

## Local spin operators for fermion simulations

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(Received 6 June 2016; published 14 September 2016)

Digital quantum simulation of fermionic systems is important in the context of chemistry and physics. Simulating fermionic models on general purpose quantum computers requires imposing a fermionic algebra on qubits. The previously studied Jordan-Wigner and Bravyi-Kitaev transformations are two techniques for accomplishing this task. Here, we reexamine an auxiliary fermion construction which maps fermionic operators to local operators on qubits. The local simulation is performed by relaxing the requirement that the number of qubits should match the number of single-particle states. Instead, auxiliary sites are introduced to enable nonconsecutive fermionic couplings to be simulated with constant low-rank tensor products on qubits. The additional number of auxiliary qubits required per fermionic degree of freedom depends only on the degree of connectivity of the Hamiltonian. We connect the auxiliary fermion construction to topological models and give examples of the construction.

DOI: [10.1103/PhysRevA.94.030301](https://doi.org/10.1103/PhysRevA.94.030301)

Quantum simulations have been a driver of quantum computing research since the earliest days of quantum computing [1]. In particular, the electronic structure of interacting fermions is often highlighted as a prime application area [2] with implications for quantum chemistry [3–5] and condensed matter [6,7]. Here, we contribute to this research direction with an alternative encoding of fermions in qubits.

Quantum computing is usually done using distinguishable two-level qubit systems. Thus, quantum computer simulations of fermions require imposing the fermionic statistics on the qubit system through an encoding. Examples of such encodings include the first quantized encoding [8,9], the Bravyi-Kitaev encoding [10–12], and the Jordan-Wigner encoding [4,13]. The manipulation and extraction of the physical features of a fermionic model then depend directly on the mapping employed.

In this Rapid Communication, we study an auxiliary fermion encoding scheme for fermionic Hamiltonians that introduces additional degrees of freedom, but is manipulated with only local qubit operators [14–16]. The previously introduced auxiliary fermion scheme [14–16] is elaborated and generalized in the context of quantum simulation with the previous constructions recovered as specific cases of the framework.

Of particular relevance to understanding the present work is the Jordan-Wigner (JW) mapping. This encoding [4,13,17,18]

maps one-dimensional nearest-neighbor fermionic Hamiltonians to nearest-neighbor operators on qubits. On higher-dimensional lattices, however, manipulation of the fermionic state requires nonlocal qubit operators after the Jordan-Wigner transform. The cost of simulating such nonlocal qubit operators can be reduced using circuit optimization [19] or teleportation techniques [20]. We may also reduce the locality of the qubit simulation operators by changing the mapping itself.

One example of such optimization is the Bravyi-Kitaev (BK) encoding, which requires only a logarithmic overhead in the number of qubit operators per fermionic operator [10–12]. Both BK and JW require the same number of qubits as fermionic sites to encode states. This contrasts with the present method, which increases the number of qubits that the fermionic system is mapped to. Nevertheless, trading the increased dimension for reduction to a local qubit Hamiltonian is still a desirable feature for quantum simulations in scenarios with restricted quantum control.

Before giving the expression for the Jordan-Wigner transformation, consider the occupation representation of a fermionic state,

$$|n_0, n_1, n_2, \dots, n_{N-1}\rangle = \prod_{i=0}^{N-1} (a_i^\dagger)^{n_i} |\Omega\rangle, \quad (1)$$

where  $|\Omega\rangle$  is the fermionic vacuum. The linear indexing of the sites is necessary to uniquely specify the vacuum and is not reflective of physical considerations. Creation and annihilation

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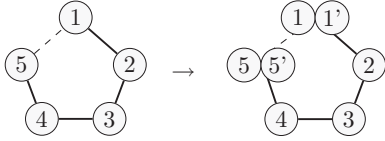


FIG. 1. Auxiliary sites are introduced in order to cancel strings of  $Z$  operators on nonlocal couplings. In the graph above, we add auxiliary fermionic sites  $1'$  and  $5'$  for sites  $1$  and  $5$ , as the fermionic coupling (dashed line) would map into nonlocal coupling on qubits with Jordan-Wigner transformation. The fermionic auxiliary sites are ordered right after the sites of the original model—in the graph above, the ordering changes as  $12345 \rightarrow 11'23455'$  with the introduction of the auxiliary sites. We assumed no knowledge about the excitation parity sector of the model.

operators satisfy the fermionic algebra

$$[a_i, a_j]_+ = [a_i^\dagger, a_j^\dagger]_+ = 0, \quad [a_i, a_j^\dagger]_+ = \delta_{ij}. \quad (2)$$

Consequently, the action of the annihilation operator is

$$a_j |n_0, \dots, n_j, \dots, n_{N-1}\rangle = \delta_{n_j, 1} (-1)^{\Gamma_{jn}} |n_0, \dots, (n_j - 1), \dots, n_{N-1}\rangle, \quad (3)$$

with a nontrivial phase factor given by  $\Gamma_{jn} = \sum_{i=0}^{j-1} n_i$ . The JW transform from  $N$  fermionic sites to  $N$  qubits preserves the fermionic algebra with tensor products of qubit operators,

$$a_j = \bigotimes_{i=0}^{j-1} Z_i \otimes A_j \quad \text{for some } 0 \leq j < N, \quad (4)$$

where  $A_j = (X_j + iY_j)/2$  is the single-qubit lowering operator acting on the  $j$ th qubit. The qubits store the fermionic occupancies, thus the vacuum state for the Jordan-Wigner transformed operators is  $|\Omega\rangle = |0 \dots 0\rangle$  with  $Z|0\rangle = |0\rangle$ . The JW transformation of the fermionic nearest-neighbor hopping term  $a_p^\dagger a_q$  for  $p < q$  is given by

$$a_p^\dagger a_q = A_p^\dagger \otimes \left( \bigotimes_{i=p+1}^{q-1} Z_i \right) \otimes A_q. \quad (5)$$

This operator contains  $|q - p| - 1$  qubit  $Z$  operators in its qubit representation. Thus, the qubit Hamiltonian is local only when the fermionic Hamiltonian has consecutively ordered couplings. Exemplary cases are one-dimensional nearest-neighbor models, such as the one-dimensional Hubbard model. In general, however, the Hamiltonian will have nonlocal qubit terms, as we will illustrate by example later in the text.

*Overview of simulation algorithm.* Before delving into technical details, we give a high level summary of the auxiliary fermion simulation algorithm for systems with  $N$  single-particle sites. The sites can be any single-particle wave function, e.g., plane waves, atomic orbitals, delta functions, etc.

(1) Consider a fermionic Hamiltonian with given coupling strengths. For each site  $p$ , compute  $D_p$  as the number of sites it couples to. Introduce  $\text{ceil}(D_p/2)$  additional (auxiliary) fermionic sites indexed adjacent to  $p$  (Fig. 1).

(2) Construct an initial  $N_f$  fermion state with the correctly initialized auxiliary sites.

(3) Convert the fermionic Hamiltonian to qubit representation. After the conversion, the one-body terms affect at most  $2\text{ceil}(D/2)$  qubits with  $D = \max D_p$ . Two-body terms affect at most  $4\text{ceil}(D/2)$  qubits.

(4) The same conversion can be applied to correlation functions and other physically interesting observables.

For example, nearest-neighbor fermionic hopping on a square lattice represented with qubits will be at most four-local, in contrast to JW, where it would have been up to  $(\sqrt{N} + 1)$  local.

The auxiliary fermion method reduces the tensor locality of the Hamiltonian terms as compared to the other methods. However, this is irrespective of the spatial locality of the qubits. Thus, the implementation on quantum hardware will depend on the specific layout and capabilities of the experimental system.

The remainder of this Rapid Communication is structured as follows: First we derive the general form for the auxiliary couplings. We then analyze the spatial requirements of the model and illustrate the construction with two examples. This is followed by discussion of state preparation.

*Auxiliary coupling terms.* The method for achieving qubit locality for operators is to replace  $h_{pq}^{\text{old}} = a_p^\dagger a_q + a_q^\dagger a_p \mapsto h_{pq} = a_p^\dagger M_{\text{aux}}(pq) a_q + a_q^\dagger M_{\text{aux}}(pq) a_p$  in the fermionic model for sites  $p$  and  $q$  separated along the linear indexing. The generalization to two-body four-point or higher coupling terms follows naturally:  $a_p^\dagger a_q a_r^\dagger a_s \mapsto a_p^\dagger M_{\text{aux}}(pq) a_q a_r^\dagger M_{\text{aux}}(rs) a_s$ . Here,  $M_{\text{aux}}(ij)$  is an operator on auxiliary fermionic sites introduced to cancel the JW nonlocal  $Z$  chains without changing the physics of the original fermionic model. As detailed below, the vacuum state  $|\Omega\rangle$  is also modified to achieve the desired fermionic statistics.

We now define  $M_{\text{aux}}(ij)$  by imposing a set of algebraic constraints. Since we increased the dimension of the Hilbert space by introducing the auxiliary fermionic sites, not every qubit state will correspond to a physical state of the fermionic system. We therefore impose that the physical fermionic states on qubits correspond to  $+1$  eigenstates of all  $M_{\text{aux}}(ij)$ . In other words,  $M_{\text{aux}}$  operators *stabilize* a physical subspace. It follows that any two  $M_{\text{aux}}$  will commute on this subspace. We also insist for all  $p$  that  $[M_{\text{aux}}, a_p] = 0$ , implying  $a_p^\dagger M_{\text{aux}} a_q |\Omega\rangle = a_p^\dagger a_q M_{\text{aux}} |\Omega\rangle = a_p^\dagger a_q |\Omega\rangle$ . This condition allows us to simulate the auxiliary fermions without any effect on the original fermionic system. To allow state preparation in the encoding, we require  $M_{\text{aux}}$  to correspond to an observable with  $\pm 1$  eigenvalues—hence all  $M_{\text{aux}}$  are Hermitian and  $M_{\text{aux}}^2 = \mathbf{1}$ . Suppose we take decomposition  $M_{\text{aux}}(pq) = i b_{p'} c_{q'}$ , where the primed indices label the auxiliary fermionic sites. The following then defines  $M_{\text{aux}}$  with the above properties,

$$b_{p'} = (e^{-i\theta} a_{p'} + e^{i\theta} a_{p'}^\dagger), \quad c_{q'} = (e^{-i\phi} a_{q'} + e^{i\phi} a_{q'}^\dagger),$$

for any real parameters  $\theta, \phi$ . Previous constructions of  $M_{\text{aux}}$  found in the literature [14–16] correspond to  $b_{p'}$  and  $c_{q'}$  as  $(a_{p'} + a_{p'}^\dagger)$  or  $-i(a_{p'} - a_{p'}^\dagger)$ , i.e.,  $\theta$  and  $\phi$  are 0 or  $\pi/2$ . Note that these choices coincide with the definition of Majorana fermions. In general, we can represent these operators on

qubits through a JW transform as

$$b_{p'} = \left( \bigotimes_{i=0}^{p'-1} Z_i \right) \otimes B_{p'}, \quad c_{q'} = \left( \bigotimes_{i=0}^{q'-1} Z_i \right) \otimes C_{q'},$$

with  $B_{p'} = [\cos \theta X + \sin \theta Y]_{p'}$  and  $C_{q'} = [\cos \phi X + \sin \phi Y]_{q'}$  being single-qubit operators acting on auxiliary sites  $p'$  and  $q'$ .

The eigenstates of  $B_{p'}$  are

$$|\pm_\theta\rangle = \frac{|0\rangle \pm e^{i\theta}|1\rangle}{\sqrt{2}}. \quad (6)$$

The specific relationship between choices for  $\theta$  and  $\phi$  will be detailed below.

Before proceeding further, we give further intuition behind the operator locality reduction achieved by the scheme. The fermionic phase factor gives rise to the nonlocality of the JW transform. In the occupation number basis, Eq. (1), the fermionic sites are in a fixed ordering. All other site orderings map back to this state with either a  $+1$  or  $-1$  phase factor. The JW operator chains compute this reordering factor. In this model, the reordering factor is computed using the code space of  $\{M_{\text{aux}}(pq)\}$ . Consider the action of  $\hat{K} = \prod_i^{N_f} a_{k_i}^\dagger$  on the vacuum state. With the JW representation [Eq. (4)] of  $\hat{K}$ , the auxiliary site  $j'$  will store parity  $p_j = \sum_{k=j+1}^N n_k$ . This follows from Eq. (6) since  $Z|\pm_\theta\rangle = |\mp_\theta\rangle$ . Thus, the information about the parity is stored locally in the correlation of the  $i'$  and  $j'$  qubits with values of  $s_i, s_j \in \{+, -\}$ . The product  $s_i s_j$  hence gives the phase factor associated with the reordering needed to implement  $a_i^\dagger a_j + a_j^\dagger a_i$ .

*Spatial requirements.* The number of additional auxiliary fermionic sites will depend on how the coupling graph differs from the linear indexing graph. In the linear graph all fermionic sites have only two neighbors. Whenever a fermion participates in nonlocal couplings involving  $D > 2$  other fermionic sites, then the present model requires  $\text{ceil}(D/2)$  auxiliary fermions to be introduced for completely local simulation. As the number of auxiliary fermionic sites increases, the operator locality must also increase. The creation or annihilation of a fermion at a site requires that all auxiliary sites affiliated with that site also be updated. Next, we show that each auxiliary site can couple up to two nonlocal neighbors.

We let  $B_\perp$  be the orthogonal partner to  $Z$  and  $B$ , such that  $\text{Tr}(ZB) = \text{Tr}(ZB_\perp) = \text{Tr}(BB_\perp) = 0$ . It follows from anticommutation that  $\pm iBZ = B_\perp$ . Since the qubit operators  $B$  and  $Z$  have only one mutually orthogonal partner, at most two nonlocal couplings can be connected to a single auxiliary mode.

We divide the analysis into two cases (assume that  $p < q < r$ ), first with  $M_{\text{aux}}(pq)$  and  $M_{\text{aux}}(pr)$  and second with  $M_{\text{aux}}(pq)$  and  $M_{\text{aux}}(qr)$ . These are the only two relevant cases because the indexing is linear. Then  $M_{\text{aux}}(pq)$  is given by

$$\begin{array}{c|ccc} M_{\text{aux}}(pq) & p & p' & q & q' \\ \hline ib_{p'} & Z & iB_\perp & & \\ c_{q'} & Z & Z & Z \dots Z & Z & C \\ \hline ib_{p'}c_{q'} & \mathbf{1} & B & Z \dots Z & Z & C \end{array} \quad (7)$$

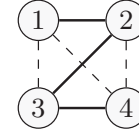


FIG. 2. The  $K_4$  graph is the completely connected graph with four sites. The solid lines indicate the linear indexing and the dashed edges indicate nonlocal couplings.

In the first case, the auxiliary couplings share a common node  $p$ . One can therefore write the qubit operators as

$$\begin{array}{c|ccc} & p' & q' & r' \\ \hline M_{\text{aux}}(pq) & B & Z \dots Z & C \\ M_{\text{aux}}(pr) & B' & Z \dots Z & Z & Z \dots Z & C' \end{array} \quad (8)$$

The operators  $B', C'$  can differ from  $B, C$ . Since  $C$  and  $Z$  anticommute, for  $M_{\text{aux}}(pq)$  and  $M_{\text{aux}}(pr)$  to commute,  $B$  and  $B'$  must also anticommute. Since  $\text{Tr}([B, B']_+) = 2 \text{Tr}(BB') = 0$ , it follows that  $B'$  must be orthogonal to  $B$  in the Hilbert-Schmidt norm. However, we have already shown that  $(B_\perp)_\perp = \pm B$ , and therefore  $B' = \pm B_\perp$ . In the second case, where the nonlocal links share a common site  $q$ , the operator acting on  $q$  must be the same for both of the auxiliary couplings since the two couplings will only overlap at  $q$ .

*Examples.* As a simple example, let us consider the simulation of the completely connected four-site fermionic system depicted in Fig. 2. First, we must choose a basis for the  $M_{\text{aux}}$  operators, construct the invariant vacuum state, and finally we can give expressions for one-body and two-body couplings.

Without loss of generality, we fix the  $\alpha$  parameter for the auxiliary couplings such that

$$\begin{array}{c|cccccc} & 1 & 1' & 2 & 2' & 3 & 3' & 4 & 4' \\ \hline M_{13} & & X & Z & Z & Z & X & & \\ M_{14} & & Y & Z & Z & Z & Z & Z & Y \\ M_{24} & & & & X & Z & Z & Z & X \end{array} \quad (9)$$

Note that the choice of  $M_{13}$  and  $M_{14}$  fix  $M_{24}$  by the commutation requirements.

Nonlocal one-body terms for the  $K_4$  graph follow from Eqs. (4) and (9):

$$\begin{array}{c|cccccc} & 1 & 1' & 2 & 2' & 3 & 3' & 4 & 4' \\ \hline a_1^\dagger M_{13} a_3 & A^\dagger & -iY & & & A & X & & \\ a_2^\dagger M_{24} a_4 & & & A^\dagger & -iY & & & A & X \\ a_1^\dagger M_{14} a_4 & A^\dagger & iX & & & & & A & Y \end{array} \quad (10)$$

The remaining local hopping terms are of the form  $a_p^\dagger a_{p+1} = A_p^\dagger \otimes Z_{p'} \otimes A_{p+1}$ . The one-local number operator is given by  $a_k^\dagger a_k = (\mathbf{1} - Z_k)/2$ . The two-body terms consisting of two-point couplings, e.g.,  $a_i^\dagger a_j^\dagger a_j a_i$ , are straightforward products of the qubit representations of  $a_i^\dagger a_i$  and  $a_j^\dagger a_j$ .

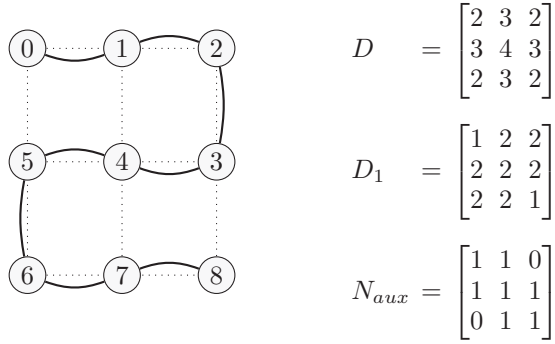


FIG. 3. The two-dimensional (2D) Hubbard model provides an illustration of the advantage of the auxiliary fermion simulations over Jordan-Wigner and Bravyi-Kitaev transformed operators. On the left, the  $L = 3$  model is depicted with linear indexing graph  $G_1$  in curved bold lines and with dotted lines indicating the Hubbard coupling graph  $G$ . On the right,  $D = \deg(G)$  is the degree of the sites in  $G$ , similarly  $D_1 = \deg(G_1)$ . Their difference gives the nonlocal degree  $D_{nl}$ . This translates into the number of auxiliary fermions needed at each site following  $N_{aux} = \text{ceil}(D_{nl}/2)$ .

Similarly, three-point interactions, e.g.,  $a_i^\dagger a_k a_j^\dagger a_j$ , are also products of the qubit representation of  $a_j^\dagger a_j$  and  $a_i^\dagger M_{aux}(ik) a_k$ , when  $i$  and  $k$  have nonconsecutive indices. The four-point interactions do not require the auxiliary coupling due to anticommutation relations.

Consider the term  $a_1^\dagger a_4^\dagger a_2 a_3$  which occurs in the quantum simulation of molecular hydrogen using a minimal basis [4]. Here, we can avoid the use of auxiliary qubits by rearranging the term as  $a_1^\dagger a_2 a_4^\dagger a_3$ . Now the term is a product of linearly local hopping terms, each of which can be simulated without appeal to the auxiliary couplings. This points out the importance of exercising the commutation relations to minimize the tensor weight of the simulated term.

While this example illustrates the model, it is not chosen to highlight the decisive advantages of the scheme. In fact, the Jordan-Wigner and Bravyi-Kitaev Hamiltonian on four sites also only has fourth-order tensor products, but requires half as many qubits. When more nonlocal couplings are present, the auxiliary fermion model will offer decisive advantages, as illustrated with the next example.

The second example is square lattices with  $N = L^d$  in  $d = 2$  and  $d = 3$  dimensions. In our analysis, we only consider  $L \rightarrow \infty$  bulk terms, but see Fig. 3 for an  $L = 3$  example. Each bulk site has  $2d$  neighbors. Subtracting the linear degree of 2, each site participates in  $2d - 2$  nonlocal couplings. By the arguments given earlier,  $d - 1$  auxiliary sites are needed for each site in the bulk. The maximum tensor product needed for the local simulation of hopping terms involves  $2d - 2$  qubit operators. Note that this is independent of  $L$  as the simulation now only depends on the local properties of the coupling graph.

*State preparation.* The model is closely connected to topological models found in error correction codes [21]. To have robust error correction, topological structures are used to store information as nonlocally as possible.

However, here we are attempting to store information strictly locally.

To highlight this overlap, a simple expression for the projected vacuum state can be borrowed from topologically nontrivial models [22]:

$$|\Omega\rangle = \prod_{(pq) \in E} \frac{\mathbf{1} + M_{aux}(pq)}{\sqrt{2}} |0 \dots 0\rangle. \quad (11)$$

Because we imposed  $M_{aux}(pq)^2 = \mathbf{1}$  and  $M_{aux} = M_{aux}^\dagger$ , this is a product of projectors. We begin by creating the state  $|00 \dots 0\rangle$  and proceed to projectively measure each auxiliary coupling. If the measurement outcome for an auxiliary coupling, say,  $M_{aux}(pq)$ , is  $-1$ , then changing its sign is a matter of applying  $Z_{p'}$  or applying  $Z_{q'}$  to the measured state. When the site participates in two nonlocal couplings, the error will propagate to the other nonlocal coupling. Therefore, it is simplest if an auxiliary site with only one nonlocal nearest neighbor is chosen. Otherwise, one should follow the linked chain of nonlocal sites applying the  $Z$  operator at each end point until the linked chain ends. This is possible as long as no closed loops of auxiliary couplings are present.

In the previous auxiliary fermion method introduced in Ref. [15], additional terms must be included to ensure that the phase around the closed loops of coupled auxiliary fermions is correct. This is an additional complication we need not consider by limiting our attention to encodings with no closed loops. Note that the no closed-loop restriction is not a serious limitation. For any closed loop of nonlocal couplings, e.g.,  $\{M_{aux}(pq), M_{aux}(qr), \dots, M_{aux}(sp)\}$ , we can take  $M_{aux}(p+1, q)$  instead of  $M_{aux}(pq)$ . The coupling from  $p$  to  $p+1$  can be done locally, allowing nearly the same connectivity to be achieved. Thus, we may now ignore nontrivial Wilson loops considered in Ref. [15].

It is interesting to note that both the vacuum state in Eq. (11) and the completely filled states are invariant under  $M_{ij}$ . Note that this must be true as  $b_m^\dagger = a_m$  is the hole creation operator with respect to the filled vacuum state. Hence, the action of  $\{b_m^\dagger, b_k\}$  must also be antisymmetric.

Lastly, consider the preparation of Fock states with  $N_f$  fermions. This is accomplished most straightforwardly by applying the JW representation of  $\hat{K} = \prod_i^{N_f} a_i^\dagger$  on the vacuum state. The action on the state can be simplified when both the desired state and auxiliary sites are known beforehand. In this case, the occupied sites can be acted upon with  $X$ . The auxiliary site  $k'$  is acted upon with  $Z^p$ , where  $p$  is the parity of occupied sites to the right of  $k'$ .

*Concluding remarks.* In this work, we have studied the auxiliary fermion scheme for encoding fermionic states which enables highly localized manipulation. This encoding is designed to make information as accessible as possible.

Future work will consider the possibility of a trade-off between robustness against noise and the locality of encoding. The auxiliary fermionic system may be easier for both experimentalists and noise sources to modify the information. While the Jordan-Wigner encoding requires nonlocal manipulation of the state, a recent numerical analysis suggests that it is more robust against noise than the Bravyi-Kitaev encoding [23]. The present Rapid Communication has not considered

the effects of noise akin to a fault-tolerant setting [20]. Within this framework, the auxiliary fermion scheme represents an important improvement over the Jordan-Wigner and Bravyi-Kitaev schemes.

Other direction of this work are the comparison against related ideas for reducing the tensor product rank of fermionic simulations [10,24,25] and applications to adiabatic computation [26,27].

## ACKNOWLEDGMENTS

This work was supported through the ERC Grants QUTE and SIMCOFE and by the Swiss National Science Foundation through NCCR QSIT. We thank Frank Verstraete, Lei Wang, Ye-Hua Liu, and Alexey Soluyanov for useful discussions, and Peter Love for comments on the manuscript.

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