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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 Rungta[3]

[1]*Department of Physics and NMR Research Centre, Indian Institute of Science, Bangalore, India*

[2]*Nuclear Science and Engineering Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

[3]*Indian 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 $\mathcal{H}_{\rm int}$ and a time-dependent part $\mathcal{H}_{\rm ext}(t)$ [3] that can be experimentally controlled such that the following holds to arbitrary precision [4]:

$$U \approx U_{\rm sim} = \mathcal{T} \exp\left[-i \int_0^\tau dt[\mathcal{H}_{\rm int} + \mathcal{H}_{\rm ext}(t)]\right], \qquad (1)$$

where τ 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 $\mathcal{H}_{\rm ext}$ is in general a challenge [6].

In practice, the simulation is constructed by decomposing U into a product of unitary evolution operators U_j: $U_{\rm sim} = U_1 U_2 \ldots U_m$ [4] for a sequence of time steps δ_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 τ 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 $U \approx U_{\rm sim}$ 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 $O(\Delta\tau^{3/2})$ [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 $\mathbf{B}$ by representing it as a *vector* $\overline{U} = [c_1, c_2, \ldots, c_N]$, since $U = \sum c_j B_j$, where $B_j \in \mathbf{B}$ and $N = 4^n$. A PD, $U = \prod_k^m \exp(i\theta_k B_k)$, 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 $\overline{U} \to [1,0,\ldots,0]$. 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

*ashokaj@mit.edu

U, hence increasing the size of the PD. This can be used to develop appropriate techniques to control the errors.

Other algorithms for simulation have been suggested previously. Reference [14], for example, uses Given's rotations [15,16] to product-decompose U in terms of $\mathrm{C}^{n-1}\mathrm{NOT}$ (controlled-NOT) and controlled-PHASE gates. Here, we have explored the usefulness of the Pauli operator basis [17] for the decomposition. The advantage is that gates from this basis can be implemented in certain spin-based QIPs in a time optimal manner [3,18]. Moreover, other optimal control techniques [9,10] 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 PPD 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 PPD 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 $B_j = 2J\sqrt{(2j-1)(2n-2j+1)}$, the Ising Hamiltonian $\mathcal{H}_I$ of the chain is given as

$$\mathcal{H}_I = \sum_{j=1}^{n-1} J_j Z_j Z_{(j+1)} + \sum_{j=1}^{n} B_j X_j, \tag{2}$$

where $\{\mathbb{1}, X, Y, Z\}$ denote spin-1/2 Pauli matrices, e.g., $X = \frac{1}{2}\sigma_X$. 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 $t = \frac{\pi}{4J}$:

$$U_I|\psi_1\rangle|\psi_2 \cdots \psi_{n-1}\rangle|0\rangle = \frac{1}{\sqrt{2}}[|0\rangle|\psi_{n-1} \cdots \psi_2\rangle|\psi_1\rangle + i|1\rangle|\psi_{n-1}^{\perp} \cdots \psi_2^{\perp}\rangle(X|\psi_1\rangle)], \tag{3}$$

where $\langle\psi_i^{\perp}|\psi_i\rangle = 0\ \forall i$. 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 $\overline{U}_B = [u_{\mathbb{1}}, u_X, u_Y, u_Z]^T$ in the four-dimensional vector space with basis $\mathbf{B} = \{\mathbb{1}, X, Y, Z\}$, 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., $u_X = \mathrm{Tr}(X^{\dagger}U)$. More importantly, Clifford algebra ensures that the basis forms a *group* up to a phase, which we denote as $G_0 \equiv \mathbf{B}$. We define the norm (squared length) of U in space G_0 as

$$\|\overline{U}\|_{G_0} = \mathrm{Tr}(U^{\dagger}U) = \sum_{j \in G_0} |u_j|^2 = 1. \tag{4}$$

We recursively use the fact that one can express $\overline{U}_{G_0}$ in an effective two-component form $\overline{U}_{G_0} = [\overline{U}_{G_1}, \overline{U}_{\widetilde{G}_1}]^T$ by choosing two orthogonal subspaces of G_0, for instance, $G_1 = \{\mathbb{1}, X\}$ and $\widetilde{G}_1 = (G_0 - G_1) = \{Y, Z\}$. G_1 is necessarily chosen to be a proper *subgroup* of G_0, and $\widetilde{G}_1$ is a coset. This allows us to decompose the norm as

$$\|\overline{U}\|_{G_0} = \|\overline{U}\|_{G_1} + \|\overline{U}\|_{\widetilde{G}_1}. \tag{5}$$

The algorithm obtains the PD in terms of the unitaries (gates) generated by the basis elements of $\mathbf{B}$. To do so, it rotates $\overline{U}_{G_0}$ to $\overline{U}'_{G_1}$, and since G_1 is *closed* under the product operation, the elements of $\widetilde{G}_1$ have no further role to play. The desired rotations are obtained by first product-decomposing U (for example) into $U' = U_Y U_Z U$, where the gates $U_Z \equiv \exp(i\phi_Z Z)$ and $U_Y \equiv \exp(i\phi_Y Y)$ are chosen with appropriate angles ϕ_Z and ϕ_Y such that U' has no support in $\widetilde{G}_1$—we call such gates *orthogonal rotations*. To obtain the angles (equivalently, the time of evolution), note that the product $U_Z U$ in the vector representation is simply the following linear transformation of $\overline{U}$,

$$\exp(i\phi Z) : \overline{U} \to \left(\cos\frac{\phi}{2}\mathbf{1}_{4\times 4} + i\sin\frac{\phi}{2}\hat{P}_Z\right)\overline{U}, \tag{6}$$

where $\hat{P}_Z$ is a permutation matrix such that $\overline{\sigma_Z U} = [u_Z, -iu_Y, iu_X, u_{\mathbb{1}}]^T = \hat{P}_Z\overline{U}$. We first choose ϕ_Z that maximizes Δ_{G_1}, the *increase* in norm of $U_Z U$ in G_1:

$$\begin{aligned}\Delta_{G_1} &= \|\exp(i\phi_Z Z)\overline{U}\|_{G_1} - \|\overline{U}\|_{G_1} \\ &= \sin^2\frac{\phi_Z}{2}(-\overline{U}^{\dagger}\hat{P}_R\overline{U}) + \frac{1}{2}\sin\phi_Z(-i\overline{U}^{\dagger}\hat{P}_Z\hat{P}_R\overline{U}),\end{aligned} \tag{7}$$

where $\hat{P}_R = \mathrm{diag}(\mathbf{1}_{G_1}, -\mathbf{1}_{\widetilde{G}_1})$ is a reflection matrix about G_1. The optimal ϕ_Z is then a function of U [30]:

$$\theta_Z[U] \equiv \phi_Z|_{\max} = \tan^{-1}\left(\frac{-i\overline{U}^{\dagger}\hat{P}_Z\hat{P}_R\overline{U}}{\overline{U}^{\dagger}\hat{P}_R\overline{U}}\right), \tag{8}$$

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 $U_Y U_Z$ rotate $\overline{U}_{G_0}$ to $\overline{U}'_{G_1} = [\overline{U}'_{G_1}, \mathbf{0}_{\widetilde{G}_1}]^T$. The PD $U = U_X U_Y U_Z$ is completed by obtaining U_X such that $U_X U_Y U_Z U = \mathbb{1} \equiv [1,0,0,0]^T$.

The above can be generalized to an n-qubit unitary U. Now basis $\mathbf{B}$ contains 4^n operators, and to within a phase, $G_0 \equiv \mathbf{B}$ forms a group under product operation. In summary, the PD of the U is achieved by iteratively rotating the vector $\overline{U}_{G_0}$ 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 Δ_G to the desired subspace is chosen *first* (or, the B_j 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 extended the PD to any size. We now demonstrate the above by explicitly product-decomposing the QST unitary.

The PPD of QST unitary. First consider the 3-qubit QST U_I, which can be represented as the vector $\overline{U}_{G_0} = 1/2\sqrt{2}[1,-i,1,1,1,-i,i,i]^T$ in the space spanned by G_0:

$$\{\mathbb{1}, X_2, X_1X_3, Y_1Y_3, Z_1Z_3, X_1X_2X_3, Y_1X_2Y_3, Z_1X_2Z_3\}.$$

Divide G_0 into two orthogonal subspaces: a subgroup $G_1 = \{\mathbb{1}, X_2, Z_1Z_3, Z_1X_2Z_3\}$, and its coset space $\widetilde{G}_1 = G_0 - G_1$. The algorithm generates a single orthogonal rotation $\exp(-i\frac{\pi}{2}Y_1X_2Y_3)$ in the space $\widetilde{G}_1$ that rotates $\overline{U}_{G_0}$ to $\overline{U}'_{G_1} = 1/2[1,-i,1,1,0,0,0,0]^T$. Now a further iteration gives the following PD:

$$U_I = \exp\left(-i\frac{\pi}{2}X_2\right)\exp\left(i\frac{\pi}{2}Z_1X_2Z_3\right)\exp\left(i\frac{\pi}{2}Y_1X_2Y_3\right).$$

Similarly, the PD for the 5-qubit U_I,

$$U_I = \exp\left(-i\frac{\pi}{2}X_3\right)\exp\left(i\frac{\pi}{2}Z_2X_3Z_4\right)\exp\left(i\frac{\pi}{2}Y_2X_3Y_4\right) \times \exp\left(i\frac{\pi}{2}Z_1X_2X_3X_4Z_5\right)\exp\left(i\frac{\pi}{2}Y_1X_2X_3X_4Y_5\right).$$

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 $\widetilde{G}_1$, there exists a single orthogonal rotation in $\widetilde{G}_1$ 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_I scales linearly with n. Inductively, the PPD of an n-qubit U_I is given as

$$U_I = \prod_{k=1}^{\lfloor n/2\rfloor}\exp\left(i\frac{\pi}{2}Y_kY_{(n-k+1)}\bigotimes_{j=k+1}^{n-k}X_j\right) \times \exp\left(i\frac{\pi}{2}Z_kZ_{(n-k+1)}\bigotimes_{j=k+1}^{n-k}X_j\right) \times \begin{cases}\exp\left(-i\frac{\pi}{2}X_{(n+1)/2}\right) & n \text{ odd},\\ \mathbf{1} & n \text{ even}.\end{cases} \quad (9)$$

NMR simulation of U_I. We used liquid state NMR to simulate the QST protocol [24,26,27] in a 3-qubit system ^{13}CHFBr$_2$, 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.

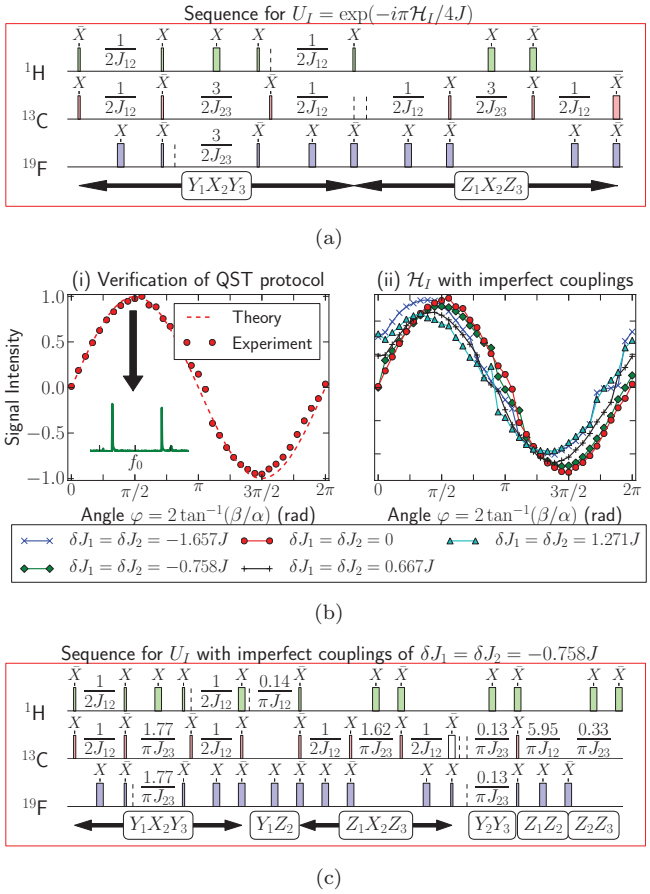

FIG. 1. (Color online) (a) Simplified pulse sequence for U_I. Filled wide and narrow bars are π and $\pi/2$ pulses, respectively. The dotted lines delineate periods of Hahn echo refocusing. The numbers between pulses are delays, with $J_{12} = J_{HC}$ and $J_{23} = |J_{FC}|$. (b)(i) Theoretical (line) and experimental (points) normalized signal intensity on the third qubit, obtained as the average intensity of the spectral lines corresponding to the state $(|00\rangle + i|11\rangle)|\psi_I\rangle$ (shown in the inset for $\varphi = \pi/2$). Here $f_0 = -40.26$ kHz (-85.6 ppm). (ii) Experimental signal intensity on the third qubit for different static errors in $\mathcal{H}_I$ couplings. A representative pulse sequence used in (ii) is shown in (c). The unfilled bar is a 103.47° $\bar{X}$ pulse.

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_iB_j, can be realized by using [5]: $\exp(-\tau[B_i,B_j]) = \exp(i\frac{\pi}{2}B_i)\exp(i\tau B_j)\exp(-i\frac{\pi}{2}B_i)$. 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_I [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 $|\psi_I 00\rangle$, and is created from the $|000\rangle$ pseudopure state (created by spatial averaging [35]) by using a $\varphi = 2\tan^{-1}(\beta/\alpha)$ 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 CNOT(1,3) gate (see Ref. [36]) to force the system to $(|00\rangle + i|11\rangle)|\psi_I\rangle$. The state of the third qubit is measured with the receiver coil in the Y direction. The results [Fig. 1(b)i] show excellent agreement with $\sin\varphi$ [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 static disorder 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)ii] 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 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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