

## Unitary circuits for strongly correlated fermions

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We introduce a scheme for efficiently describing pure states of strongly correlated fermions in higher dimensions using unitary circuits featuring a causal cone. A local way of computing local expectation values is presented. We formulate a dynamical reordering scheme, corresponding to time-adaptive Jordan-Wigner transformation, that avoids nonlocal string operators. Primitives of such a reordering scheme are highlighted. Fermionic unitary circuits can be contracted with the same complexity as in the spin case. The scheme gives rise to a variational description of fermionic models not suffering from a sign problem. We present numerical examples in a  $9 \times 9$  and  $6 \times 6$  fermionic lattice model to show the functioning of the approach.

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Strongly correlated quantum lattice models still pose some of the most intriguing problems in quantum physics, presumably being at the basis of phenomena such as high-temperature superconductivity [1]. To describe such models theoretically is often very difficult, an obvious obstacle being the prohibitive dimension of Hilbert space even for moderately sized systems when naively representing ground states. In recent years, it has increasingly become clear, however, that typical ground states of physically meaningful local models are lurking in some corner of Hilbert space, one that can often even be identified [2–12]. Hence to faithfully describe such a state, even though it may be impossible to parametrize the entire physical space, one merely has to parametrize those quantum states from the relevant set, requiring significantly fewer parameters. The most prominent and, to date, most powerful incarnation of this idea is provided by the density-matrix renormalization group (DMRG) method [2,3], requiring only linearly many parameters in the system size, but still giving an exceptionally good description of gapped one-dimensional spin chains and a very reasonable one for critical chains.

To realize such an idea in higher-dimensional systems is significantly more difficult, although progress has been made in recent years [3–13], specifically when it comes to generalizing DMRG ideas to higher dimensions, including variations of tensor product states or projected entangled pair states variants with graph enhancement, or the promising multiscale entanglement renormalization (MERA). This is a scale-invariant approach related to renormalization that has been proposed in Ref. [6] and implemented in Refs. [7–11]. Area laws [12] often point to the part of Hilbert space that is being occupied.

To describe higher dimensional fermionic systems, such as the Fermi-Hubbard model itself [1], in such a fashion, appears particularly promising, but also particularly challenging. Here, other key methods of describing quantum lattice models like the powerful quantum Monte Carlo method are hampered by the sign problem [14]. Surely, fermionic models can readily be represented as spin models, yet at the expense of losing locality (or by increasing the locality region of Hamiltonians [15]). If

one considers the term  $f_j^\dagger f_k$ ,  $j < k$ , then its spin representation under the Jordan-Wigner transformation (JWT) is

$$\sigma_j^- \otimes \bigotimes_{j < l < k} \sigma_l^z \otimes \sigma_k^+.$$

For a pair of nearest-neighbor sites  $\langle j, k \rangle$  on a  $d \times d$  lattice, the occurring string operator that is supported not only on the spins associated with  $j$  and  $k$ , but in fact on all spins between  $j$  and  $k$ , will typically have a length linear in  $d$ . It should be clear that no order can be chosen to let this apparent problem disappear.

In this work, we present a method for studying strongly correlated fermionic models using quantum circuits, that is, circuits of fermionic gates, in a way that is not overburdened by string operators: When describing the system and computing local expectation values, one has to deal with operators having support identical to that of a corresponding spin system (fermionic gates of the circuit replaced by regular ones), and strings can be made to disappear. The key point is to acknowledge that while any fixed order will give rise to the aforementioned problem, we are not necessarily forced to pick any order in the first place. Instead, one can employ a dynamical reordering of the fermionic modes in the essential part of the lattice, reordering and projecting out particles “on the fly,” in dynamical JWTs. We show that this can be consistently done, not altering expectation values of parity-preserving operators. In this way, we find that to describe fermionic lattice models is, in this sense, just as hard or easy as describing spin models, with unaltered contraction complexity.

*Fermions.* We first prepare the ground of the dynamical reordering idea. The algebra  $\mathcal{G}(L)$  of a set of  $n$  fermionic modes is spanned by products of anticommuting fermionic operators  $\{f_j, f_j^\dagger : j = 1, \dots, n\}$ , with  $\{f_j, f_k\} = 0$ ,  $\{f_j, f_k^\dagger\} = \delta_{j,k}$ . Physical operators form the subalgebra  $\mathcal{F}(L)$ , the so-called physical algebra, of operators respecting the fermion number parity [16,17]. In practical terms, this means that they are even polynomials in the fermionic creation and annihilation operators. Hence, the physical algebra splits into a direct sum

of an even and an odd part,  $\mathcal{F}(L) = \mathcal{F}^{(\text{even})}(L) \oplus \mathcal{F}^{(\text{odd})}(L)$ . For a subset  $I \subset L$  of some sites, one similarly finds the physical algebra  $\mathcal{F}(I)$ .

*Fermionic unitary circuits and multiscale entanglement renormalization.* A fermionic unitary is a parity-preserving unitary gate acting on fermionic modes,  $U = \exp(iH)$ , where  $H \in \mathcal{F}(L)$  is a hermitian operator. In a circuit [6–9], unitaries will typically not have support on the entire lattice, but will be local; that is, it will have a small support  $I$  independent of  $n$  such that  $U \in \mathcal{F}(I)$ . A fermionic unitary circuit is an ordered product of fermionic unitaries. For most of this work, we in fact consider conjugation, in particular, for the evaluation of expectation values of local observables  $A \in \mathcal{F}(L)$ , with respect to states that have been prepared by applying a fermionic unitary circuit to the vacuum  $|\phi\rangle$ ,

$$E = \langle \phi | \dots U_2 U_1 A U_1^\dagger U_2^\dagger \dots | \phi \rangle, \quad (1)$$

or by applying it to some other with odd fermion number parity, for example,  $f_n^\dagger |\phi\rangle$  instead of  $|\phi\rangle$ . In fact, there is a natural discrete time label  $t$  in a circuit, in that  $t = 0, \dots, T$  labels the time at which a single gate is being applied. What is more, we focus on circuits that feature a causal cone (see Fig. 1), most prominently present in the MERA in the original sense of Ref. [6]: The cone is formed by those unitaries in a circuit that cannot be sequentially canceled with their conjugates from the dual vector in Eq. (1) due to the presence of a local observable  $A$  that is supported only on a few sites, typically nearest neighbors. Efficient schemes will have a causal cone of a fixed width, in that a local operator will only touch a constant number of unitaries for each time step. The sequence of sequentially computing the expectation values respecting the discrete time order gives rise to a contraction. We can also allow for tensors different from unitary gates and partial traces. We also allow time steps where partial projections are applied onto the fermionic vacuum in some mode.

We now turn to aspects that are specific for fermions. A first key property from the elements of disjoint subalgebras  $U \in \mathcal{F}(I)$  and  $V \in \mathcal{F}(J)$ ,  $I \cap J = \emptyset$ , respecting parity, is that their elements commute,  $[U, V] = 0$ . This has the important

consequence that, just as for spin systems, all unitaries outside a causal cone can be canceled, and the fermionic variant inherits the same cone as the spin system. We now see that the computation of the expectation value Eq. (1) can be done without having to deal with string operators outside the cone.

*Jordan-Wigner transformations.* Fermionic operators are encoded in an occupation number representation, a representation necessarily depending on the chosen order of the fermionic modes. As we will later make updates with different fermionic orderings at different times, it makes sense to first highlight the status of the JWT. For the entire system  $L$  one can take some order  $O$  corresponding to an element of the symmetric group  $S_n$ , for example, the trivial order  $O = (1, \dots, n)$ . For this order  $O$ , a basis for the Hilbert space is given in the occupation number representation,  $|i_1, \dots, i_n\rangle_O = (f_{O_1}^\dagger)^{i_1} \dots (f_{O_n}^\dagger)^{i_n} |\phi\rangle$ , giving an identification of the total Hilbert space with the  $(\mathbb{C}^2)^{\otimes n}$ , the Hilbert space of  $n$  spins 1/2. Expressing fermionic operators in the occupation number representation amounts to a map  $J_O : \mathcal{G}(L) \rightarrow M(L)$ , where  $M(L)$  is the algebra of linear operators on  $(\mathbb{C}^2)^{\otimes n}$ . This map is the well-known JWT, depending on  $L$  and the chosen order  $O \in S_n$  of the fermionic modes; for example,

$$J_O(f_{O_k}) = \left( \bigotimes_{l=1}^{k-1} \sigma_l^z \right) \otimes \sigma_k^+, \quad (2)$$

where  $\sigma_k^{x,y,z}$  denote the familiar Pauli operators and  $\sigma_j^+ = (\sigma_j^x + i\sigma_j^y)/2$ . In this light, a JWT simply gives fermionic operators in the occupation number (or spin) representation for a given ordering  $O$ . We hence identify local fermionic operators with nonlocal operators in the respective spin systems. Also, physical operators contain strings that depend on the order chosen. Consider a local physical operator acting on sites  $I$ , the spin representation will in general also be supported on the spins in between with respect to order  $O$ . For example, for the local fermionic number operator, one finds  $J_O(f_{O_j}^\dagger f_{O_j}) = \sigma_j^z$ , but the occupation number representation of  $f_{O_j}^\dagger f_{O_k}$ ,

$$J_O(f_{O_j}^\dagger f_{O_k}) = \sigma_j^- \otimes \bigotimes_{j < l < k} \sigma_l^z \otimes \sigma_k^+, \quad (3)$$

with  $j < k$ , contains a string of Pauli operators on  $[j, k]$ .

For operators  $A \in \mathcal{F}(L)$  parity conservation manifests itself in the occupation number representation for an  $O$  as follows: Splitting the occupation number basis into two parts, depending on the parity of  $\sum_k i_k$ , the spin representation  $a = J_O(A)$  of  $A$  attains the form  $a = a^{(\text{even})} \oplus a^{(\text{odd})}$ .

*Dynamical reordering.* We now describe a new scheme to contract a fermionic unitary circuit, henceforth called dynamical reordering, and demonstrate that the contraction can be done with essentially the same complexity compared to the corresponding spin circuit: We take the “time order” in contracting, with  $t = 0$  corresponding to the local operator  $A$  itself. In turn, in our fermionic variant of the MERA [6], the top layer with largest  $t$  defines the parity, similar to fixing the topological degrees of freedom in Kitaev’s toric code [18]. The general idea of dynamical reordering is to order only the modes we are currently using at a time  $t$  in a nontrivial fashion with order  $O^t$  explicitly dependent on  $t$ . As we proceed, new

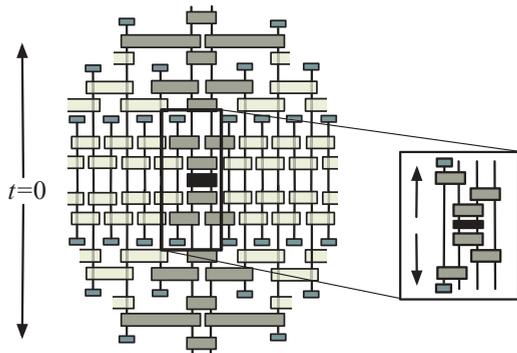


FIG. 1. (Color online) Example for the evaluation of a local observable (black box) with respect to a fermionic MERA (gray boxes). Each gray box represents a single fermionic unitary. Dark gray boxes make up the causal cone of the observable; all others lie outside of it and cancel each other. Only for conceptual clarity, a 1D MERA is depicted, not a 2D one, for which dynamical reordering becomes relevant.

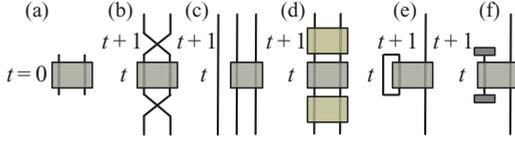


FIG. 2. (Color online) The basic primitives of (a) representing local operators, (b) reordering fermionic modes, (c) adding fermionic modes, (d) conjugating with unitaries, (e) doing partial traces, and (f) generating partial projections.

modes appear in the causal cone, and they are added to the description. When they are discarded due to projection, they are removed from the description  $O^t$  as  $t$  evolves. Hence, we arrive at an entirely local description of the fermionic tensor network, using the subsequent rules (see Fig. 2).

(a) *Local representation of fermionic local operators:* Consider a local operator  $A \in \mathcal{F}(I)$ ; that is, it is an even polynomial in the operators  $\{f_j, f_j^\dagger\}$  for  $j \in I$ . The spin representation of the fermionic operator  $A$  in order  $O$  is given by  $a = J_O(A)$ . This representation only involves  $k = |I|$  spins.

(b) *Reordering of fermionic modes:* Consider some fermionic operator  $A$  and an order  $O^t$  at time  $t$ . The new spin representation at a time  $t+1$  in the new order  $O^{t+1}$  reads  $J_{O^{t+1}}(A) = p J_{O^t}(A) p$ , with  $p = \prod_i \mathbb{1} \otimes s_{O_i^t, O_{i+1}^t} \otimes \mathbb{1}$ ,  $s_{O_i^t, O_{i+1}^t} = |0,0\rangle\langle 0,0| + |0,1\rangle\langle 1,0| + |1,0\rangle\langle 0,1| - |1,1\rangle\langle 1,1|$ , where the  $i$  are chosen such that the corresponding sequence of nearest-neighbor pair permutations of modes gives rise to the overall permutation  $O^{t+1} = \pi(O^t)$ ; so familiar fermionic swaps can be applied to the local spin representation.

(c) *Prepending of fermionic modes:* Let us have an operator  $A$  at some time  $t$ , represented as  $a = J_{O^t}(A)$  in the order  $O^t$ . We now just prepend a new fermionic mode, yielding the new order  $O^{t+1} = (k, O^t)$ . Then the new representation of  $a' = J_{O^{t+1}}(A)$  is, in the even and odd sectors, given by

$$(a')^{\text{even or odd}} = |0\rangle\langle 0| \otimes a^{\text{even or odd}} + |1\rangle\langle 1| \otimes a^{\text{odd or even}}. \quad (4)$$

(d) *Conjugation with fermionic unitaries having the same support:* Consider a subset of modes  $I$  at time  $t$ . Let  $U, A \in \mathcal{F}(I)$  be fermionic operators with support in  $I$ . Then  $J_{O^{t+1}}(UAU^\dagger) = J_{O^t}(U) J_{O^t}(A) J_{O^t}(U^\dagger)$  if the same order  $O^{t+1} = O^t$  is taken. If  $U$  is stored in a different order, the permutation rule has to be applied first.

(e) *Partial trace over the first mode:* Let us have some operator  $A$  at time  $t$  in order  $O^t$ , and we trace out the first mode  $O_1^t$ ; that is,  $O^t = (O_1^t, O^{t+1})$ . Then the spin representation of the resulting fermionic operator is, with  $k = |O^t|$ ,

$$J_{O^{t+1}}(\text{tr}_{O_1^t} A) = \sum \langle i_1, j_2, \dots, j_k | J_{O^t}(A) | i_1, i_2, \dots, i_k \rangle \times |j_2, \dots, j_k\rangle \langle i_2, \dots, i_k|. \quad (5)$$

(f) *Partial projection over the first mode:* Let us consider the same orderings  $O^t$  and  $O^{t+1}$  as for rule (e), but instead of tracing out mode  $r = O_1^t$  from operator  $A$ , we now want the projection of the mode to the empty state or that of a filled mode. The corresponding projectors in  $\mathcal{F}(I)$  are  $P_r^{(0)} = f_r f_r^\dagger$  and  $P_r^{(1)} = f_r^\dagger f_r$ , respectively, so that the projected fermionic

operators are  $P_r^{(i)} A P_r^{(i)}$ ,  $i = 0, 1$ . Applying this to Eq. (5), we find

$$J_{O^{t+1}}(\text{tr}_r P_r^{(i)} A P_r^{(i)}) = \sum |j_2, \dots, j_k\rangle \langle i_2, \dots, i_k | \langle i_1, j_2, \dots, j_k | \times J_{O^t}(A) | i_1, i_2, \dots, i_k \rangle. \quad (6)$$

The main point now is that if one follows this recipe of rules (a)–(f), and keeps only local descriptions at each time, involving the nontrivial support, one gets a value identical to Eq. (1), as if one had performed a global JWT and computed it—then with a significant overhead in complexity. To prove the reordering rule for two modes with labels  $j, k$  with  $j = O_i^t$  and  $k = O_{i+1}^t$ , that is, two modes neighboring in the order  $O^t$ , we need to show  $J_{O^t}(S_{j,k} A S_{j,k}^\dagger) = s_{j,k} J_{O^t}(A) s_{j,k}^\dagger = J_{O^{t+1}}(A)$ , where  $S_{j,k}$  acts as  $S_{j,k} f_j S_{j,k}^\dagger = f_k$  and  $S_{j,k} f_k S_{j,k}^\dagger = f_j$ . One finds  $S_{j,k} = \mathbb{1} - f_j^\dagger f_j - f_k^\dagger f_k + f_j^\dagger f_k + f_k^\dagger f_j$  [16,19]. The reordering rule for more than two modes follows by iteration. To derive the rule of adding modes, note that the local JWT gives  $J_{O^t}(f_{O_i^t}) = (\otimes_{l=1}^{i-1} \sigma_l^z) \otimes \sigma_i^+$ , and hence we obtain for  $O^{t+1} = (i, O^t)$  that  $J_{O^{t+1}}(f_{O_{i+1}^t}) = J_{O^{t+1}}(f_{O_i^t}) = \sigma_i^z \otimes J_{O^t}(f_{O_i^t})$ . Exploiting the conservation of the fermion number parity for any  $A \in \mathcal{F}(I)$ ,  $J_{O^{t+1}}(A) = \sum_\nu (\sigma_i^z)^{2\nu} \otimes J_{O^t}(A_\nu) = \mathbb{1} \otimes J_{O^t}(A)$ , where  $A_\nu$  collects all monomial terms of degree  $2\nu$  such that  $A = \sum_\nu A_\nu$ . With  $a' = J_{O^{t+1}}(A)$  and  $a = J_{O^t}(A)$ , for the even and odd sectors, this gives Eqs. (4). To show Eq. (5), note that for any operator  $B$  not acting on mode  $O_1$ , that is,  $B \in \mathcal{F}(I \setminus \{O_1\})$ , matrix elements obey  $\langle i_1, \dots, i_k | B | j_1, \dots, j_k \rangle_{O^t} = \delta_{i_1, j_1} \langle i_2, \dots, i_k | B | j_2, \dots, j_k \rangle_{O^t}$ , where  $O = (O_1, O')$  and  $k = |O|$ . With

$$\text{tr}_{O_1}(A) = \langle j_1, j_2, \dots, j_k | O A | j_1, i_2, \dots, i_k \rangle_{O'} | j_2, \dots, j_k \rangle_{O'} \times \langle i_2, \dots, i_k |_{O'}, \quad (7)$$

it follows that  $\text{tr}(AB) = \text{tr}[\text{tr}_{O_1}(A)B]$  for any  $A \in \mathcal{F}(I)$ . This means that  $\text{tr}_{O_1}$  is the fermionic partial trace for mode  $O_1$ . The resulting occupation number representation  $J_{O'}(\text{tr}_{O_1} A)$  of the partial trace is given in Eq. (5). Rules (c), (e), and (f) were given for the case where only the very first mode  $O_1$  of the ordering is affected. Combining those rules with the rule for reordering modes, they are generalized to the case where an arbitrary mode  $O_j$  is affected. In the corresponding expressions this results in extra sign factors. For the generalization of rule (d), note that when one wants to perform a contraction in which the support is not the same for the two involved operators, one can add the corresponding modes in both operators, reorder and apply (d). With these basic building blocks, we can thus contract fermionic tensor networks and also build, for example, reduced density matrices [8].

*Observation (computing expectation values).* When computing expectation values  $E = \langle \Psi | \dots U_2 U_1 H U_1^\dagger U_2^\dagger \dots | \Psi \rangle$  where  $U = U_1 U_2 \dots$  is a fermionic circuit on an elementary state vector  $|\Psi\rangle$ , then the support of the causal cone at each time step is exactly the same as if one had a spin system with the same topology. Hence, a fermionic circuit acting on a higher-dimensional fermionic system can be described entirely locally with the same time and memory complexity.

This observation renders known algorithms useful even in the case of strongly correlated fermions, with little

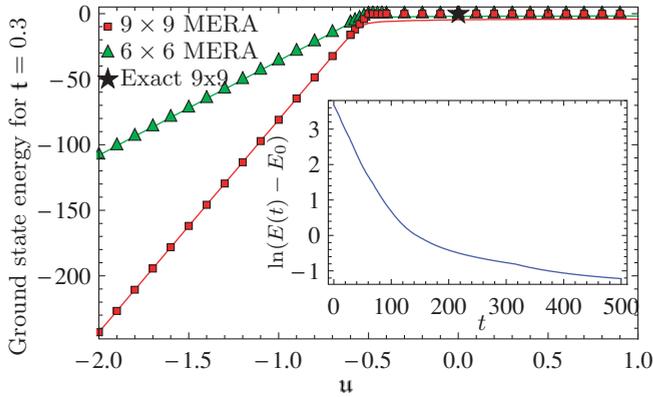


FIG. 3. (Color online) Numerical examples of the ground-state energy  $E_0$  for several  $9 \times 9$  and  $6 \times 6$  (boxes and triangles) instances of strongly correlated fermionic models,  $H = t \sum_{(j,k)} (f_j^\dagger f_k + \text{H.c.}) + \sum_j J_j^\dagger f_j + u \sum_{(j,k)} f_j^\dagger f_j f_k^\dagger f_k$ ; the free models  $u = 0$  are marked. As the MERA ansatz is a truly variational ansatz, providing upper bounds to the energy, success is guaranteed by giving lower bounds as provided by Anderson bounds (lines). This is based on an exact diagonalization of  $5 \times 5$  fermionic models, taking care of arising string operators. Even for this lowest order 2D MERA, in which, in each renormalization step, nine fermionic modes are mapped to one, we find an impressive precision. The inset shows the convergence in time for a  $9 \times 9$  free model ( $u = 0$ ,  $t = 0.3$ ) in a minimization using imaginary time evolution. In the same way, correlators and on-site properties can be efficiently computed.

modification. Notably, for MERA, the computational effort for the computation of a local expectation value scales as  $O(\log l)$  in an  $l^D$  cubic lattice and polynomially in the refinement parameter [6], hence giving rise to an indeed efficient algorithm, up to, at most, a small constant, the same as for bosons or spins. It is noteworthy that the entire machinery developed for spin systems can, with slight modification,

be used here. The preceding observation is independent of whether the system is free or strongly correlated. As it turns out, general fermionic gates also can be taken account, by directly contracting appropriately ordered fermionic operators. One can show that the computational requirements remain unchanged, giving rise to a general theory of fermionic tensor networks.

*Time evolution.* One also finds the following: For the time evolution, both real and imaginary, of local fermionic Hamiltonians, we aim at determining updates of each the fermionic unitaries forming the circuit such that  $(U_1)^\dagger (U_2)^\dagger \dots |\psi\rangle$  is an optimal approximation to the evolved  $\exp(xH) U_1^\dagger U_2^\dagger \dots |\psi\rangle$ , again with the same complexity as for a qubit system.

*Numerical implementation.* We have realized a scalable numerical implementation of this idea, applied to two-dimensional fermionic lattice models. To show the functioning of this approach as a proof of principle, we present benchmark examples in Fig. 3.

*Summary.* In this work, we have introduced a notion of time-adaptive JWTs allowing us to contract fermionic unitary circuits with the same complexity as for the corresponding spin model. This opens up a way to efficiently describe fermionic higher-dimensional models without intrinsic algorithmic problems, such as the sign problem in quantum Monte Carlo sampling. It is the hope that this work stimulates further interest in numerically assessing strongly correlated fermionic models using unitary circuits.

*Note added.* Recently, further approaches to the problem have appeared [21].

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