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Warp-Drive Quantum Computation

Mikio Nakahara[1], Juha J. Vartiainen[2], Yasushi Kondo[1], Shogo Tanimura[3], and Kazuya Hata[1]
[1]*Department of Physics, Kinki University, Higashi-Osaka 577-8502, Japan*
[2]*Materials Physics Laboratory, POB 2200, FIN-02015 HUT, Helsinki University of Technology, Finland*
[3]*Graduate School of Engineering, Osaka City University, Sumiyoshi-ku, Osaka 558-8585, Japan*

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Recently it has been shown that time optimal quantum computation is attained using the Cartan decomposition of a unitary matrix. We extend this approach by noting that the unitary group is compact. This allows us to reduce the execution time of a quantum algorithm $U_{\rm alg}$ further by adding an extra gate W to it. This gate W sends $U_{\rm alg}$ to another algorithm $WU_{\rm alg}$ which is executable in a shorter time than $U_{\rm alg}$. We call this technique warp-drive. Here we show both theoretically and experimentally that the warp-drive reduces the execution time of Grover's algorithm implemented with a two-qubit NMR quantum computer. Warp-drive is potentially a powerful tool in accelerating algorithms and reducing errors in any realization of a quantum computer.

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Quantum computing is an emerging discipline based on encoding information into a quantum-mechanical system [1, 2]. There a quantum algorithm is expressed in a form of a unitary matrix

$$U_{\rm alg} = \mathcal{T} \exp\left[-\frac{i}{\hbar}\int_0^T \mathcal{H}(\gamma(t))dt\right], \qquad (1)$$

where $\mathcal{T}$ stands for time-ordered product, $\gamma(t)$ denotes collectively the control parameters of the Hamiltonian $\mathcal{H}$ at time t. This unitary matrix is often implemented in terms of so-called elementary gates, such as U(2) gates and CNOT gates [3, 4, 5]. It is possible, instead, to directly implement a given unitary matrix without decomposing it into these elementary gates. It is expected that this will reduce the execution time required in general. One method for direct implementation is to employ numerical optimization of the control parameters of the Hamiltonian [6, 7, 8]. The other method is to use the Cartan decomposition of the group $\mathrm{SU}(2^n)$, to which an n-qubit matrix representation of a quantum algorithm belongs [9, 10]. The latter approach, which is adopted here, is successfully demonstrated recently using an NMR quantum computer, whose pseudopure state is generated by cyclic permutations of state population [11]. It should be noted that exact optimal implementation of a quantum algorithm has been achieved in holonomic quantum computation in an idealized case [12].

A warp-drive is a fictitious gadget with which two remote points in space are connected [13]. It is the purpose of the present Letter to demonstrate, both theoretically and experimentally, that a similar technique may be employed to shorten the execution time of a quantum algorithm. A time optimal implementation of the quantum algorithm is equivalent to navigating along the time optimal path from the identity operator to the point $U_{\rm alg}$ in $\mathrm{SU}(2^n)$ by tuning the parameters $\gamma(t)$ in the Hamiltonian. We show below that an additional permutation matrix W of the basis vectors, when added after $U_{\rm alg}$, sends it to a point $WU_{\rm alg}$ near the identity matrix I so that it takes a shorter time to follow the time optimal path connecting I with $WU_{\rm alg}$ than I with $U_{\rm alg}$, see Fig. 1. Therefore we have "warp-driven" $U_{\rm alg}$ to $WU_{\rm alg}$ by adding W. Although it might seem counterintuitive that the execution time is reduced by adding an extra gate, this is the case since the unitary group $\mathrm{SU}(2^n)$ is compact. Let us consider navigating on a sphere S^2, which is also a compact space. Suppose we leave from

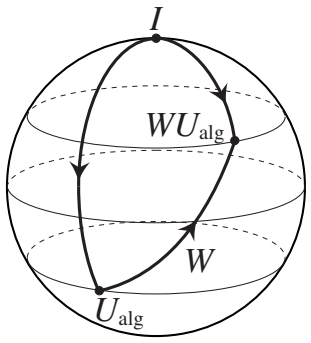

FIG. 1: Conceptual diagram showing the effect of a warp-drive gate W in a compact space SU(4). A matrix $U_{\rm alg}$ is sent to $WU_{\rm alg}$ which is reachable from the unit matrix I in a shorter execution time. The curves connecting these matrices represent time optimal paths.

a point O on the equator toward west. Then we will eventually arrive at the antipodal point. The distance between O and us will be shorter and shorter as we further circumnavigate the sphere. This is what happens when an extra gate is added.

In an NMR quantum computer, a one-qubit operation may be carried out in a short time on the order $10\,\mu$s while a two-qubit entangling operation takes time typically $\sim 10\,$ms. Thus one-qubit operation time may be ignored in estimating the overall execution time. Let us consider a molecule with two heteronucleus spins for definiteness, whose Hamiltonian, in the rotating frame with respective Larmor frequency, is

$$\begin{aligned}\mathcal{H}(\gamma) &= -\omega_{11}\left[\cos\phi_1(\sigma_x\otimes I_2/2)+\sin\phi_1(\sigma_y\otimes I_2/2)\right]\\ &\quad -\omega_{12}\left[\cos\phi_2(I_2\otimes\sigma_x/2)+\sin\phi_2(I_2\otimes\sigma_y/2)\right]\\ &\quad +2\pi J\sigma_z\otimes\sigma_z/4, \end{aligned} \tag{2}$$

where ω_{1i} and ϕ_i are the control parameters denoting the amplitude and the angle in the xy-plane of the external rf fields, respectively. Above J denotes the spin-spin coupling constant. Typically we have $\omega_{1i}\gg J$, which justifies the above assumption of negligible one-qubit operation time compared to two-qubit operation time. Neglecting one-qubit operation time in evaluating the execution time amounts to identifying the matrices U_1 and U_2 which differ by an element of $K\equiv \mathrm{SU}(2)\otimes\mathrm{SU}(2)$. Thus the relevant space for evaluating the time optimal path is the coset space $\mathrm{SU}(4)/\mathrm{SU}(2)\otimes\mathrm{SU}(2)$. To find the time optimal path connecting the unit matrix I and the matrix $U_{\rm alg}$, therefore, amounts to finding the time optimal path connecting cosets $[I]$ and $[U_{\rm alg}]$, where $[U]\equiv\{kU|k\in K\}$. The Lie algebra $\mathfrak{su}(4)$ of SU(4) is decomposed as $\mathfrak{su}(4)=\mathfrak{k}\oplus\mathfrak{p}$ [14], where

$$\mathfrak{k} = \mathrm{Span}(\{iI\otimes\sigma_j/2, i\sigma_j\otimes I/2\}),\ (j=x,y,z) \tag{3}$$

$$\mathfrak{p} = \mathfrak{k}^{\perp} = \mathrm{Span}(\{i\sigma_j\otimes\sigma_k/4\}),\ (j,k=x,y,z). \tag{4}$$

Note that they satisfy the commutation relations

$$[\mathfrak{k},\mathfrak{k}]\subset\mathfrak{k},\qquad [\mathfrak{p},\mathfrak{k}]\subset\mathfrak{p},\qquad [\mathfrak{p},\mathfrak{p}]\subset\mathfrak{k}. \tag{5}$$

The decomposition of a Lie algebra $\mathfrak{g}$ into $\mathfrak{k}$ and $\mathfrak{p}$, satisfying the above commutation relation, is called the Cartan decomposition. The Cartan subalgebra $\mathfrak{h}=\mathrm{Span}(\{i\sigma_j\otimes\sigma_j/4\})\subset\mathfrak{p}$ plays an important role in the following construction. A general theorem of Lie algebras proves that any element $U_{\rm alg}\in\mathrm{SU}(4)$ has a KP decomposition $U_{\rm alg}=kp, k\in K\equiv\exp\mathfrak{k}$ and $p\in P\equiv\exp\mathfrak{p}$. Moreover, any matrix $p\in P$ is rewritten in the conjugate form $p=k_1^{\dagger}hk_1$, where $k_1\in K$ and h is an element of the Cartan subgroup H of SU(4),

$$H\equiv\exp\mathfrak{h}=\left\{\exp\left(i\sum_{j=x,y,z}\frac{\alpha_j}{4}\sigma_j\otimes\sigma_j\right)\Big|\alpha_j\in\mathbb{R}\right\}. \tag{6}$$

Therefore we have a corresponding Cartan decomposition for a group element as $U_{\rm alg}=k_2hk_1$, where $k_i\in K$ and $h\in H$. The implementation of a quantum algorithm based on a Cartan decomposition requires shorter execution time in general [9, 10, 11].

To be more concrete, let us consider implementing two-qubit Grover's database search algorithm U_{ij} with an NMR quantum computer. The data is encoded in one of the basis vectors $|00\rangle,|01\rangle,|10\rangle,|11\rangle$ and the gate U_{ij} picks out a particular binary basis vector $|ij\rangle$ as a "target file" [15, 16]. Here we restrict ourselves within U_{10} which picks out the file $|10\rangle$ with a single step. The unitary matrix representing this algorithm takes the form

$$U_{10}=\begin{pmatrix}0&1&0&0\\0&0&0&-1\\-1&0&0&0\\0&0&-1&0\end{pmatrix}. \tag{7}$$

The Cartan decomposition of an arbitrary $U\in\mathrm{SU}(4)$ is carried out explicitly as follows. We first introduce the Bell basis [17]

$$\begin{aligned}|\Psi_0\rangle&=(1/\sqrt{2})(|00\rangle+|11\rangle),\\ |\Psi_1\rangle&=(i/\sqrt{2})(|01\rangle+|10\rangle),\\ |\Psi_2\rangle&=(1/\sqrt{2})(|01\rangle-|10\rangle),\\ |\Psi_3\rangle&=(i/\sqrt{2})(|00\rangle-|11\rangle).\end{aligned} \tag{8}$$

The transformation rule of a matrix U with respect to the standard binary basis $|00\rangle,|01\rangle,|10\rangle,|11\rangle$ into that with the Bell basis $|\Psi_i\rangle$ is $U\to U_B\equiv Q^{\dagger}UQ$, where

$$Q=\frac{1}{\sqrt{2}}\begin{pmatrix}1&0&0&i\\0&i&1&0\\0&i&-1&0\\1&0&0&-i\end{pmatrix}. \tag{9}$$

The matrix Q defines an isomorphism between $K=\mathrm{SU}(2)\otimes\mathrm{SU}(2)$ and SO(4) and is used to classify two-qubit gates [17, 18]. Namely, it is easy to verify that $Q^{\dagger}kQ\in\mathrm{SO}(4)$ for $k\in K$. Moreover, Q diagonalizes the elements of the Cartan subgroup, viz $Q^{\dagger}hQ=\mathrm{diag}(e^{i\theta_0},e^{i\theta_1},e^{i\theta_2},e^{i\theta_3})$ for $h\in H$. Therefore we find for $U=k_2hk_1$ that

$$U_B=Q^{\dagger}UQ=Q^{\dagger}k_2Q\cdot Q^{\dagger}hQ\cdot Q^{\dagger}k_2Q=O_2h_DO_1,$$

where $O_i\equiv Q^{\dagger}k_iQ\in\mathrm{SO}(4)$ and $h_D\equiv Q^{\dagger}hQ$ is a diagonal matrix. From $U_B^TU_B=O_1^Th_D^2O_1$, we notice that $U_B^TU_B$ is diagonalized by O_1 and its eigenvalues form the diagonal elements of h_D^2. Finally O_2 is found as $O_2=U_B(h_DO_1)^{-1}$.

We apply the above strategy to find the Cartan decomposition $U_{10}=k_2hk_1$. An example of the time optimal control is

$$\begin{aligned}k_1 &= I_2\otimes I_2,\\ h &= e^{i(\pi/4)(\sigma_x\otimes\sigma_x-\sigma_y\otimes\sigma_y)},\\ k_2 &= e^{-i(\pi/4)\sigma_z}\otimes e^{i(\pi/2\sqrt{2})(\sigma_x+\sigma_y)}.\end{aligned} \tag{10}$$

To implement this decomposition with an NMR quantum computer, such terms as $e^{i(\pi/4)(\sigma_x\otimes\sigma_x)}$ must be rewritten

TABLE I: time optimal pulse sequences for Grover's algorithm U_{10} and the warp-driven algorithm, W_4U_{10}. The hydrogen nucleus is the qubit 1 while the carbon nucleus is the qubit 2. Here X (Xm) and Y (Ym) denote $\pi/2$-pulse around x ($-x$) and y ($-y$) axis, respectively. The symbol Pi(θ) denotes a π-pulse around a vector $(\cos\theta, \sin\theta, 0)$ in the Bloch sphere. The symbol $(1/2J)$ indicates the length of the idle time, during which no external pulses are applied. The number of pulses is reduced from 10 to 4 and the execution time is halved by adding the extra gate W_4.

Gate	Pulse sequence								Execution Time
U_{10}	1: X	$(1/2J)$	Xm	Y	$(1/2J)$	X	Ym		$1/J$
	2: X	$(1/2J)$	Xm	Ym	$(1/2J)$	Y	Pi($\pi/2$)		
W_4U_{10}	1:		Xm	Pi($-\pi/4$)	$(1/2J)$	X			$1/2J$
	2:				$(1/2J)$	Pi(π)			

in favor of the subset of generators of SU(4) in the Hamiltonian (1). We verify, for example, that

$$e^{i(\pi/4)(\sigma_x\otimes\sigma_x)} = [e^{i(\pi/4)\sigma_x}\otimes e^{-i(\pi/4)\sigma_y}]e^{i(\pi/4)(\sigma_z\otimes\sigma_z)} \times[e^{-i(\pi/4)\sigma_x}\otimes e^{i(\pi/4)\sigma_y}]. \quad (11)$$

The extra gate W which possibly shortens the execution time must be simple enough so that we can deduce the output of $U_{\rm alg}$ efficiently from that of $WU_{\rm alg}$ using classical computation only. We call such gates warp-drive gates. Since a matrix $U_{\rm alg}$ is an element of a compact group U(2^n), there always exist such warp-drive gates which will reduce the execution time. In the present work, we choose the permutation matrices of the binary basis vectors as candidates for such gates. Since there are four basis vectors, there are $4! = 24$ permutation matrices. Note that we are not required to examine all of 24 permutations since 18 of them are obtained by applying one-qubit rotations on the following six permutations:

$$\begin{aligned} W_0 &= I_4,\ W_1 = U^{12}_{\rm CNOT},\ W_2 = U^{21}_{\rm CNOT}, \\ W_3 &= U_{\rm SWAP},\ W_4 = U_{\rm cp} \equiv U^{12}_{\rm CNOT}U^{21}_{\rm CNOT}, \\ W_5 &= U^2_{\rm cp} \equiv U^{21}_{\rm CNOT}U^{12}_{\rm CNOT}, \end{aligned} \quad (12)$$

where $U_{\rm SWAP}$ represents the swap gate and $U^{ij}_{\rm CNOT}$ is the CNOT gate whose control bit is i while the target bit is j. The matrices $U_{\rm cp}$ and $U^2_{\rm cp}$ have been utilized to cyclically permute the state populations to generate pseudopure states [19].

We have optimized the execution time of the matrices W_iU_{10} ($0 \le i \le 5$) by utilizing the Cartan decomposition outlined above and found that the execution time is $1/J$ for $i = 0, 1$ and 2 while $1/2J$ for $i = 3, 4$ and 5. A time optimal control for the warp-driven gate $W_4U_{10} = k_2hk_1$ is

$$\begin{aligned} k_1 &= e^{i(\pi/2\sqrt{2})(\sigma_x-\sigma_z)}\otimes e^{i(\pi/4)\sigma_x}, \\ h &= e^{i(\pi/4)\sigma_y\otimes\sigma_y}, \\ k_2 &= I\otimes e^{i\pi\sigma_x/4}. \end{aligned} \quad (13)$$

Therefore the execution time T satisfies $\pi JT/2 = \pi/4$, yielding $T = 1/2J$. Since the decomposition (13) contains generators which do not exist in the Hamiltonian, a trick similar to (11) must be employed. The one-qubit gates are realized using rf-pulses in an NMR quantum computer. Table I shows the actual NMR pulse sequences derived from the Cartan decompositions of U_{10} and W_4U_{10}. We call the hydrogen nucleus and the carbon nucleus as qubit 1 and qubit 2, respectively, in Table I and the rest of this Letter. In spite of the extra gate W_4, the latter requires less pulses and half of the execution time required for the former. The permutation W_4 maps the binary basis vectors as $W_4 : |10\rangle \mapsto |11\rangle$, and accordingly the output state of W_4U_{10} upon acting the initial state $|00\rangle$ is $|11\rangle$.

In our experiments, a 0.6 ml, 200 mM sample of carbon-13 labeled chloroform (Cambridge Isotope) in d-6 acetone has been employed as a two-qubit molecule and data were taken at room temperature with a JEOL ECA-500 NMR spectrometer, whose hydrogen Larmor frequency is approximately 500 MHz. The measured spin-spin coupling constant is $J = 215.5$ Hz and the transverse relaxation time is $T_2 \sim 7.5$ s for the hydrogen nucleus and $T_2 \sim 0.30$ s for the carbon nucleus. The longitudinal relaxation time is measured to be $T_1 \sim 20$ s for both nuclei. The initial state $|00\rangle$ is prepared as a pseudopure state generated by the field gradient method [20].

Figure 2 shows our experimental result. The spectra for the ^{13}C nucleus (qubit 2) are shown in the panels. The spin states of both nuclei are inferred from these spectra. The position of the peak depends on the state of the qubit

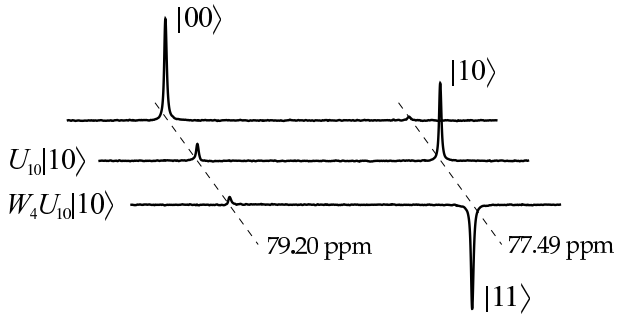

FIG. 2: NMR spectra obtained by applying a reading pulse to the ^{13}C nucleus. The rear row shows the pseudopure initial state $|00\rangle$ while the middle row indicates the state $|10\rangle$ obtained by executing U_{10} on $|00\rangle$. Finally the front row shows the spectrum obtained from warp-drive quantum computing W_4U_{10}, where the peak corresponds to $|11\rangle$.

1: peaks at 77.49 ppm (part per million) and 79.20 ppm stand for the states $|1\rangle$ and $|0\rangle$, respectively, of the qubit 1. The positive (negative) amplitude indicates qubit 2 being in the state $|0\rangle$ ($|1\rangle$). Thus the peak in the rear row shows the initial pseudopure state is $|00\rangle$ while the peak in the middle row tells us that the execution of Grover's algorithm U_{10} generates the state $|10\rangle$. Finally the front row shows the spectrum obtained after the execution of the warp-driven gate W_4U_{10}. The peak shows that the resulting state is $|11\rangle$, from which the output of $U_{10}|00\rangle$ is easily deduced as $|10\rangle$. The spectrum obtained with the warp-driven gate is sharper than that with the original U_{10} gate. The undesirable peak at $|00\rangle$ is also improved by the warp-drive. Smaller number of gates and reduced execution time account for these improvements.

We have also examined the effect of the warp-drives for Grover's algorithms other than U_{10} and found that the execution times remain unchanged for $W_{0,1,2}$ while they are halved for $W_{3,4,5}$. It should not be expected, however, that the latter gates reduce the execution time of an arbitrary two-qubit gate: clearly, such a "universal warp-drive" which reduces execution time of an arbitrary quantum algorithm does not exist. In view of the compactness of the unitary group, however, there exists a finite set of simple unitary transformations, such that the execution time of any quantum algorithm is reduced by properly chosen elements of the set. We expect that the set of permutation matrices, or certain subset thereof, is such a "universal warp-drive set".

In summary, we have demonstrated both theoretically and experimentally that a quantum algorithm may be accelerated by adding an extra gate to it. We took advantage of the compactness of the group SU(4) and found the time optimal control parameters utilizing the Cartan decomposition for it. When applied to two-qubit Grover's algorithm in the NMR experiment the execution time is found to be halved along with a reduction in the number of the gate pulses from 10 to 4. As a result, application of warp-drive quantum computing sharpens the NMR spectrum and reduces the spurious peak, implying reduction in decoherence and gate operation errors. How reductions in the execution time and the number of gate pulses scales with the number of qubits remains a challenging problem.

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