Time-optimal synthesis of unitary transformations in coupled fast and slow qubit system

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In this paper, we study time-optimal control problems related to system of two coupled qubits where the time scales involved in performing unitary transformations on each qubit are significantly different. In particular, we address the case where unitary transformations produced by evolutions of the coupling take much longer time as compared to the time required to produce unitary transformations on the first qubit but much shorter time as compared to the time to produce unitary transformations on the second qubit. We present a canonical decomposition of SU(4) in terms of the subgroup SU(2) × SU(2) × U(1), which is natural in understanding the time-optimal control problem of such a coupled qubit system with significantly different time scales. A typical setting involves dynamics of a coupled electron-nuclear spin system in pulsed electron paramagnetic resonance experiments at high fields. Using the proposed canonical decomposition, we give time-optimal control algorithms to synthesize various unitary transformations of interest in coherent spectroscopy and quantum information processing.

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I. INTRODUCTION

The synthesis of unitary transformations using time-efficient control algorithms is a well studied problem in quantum information processing and coherent spectroscopy. Time-efficient control algorithms can reduce decoherence effects in experimental realizations, and the study of such control algorithms is related to the complexity of quantum algorithms (see, e.g., [1, 2, 3]). Significant literature in this subject treat the case where unitary transformations on single qubits take negligible time compared to transformations interacting between different qubits. This particular assumption is very realistic for nuclear spins in nuclear magnetic resonance (NMR) spectroscopy. Under this assumption, Ref. [4] (see also [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]) presents time-optimal control algorithms to synthesize arbitrary unitary transformations on a system of two qubits. Further progress in the case of multiple qubits is reported in [25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42].

In this work, we consider a coupled qubit system where local unitary transformations on the first qubit take significantly less time than local transformations on the second one. In addition, we assume that the coupling evolution is much slower than transformations on the first qubit but much faster than transformations on the second one. We present a canonical decomposition of SU(4) in terms of the subgroup SU(2) × SU(2) × U(1) reflecting the significantly different time scales immanent in the system. Employing this canonical decomposition, we derive time-optimal control algorithms to synthesize various unitary transformations. Our methods are applicable to coupled electron-nuclear spin systems occurring in pulsed electron paramagnetic resonance (EPR) experiments at high fields, where the Rabi frequency of the electron is much larger than the hyperfine coupling which is further much larger than the Rabi frequency of the nucleus.

The main results of this paper are as follows. Let $S_u$ and $I_r$ represent spin operators for the fast (electron spin) and slow (nuclear spin) qubit, respectively. Any unitary transformation $G ∈ SU(4)$ on the coupled spin system can be decomposed as

$$G = K_1 \exp(t_1 S_u^z I_r + t_2 S_u^z I_r)K_2,$$

where $S_u^z I_r$ and $S_u^z I_r$ correspond to $z$-rotations of the slow qubit, conditioned, respectively, on the up or down state of the fast qubit. The elements $K_1$ and $K_2$ are rotations synthesized by rapid manipulations of the fast qubit in conjunction with the evolution of the natural Hamiltonian. The elements $K_1$ and $K_2$ belong to the subgroup SU(2) × SU(2) × U(1), and in appropriately chosen basis correspond to block-diagonal special unitary matrices with 2×2-dimensional blocks of unitary matrices.

The minimum time to produce any unitary transformation $G$ is the smallest value of $(|t_1| + |t_2|)/\omega_f^I$, where $\omega_f^I$ is the maximum achievable Rabi frequency of the nucleus and $(t_1, t_2)^T$ is a pair satisfying Eq. (1). Synthesizing $K_1$ and $K_2$ takes negligible time on the time scale governed by $\omega_f^I$. 

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The paper is organized as follows. In Sec. III we recall the physical details of our model system exemplified by a coupled electron-nuclear spin system. The Lie-algebraic structure of our model is described in Sec. III which is used to derive control algorithms (pulse sequences) for synthesizing arbitrary unitary transformations in our coupled spin system. In Sec. IV we present examples. We prove the time-optimality of our control algorithms in Sec. V and some details of the proof are given in Appendix A.

Our work draws some results from the theory of Lie groups, which are explained as needed. We refer to [43] for general reference. To make the paper broadly accessible, we work with explicit matrix representations of Lie groups and Lie algebras.

II. PHYSICAL MODEL

As our model system, we consider two coupled qubits. We introduce the operators $S_\mu$ and $I_\nu$ which correspond to operators on the first and second qubit, respectively. In particular, these operators are defined by $S_\mu := (\sigma_\mu \otimes \text{id}_2)/2$ and $I_\nu = (\text{id}_2 \otimes \sigma_\nu)/2$ (see [44]), where $\sigma_\mu := (0 \ 1)/\sqrt{2}$, and $\sigma_\nu := (1 \ 0)/\sqrt{2}$ are the Pauli matrices and $\text{id}_2 := (1 \ 0 0 \ 1)/2$ is the 2×2-dimensional identity matrix. In the remaining text, let $\mu, \nu \in \{x, y, z\}$ and $\gamma \in \{x, y\}$.

In an experimental setting using an electron-nuclear spin system, the first qubit is represented by the electron spin (of spin 1/2). Similarly, the second qubit is represented by the nuclear spin (of spin 1/2). We assume that in the presence of a static magnetic field pointing in the z-direction, the free evolution is governed in the lab frame by a Hamiltonian of the form

$$H_0^\text{lab} = \omega_S S_z + \omega I_z + J(2S_z I_z),$$

where $\omega_S$ and $\omega I$ represents the natural precession frequency of, respectively, the first qubit and second qubit and $J$ is the coupling strength. We assume that

$$\omega_S \gg \omega I \gg J.$$  \hspace{1cm} (3)

This assumption is motivated by coupled electron-nuclear spin system occurring in EPR experiments at high fields (see, e.g., Sect. 3.5 of [44]). The time scales in Eq. (3) ensure that the hyperfine coupling Hamiltonian between the spins averages to the Ising Hamiltonian $2S_z I_z$, as in Eq. (2). This is the so-called high field limit.

The first and second qubit are controlled by transverse oscillating fields, which result in the corresponding control Hamiltonian given by $H_\text{lab}^S + H_\text{lab}^I$, where

$$H_\text{lab}^S = 2\omega_S^*(t) \cos[\omega_S^* t + \phi_S(t)] S_x$$

is the control Hamiltonian of the first qubit and

$$H_\text{lab}^I = 2\omega_I^*(t) \cos[\omega_I^* t + \phi_I(t)] I_x$$

is the control Hamiltonian of the second qubit. The amplitude, frequency, and phase of the control function w.r.t. the first qubit are represented by $\omega_S^*(t)$, $\omega_S^*$, and $\phi_S(t)$ respectively. Similarly, $\omega_I^*(t)$, $\omega_I^*$, and $\phi_I(t)$ represents the amplitude, frequency, and phase of the control function w.r.t. the second qubit. We use $\omega_S^*$ and $\omega_I^*$ to denote the maximal possible values of $\omega_S^*(t)$ and $\omega_I^*(t)$. In our model system, we assume that

$$\omega_S^* \ll J \ll \omega_I^*.$$  \hspace{1cm} (5)

Therefore, we refer to the first qubit as the fast qubit and the second qubit as the slow qubit.

We choose $\omega_S^* = \omega_S$ and $\omega_I^* = \omega I$. In a double rotating frame, rotating with the first and second qubit at frequency $\omega_S^*$ and $\omega_I^*$, the transformations $U_{\text{lab}}(t)$ and $U_{\text{rot}}(t)$ describe, respectively, a unitary transformation in the lab frame and the double rotating frame. We have

$$U_{\text{lab}}(t) = \exp(-it\omega_S^* S_z) \exp(-it\omega_I^* I_z) U_{\text{rot}}(t).$$

Using the rotating wave approximation, the Hamiltonians $H_0^\text{lab}$, $H_0^\text{lab}$, and $H_0^\text{lab}$ transform, respectively, to

$$H_0 = JI_z + J(2S_z I_z),$$

$$H_S = \omega_S^* S_z \cos \phi_S(t) + S_y \sin \phi_S(t),$$

and

$$H_I = \omega_I^* I_z \cos \phi_I(t) + I_y \sin \phi_I(t).$$

In absence of any irradiation on qubits, the system evolves under the free Hamiltonian $-iH_0$. From the time scales in Eq. (5), we can synthesize any unitary transformation of the form $\exp(-itS_\mu)$ in arbitrarily small time as compared to the evolution under $H_0$ or $H_0 + H_I$.

Let us define the operators,

$$S^d = (\text{id}_4/2 + S_z) = \begin{pmatrix} \text{id}_2 & 0_2 \\ 0_2 & \text{id}_2 \end{pmatrix},$$

and

$$S^n = (\text{id}_4/2 - S_z) = \begin{pmatrix} 0_2 & 0_2 \\ 0_2 & \text{id}_2 \end{pmatrix},$$

where $\text{id}_d$ is the $d \times d$-dimensional identity matrix and $0_2$ is the $2 \times 2$-dimensional zero matrix. Note that $H_0 = 2JS^d I_z$, and the system is described by the Hamiltonian $H_0 + H_I = 2JS^d I_z + w_I^*(t)(S^n + S^d)(I_z \cos \phi_I + I_y \sin \phi_I)$.

Since $J \gg w_I^*(t)$, and $S^n I_z$, does not commute with $S^d I_z$, the above Hamiltonian gets in the first order approximation truncated to

$$H^n(\phi_I) = 2JS^n I_z + w_I^*(t)S^n(I_z \cos \phi_I + I_y \sin \phi_I).$$

Similarly, we can prepare an Hamiltonian

$$H^d(\phi_I) = 2JS^d I_z + w_I^*(t)S^d(I_z \cos \phi_I + I_y \sin \phi_I).$$
by using $H^3(\phi_1) = \exp(i\pi S_x)H^\alpha(\phi_1)\exp(-i\pi S_x)$. 

The Hamiltonians $H^\alpha(\phi_1)$ and $H^3(\phi_1)$, operate on the slow qubit and induce transitions $\alpha\alpha \leftrightarrow \alpha\beta$ and $\beta\alpha \leftrightarrow \beta\beta$ of the nuclear spin as shown in Fig. 1 (cp. Table 6.1.1 of [46]). The $\alpha$ and $\beta$ states of the spins denote their orientation along and opposite to the static magnetic field, respectively. For the electron spin, the $\beta$ state has lower energy than the $\alpha$ state as its gyromagnetic ratio is negative. Similarly, for the nuclear spin, the $\alpha$ state has lower energy than the $\beta$ state as its gyromagnetic ratio is positive (as for a proton). We remark that the energy of any irradiation on the two qubits, the system evolves under the Hamiltonian $-iH_0$, where $a$ takes the form

$$a = \begin{pmatrix} 0 & a_1 & 0 & 0 \\ a_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & a_2 \\ 0 & 0 & a_2 & 0 \end{pmatrix}. $$

We obtain the Lie group $A = \exp(a)$ corresponding to the Abelian algebra $a$. From a Cartan decomposition of a real semisimple Lie-algebra as satisfying Eqs. (9)-(10), we obtain a decomposition of the compact Lie group $G = KAK$ (see, e.g., \cite{43}, Chap. V, Thm. 6.7):

**Lemma 3.** Any element $G \in SU(4)$, can be written as

$$G = K_1 \exp\{t_1(-iS^3 I_x) + t_2(-iS^\alpha I_x)\}K_2, $$

where $t_1, t_2 \in \mathbb{R}$ and $K_1, K_2 \in K$. 

**Remark 1.** The computation of KAK decompositions was analyzed in Refs. \cite{48, 50-51, 52}. In this work, we consider the Cartan decomposition, which corresponds...
to the type AIII in the classification of possible Cartan decompositions (see, e.g., pp. 451–452 of Ref. [43]).

Transforming all elements $G \in G$ to SWAP·$G$·SWAP, where

$$SWAP = \exp(-i\pi S \cdot I) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$S = (S_x, S_y, S_z)^T$, and $I = (I_x, I_y, I_z)^T$, the KAK decomposition is given in explicit matrices by

$$(U_1 \ 0_2) \exp \left[ -\frac{i}{2} \begin{pmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & a_2 & 0 \\ 0 & 0 & 0 & a_1 \end{pmatrix} \right] (U_3 \ 0_2) \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & c_1 & -iS_1 & 0 \\ 0 & -iS_2 & 0 & c_2 \\ 0 & 0 & c_2 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & c_1 & 0 & 0 \\ 0 & 0 & c_1 & 0 \\ 0 & 0 & 0 & c_2 \end{pmatrix} (U_4 \ 0_2),$$

where $s_j = \sin(a_j/2)$ and $c_j = \cos(a_j/2)$. In particular, the Lie group $K$ is given in this basis by block-diagonal unitary transformations, where $0_2$ is the $2\times2$-dimensional zero matrix and $U_1, U_2$ (and $U_3, U_4$) are $2\times2$-dimensional unitary matrices such that the product of their determinants is one. The considered KAK decomposition is equivalent to the cosine-sine decomposition [53, 54, 55].

Remark 2. In Ref. [4], a different Cartan decomposition is considered. In that case, the subalgebra $t$ is given by the elements $-iS_\mu$ and $-iI_\nu$ and corresponds to unitary transformations on single qubits of a coupled two-qubit system. Synthesizing unitary transformations on single qubits is assumed in Ref. [4] to take significantly less time, as compared to unitary transformations which interact between different qubits.

Since elements of $K$ can be synthesized in negligible time, we obtain as the main result of this paper that the minimum time to synthesize any element $G \in SU(4)$ is the minimum value of $|t_1| + |t_2|/\omega_i$ such that $(t_1, t_2)^T$ is a pair satisfying Eq. (11). We defer the proof of this fact to Sec. [V]. Let us describe how to use the KAK decomposition of $G$, to synthesize an arbitrary transformation using only the generators $-iS_\mu$, $-iH^\alpha(\phi_I)$, and $-iH_0$.

The Lie algebra $\mathfrak{k}$ decomposes to $\mathfrak{t}_1 \oplus \mathfrak{p}_1$, where $\mathfrak{t}_1$ is a subalgebra, composed of operators $-iS_\mu$ and $-iS_\nu I_\nu$, and $\mathfrak{p}_1$ is generated by $-I_2$, which commutes with all elements of $\mathfrak{t}_1$. The Lie algebra $\mathfrak{t}_2$ can be further subdivided by a Cartan decomposition $\mathfrak{t}_2 = \mathfrak{t}_2 \oplus \mathfrak{p}_2$. The subalgebra $\mathfrak{t}_2$ is generated by the operators $-iS_\mu$, and the subspace $\mathfrak{p}_2$ consists of the operators $-i2S_\mu I_2$. Therefore, similar as in Lemma 3, we obtain a decomposition of $K$.

Lemma 4. Each element $K_j \in K$ can be decomposed as $K_j = \exp(-i\tau_{J_2} - i\tau_{J_2} I_2 J_2 - i\tau_{J_2} S_2 I_2 L_2 - i\tau_{J_2} 2S_2 I_2 L_2) = \exp[-i(\tau_{J_2} - \tau_{J_2}) I_2 L_2 - i\tau_{J_2} H_0(J_2) L_2]$, (12)

where $\tau_{J_2} \in \mathbb{R}$ and $L_2 \in K_2 = \exp(\mathfrak{t}_2)$.

Using an Euler angle decomposition (see, e.g., pp. 454–455 of Ref. [50]), the elements $L_j \in K_2$ are given as

$$L_j = \exp(-i\theta_{3,1} S_z) \exp(-i\theta_{3,2} S_z) \exp(-i\theta_{3,3} S_z) = \exp[-i(\theta_{3,1} + \theta_{3,3}) S_z] \exp[-i\theta_{3,2} R(\theta_{3,3})],$$

(13)

where $R(\theta_{3,3}) = S_x \cos \theta_{3,3} - S_y \sin \theta_{3,3}$.

Similarly, any element $A$ of the subgroup $\Lambda$ can be written as $A = \exp[t_1(-iS_0(I_2) + t_2(-iS_0(I_2))] = \exp[-i(t_1 S_0^*) H_0^{i2} / J] e^{-it_1 H_{3}^i / J} e^{-it_2 H_{3}^i / J_0^i} e^{-it_2 H_0 / J_0^i}$, (14)

for $t_3 = 2Jt_1/t_4$ mod $4\pi$ and $t_4 = J(t_1 - t_2)/t_4$ mod $2\pi \geq 0$. This follows by substituting for expressions of $H_0$, $H^\alpha(\phi_I)$, and $H^3(\phi_I)$ (see Eqs. (7–8)). Combining Eqs. (12–14), a complete decomposition of an element $G \in SU(4)$, can be written as $K_1 K_2 = e^{-i\omega S_\mu} e^{-iw_1 H_0 / J} R_1 e^{-i\tau H_0 / J} R_2 e^{-i\tau H_0 / J} R_3 e^{-i\tau H_0 / J} R_4$, where all the transformations $R_j$ operate on the fast qubit. In particular, we have $R_4 = \exp[-i\theta_{3,2} R(\theta_{3,3})], R_3 = \exp[-i\theta_{3,2} R(v_0)], R_2 = \exp[-i\theta_{3,3} R(v_1)], R_1 = \exp[-i\theta_{3,1} R(v_2)], v_3 = \theta_{3,3} + \theta_{3,4}, v_2 = \theta_{3,3} + v_3, v_1 = \theta_{3,3} + v_2, v_0 = \theta_{3,3} + v_1, t = \tau_{J_2} - \tau_{J_3}$, and $w = \tau_{J_2} - \tau_{J_3} - \tau_{J_4} - \tau_{J_5}$. The time to produce $G$ is essentially $(t_1 + t_2) + t_4$. Note that Eq. (12) = $e^{-i\omega S_\mu} e^{-iw_1 H_0 / (2J)} e^{-i\omega S_\mu} e^{-iw_0 H_0 / (2J)}$.

Transformations on the fast qubit such as $\exp(-i\omega S_\mu)$ are significantly faster. Figure [2] shows the canonical pulse sequence realizing any unitary transformation as a sequence of rotations under $-iH_0$, $-iH^3(\phi_I)$, and $-iS_\mu$.

FIG. 2: The figure shows a canonical pulse sequence for synthesizing unitary transformations in the coupled qubit system. Let $\vec{R}_2 = R_2 \exp(i\pi S_z)$ and $R_0 = \exp(-i\omega S_\mu) \exp(-i\pi S_z)$. Since $1/J \ll 1/w_i^f$, the length of the time intervals $t_j/w_i^f$ is larger as depicted. Refer to the text for details.
IV. EXAMPLES

We introduce the unitary transformations CNOT[1, 2], CNOT[2, 1], and SWAP which are given as follows

\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
\quad \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0
\end{pmatrix}
, \quad \text{and} \quad \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
.
\]

Let \(c \in \{1, 3, -1, -3\}\). The elements of SU(4) corresponding to the transformation CNOT[2, 1] are given by \(\exp[i\pi(-i2S_z I_x + iS_z + iI_x)/2]\), which is equal to \(\exp(i\pi/4)\)CNOT[2, 1]. For CNOT[1, 2] and SWAP we obtain the elements \(\exp[i\pi(-i2S_z I_x + iS_z + iI_x)/2]\) and \(\exp[i\pi(2S_y I_x + i2S_y I_y + i2S_z I_z)/2]\), which are equal to \(\exp(ic\pi/4)\)CNOT[1, 2] and \(\exp(ic\pi/4)\)SWAP, respectively. These different instances of unitary transformations result from the irrelevance of the global phase in quantum mechanics and can be described mathematically by multiplying with elements of the (finite) center of G. The center consists of those elements which commute with all elements of G. To find the time-optimal control algorithm, we may have to consider multiplying with different elements of the center.

As \(\exp(ic\pi/4)\)CNOT[2, 1] is an element of K, it takes negligible time to synthesize CNOT[2, 1]. In strong contrast, \(\exp(ic\pi/4)\)CNOT[1, 2] is not contained in K. Using the KAK decomposition, both \(\exp(ic\pi/4)\)CNOT[1, 2] and \(\exp(ic\pi/4)\)SWAP correspond to the same generator of A, given by \(\pi(iS_\alpha + 0(-iS_\alpha))\), and the minimum time to synthesize each of them is equal to \(t_{\min} = \pi\). This is still the optimal time if we consider to multiply with different elements of the center.

We explicitly state the control algorithms: The unitary transformation \(\exp(ic\pi/4)\)CNOT[1, 2] is given by

\[
\exp(i\pi S_z /2) \exp(i I_z) \exp(-i\pi S_\alpha I_z) \exp(-i\pi I_z)
= \exp(i\pi S_z /2) \exp(-it' H_0 / J) \exp \left[-i\pi H_0 (\pi)/w_I t' \right],
\]

where \(t' = -\pi J / w_I \mod 2\pi \geq 0\). Similarly, the unitary transformation \(\exp(ic\pi/4)\)SWAP is given by

\[
e^{ic\pi/4} \text{CNOT}[2, 1] e^{ic\pi/4} \text{CNOT}[1, 2] e^{-ic\pi/4} \text{CNOT}[2, 1]
= e^{i\pi S_z /2} e^{-i\pi S_\alpha /2} e^{-i\pi H_0 / (2J)} e^{i\pi S_z /2} e^{-i\pi H_0 / J} \times \exp \left[-i\pi H_0 (\pi)/w_I t' \right] e^{-i\pi S_z /2} e^{-i\pi H_0 / (2J)} e^{-i\pi S_\alpha /2}.
\]

The corresponding pulse sequences are given in Fig. 3

V. PROOF OF TIME-OPTIMALITY

In this section, we prove the time-optimality of the given control algorithms in order to synthesize unitary transformations in coupled fast and slow qubit system. As expected, the maximal amplitude \(\omega_I t'\) (see Eq. 6) determines the optimal time.

FIG. 3: The figure shows the pulse sequences for synthesizing the unitary transformations (a) \(\exp(i\pi/4)\)CNOT[1, 2] and (b) \(\exp(i\pi/4)\)SWAP, where \(R_5 = \exp(i\pi S_z /2) \exp(-i\pi S_\alpha /2)\). Since \(1/J \ll 1/w_I t'\), the length of the time intervals \(\pi w_I t'\) is larger as depicted. Refer to the text for details.

A. The simple case

All control algorithms, synthesizing a unitary transformation in time \(t = \sum_j t_j\), can be written in the form

\[
K_{n+1} \exp[-it \alpha J] K_n \cdots K_1 \exp[-it_1 \alpha J] K_1,
\]

where \(K_j \in K\) take negligible time to be synthesized as compared to the evolution under \(H_0\). We can rewrite Eq. (15) as

\[
K_{n+1} \exp[-it_n \beta J] K_n \cdots K_2 \exp[-it_1 \beta J] K_1,
\]

where \(K_j \in K\). Equation (16) can be rewritten as

\[
\tilde{K}_{n+1} \exp(p_n \cdots \exp(p_1),
\]

where \(\tilde{p}_j = \tilde{K}_j(-it_2 \beta J) \tilde{K}_j^{-1}\) and \(\tilde{K}_j\) are suitable elements of K. We observe that the elements \(\tilde{p}_j\) are contained in \(p\). This follows from the Campbell-Baker-Hausdorff formula (see, e.g., Appendix B.4 of Ref. 44) and the fact that \([t, p] \in p\) (see Eq. 10). It was shown in Ref. 4 that for all time-optimal control algorithms the elements \(\tilde{K}_j\) can be chosen such that all \(\tilde{p}_j\) commute. Therefore, all \(\tilde{p}_j\) belong to a maximal Abelian subalgebra inside \(p\), and we can find one \(K_0 \in K\) such that \(K_0 \tilde{p}_j K_0^{-1} \in a\) for all \(j\). Using this result and results of Eq. (20) below, we can rewrite Eq. (17) in the form

\[
\tilde{K}_2 \exp(t_n p_n) \cdots \exp(t_1 p_1) \tilde{K}_1,
\]

where \(p_j = (\beta_j(-iS_\alpha I_x) + \alpha_j(-iS_\alpha I_x))\)

\[
(\beta_j, \alpha_j)^T \in \{(-1, 0)^T, (1, 0)^T, (0, -1)^T, (0, 1)^T\}
\]

and \(K_1, \tilde{K}_2 \in K\). Equation (18) can be simplified to

\[
\tilde{K}_2 \exp(\tilde{\beta}(-iS_\alpha I_x) + \alpha(-iS_\alpha I_x)) \tilde{K}_1,
\]

where \(\alpha = \sum_j \alpha_j t_j\) and \(\tilde{\beta} = \sum_j \beta_j t_j\). Assume that the unitary transformation to be synthesized is given
by one of its KAK decompositions $K_0 \exp[a_1(-iS^\beta I_x) + a_2(-iS^\alpha I_y)]K_0$, where $a_1, a_2 \in \mathbb{R}$ and $K_0 \in K$. We remark that the KAK decomposition is not unique, and we prove in Sec. A.2 that different KAK decompositions $K_6 \exp[a'_1(-iS^\beta I_x) + a'_2(-iS^\alpha I_y)]K_5$ correspond to all values $a'_j = a_j + 2\pi z_j$, where $z_j \in \mathbb{Z}$ and $K_5, K_6 \in K$. We can choose $a_1$ and $a_2$ as those values of $a'_1$ and $a'_2$ such that $|a_1| + |a_2|$ is minimal. If $|a_1| + |a_2| > t$, we cannot synthesize the unitary transformation in time $t$ since all time-optimal control algorithms are equal to Eq. (19) and $|a_1| + |\beta| = \sum_j |\alpha_j| + \sum_j |\beta_j| t_j = \sum_j |\alpha_j| + \beta \sum_j t_j = t$. For $|a_1| + |\beta| \leq t$, we can use the control algorithm $\exp(-i\tilde{a}_1 S^\beta I_x) \exp(-i\pi S^\alpha I_y) \exp(-i\tilde{a}_2 S^\beta I_x)$ to synthesize the unitary transformation in time $|a_1| + |\beta|$. 

B. The general case

Until now, we have assumed that in Eq. (3), $\omega'_j = \omega_{j-1}^{-1}$, i.e., we irradiate on the transition $\alpha \leftrightarrow \beta$. More generally, we can irradiate on both transitions $\alpha \leftrightarrow \beta$ and $\beta \leftrightarrow \alpha$. Hence, we substitute Eq. (3) by

$$H_{\text{lab}}^\text{lab}(t') = 2\omega'_j (t') \{b_2 \cos(\omega_{j-1} t') + \phi_2(t')\} I_x + b_1 \cos(\omega_{j-1} t') \phi_1(t') I_y,$$

where $|b_1| + |b_2| \leq 1$ (this ensures that the peak amplitude is $2\omega'_j$). Transforming into a double rotating frame by $U_{\text{lab}}(t') = \exp(-it' \omega S Z) \exp(-it' (\omega_1 + J2I_2 S_2)) U_{\text{rot}}(t')$, the evolution under the control Hamiltonian for time $t'$ (with constant $\omega'_j, \phi_1, \phi_2 \in \mathbb{R}$) generates a net rotation $K_1^T \exp(-it' (b_1 S^\beta I_p + b_2 S^\alpha I_q))$, where $I_p = I_x \cos(\phi_1) + I_y \sin(\phi_1)$, $I_q = I_x \cos(\phi_2) + I_y \sin(\phi_2)$, and $K_1^T \in K$. This can be rewritten as $K_1^T \exp(-ib_1 S^\beta I_p) K_2^T$, where $b = b_1(-iS^\beta I_x) + b_2(-iS^\alpha I_y) \in a$, $K_1', K_2' \in K$, and $t = t' \omega'_j$. Therefore, any control algorithm generates in time $t$, a transformation (written as in Eq. (16))

$$K_{n+1} \exp[-it_{n} b] K_{n} \cdots K_2 \exp[-it_1 b] K_1,$$

where $t_j$ is given in units of $1/\omega_j$ and $\sum_j t_j = t$. This generalizes the case of $b_1 = 1$ and $b_2 = 0$, treated in Sec. V.A.

Similarly as in Sec. V.A, we obtain time-optimal control algorithms as in Eq. (17), where $p_j = K_j b K_j^{-1}$ and $K_j$ are suitable elements of $K$. Therefore, Eq. (17) can be transformed to Eq. (18), where the commuting elements $p_j = \beta_j (-iS^\beta I_x) + \alpha_j (-iS^\alpha I_y)$ are contained in the Weyl orbit $\mathcal{W}(b) = \{K b K^{-1} : K \in K \cap a, \text{ i.e., } (\beta_j, \alpha_j) T\}$ is an element of the set

$$\{(b_1, b_2) T, (b_1, -b_2) T, (-b_1, b_2) T, (-b_1, -b_2) T, (b_2, b_1) T, (-b_2, b_1) T, (-b_2, -b_1) T\}.$$ (20)

The Weyl orbit is induced by the map $(K, b) \mapsto K b K^{-1}$, where $b \in a$ and the elements $K \in K$ are

$$\{i d_4 \exp(-i\pi S^\alpha I_y) \exp(-i\pi S^\beta I_x) \exp(-i\pi I_z),$$

$$\exp(-i\pi S_x), \exp(-i\pi S_y) \exp(-i\pi S^\alpha I_y),$$

$$\exp(-i\pi S_x) \exp(-i\pi S^\beta I_x) \exp(-i\pi S_z)\}.$$ (21)

As before, Equation (15) can be simplified to Eq. (19), and we obtain $|\alpha_1| + |\beta| \leq t \max(|b_1|, |b_2|)$. Furthermore, $\max(|\alpha|, |\beta|) \leq t \max(|b_1|, |b_2|)$. When the pairs $(a_1, a_2)^T$ and $(b_1, b_2)^T$ satisfy $\max(|a_1|, |a_2|) \leq \max(|b_1|, |b_2|)$ and $|a_1| + |a_2| \leq |b_1| + |b_2|$, then we say $(a_1, a_2)^T$ is $r$-majorized $(b_1, b_2)^T$, i.e., $(a_1, a_2)^T \leq_r (b_1, b_2)^T$. The notion of $r$-majorization is equivalent to the condition that one element of $a$ is contained in the convex closure of the Weyl orbit of another one (for a proof see Appendix A).

Given any unitary transformation $G \in G$, let $t_{\text{opt}}$ be the smallest possible time such that

$$(a_1, a_2)^T \leq_r t_{\text{opt}} (b_1, b_2)^T$$

and $G = K_2 \exp[a_1(-iS^\beta I_x) + a_2(-iS^\alpha I_y)] K_1$, where $K_2 \in K$. Again, the KAK decomposition is not unique, and different KAK decompositions correspond to all values $a'_j = a_j + 2\pi z_j$, where $z_j \in \mathbb{Z}$ (see Sec. A.2). Let us choose $a_j$ as an element of $[-\pi, \pi]$. We prove in Appendix A.3 that for such a choice of $a_j$, the equation $(a_1, a_2)^T \leq_r (b_1, b_2)^T$ holds for all $a_1, a_2 \in Z$. This implies that the smallest $t_{\text{opt}}$ in Eq. (22) can be achieved for $a_1, a_2 \in [-\pi, \pi]$.

Then $G$ cannot be synthesized in time $t$ less than $t_{\text{opt}}$, as for such a control algorithm the equation $(\bar{a}, \bar{\beta})^T \leq_r t_{\text{opt}} (b_1, b_2)^T$ would hold, and this would contradict the minimality of $t_{\text{opt}}$. In addition, $G$ can be synthesized in time $t$ greater than or equal to $t_{\text{opt}}$: It follows from $(a_1, a_2)^T \leq_r t_{\text{opt}} (b_1, b_2)^T$ that $(a_1, a_2)^T$ is contained in the convex closure of the Weyl orbit of $t_{\text{opt}} (b_1, b_2)^T$ (see Appendix A.1) and we can synthesize $G$ by convex combinations of elements of the Weyl orbit of $t_{\text{opt}} (b_1, b_2)^T$.

Remark 3. Note, since $(b_1, b_2) \leq_r (1, 0)$, it follows that the minimum time to produce any unitary transformation can be obtained when all rf-amplitude is used to irradiate only on one nuclear transition (say $\alpha \alpha \leftrightarrow \beta \beta$ as in Fig. 11) as described earlier. This justifies our initial choice of irradiating only on one nuclear transition.

VI. CONCLUSION

In this paper, we presented time-optimal control algorithms to synthesize arbitrary unitary transformations for coupled fast and slow qubit systems. These control algorithms are applicable to electron-nuclear spin systems in pulsed EPR experiments at high fields. Explicit examples were given for CNOT and SWAP. Recently, controllability results have appeared for coupled electron-nuclear spin systems at low fields [57, 58]. where it is
shown that it is possible to synthesize any unitary transformation on the electron-spin system by only manipulating the electron. New methods need to be developed to obtain time-optimal control algorithms in these settings.

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APPENDIX A: PROOFS

1. Convex closure of Weyl orbits

Assume that \(a = a_1(-iS^3 I_a) + a_2(-iS^0 I_a)\) and \(b = b_1(-iS^3 I_b) + b_2(-iS^0 I_b)\) are elements of \(a\). We prove that \((a_1, a_2)^T\) is contained in the convex closure of the Weyl orbit of \((b_1, b_2)^T\) if \((a_1, a_2)^T \preceq_r (b_1, b_2)^T\).

Suppose \((a_1, a_2)^T\) is contained in the convex closure of the Weyl orbit of \((b_1, b_2)^T\). Assume that \(|b_1| \geq |b_2|\). Then, \((a_1, a_2)^T = \sum_j w_j (b_{1j}, b_{2j})^T\), where \((b_{1j}, b_{2j})^T\) belongs to the set in Eq. (20) \((w_j \geq 0 \text{ and } \sum_j w_j = 1)\). It follows that \(|b_{1j}| \leq |b_1| \text{ and } |b_{2j}| \leq |b_2|\). Therefore, \(|a_1| \leq |b_1| \text{ and } |a_2| \leq |b_2|\), implying \(\max\{|a_1|, |a_2|\} \leq \max\{|b_1|, |b_2|\}\). Also note, \(|a_1| + |a_2| \leq \sum_j w_j (|b_{1j}| + |b_{2j}|) = |b_1| + |b_2|\).

Suppose that \((a_1, a_2)^T \preceq_r (b_1, b_2)^T\). The conditions \(\max\{|a_1|, |a_2|\} \leq \max\{|b_1|, |b_2|\}\) and \(|a_1| + |a_2| \leq |b_1| + |b_2|\) are equivalent to \((|a_1|, |a_2|)^T\) being weakly submajorized by \((|b_1|, |b_2|)^T\). Thus, we obtain from Prop. 4.C.2. of Ref. 59 that \((|a_1|, |a_2|)^T = e_1(|b_1|, |b_2|)^T + e_2(|b_1|, |b_1|)^T + e_3(|b_1|, |0|)^T + e_4(0, |b_1|)^T + e_5(|b_2|, |0|)^T + e_6(0, |b_2|)^T = f_1(|b_1|, |b_2|)^T + f_2(|b_1|, |b_1|)^T + f_3(|b_1|, |b_2|)^T + f_4(|b_2|, |b_1|)^T + f_5(|b_2|, |b_2|)^T + f_6(0, |b_2|)^T = 0\), where \(e_j \geq 0, \sum_j e_j = 1, f_1 = e_1 + (e_3 + e_6)/2, f_2 = e_2 + (e_4 + e_5)/2, \text{ and } f_k = e_k/2 \text{ for } k \in \{3, 4, 5, 6\}\). In particular, we have that \(f_j \geq 0 \text{ for all } j\) and \(\sum_j f_j = 1\).

It follows that \((a_1, a_2)^T = (e_1|a_1|, e_2|a_2|)^T = f_1(e_3 b_1, e_4 b_2)^T + f_2(e_5 b_2, e_6 b_1)^T + f_3(e_7 b_1, e_8 b_2)^T + f_4(e_9 b_2, e_{10} b_1)^T + f_5(e_{11} b_2, e_{12} b_1)^T + f_6(e_{13} b_1, e_{14} b_2)^T\), for appropriate choices of \(e_j \in \{1, -1\}\). We conclude the proof by consulting Eq. (20). A Lie-theoretic proof can be obtained by following Thm. 2 of Ref. 10.

2. KAK decomposition for elements of \(A\)

We prove that the elements \(\exp(a') \in A\) equal to \(K_1 \exp(a) K_2\) are given by the elements \((a_1', a_2')^T = (a_1, a_2)^T + 2\pi (z_1, z_2)^T\), where \(K_j \in K, a' = a_1'(-iS^3 I_a) + a_2'(-iS^0 I_a), a = a_1(-iS^3 I_a) + a_2(-iS^0 I_a)\), and \(z_j \in \mathbb{Z}\).

We can choose \(a' = K(a + k)K^{-1}\), where \(K\) is an element of Eq. (21) and \(k \in \{q \in a \exp(q) \in K\}\) (cp. Ref. 10, Lemma 2, and Ref. 17, Prop. 4). Using the ansatz \(\exp(a_1'(-iS^3 I_a) + a_2'(-iS^0 I_a) = id_4, \text{ where } a_1', a_2' \in \mathbb{R}, \text{ we obtain that } a_1', a_2' \in \{4\pi z : z \in \mathbb{Z}\}\). It is a consequence of Thm. 8.5, Chap. VII, of Ref. 18 that \(|q \in a \exp(q) \in K\) is equal to \(|q_1(-iS^3 I_a) + q_2(-iS^0 I_a) : q_1, q_2 \in \{2\pi z : z \in \mathbb{Z}\}\). This completes the proof. We remark that \(\exp(2\pi z_1(-iS^3 I_a) + 2\pi z_2(-iS^0 I_a)) = \exp(2\pi z_1(-iS^3 I_a) + 2\pi z_2(-iS^0 I_a))\) for all \(z_j \in \mathbb{Z}\), where \(2\pi z_1(-iS^3 I_a) + 2\pi z_2(-iS^0 I_a) \in \mathfrak{t}\).

3. Proof of a majorization relation

We prove that \((a_1, a_2)^T \preceq_r (a_1, a_2)^T + 2\pi (z_1, z_2)^T\) holds for all \(z_1, z_2 \in \mathbb{Z}\), if we assume that \(a_1, a_2 \in [-\pi, \pi]\).

As the case \(z_1 = z_2 = 0\) is trivial, we assume that \(|z_1| > 0\) or \(|z_2| > 0\). We obtain that \(\max\{|a_1+2\pi z_1|, |a_2+2\pi z_2|\} \geq 2\pi - \pi = \pi \geq \max\{|a_1|, |a_2|\}\), and the first condition in the definition of \(r\)-majorization is satisfied. The second condition \(|a_1+2\pi z_1|+|a_2+2\pi z_2| \geq |a_1|+|a_2|\) follows from the fact that \(|a_1+2\pi z_1| \geq |a_1|\) is always true. In particular, this is trivial for \(z_j = 0\) and it is a consequence of \(|a_j+2\pi z_j| \geq |(2\pi z_j-|a_j|)| \geq \pi \geq |a_j|\) in all other cases. The result follows.

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