Algorithmic approach to simulate Hamiltonian dynamics and an NMR simulation of quantum state transfer

Ashok Ajoy,1,2,* Rama Koteswara Rao,1 Anil Kumar,1 and Pranaw Rungta3
1Department of Physics and NMR Research Centre, Indian Institute of Science, Bangalore, India
2Nuclear Science and Engineering Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
3Indian Institute of Science Education and Research Mohali, Sector-26 Chandigarh, India

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We propose an iterative algorithm to simulate the dynamics generated by any n-qubit Hamiltonian. The simulation entails decomposing the unitary time evolution operator U (unitary) into a product of different time-step unitaries. The algorithm product-decomposes U in a chosen operator basis by identifying a certain symmetry of U that is intimately related to the number of gates in the decomposition. We illustrate the algorithm by first obtaining a polynomial decomposition in the Pauli basis of the n-qubit quantum state transfer unitary by Di Franco et al. [Phys. Rev. Lett. 101, 230502 (2008)] that transports quantum information from one end of a spin chain to the other, and then implement it in nuclear magnetic resonance to demonstrate that the decomposition is experimentally viable. We further experimentally test the resilience of the state transfer to static errors in the coupling parameters of the simulated Hamiltonian. This is done by decomposing and simulating the corresponding imperfect unitaries.

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Introduction. Feynman [1] has stated that it should be possible to manipulate the Hamiltonian of one quantum system to simulate the dynamics of another, exponentially faster than a classical computer. This serves as one of the main motivations for building a quantum information processor (QIP) [2]. More precisely, simulation is the desire to mimic the unitary dynamics U of an n-qubit Hamiltonian \( \mathcal{H} \), and if the physical resources required for the simulation scale polynomially with the problem size \( n \), then it is said to be efficient [2].

The Hamiltonian of any QIP is the sum of an intrinsic part \( \mathcal{H}_{\text{int}} \) and a time-dependent part \( \mathcal{H}_{\text{ext}}(t) \) [3] that can be experimentally controlled such that the following holds to arbitrary precision [4]:

\[
U \approx U_{\text{sim}} = \mathcal{T} \exp \left[ -i \int_0^\tau dt [\mathcal{H}_{\text{int}} + \mathcal{H}_{\text{ext}}(t)] \right],
\]

where \( \tau \) is the simulation time and \( \mathcal{T} \) is the Dyson time-ordering operator. A QIP allows universal control if it can simulate any unitary dynamics [5]. However, finding the requisite efficient set of controls \( \mathcal{H}_{\text{ext}} \) is in general a challenge [6].

In practice, the simulation is constructed by decomposing \( U \) into a product of unitary evolution operators \( U_j \): \( U_{\text{sim}} = U_1 U_2 \ldots U_m \) [4] for a sequence of time steps \( \delta_j \) with \( \sum_{j=1}^m \delta_j = \tau \). A polynomial product decomposition (PPD) of \( U \) is a decomposition such that \( m \) scales polynomially with the problem size \( n \). Clearly, a PPD is necessary for a simulation to be efficient. Efficiency also entails that each \( U_j \) (or gates) be implemented so that the amount of physical resources (spatial cost) and the implementation time (temporal cost) are small—i.e., the total cost incurred scales polynomially with \( m \). Moreover, inevitable decoherence processes in the QIP [7] could impose further efficiency constraints.

For certain unitaries a PPD may not exist in principle [4]. In this case, or when the PPD of \( U \) is not known, one resorts to approximate methods. This entails resolving \( \tau \) into a finer time steps \( \Delta \tau \), and then by assuming \( \Delta \tau \approx 0 \) one expands \( U \) onto a product decomposition (PD). Consequently, both the total cost (the number of time steps) and the precision \( U \approx U_{\text{sim}} \) become \( \Delta \tau \) dependent: If one increases (decreases) the precision, then the total temporal cost also increases (decreases). For instance, the use [2] of the Suzuki-Trotter expansion [8] limits the precision to \( O(\Delta \tau^{1/2}) \) [5]. This has motivated numerical optimization methods to achieve the desired balance between the precision and time [9,10], but their inherent computationally intensive nature restricts them to small \( n \), and they generally cannot be easily extended to arbitrary \( n \).

In this Rapid Communication, we not only propose an algorithm to exactly product-decompose any \( U \), but perhaps more importantly the algorithm also allows one to search for an efficient PPD. The algorithm first studies the support of \( U \) in a basis \( \mathcal{B} \) by representing it as a vector \( \mathcal{U} = [c_1, c_2, \ldots, c_N] \), since \( U = \sum_j c_j B_j \), where \( B_j \in \mathcal{B} \) and \( N = 4^n \). A PD, \( U = \prod_k \exp(i \theta_k B_k) \), is then obtained by systematically using the unitaries \( \exp(i \theta_k B_k) \) (gates) generated by the basis operators \( B_k \) to iteratively rotate \( \mathcal{U} \rightarrow [1,0,\ldots,0] \). The PD is derived for arbitrary \( n \) in an inductive manner, by extrapolating the symmetry in the PD for small \( n \). In principle, our algorithm allows any basis at the start: If a PPD is not obtained for one choice, then a different basis may be tried. Note, however, that any random search for such bases is bound to be inefficient since the optimal search algorithm of Grover [11] is nonpolynomial and hence inefficient. Since a PPD is realized when the PD consists of a polynomial number of gates, this may be interpreted to mean that \( U \) has a large symmetry in the sense that it is the composition of a “few” rotations, the quantum Fourier transform unitary [12,13] being a famous example.

We note that our algorithm also enables one to understand how errors and noise affect the simulation of the unitary \( U \). The errors manifest themselves by reducing the symmetry of
the error results in a PD that scales faster in terms of \( c^{n-1} \). This is done by introducing specific errors in the protocol which is then simulated by our algorithm. We explicitly demonstrate how introducing certain kind of errors [28,29] against certain kind of errors can also be modularized in our algorithm to further reduce the total cost of simulation. Note, however, that the Pauli basis will not lead to a PPD for all \( U \), and for a given QIP, there may exist several efficient bases. Recently Ref. [19] employed our algorithm to experimentally simulate the quantum no-hiding theorem [20].

We explain the essential ingredients in the algorithm, including the role of symmetries, by explicitly product-decomposing (and simulating) the unitary that causes quantum state transfer (QST) in a linear spin-1/2 chain [21]. QST allows the chain to act equivalent to a “wire” in a spin-based QIP architecture [22]. Simulation is motivated because the spin chains, as required for QST, are normally hard to manufacture [22]. We first obtain a PD in the Pauli basis of a remarkable QST protocol by Di Franco et al. [23] that inherently does not require the chain to be initialized [23,24]. We then experimentally simulate it in a nuclear magnetic resonance (NMR) QIP [25–27].

We also use the PD to investigate the protocol’s robustness against certain kind of errors [28,29]. This is done by introducing specific errors in the protocol which is then simulated by our algorithm. We explicitly demonstrate how the error results in a PD that scales faster than the PPD of the error-free protocol.

The QST protocol [23]. Given an \( n \)-qubit chain and couplings between the qubits \( J_{J} = 2J/\sqrt{4J(n-J)} \) and \( B_{J} = 2\sqrt{2J(n-1)(2n-2J+1)} \), the Ising Hamiltonian \( \mathcal{H}_{I} \) of the chain is given as

\[
\mathcal{H}_{I} = \sum_{j=1}^{n} J_{j} Z_{j} Z_{j+1} + \sum_{j=1}^{n} B_{j} X_{j},
\]

where \([X,Y,Z]\) denote spin-1/2 Pauli matrices, e.g., \( X = i\sigma_{X} \). Let \( |\psi_{1}\rangle \cdots |\psi_{n}\rangle \) be the initial state of the chain, then QST is achieved by evolving \( U_{I} = \exp(-i\mathcal{H}_{I}t) \) for \( t = \frac{\pi}{\mathcal{F}} \):

\[
U_{I} |\psi_{1}\rangle |\psi_{2} \cdots \psi_{n-1}\rangle |0\rangle = \frac{1}{\sqrt{2}} |[0]|\psi_{n-1} \cdots \psi_{2}\rangle |\psi_{1}\rangle + i |[0]|\psi_{n-1} \cdots \psi_{2}\rangle |X\rangle |\psi_{1}\rangle,
\]

where \( \langle \psi_{i} | \psi_{i} \rangle = 0 \) \( \forall i \). A state locally equivalent to \( |\psi_{1}\rangle \) is then recovered at the end of the chain by measuring the first qubit in the Z basis.

The algorithm. Consider a 1-qubit \( U \) as an example. It can be represented as a column vector \( \mathcal{U}_{B} = [u_{\bar{z}}, u_{X}, u_{Y}, u_{Z}]^{T} \) in the four-dimensional vector space with basis \( B = [1, X, Y, Z] \), and where the subscript \( B \) denotes that it supports the hyperplane where the vector lies. The coefficients \( u_{j} \) can be deduced via the orthogonality of the basis, e.g., \( u_{X} = \Tr(X^{T}U) \). More importantly, Clifford algebra ensures that the basis forms a group up to a phase, which we denote as \( G_{0} \equiv B \). We define the norm (squared length) of \( U \) in space \( G_{0} \) as

\[
\|\mathcal{U}\|_{G_{0}} = \Tr(U^{+}U) = \sum_{j \in G_{0}} |u_{j}|^{2} = 1.
\]

We recursively use the fact that one can express \( \mathcal{U}_{G_{0}} \) in an effective two-component form \( \mathcal{U}_{G_{1}} = [\mathcal{U}_{G_{0}}, \tilde{\mathcal{U}}_{G_{1}}]^{T} \) by choosing two orthogonal subspaces of \( G_{0} \), for instance, \( G_{1} = [1, X] \) and \( \tilde{G}_{1} = (G_{0} - G_{1}) = [Y, Z] \), \( G_{1} \) is necessarily chosen to be a proper subgroup of \( G_{0} \), and \( \tilde{G}_{1} \) is a coset. This allows us to decompose the norm as

\[
\|\mathcal{U}\|_{G_{0}} = \|\mathcal{U}\|_{G_{1}} + \|\mathcal{U}\|_{\tilde{G}_{1}}.
\]

The algorithm obtains the PD in terms of the unitaries (gates) generated by the basis elements of \( B \). To do so, it rotates \( \mathcal{U}_{G_{0}} \) to \( \mathcal{U}_{\tilde{G}_{1}} \), and since \( \tilde{G}_{1} \) is closed under the product operation, the elements of \( \tilde{G}_{1} \) have no further role to play. The desired rotations are obtained by first product-decomposing \( U \) (for example) into \( U = U_{1} U_{2} U_{3} \), where the gates \( U_{2} = \exp(i\phi_{Z} Z) \) and \( U_{3} = \exp(i\phi_{Y} Y) \) are chosen with appropriate angles \( \phi_{Z} \) and \( \phi_{Y} \) such that \( U_{1} \) has no support in \( \tilde{G}_{1} \)---we call such gates orthogonal rotations. To obtain the angles (equivalently, the time of evolution), note that the product \( U_{2} U_{3} \) in the vector representation is simply the following linear transformation of \( U \):

\[
\exp(i\phi_{Z} Z) : \mathcal{U} \rightarrow \left( \cos \frac{\phi_{Z}}{2} 1_{4} + i \sin \frac{\phi_{Z}}{2} \tilde{P}_{Z} \right) \mathcal{U},
\]

where \( \tilde{P}_{Z} = \text{perm} \mathcal{U} - \mathcal{U} \) is a permutation matrix such that \( \mathcal{U} = [u_{\bar{z}}, -iu_{Y}, iu_{X}, u_{Z}]^{T} = \tilde{P}_{Z} \mathcal{U} \). We first choose \( \phi_{Z} \) that maximizes \( \Delta_{G_{1}} \), the increase in norm of \( U_{2} U_{3} \) in \( G_{1} \):

\[
\Delta_{G_{1}} = \| \exp(i\phi_{Z} Z) \mathcal{U} \|_{G_{1}} - \| \mathcal{U} \|_{G_{1}},
\]

\[
= \sin^{2} \frac{\phi_{Z}}{2} \left( -\tilde{P}_{Z} \tilde{P}_{Z} \mathcal{U} \right) + \frac{1}{2} \sin \phi_{Z} (-i\tilde{U}) \tilde{P}_{Z} \tilde{P}_{Z} \mathcal{U},
\]

where \( \tilde{P}_{Z} = \text{diag}(1_{G_{0}}, -1_{G_{0}}) \) is a reflection matrix about \( G_{1} \). The optimal \( \phi_{Z} \) is then a function of \( U \) [30]:

\[
\theta_{Z}[U] \equiv \phi_{Z}\max = \tan^{-1} \left( -\frac{\mathcal{U}^{+} \tilde{P}_{Z} \tilde{P}_{Z} \mathcal{U}}{\mathcal{U}^{+} \tilde{P}_{Z} \mathcal{U}} \right),
\]

since \( \theta_{Z}[\exp(i\theta_{Z} Z) U] = 0 \). Similarly \( \phi_{Y} = \theta_{Y} \) when \( \theta_{Y}[\exp(i\theta_{Y} Y) \exp(i\theta_{Z} Z) U] = 0 \). The orthogonal rotations \( U_{1} U_{2} U_{3} \) rotate \( \mathcal{U}_{G_{0}} \) to \( \tilde{G}_{1} = [\tilde{U}_{G_{1}}, 0_{G_{0}}]^{T} \). The PD \( U = U_{1} U_{2} U_{3} \) is completed by obtaining \( U_{X} \) such that \( U_{X} U_{1} U_{2} U_{3} U = 1 \equiv [1, 0, 0, 0]^{T} \).

The above can be generalized to an \( n \)-qubit unitary \( U \). Now basis \( P \) contains \( 4^{n} \) operators, and to within a phase, \( G_{0} \equiv B \) forms a group under product operation. In summary, the PD of the \( U \) is achieved by iteratively rotating the vector \( \mathcal{U}_{G_{0}} \) via orthogonal rotations to smaller and smaller (subgroup) subspaces until the PD is completed.

The rotations are essentially deduced by diagonalizing \( U \) in two-component form, analogous to determining the eigenvectors in “coupled two-level problems” in quantum mechanics. More importantly, the order of the rotations are chosen to minimize the number of terms (gates) in the PD.
This is done through dynamic programming [31]: At each step, the orthogonal rotation that causes the maximum transfer of norm $\Delta_{G}$ to the desired subspace is chosen first (or, the $B_{i}$ that has the maximum “off-diagonal” contribution to the two-component matrix is extinguished first).

In order to minimize the time to obtain a PD for a $U$ of arbitrary size, we will product-decompose $U$ for small sizes, and identify the structural symmetry in the form of the PD. We will then use the pattern identified to inductively extend the PD to any size. We now demonstrate the above by explicitly product-decomposing the QST unitary.

The PD of QST unitary. First consider the 3-qubit QST $U_{1}$, which can be represented as the vector $U_{G_{0}} = 1/2\sqrt{2}$ [1,−1,1,1,−1,1,1]T in the space spanned by $G_{0}$:

$$\{1,X_{2},X_{1}X_{2},Y_{1}Y_{2},Z_{1}Z_{2},Z_{1}X_{2}Y_{1},X_{1}X_{2}Y_{1},X_{1}X_{2}Z_{1}\}.$$ 

Divide $G_{0}$ into two orthogonal subspaces: a subgroup $G_{1} = \{1, X_{2}, Z_{1}Z_{2}, Z_{1}X_{2}, Y_{1}\}$, and its coset space $G_{1} = G_{0} - G_{1}$. The algorithm generates a single orthogonal rotation $\exp(-i\frac{\pi}{2}Y_{1}Y_{2}Y_{3})$ in the space $G_{1}$ that rotates $U_{G_{0}}$ to $U_{G_{1}} = 1/2\sqrt{2}[1,−1,1,1,0,0,0,0]T$. Now a further iteration gives the following PD:

$$U_{1} = \exp\left(-i\frac{\pi}{2}X_{2}\right) \exp\left(i\frac{\pi}{2}Z_{1}X_{2}Z_{3}\right) \exp\left(i\frac{\pi}{2}Y_{1}X_{2}Y_{3}\right).$$

Similarly, the PD for the 5-qubit $U_{1}$,

$$U_{1} = \exp\left(-i\frac{\pi}{2}X_{3}\right) \exp\left(i\frac{\pi}{2}Z_{2}X_{3}Z_{4}\right) \exp\left(i\frac{\pi}{2}Y_{2}X_{3}Y_{4}\right) \times \exp\left(i\frac{\pi}{2}Z_{1}X_{2}X_{3}X_{4}X_{5}\right) \exp\left(i\frac{\pi}{2}Y_{1}X_{2}X_{3}X_{4}X_{5}\right).$$

The above PDs are seen to exhibit the following pattern: The QST is mirror symmetric about the center of the chain [32]. For any equal division of $G_{0}$ into $G_{1}$ and $G_{1}$, there exists a single orthogonal rotation in $G_{1}$ that causes maximum transfer of the norm such that the resulting unitary has no support in the coset space. This property is invariant under further iterations. Thus the decomposition of $U_{1}$ scales linearly with $n$. Inductively, the PPD of an $n$-qubit $U_{1}$ is given as

$$U_{1} = \prod_{k=1}^{[\frac{n}{2}]} \exp\left(i\frac{\pi}{2}Y_{k}X_{(n-k+1)}X_{j}\right) \times \exp\left(i\frac{\pi}{2}Z_{k}X_{(n-k+1)}X_{j}\right) \times \begin{cases} \exp\left(-i\frac{\pi}{2}X_{(a+1)/2}\right) & n \text{ odd,} \\ 1 & n \text{ even.} \end{cases}$$

NMR simulation of $U_{1}$. We used liquid state NMR to simulate the QST protocol [24,26,27] in a 3-qubit system $^{13}$CHFB$_2$, where $^{1}H$, $^{13}$C, and $^{19}$F are the qubits. Our motivation is to study experimental viability of the PD and its scaling. Experiments were performed at room temperature in a 11.7-T magnetic field with the resonance frequencies 500 MHz ($^{1}H$), 125 MHz ($^{13}$C), and 470 MHz ($^{19}$F). The couplings between the qubits were $J_{HC} = 224.5$ Hz, $J_{HF} = 49.7$ Hz, and $J_{FC} = -310.9$ Hz.

The gates in the PPD [Eq. (9)] are implemented by using NMR pulse sequences [17] as the controls. To do so, note that the rotations generated by any basis operators, such as $B_{i}B_{j}$, can be realized by using [5]: $\exp(-i\tau[B_{i}, B_{j}]) = \exp(i\frac{\pi}{2}B_{i}) \exp(i\tau B_{j}) \exp(-i\frac{\pi}{2}B_{i})$. Thus orthogonal rotations by elements of $B$ are implemented by using hard pulses alone, by Hahn echo refocusing [33,34], or by a combination of both. Piecing together these sequences leads to the implementation of $U_{1}$ [Fig. 1(a)] [30]. In Eq. (9) the multiqubit operators act only on contiguous qubit positions. Hence they can be constructed only by using nearest-neighbor couplings. The non-nearest-neighbor couplings are refocused during the simulation time and $^{1}H$, $^{13}$C, and $^{19}$F (in that order) form the requisite 3-qubit chain. Let $|\psi_{i}\rangle = \alpha|0\rangle + \beta|1\rangle$ be the initial state of the first qubit, which is to be transferred along the spin chain. Although the protocol allows the state of the second qubit to be arbitrary,
we fix its initial state to $|0\rangle$ for ease of measurement. Thus the initial state of the chain is $|\psi_f\rangle_0$, and is created from the $|000\rangle$ pseudopure state (created by spatial averaging [35]) by using a $\alpha = 2\tan^{-1}(\beta/\alpha)$ X pulse on the first qubit. The pulse sequence corresponding to the PPD of $U_I$ [Fig. 1(a)] is then applied. Since projective measurement is not possible in a bulk-ensemble QIP such as NMR [6], the readout of the final state of the spin chain is done by applying a $\text{CNOT}(1,3)$ gate (see Ref. [36]) to force the system to $|000\rangle + i|111\rangle|\psi_f\rangle_1$. The state of the third qubit is measured with the receiver coil in the $Y$ direction. The results [Fig. 1(b)] show excellent agreement with sin $\langle\psi| [30], which indeed confirms the QST.

To see the role of symmetry in the study of the robustness of the PPD (thus of the protocol) to coupling errors, we consider the simplest case of disorder static field in the engineered couplings [28,37], where the deviations of the couplings from their ideal values are independent of qubit position, i.e., $\delta J_1 = \delta J_2$. A representative example of the pulse sequence for this simulation is shown in Fig. 1(c) [30]. The experimental results [Fig. 1(b)] show that the state recovered is corrupted by an additional phase, and the degree of corruption increases with the error of couplings. Hence, the transfer fidelity—characterized by how closely the final state reproduces the initial state—decreases with the error of couplings.

Figure 1(c) demonstrates that the PD of the protocol with coupling error destroys the structural symmetry [38] of the error-free PD [30]. Consequently, the size of the PD scales faster with the system size, hence incurring higher simulation cost. In conclusion, our work strongly suggests that the structural symmetry of $U$ in a given basis is intimately related to the scaling of the corresponding PD. Any algorithm that unravels the symmetry in $U$ can therefore most economically simulate it.

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