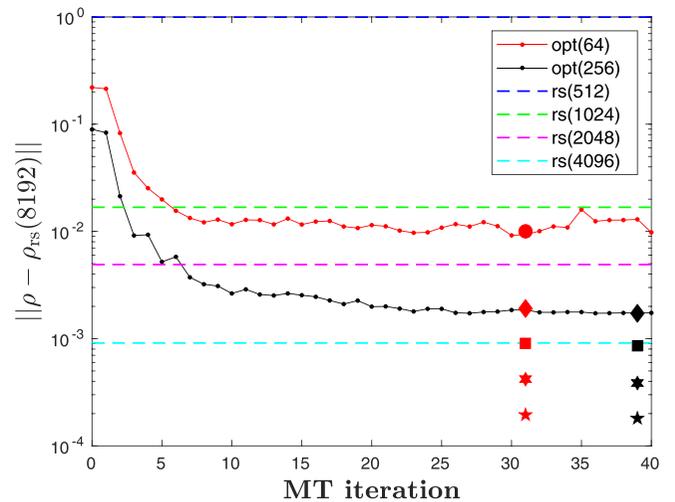


FIG. 3. Error norm of the one-particle reduced density matrix with respect to the reference obtained with the real-space basis with $D = 8192$. Red and black symbols show result for $D = 64, 256, 512, 1024, 2048$ but using the optimized basis for $D_{\text{opt}} = 64$ and 256 , respectively. For both quantities reference data obtained with the real-space basis for various D values up to 8192 are shown with dashed lines and labeled as $\text{rs}(D)$.

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APPENDIX

In this Appendix, we present additional numerical data complementing the findings of the main text together with further scaling properties obtained for larger system sizes as well as further conceptual considerations.

1. Error analysis of the one particle reduced density matrix

To investigate how faithfully information beyond the ground-state energy can be reproduced and predicted in the optimized basis, we depict in Fig. 3 the operator norm of the difference of the one particle reduced density matrix $\widehat{\rho}^{(1)}(D_{\text{opt}})$ over the mode transformation iterations and the real-space reference data $\rho^{(1)}(8192)$. Using the optimized basis, we also show the result for $\rho^{(1)}(D_{\text{opt}}, D)$ with increasing bond dimension D , using different symbols. These latter data sets are basically the same for $D_{\text{opt}} = 64$ and 256 , thus the optimal basis has already been obtained with the lower D_{opt} value (see Fig. 3). The error norms obtained with the real-space basis are again much larger as indicated by the dashed lines. The error norm is less meaningful for very large bond

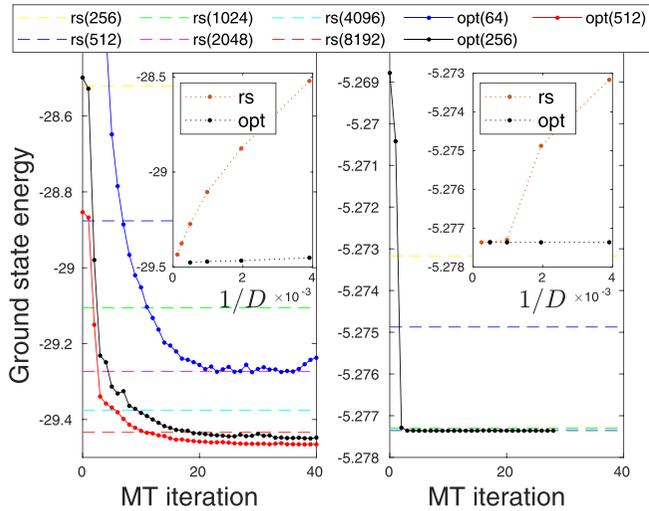


FIG. 4. Convergence of the ground-state energy for the half-filled 8×8 spinless fermion model as a function of mode transformation iterations for fixed bond dimension of $D_{\text{opt}} = 64, 256,$ and 512 is shown by blue, red and black curves, respectively, for $V = 1$ (left panel) and for $V = 8$ (right panel). Reference data obtained in the real-space basis for D up to 8192 are shown with dashed lines. In the inset, the scaling of $E(D)$ and $\tilde{E}(256, D)$ with the inverse bond dimension is shown.

dimensions since $\tilde{E}(256, 4096)$ is below $E(8192)$ rendering $\rho^{(1)}(256, 4096)$ potentially more accurate than $\rho^{(1)}(8192)$.

2. Further numerical results for the ground-state energy of the half-filled $N \times N$ spinless fermion model

In Fig. 4, we present further numerical results for the ground-state energy of the half-filled 8×8 spinless fermion model, and obtained bond energies are summarized up to lattice sizes 10×10 in Table I.

3. Complexity theoretic insights into dimensional reduction in description

The main point of this work is to provide evidence for the observation that an effective dimension reduction in description can lead to a substantially improved classical simulation of strongly correlated quantum systems: A one-dimensional tensor network ansatz can capture two-dimensional strongly correlated models well, if the prejudice is overcome that the mapping to one spatial dimension has to be spatially local. The main text shows that such an effective dimension reduction on the level of description is possible, leading to substantially improved descriptions over standard one-dimensional embeddings. In the subsequent subsections, we provide further evidence for this at hand of discussing entanglement entropies and energies.

Having said that, we insist on an effective dimension reduction in description, that is, on the level of the variational ansatz capturing the strongly correlated quantum system at hand. On the level of Hamiltonians and concomitant ground states to polynomial accuracy, a full efficient reduction to a one-dimensional system is in general infeasible, as obstructions of computational complexity are in the way. In the light

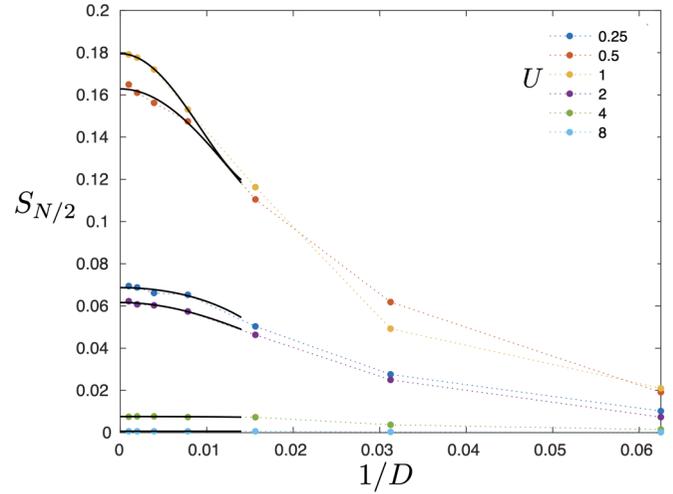


FIG. 5. Half chain block entropy obtained for the 6×6 spinless fermion model as a function of inverse bond dimension for various interaction strengths, including a fit to the data. The solid line is a fit defined by Eq. (A2).

of this observation, it is even more interesting that the effective dimension reduction in description provides so convincing results. In the following, we elaborate more on this conceptual obstruction.

Consider as input to the problem a family of general strongly correlated fermionic systems with Hamiltonian

$$H = \sum_{i,j=1}^n t_{i,j} c_i^\dagger c_j + \sum_{i,j,k,l=1}^n v_{i,j,k,l} c_i^\dagger c_j^\dagger c_l c_k \quad (\text{A1})$$

as above. Under a mode transformation defined by a $U \in U(n)$ such a Hamiltonian transforms to a new local (quartic) Hamiltonian of the same form, albeit no longer necessarily a geometrically local one even if the original Hamiltonian has been geometrically local. It has been shown in Ref. [57] that to approximate the ground-state energy of such a model to polynomial accuracy is QMA-hard (“quantum Merlin-Arthur”), in a complexity-theoretic language [58]. This implies in particular that it is NP-hard, so no polynomial time algorithm exists unless $\text{NP} = \text{P}$. If one could find a mode transformation $U \in U(n)$ in polynomial time that transforms the ground state to a quantum state that is approximated by a matrix-product-state up to an error in trace norm that scales suitably polynomially in n , then one could find a polynomial time algorithm that provides an efficient classical solution to a QMA-hard problem, which leads to a contradiction unless $\text{QMA} = \text{P}$. Therefore, on the level of Hamiltonians and accompanying exact ground states, a full dimension reduction to one-dimensional problems is in general implausible.

4. Further numerical results for the ground-state block entropy profiles of the half-filled 8×8 spinless fermion model

In this section, we elaborate in more detail on the entropy reduction by means of mode transformations as discussed in the main text, to further corroborate our main claims. Figure 5 shows the (von Neumann) entanglement entropy of a half chain for an $N \times N$ lattice for $N = 6$, so $n = N^2$ fermionic modes, as a function of the inverse bond dimension D , for

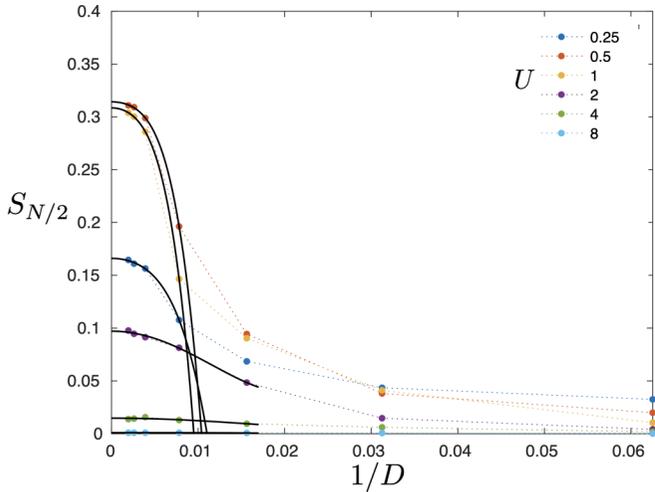


FIG. 6. Similar to Fig. 5, but for the 8×8 spinless fermion model.

several values of the interaction U . Depicted are the raw data, as well as a fit to the function $x \mapsto y(x)$ defined as

$$y = a + b\frac{1}{x^2} + c\frac{1}{x^4}, \quad (\text{A2})$$

for suitable real a, b, c , signifying the interesting regime for large bond dimension D . The striking insight is that not only is the entanglement entropy drastically reduced, compared to the values without mode transformation. But in fact, the values for the entanglement entropy saturate for large bond dimensions D , instead of being divergent. This is a convincing illustration of the power of mode transformations to reduce the entanglement entropy in this dimension reduction in description. Figure 6 shows the same plot for $N = 8$, with compatible findings.

5. Further computational aspects

The reference real-space DMRG data has been generated by fixing the bond dimension D from the very beginning of the DMRG calculations, the residual error threshold in the Lanczos and Davidson diagonalization steps has been set to be 10^{-9} and we have used some 13–15 sweeps. The maximum value of the truncation error has been in the range of 10^{-6} – 10^{-7} . The half-chain (von Neumann) entanglement entropy data via mode optimization up to $D = 1024$ is shown in Figs. 3 and 4, and it has been obtained with similar settings, but using 7–9 sweeps and 60 iterations of mode transformations. On the practical side, the effective Hamiltonian in the DMRG treatment gets more dense, i.e., additional terms are generated during the course of mode optimization which require substantial more computational efforts. However, the tremendous reduction in the block entropy and the bond dimension largely overcompensate this. In addition, the extra terms that are generated can be applied independently during the diagonalization step. Thus, the idea of effective dimension reduction by means of mode transformation constitutes an ideal candidate for GPU based massive parallelization [59].

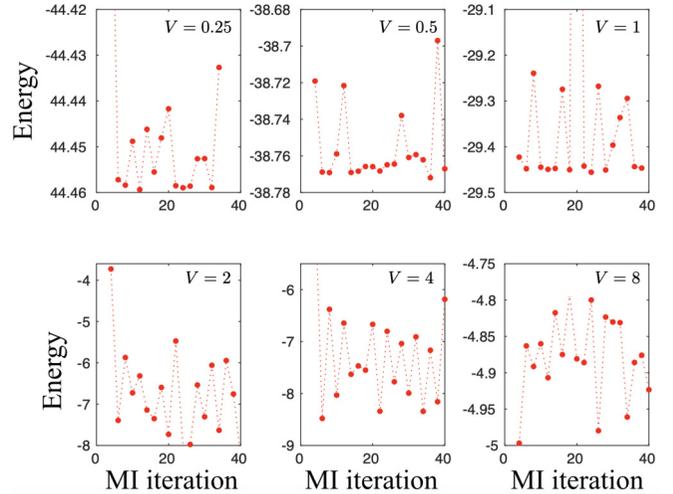


FIG. 7. Convergence of the ground-state energy for the half-filled 8×8 spinless fermion model as a function of mode transformation iterations with fixed bond dimension of $D_{\text{opt}} = 256$ for various V values if we rotate to the natural orbitals after the seventh sweep of each iteration instead of using the local updates and perform another seven sweeps to obtain a converged ground state in the current rotated basis to determine the optimal ordering for the next iteration. Therefore, each iteration based on natural orbitals corresponds to every second iteration based on fermionic mode transformation.

6. Mode transformation analysis using rotations based on natural orbitals for the half-filled 8×8 spinless fermion model

Through the course of basis optimization, the residual quantum correlations that have to be captured by the tensor network ansatz are significantly reduced (see Figs. 7 and 8). As a further proxy for this behavior, one may investigate the sum of the single mode von Neumann entropies $I_{\text{tot}} = \sum_i s_i$ that is reduced drastically, while pair-wise correlations reflected by $I_{i,j}$ get very much localized (for additional numerical data see Fig. 8). In addition, the investigation of the one-particle reduced density matrix shows that the optimized basis converges to the natural orbital basis as λ_i and $\langle n_i \rangle$ tend to lie on the top of each other (Fig. 8). Therefore, here the final basis is the natural orbital basis, but the underlying basis has been systematically rotated by each mode transformation iterations.

Since the final basis is the natural orbital basis (see Fig. 8), one might think that a natural step is to aim at identifying a globally optimal single-particle basis could be more directly based on natural orbitals, i.e., by instead of using the local updates to the single-particle basis one could rotate to the natural orbitals at the end of each mode transformation iteration. Such an approach has already been tested for quantum chemical applications [55], but a very unstable performance has been reported. In fact, we have also found that in the small- V limit such an approach works acceptably, but for larger V values it breaks down (see Fig. 7). The reason is that for small V the optimal orbitals are Hartree-Fock like orbitals, while for large V values localized orbitals seem to be more optimal. Our novel method based on fermionic mode transformation is, however, stable for all V values. Importantly, it can also be used in general for interacting quantum many body systems.

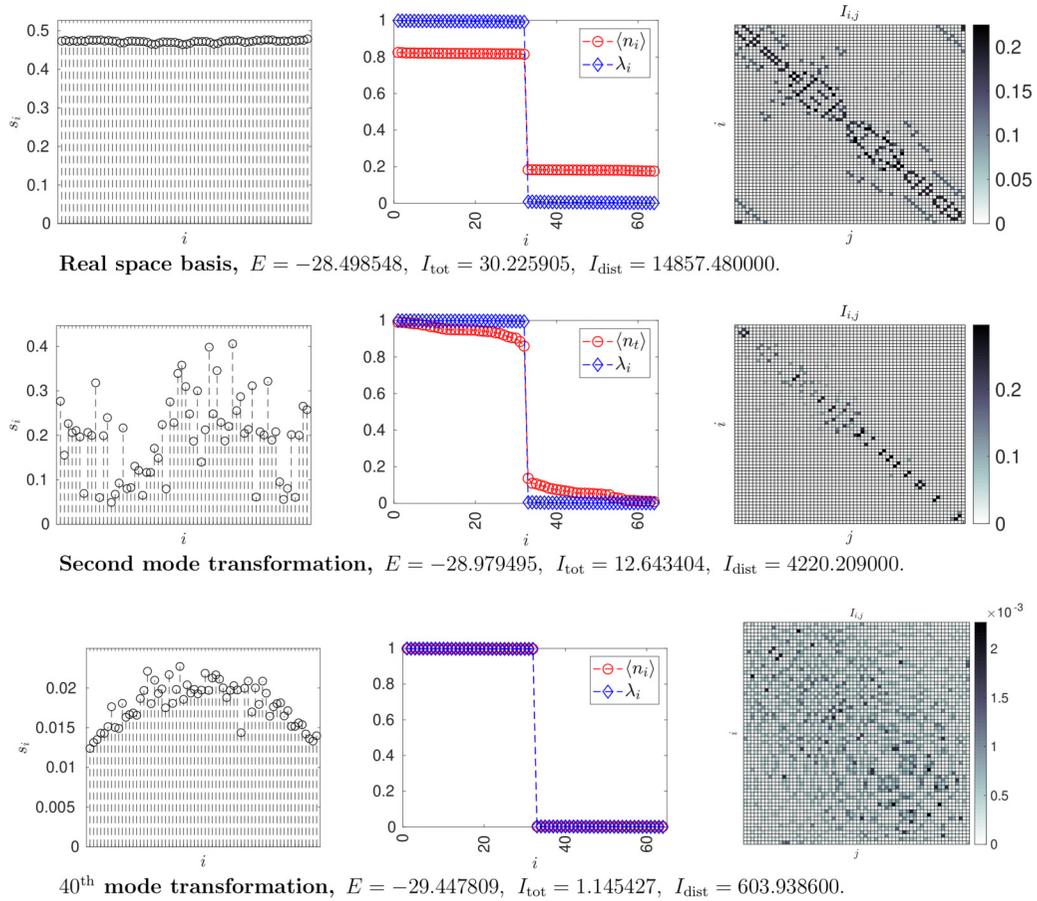


FIG. 8. Site entropy profiles $\{s_i\}$, sorted values of the natural orbital occupation numbers $\{\lambda_i\}$, occupation numbers $\{n_i\}$ and mutual informations $\{I_{i,j}\}$ for the real-space basis (first row), and for the 2nd and 40th mode transformation iterations for the half-filled 8×8 spinless fermion model for $V = 1$ and $D_{\text{opt}} = 256$. The ground-state energy, the sum of the site entropy I_{tot} , and the entanglement distance $I_{\text{dist}} = \sum_{i,j} I_{i,j} |i - j|^2$, are printed below the corresponding panels.

- [1] R. Orus, A practical introduction to tensor networks: Matrix-product states and projected entangled pair states, *Ann. Phys.* **349**, 117 (2014).
- [2] F. Verstraete, J. I. Cirac, and V. Murg, Matrix-product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems, *Adv. Phys.* **57**, 143 (2008).
- [3] J. Eisert, Entanglement and tensor network states, *Mod. Sim.* **3**, 520 (2013).
- [4] S. Szalay, M. Pfeffer, V. Murg, G. Barcza, F. Verstraete, R. Schneider, and Ö. Legeza, Tensor product methods and entanglement optimization for *ab initio* quantum chemistry, *Int. J. Quant. Chem.* **115**, 1342 (2015).
- [5] J. Eisert, M. Cramer, and M. B. Plenio, Area laws for the entanglement entropy, *Rev. Mod. Phys.* **82**, 277 (2010).
- [6] S. R. White, Density Matrix Formulation for Quantum Renormalization Groups, *Phys. Rev. Lett.* **69**, 2863 (1992).
- [7] S. R. White and R. M. Noack, Real-Space Quantum Renormalization Groups, *Phys. Rev. Lett.* **68**, 3487 (1992).
- [8] U. Schollwöck, The density-matrix renormalization group in the age of matrix-product states, *Ann. Phys.* **326**, 96 (2011).
- [9] M. Fannes, B. Nachtergaele, and R. F. Werner, Finitely correlated states on quantum spin chains, *Commun. Math. Phys.* **144**, 443 (1992).
- [10] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Matrix-product state representations, *Quantum Info. Comput.* **7**, 401 (2007).
- [11] S. Rommer and S. Östlund, Class of ansatz wave functions for one-dimensional spin systems and their relation to the density matrix renormalization group, *Phys. Rev. B* **55**, 2164 (1997).
- [12] M. B. Hastings, An area law for one-dimensional quantum systems, *J. Stat. Mech.* (2007) P08024.
- [13] I. Arad, A. Kitaev, Z. Landau, and U. Vazirani, An area law and sub-exponential algorithm for 1d systems, [arxiv:1301.1162](https://arxiv.org/abs/1301.1162).
- [14] N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, Entropy Scaling and Simulability by Matrix-Product States, *Phys. Rev. Lett.* **100**, 030504 (2008).
- [15] U. Schollwöck, The density-matrix renormalization group, *Rev. Mod. Phys.* **77**, 259 (2005).
- [16] T. Nishino, Unofficial DMRG, MPS, TPS, and MERA home page, <http://quattro.phys.sci.kobe-u.ac.jp/dmrg/condmat.html>.

- [17] G. Vidal, Efficient Classical Simulation of Slightly Entangled Quantum Computations, *Phys. Rev. Lett.* **91**, 147902 (2003).
- [18] A. J. Daley, C. Kollath, U. Schollwöck, and G. Vidal, Time-dependent density-matrix renormalization-group using adaptive effective Hilbert spaces, *J. Stat. Mech.* (2004) P04005.
- [19] J. Haegeman, C. Lubich, I. Oseledets, B. Vandereycken, and F. Verstraete, Unifying time evolution and optimization with matrix-product states, *Phys. Rev. B* **94**, 165116 (2016).
- [20] F. Verstraete, J. J. Garcia-Ripoll, and J. I. Cirac, Matrix-Product Density Operators: Simulation of Finite-Temperature and Dissipative Systems, *Phys. Rev. Lett.* **93**, 207204 (2004).
- [21] A. H. Werner, D. Jaschke, P. Silvi, M. Kliesch, T. Calarco, J. Eisert, and S. Montangero, Positive Tensor Network Approach for Simulating Open Quantum Many-Body Systems, *Phys. Rev. Lett.* **116**, 237201 (2016).
- [22] V. Khemani, F. Pollmann, and S. L. Sondhi, Obtaining Highly Excited Eigenstates of Many-Body Localized Hamiltonians by the Density Matrix Renormalization Group Approach, *Phys. Rev. Lett.* **116**, 247204 (2016).
- [23] F. Verstraete and J. I. Cirac, Renormalization algorithms for quantum-many body systems in two and higher dimensions, cond-mat:0407066.
- [24] T. Barthel, C. Pineda, and J. Eisert, Contraction of fermionic operator circuits and the simulation of strongly correlated fermions, *Phys. Rev. A* **80**, 042333 (2009).
- [25] C. V. Kraus, N. Schuch, F. Verstraete, and J. I. Cirac, *Phys. Rev. A* **81**, 052338 (2010).
- [26] I. Pižorn and F. Verstraete, Fermionic implementation of projected entangled pair states algorithm, *Phys. Rev. B* **81**, 245110 (2010).
- [27] C. Pineda, T. Barthel, and J. Eisert, Unitary circuits for strongly correlated fermions, *Phys. Rev. A* **81**, 050303(R) (2010).
- [28] P. Corboz, G. Evenbly, F. Verstraete, and G. Vidal, Simulation of interacting fermions with entanglement renormalization, *Phys. Rev. A* **81**, 010303(R) (2010).
- [29] P. Corboz, Improved energy extrapolation with infinite projected entangled-pair states applied to the two-dimensional Hubbard model, *Phys. Rev. B* **93**, 045116 (2016).
- [30] S. Yan, D. A. Huse, and S. R. White, Spin-liquid ground state of the $S = 1/2$ Kagome-Heisenberg antiferromagnet, *Science* **332**, 1173 (2011).
- [31] S. Depenbrock, I. P. McCulloch, and U. Schollwöck, Nature of the Spin-Liquid Ground State of the $S = 1/2$ Heisenberg Model on the Kagome Lattice, *Phys. Rev. Lett.* **109**, 067201 (2012).
- [32] E. M. Stoudenmire and S. R. White, Studying two-dimensional systems with the density matrix renormalization group, *An. Rev. Cond. Mat. Phys.* **3**, 111 (2012).
- [33] T. Xiang, Density-matrix renormalization-group method in momentum space, *Phys. Rev. B* **53**, R10445 (1996).
- [34] S. Nishimoto, E. Jeckelmann, F. Gebhard, and R. M. Noack, Application of the density matrix renormalization group in momentum space, *Phys. Rev. B* **65**, 165114 (2002).
- [35] Ö. Legeza and J. Sólyom, Optimizing the density-matrix renormalization group method using quantum information entropy, *Phys. Rev. B* **68**, 195116 (2003).
- [36] Ö. Legeza, F. Gebhard, and J. Rissler, Entanglement production by independent quantum channels, *Phys. Rev. B* **74**, 195112 (2006).
- [37] V. Murg, F. Verstraete, Ö. Legeza, and R. M. Noack, Simulating strongly correlated quantum systems with tree tensor networks, *Phys. Rev. B* **82**, 205105 (2010).
- [38] G. Ehlers, J. Sólyom, Ö. Legeza, and R. M. Noack, Entanglement structure of the Hubbard model in momentum space, *Phys. Rev. B* **92**, 235116 (2015).
- [39] J. Motruk, M. P. Zaletel, R. S. K. Mong, and F. Pollmann, Density matrix renormalization group on a cylinder in mixed real and momentum space, *Phys. Rev. B* **93**, 155139 (2016).
- [40] G. Ehlers, S. R. White, and R. M. Noack, Hybrid-space density matrix renormalization group study of the doped two-dimensional Hubbard model, *Phys. Rev. B* **95**, 125125 (2017).
- [41] C. Krumnow, L. Veis, Ö. Legeza, and J. Eisert, Fermionic Orbital Optimization in Tensor Network States, *Phys. Rev. Lett.* **117**, 210402 (2016).
- [42] C. Krumnow, Detecting and understanding efficient structures in finite fermionic systems, Ph.D. thesis, Freie Universität Berlin, 2018.
- [43] C. Krumnow, J. Eisert, and Ö. Legeza, Towards overcoming the entanglement barrier when simulating long-time evolution, [arXiv:1904.11999](https://arxiv.org/abs/1904.11999) (2019).
- [44] G. Barcza, Ö. Legeza, K. H. Marti, and M. Reiher, Quantum-information analysis of electronic states of different molecular structures, *Phys. Rev. A* **83**, 012508 (2011).
- [45] Ö. Legeza, J. Röder, and B. A. Hess, Controlling the accuracy of the density-matrix renormalization-group method: The dynamical block state selection approach, *Phys. Rev. B* **67**, 125114 (2003).
- [46] Ö. Legeza and J. Sólyom, Quantum data compression, quantum information generation, and the density-matrix renormalization-group method, *Phys. Rev. B* **70**, 205118 (2004).
- [47] Jenő Sólyom, *Fundamentals of the Physics of Solids, Normal, Broken-symmetry, and Correlated Systems* (Springer, Berlin, 2011), Vol. 3.
- [48] W. Metzner, M. Salmhofer, C. Honerkamp, V. Meden, and K. Schönhammer, Functional renormalization group approach to correlated fermion systems, *Rev. Mod. Phys.* **84**, 299 (2012).
- [49] E. Halvorsen, G. S. Uhrig, and G. Czycholl, $1/d$ corrections for interacting spinless fermions: One particle properties, *Z. Phys. B* **94**, 291 (1994).
- [50] G. S. Uhrig and R. Vlaming, Inhibition of Phase Separation and Appearance of New Phases for Interacting Spinless Fermions, *Phys. Rev. Lett.* **71**, 271 (1993).
- [51] Ö. Legeza and J. Sólyom, Two-Site Entropy and Quantum Phase Transitions in Low-Dimensional Models, *Phys. Rev. Lett.* **96**, 116401 (2006).
- [52] L. Wang, P. Corboz, and M. Troyer, Fermionic quantum critical point of spinless fermions on a honeycomb lattice, *New J. Phys.* **16**, 103008 (2014).
- [53] D. Zgid and M. Nooijen, Obtaining the two-body density matrix in the density matrix renormalization group method, *J. Chem. Phys.* **128**, 144115 (2008).

- [54] S. Capponi, Phase diagram of interacting spinless fermions on the honeycomb lattice, *J. Phys.* **29**, 043002 (2017).
- [55] J. Rissler, R. M. Noack, and S. R. White, Measuring orbital interaction using quantum information theory, *Chem. Phys.* **323**, 519 (2006).
- [56] S. R. White and R. L. Martin, *Ab initio* quantum chemistry using the density matrix renormalization group, *J. Chem. Phys.* **110**, 4127 (1999).
- [57] N. Schuch and F. Verstraete, Computational complexity of interacting electrons and fundamental limitations of density functional theory, *Nat. Phys.* **5**, 732 (2009).
- [58] S. Gharibian, Y. Huang, Z. Landau, and S. W. Shin, Quantum Hamiltonian complexity, *Found. Tr. Theor. Comp. Sc.* **10**, 159 (2015).
- [59] C. Nemes, G. Barcza, Z. Nagy, Ö. Legeza, and P. Szolgay, The density matrix renormalization group algorithm on kilo-processor architectures: Implementation and trade-offs, *Comput. Phys. Commun.* **185**, 1570 (2014).