Linear and Logarithmic Time Compositions of Quantum Many-Body Operators

F. Motzoi,[1] M. P. Kaicher,[2] and F. K. Wilhelm[2]
[1]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus, Denmark
[2]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany
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We develop a generalized framework for constructing many-body-interaction operations either in linear time or in logarithmic time with a linear number of ancilla qubits. Exact gate decompositions are given for Pauli strings, many-control Toffoli gates, number- and parity-conserving interactions, unitary coupled cluster operations, and sparse matrix generators. We provide a linear time protocol that works by creating a superposition of exponentially many different possible operator strings and then uses dynamical decoupling methodology to undo all the unwanted terms. A logarithmic time protocol overcomes the speed limit of the first by using ancilla registers to condition evolution to the support of the desired many-body interaction before using parallel chaining operations to expand the string length. The two techniques improve substantially on current strategies (reductions in time and space ranging from linear to exponential), are applicable to different physical interaction mechanisms such as CNOT, XX, and $XX + YY$, and generalize to a wide range of many-body operators.

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Introduction.—Generating multibody entanglement is the hallmark of most quantum information technologies. Such technologies promise to harness entanglement across multiple quantum registers to enable potentially significant improvements in speed or precision compared to their classical counterparts. Yet much of the difficulty in the control of quantum systems lies in the constraint that entanglement naturally arises on a local scale while scaling improvements occur as a result of wave functions spread over much larger spaces.

Quantum circuits generating entanglement across n qubits in linear or sublinear time (circuit depth) in n have been the subject of many studies, with direct use as subroutines in quantum algorithms for factoring [1,2], simulation [3–15], unstructured search [16], error correction [17], and solutions to systems of differential equations [4,11,18,19]. Much progress has been made for constructing many-body operations, either by finding architectures where commuting two-qubit interactions could be executed simultaneously on overlapping Hilbert spaces or via cases where a particular many-body gate with known or suspected sublinear implementation can be used to synthesize other many-body circuits. The former has been used for so-called *collective* Pauli operations on qubits in ion chains [20–22], while the workhorse for the latter has been the *fanout* operation [23,24], which has successfully lead to $O(\log(n))$ depth quantum circuits for various flavors of quantum adders [25–27], with related arithmetic operations [1,28].

Other many-body interactions have also been synthesized to mixed success. The ubiquitous many-control CNOT has found general linear-depth implementations, though with a relatively large prefactor [29–31]. Likewise, operations have been sought for rotating between two arbitrary multiqubit states, use in sparse matrix generation [4,11,19,32], or, equivalently, pairwise inversion of opposing spins in the unitary couple cluster (UCC) theory [33–37]. Here, proposals have typically involved (based on intended application) either multicontrol CNOT and arithmetic gates with linear ancillary memory [11,19] or Trotter decomposition of the dynamics into (exponentially many) Pauli-string factors but with no ancillas.

In this Letter, we provide a formalism on how to directly compose a wide class of such many-body entangling operations (generated each by an equivalent Hermitian many-body operator $\bar{H}$) via two-(or few-)local interactions and for which the above discussed protocols and algorithms form important examples of its application. We aim to minimize two standard figures of merit of the generic circuit, namely, its *depth*, defined as the number of layers of gates acting simultaneously on disjoint sets of qubits, and its *width*, defined as the total number of qubits acted on by the circuit [38]. We find a width-optimized general algorithm, which we label the *decoupling protocol*, to compose $\bar{H}$ with zero or constant memory overhead and depth limited to linear n scaling. Moreover, we demonstrate a depth-optimized algorithm for simulating $\bar{H}$, the *selection protocol*, which has logarithmic depth and requires at most linear memory overhead. We demonstrate the formalism towards the linear or exponential speedup of the aforementioned examples, given in our notation by equivalent Hamiltonians:

$$\bar{H} = \begin{cases} \prod_{i=1}^{n} X_i (n\text{-qubit Pauli strings}) \\ \left(\prod_{i=1}^{n} P_i\right) X_{n+1} (n\text{-controlled} X \text{gate}) \\ \prod_{i=1}^{n/2} (\sigma_{2i-1}^{+}\sigma_{2i}^{-} + \text{H.c.}) (\text{number or parity consv}) \\ \left(\prod_{i=1}^{n} \sigma_i^{+}\right) + \text{H.c.} (\text{UCC-type operators}, \\ \qquad\qquad \text{sparse matrix generators}), \end{cases}$$

where X_i, Y_i, and Z_i are Pauli operators acting on qubit i, $\sigma_j^{\pm} = (X_j \mp iY_j)/2$, and $P_i = |1\rangle\langle 1|_i$. The unitary circuit generated by the many-body composed dynamics can then be written succinctly via the notation

$$[\bar{H}]^{\alpha} \equiv \exp(-i\alpha\bar{H}), \tag{1}$$

with rotation angle α.

In order to identify the type of Hamiltonians we can compose, we first introduce notation and conventions. For simplicity, we disregard local unitary transformations between operators of the same rank. Let $\mathcal{H} = H_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$ denote a separable Hilbert space. Then $R_i = \mathbb{1}^{\otimes(i-1)} \otimes R \otimes \mathbb{1}^{\otimes(n-i)}$, where $\mathbb{1}_j$ denotes the identity on $\mathcal{H}_j$ and R ($\neq \mathbb{1}$) is a 2×2-Hermitian matrix for qubits (or $d \times d$ for qudits). We use the convention $\text{rank}(R_i) \equiv \text{rank}(R)$, thereby ignoring contributions from identities $\bigotimes_{j\neq i} \mathbb{1}_j$ on other sub-Hilbert spaces. We write a higher-rank R_i as the tensor sum $R = V(S \oplus S^{\perp})V^{\dagger}$, where V is any local unitary transformation (i.e., $S^{\perp}$ lies in the kernel of S). It is by chaining together the lower-rank S_i factors that we will be able to construct our many-body dynamics $\bar{H}$.

Many-body decoupling protocol.—Our main tool is a unitary (two- or few-body) operator $U_{j-1,j}$ which will be used to iteratively increase in length a string of Hermitian operators $S_1 S_2 \ldots S_j$ acting on the system. However, recall that generally S_j will not be full rank, and so $U_{j-1,j}$ will invariably have to also act outside the support of S. Thus, our protocol will have to execute the desired system dynamics (given by $\bar{H}$) while leaving the rest of the Hilbert space (namely, the kernels of S_j) intact. A condition to using the protocol is that a $U_{i,j}$ can be found such that

$$U_{i,j}^{\dagger} R_i U_{i,j} = S_i R_j + S_i^{\perp} + S_i R_j^{\perp}, \tag{2}$$

thereby incrementing the length of a string of nonidentity Hermitian operators by one when acting on R_i. Then, successively applying Eq. (2), one can show that the following sum of operator strings of increasing string length can be composed:

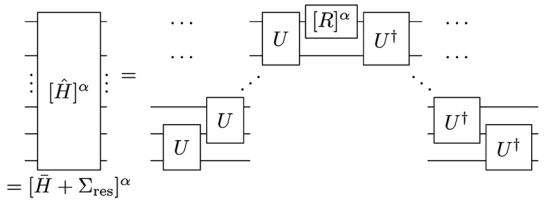

FIG. 1. Generating the unitary dynamics $[\hat{H}]^{\alpha} = [\bar{H} + \Sigma_{\text{res}}]^{\alpha}$ of Eq. (3) using one single-body and $2n$ $U_{j-1,j}$ operators.

$$\begin{aligned} \hat{H} &= \left(\prod_{j=n}^{1} U_{j,j+1}^{\dagger}\right) R_1 \left(\prod_{j=1}^{n} U_{j,j+1}\right) \\ &= \left(\prod_{i=1}^{n} S_i\right) R_{n+1} + \sum_{m=1}^{n} \left(\prod_{i=1}^{m-1} S_i\right) (S_m R_{m+1}^{\perp} + S_m^{\perp}) \\ &\equiv \bar{H} + \Sigma_{\text{res}}, \end{aligned} \tag{3}$$

as shown in Fig. 1, where $\bar{H} = (\prod_{i=1}^{n} S_i) R_{n+1}$. Therefore, composing $\bar{H}$ from two-body operators $U_{i,j}$ usually creates unwanted remainder terms Σ_{res}. However, the remainder terms commute with $\bar{H}$ while also acting as the identity on the support of R_{n+1}. Thus, we can find a one-body unitary transformation M_{n+1} such that it imparts an opposite phase to R_{n+1} (and thus $\bar{H}$) but does not change Σ_{res} [39]. The requisite dynamics can then be recovered using the decoupling sequence (cf. Fig. 2)

$$[\bar{H}]^{2\alpha} = [\hat{H}]^{\alpha} M_{n+1}^{\dagger} [\hat{H}]^{-\alpha} M_{n+1}. \tag{4}$$

Here, to construct an effective Hamiltonian $\bar{H}$ of string length $n+1$, a total of $4n$ unitary operators $U_{i,j}$ are needed. Note that if R is full rank, Eq. (2) reduces to $U_{i,j}^{\dagger} R_i U_{i,j} = R_i R_j$ and only half as many operators are used, since decoupling is not required.

Many-body selection protocol.—We now present a composition scheme that can further decrease the required circuit depth for n-body operators from a $\mathcal{O}(n)$ to a $\mathcal{O}(\log(n))$ scaling, at the cost of $n-1$ ancillas (cf. Figs. 3 and 4). Without loss of generality, we set $n = 2^m$, where $m \in \mathbb{N}$, and introduce two sets of qubit indices, namely, register qubits $q_{\text{reg}} = \{1, 2, \ldots, n+1\}$ containing the qubits of the desired string and ancilla qubits $q_{\text{anc}} = \{n+2, 2, \ldots, 2n\}$, where the latter are all initialized to the $|0\rangle$ state.

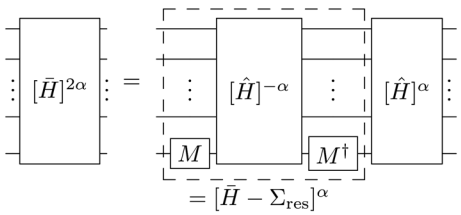

FIG. 2. Gate sequence for realizing the decoupling protocol given in Eq. (4) using $4n$ $U_{j-1,j}$ operators.

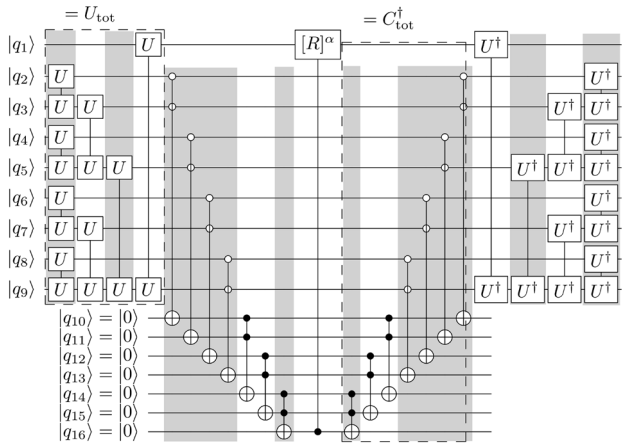

FIG. 3. Gate sequence to compose an operator string of length $n = 9$, to run in $O(\log n)$ depth. Here, we assume that $1 < \mathrm{rank}(S_i) < \mathrm{rank}(S_i + S_i^\perp)$ for $i > 1$. Small empty circles are conditioning operators (projectors) on the support of S, while solid circles are conventional Toffoli gates. The connected U are the entangling operations from Eq. (2). Since $R_1 \equiv S_1$ is applied only on the support of $S_2 \ldots S_9$, $\hat{H}$ (which is created by the $U_{i,j}$ tree structure) is also applied only on the support of $\bar{H}$.

Moreover, we introduce Toffoli-type unitary operators $C_{i,j}X_k$, whereby a NOT is applied to qubit k conditioned on the state of qubits i, j which can be either register or ancilla qubits. The operation can be written mathematically as, e.g., $C_{i,j}X_k = [S_i S_j X_k]^{\pi/2}$. For $i, j \in q_{\rm reg}$, $C_{i,j}$ essentially conditions on being in the support of both S_i and S_j. If i, $j \in q_{\rm anc}$, the operation is a standard Toffoli (or simply letting $S_i = |1\rangle\langle 1|_i$). Note that if n is not a power of 2, some $C_{i,j}X_k$ operations can have both register and ancilla qubits as controls. We define as in Fig. 3 compound operations

$$C_{\rm tot} \equiv \prod_{k=1}^{\log n} \left(\prod_{l=n-2^k+1}^{n-2^{k-1}} C_{2l+1,2l} X_{n+l+1} \right), \tag{5}$$

$$U_{\rm tot} \equiv \prod_{k=\log n}^{1} \left(\prod_{l=1}^{n/2^k} U_{l2^k+1,(l-\frac{1}{2})2^k+1} \right) U_{1,n+1}. \tag{6}$$

For the boundary case $\mathrm{rank}(S) = 1$, we set $U_{\rm tot} = \mathbb{1}$, while if S full rank, then $C_{\rm tot} = \mathbb{1}$. All the operations in the brackets can be run parallel. The full selection protocol is given by the sequence

$$[\bar{H}]^\alpha = U^\dagger_{\rm tot} C^\dagger_{\rm tot} (C[R_1]^\alpha) C_{\rm tot} U_{\rm tot}; \tag{7}$$

see Fig. 4. The middle operator is defined as $C[R_1]^\alpha = [R_1]^\alpha$ if S full rank and $[|1\rangle\langle 1|_{2n} R_1]^\alpha$ otherwise. The result of the sequence is that the many-body rotation is applied only on states that are supported by $R_1 S_2 \ldots S_n$, while identity is applied otherwise. The selection protocol improves on previous generic algorithms by quadratically reducing the space requirements [23].

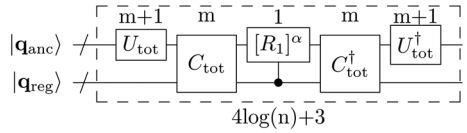

FIG. 4. Generalized version of Fig. 3, where all register (respectively, ancillary) qubits $\mathbf{q}_{\rm reg}$ and $\mathbf{q}_{\rm anc}$ are compounded to one circuit line. All operations that can be run in parallel are synthesized to one box, with the number above it indicating how many noncommutative time steps are necessary for each box. For $n = 2^m$, a string of length $n + 1$ is composed in $\mathcal{O}(\log(n))$ depth.

The following sections demonstrate how to apply the decoupling and selection protocols to existing problems, to either take advantage of specific two-body interaction mechanisms or reduce the time and gate complexity of known implementations. Further details of the derivations are given in Supplemental Material [40].

Pauli strings.—Well-known formulas exist for forming strings of Pauli operators in linear time (e.g., [41,42]), which we first reproduce using our formalism. Since Pauli operators are full rank, $\hat{H} = S_1 S_2 \ldots S_j = \bar{H}$, and there is no need for decoupling. The optimal form of $U_{i,j}$ will depend on the architecture and its natural interaction. A standard entangling operation is via $U_{i,j} = \mathrm{CNOT}_{ij}$ gates [41], which applied as in Fig. 1 produce a many-body operator (3) with $R_i = X_i$. However, this interaction is natural for neither superconducting nor trapped ion qubits. A native gate for ion-trap designs is the Mølmer-Sørensen gate (MSG), where commuting $U_{i,j} = [X_i X_j]^{\pi/4}$ [20,43] interactions can be applied simultaneously. We present a third composition with the same size as the CNOT and MSG circuits, designed for architectures with exchange gate interactions, $G_{i,j} = \frac{1}{2}(X_i X_j + Y_i Y_j)$, which is the fastest perfect entangler for most circuit-QED quantum processors [44,45], quantum dot spins coupled by a cavity [46], and nuclear spins interacting via a two-dimensional electron gas [47]. Here, $U_{i,j} = [G_{i,j}]^{-\pi/2}$ is an iSWAP gate. Using Eq. (2) and $U^\dagger_{i,j} Y_i U_{i,j} = Z_i X_i$ allows us to construct a Pauli string of length n using $2(n-1)$ iSWAPs. Since the Pauli operators are full rank, one can drastically reduce the depth of the circuit from $\mathcal{O}(n)$ to $\mathcal{O}(\log(n))$ by using (7), with $\prod_{i=1}^n S_i = U^\dagger_{\rm tot} R_1 U_{\rm tot}$, without needing any ancillary qubits. Note further that, instead of increasing the length of the string using $U_{i,j}$, one can also use the inverse operation to remove a qubit from the string, e.g., to form a disconnected string from a nearest-neighbor architecture.

Number- and parity-conserving strings.—We now turn to generating many-body operators that act conditionally only within the fixed excitation-number subspace. These are a natural fit for a two-body, exchange gate interaction, $G^+_{i,j} = \sigma^+_i \sigma^-_j + \sigma^-_i \sigma^+_j$, which has the same symmetry, noting also its rank is smaller than $\dim(\mathcal{H}_i \otimes \mathcal{H}_j)$. Defining $F^-_{i,j} = -i(\sigma^+_i \sigma^-_j - \sigma^-_i \sigma^+_j)$, we desire strings of $R_{i,j} \in \{G_{i,j}, F_{i,j}\}$. We choose $U_{i,k,l} = [Z_i G_{k,l}]^{\pi/4}$ as the

(now three-qubit) entangling operation, giving $U^\dagger_{i,k,l}G_{i,j}U_{i,k,l} = F_{i,j}G_{k,l} + G_{i,j}P_{\ker\{G_{k,l}\}}$, where $R^\perp_{k,l} = \frac{1}{2}(\mathbb{1} + Z_kZ_l)$. Following the steps in Eq. (3), one obtains

$$\hat{H} = \prod_{i=1}^{n/2} R_{2i-1,2i} + \sum_{i=1}^{n/2-1}\left(\prod_{j=1}^{i} R_{2j-1,2j}\right)R^\perp_{2i+1,2i+2}, \quad (8)$$

a many-body Hamiltonian that collectively excites and deexcites n qubits in a number-conserving way. By choosing $M_n = [Z_n]^{\pi/2}$, one can apply the decoupling sequence (4) to pick out one particular number-conserving string

$$[\bar{H}]^\alpha = \left[\prod_{i=1}^{n/2} R_{2i-1,2i}\right]^\alpha. \quad (9)$$

More generally, parity can be conserved without conserving number [13] by applying local operations (X_i) to transform operators in the string from $G_{i,j}$ to $\sigma^+_i\sigma^+_j + \sigma^-_i\sigma^-_j$. As we detail in Ref. [40], the whole sequence takes $2n-4$ $U_{i,j,k}$ gates or, equivalently, $6n-10$ iSWAPs. Half as many are required if $\hat{H}$ is used instead. Alternatively, the many-body dynamics can be generated with the selection protocol at the cost of $n-1$ ancillas. For this, we can reuse $U_{i,j,k} = C_{i,j}X_k$ for $i,j \in q_{\text{reg}}$. This total sequence uses a total of $2n-4$ entanglers $U_{i,k,l}$ and $n+4$ Toffolis in a circuit depth of $4\log(n)+3$.

Multicontrol CNOT gates.—$C_{1,\ldots,n}X_{n+1}$ gates have widespread use in quantum and reversible computation, including for circuit distillation [48], unstructured search [16], factorization [1], error correction [17], and linear equation system solvers [19]. For our construction, $U_{i,j,k} = [P_iX_jP_k]^{\pi/2}$ (a Toffoli gate with a relative phase [31], though a regular Toffoli can also be used) acts on three qubits, recalling $P_i = |1\rangle\langle 1|_i$. The chaining operation is given by $U_{i,j,k}Z_iZ_jU^\dagger_{i,j,k} = -P_iZ_jZ_k + P^\perp_iZ_j$, with $P^\perp_i = |0\rangle\langle 0|_i$. Repeated application of the chaining operation on $R_{1,2} = Z_1Z_2$ following Eq. (3) gives [40]

$$\hat{H}_n = (-1)^n\prod_{i=1}^{n} P_iZ_{n+1}Z_{n+2} - \sum_{j=1}^{n}(-1)^j\prod_{k=1}^{j-1}P_kP^\perp_jZ_{j+1}. \quad (10)$$

Choosing $M = [X]^{\pi/2}$, one can use the decoupling protocol (4) to obtain a multiqubit-controlled rotation around an arbitrary angle. For a phaseless multicontrol CNOT gate, one can compose instead the sequence

$$C_{1,\ldots,n}Z_{n+2} = [\hat{H}_n]^{\pi/2}M^\dagger_{n+1}[\hat{H}_{n-1}]^{-\pi/2}M_{n+1}, \quad (11)$$

using $4n-2$ Toffolis, cutting in half the size and depth of the long-standing construction [29–31].

A more drastic reduction results with the selection protocol, where $S_i = P_i$ and thus $\text{rank}(S) = 1$. Equation (7) simplifies to

$$C_{2,\ldots,n+1}X_1 = C^\dagger_{\text{tot}}(C_{n+1}X_1)C_{\text{tot}}, \quad (12)$$

resulting in an n-control CNOT gate using $2(n-1)$ Toffoli gates and $2\log(n)$ depth (cf. Fig. 4). This gives an exponential speedup compared to the $O(n)$ ancilla solution found in Ref. [31].

Unitary coupled cluster.—Another many-body operator which is frequently used (e.g., in quantum chemistry algorithms for computing energy landscapes) is an operator which transfers population between electronic orbitals (encoded in the qubits) while maintaining the electron number and spin. More generally, when the operator couples arbitrary many-qubit states, it corresponds to a sparse matrix off-diagonal element [19]. It takes the form

$$\text{UCC}(m,n) \equiv \prod_{i=1}^{m}\sigma^+_i\prod_{j=m+1}^{m+n}\sigma^-_j + \text{H.c.} \quad (13)$$

We have seen in the section on Pauli strings how to construct $R = \prod_{i=1}^{m+n}X_i$ using $2(m+n-1)$ entanglers. Since $\prod_{i=1}^{n+m}X_i$ contains all 2^{m+n} combinations of products of σ^+ and σ^-, we use $U = [(\prod_{i=1}^{m}P_i)(\prod_{j=m+1}^{n}P^\perp_j)X_{n+m+1}]^{\pi/2}$, which we know how to construct from the previous section on multicontrol CNOTs, computing $\hat{H} = U^\dagger RU$ to get

$$\hat{H} = \prod_{i=1}^{m+n}X_i - \left(\prod_{i=1}^{m}\sigma^+_i\prod_{j=m+1}^{m+n}\sigma^-_j + \text{H.c.}\right) + i\left(\prod_{i=1}^{m}\sigma^+_i\prod_{j=m+1}^{m+n}\sigma^-_j - \text{H.c.}\right)X_{m+n+1}. \quad (14)$$

By setting $M = [Z_{m+n+1}]^{\pi/2}$, we can apply the decoupling protocol to construct the unitary dynamics of the UCC(m,n) operator in a circuit with $m+n+1$ qubits (q_{m+n+1} is an ancillary qubit) using $4(m+n-1)$ iSWAPs and $4(m+n)$ (relative phase) Toffolis:

$$[\bar{H}]^{2\alpha} = [\hat{H}]^\alpha M^\dagger[\hat{H}]^{-\alpha}M = [\text{UCC}(m,n)]^{2\alpha}. \quad (15)$$

Conventional factorization of the UCC(m,n) terms into Pauli strings scales exponentially as $\mathcal{O}(2^{m+n-1})$ in the number of two-qubit gates cost, whereas only $36(m+n) + \mathcal{O}(1)$ iSWAPs are required when using our decoupling protocol. An even further decrease in the composition time is once again achieved if the Pauli string and multi-CNOT gates are produced using the selection protocol, down to a depth of $O(\log n)$.

Architectural considerations.—Clearly, any time and space complexity advantages will be subject to limitations set by the architecture. The presence of $O(n)$ ancillas (needed for exponential speedup) is actually fairly easy to include, as most architectures have ancillary electronic, motional, or photon bus degrees of freedom. Despite much worse lifetimes typically found in these states, the (linear) tradeoff in the error rate is more than made up by an exponential speedup in time and justifies their use for many-body gates. Note previous generic $O(\log(n))$ circuit constructions require $O(n^2)$ space [23], which may be practically infeasible. The adjacency graph of bodies that couple to each other in the architecture will also greatly impact the composition time. For many-body operators spanning much of the graph, the circuit depth can range from $O(\log(n))$ when the depth of the spanning tree is $O(\log(n))$, as in Refs. [49–55], to $O(\sqrt[d]{n})$ for d-dimensional, nearest-neighbor architectures being expected [56–58].

Conclusions.—We have developed two protocols, the decoupling and selection compositions, to generate many-body operators in $O(n)$ time for zero or constant memory overhead, and $O(\log(n))$ time for $O(n)$ ancillas, respectively. The former enhances previous constant-overhead approaches, with improvement ranging for prominent examples from linear (multicontrol CNOT) to exponential (UCC). Our construction to bring down further the runtime to $O(\log(n))$ depth also improves quadratically on the space requirements of previous generic methods. Our approach is generated directly from Hamiltonian dynamics, allowing the straightforward incorporation of different coupling mechanisms and architectures.

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