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Efficient synthesis of quantum gates on indirectly coupled spins

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Experiments in coherent nuclear and electron magnetic resonance and quantum computing in general correspond to control of quantum-mechanical systems, guiding them from initial to final target states by unitary transformations. The control inputs (pulse sequences) that accomplish these unitary transformations should take as little time as possible so as to minimize the effects of relaxation and decoherence and to optimize the sensitivity of the experiments. Here, we derive a time-optimal sequences as fundamental building blocks to synthesize unitary transformations. Such sequences can be widely implemented on various physical systems, including the simulation of effective Hamiltonians for topological quantum computing on spin lattices. Experimental demonstrations are provided for a system consisting of three nuclear spins.

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I. INTRODUCTION

The control of quantum systems has important applications in physics and chemistry. In particular, the ability to steer the state of a quantum system (or an ensemble of quantum systems) from a given initial state to a desired target state forms the basis of spectroscopic techniques such as nuclear magnetic resonance (NMR) [1], electron spin resonance (ESR) spectroscopy [2], laser coherent control [3], and quantum computing [4,5]. Experiments in coherent nuclear and electron magnetic resonance and optical spectroscopy correspond to control of quantum-mechanical ensembles, guiding them from initial to final target states by unitary transformations. The control inputs (pulse sequences) that accomplish these unitary transformations should take as little time as possible so as to minimize the effects of relaxation and decoherence and to optimize the sensitivity of the experiments. The time-optimal synthesis of unitary operators is now well understood for coupled two-spin systems [6–11]. This problem has also been recently studied in the context of linear three-spin topologies [12–19]. In this article, we use optimal control technique to design pulse sequences to efficiently generate a class of quantum gates on three-spin systems, and show that such pulse sequences have significant savings in the implementation time of trilinear Hamiltonians and synthesis of couplings between indirectly coupled qubits over conventional methods. The generalization of such pulse sequences have applications on various other systems. The article is organized as follows: in Sec. II, we first review previous results on linearly coupled three-spin systems; in Sec. III, we use optimal control techniques to design time optimal pulse sequences and show significant savings in the implementation time and applications of such pulse sequences; in Sec. IV, we show an experiment implementation of the time optimal pulse sequence on NMR; Sec. V concludes.

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II. TIME OPTIMAL CONTROL FOR THREE LINEARLY COUPLED SPINS

In this section, we give a brief review of a previous result on three linearly coupled spins [12], to which our result is to be compared.

Consider a linear spin chain of three spins (see Fig. 1) coupled by scalar couplings and assume it is possible to selectively excite each spin (perform one qubit operations in context of quantum computing). The unitary propagator U describing the evolution of the system in a suitable rotating frame is well approximated by

$$\dot{U} = -i\left(H_d + \sum_{j=1}^{6} u_j H_j\right)U, \quad U(0) = I, \tag{1}$$

where

$$H_d = 2\pi J_{12} I_{1z} I_{2z} + 2\pi J_{23} I_{2z} I_{3z}, \quad H_1 = 2\pi I_{1x},$$
$$H_2 = 2\pi I_{1y}, \quad H_3 = 2\pi I_{2x}, \quad H_4 = 2\pi I_{2y},$$
$$H_5 = 2\pi I_{3x}, \quad H_6 = 2\pi I_{3y}.$$

Here H_d describes the coupling between the spins, and is fixed by the system, H_i, $i \in \{1,2,3,4,5,6\}$ describe local controls on the spins whose strength can be tuned. We use the notation $I_{\ell\nu}$ to denote the operator which acts on the ℓth spin as I_ν and acts on other spins as identity (see [1]), for example, I_{2x} is an operator which acts on the second spin as I_x and leaves the other spins intact. The matrices $I_x := \frac{1}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}$, $I_y := \frac{1}{2}\begin{pmatrix}0&-i\\i&0\end{pmatrix}$, and $I_z := \frac{1}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ are the Pauli spin matrices. J_{12} and J_{23} represent the strength of scalar couplings between spins (1,2) and (2,3) respectively; here we will treat the important case of this problem when the couplings are both equal ($J_{12} = J_{23} = J$) and we assume that we can selectively rotate each spin at a rate much faster than the evolution of the couplings, i.e., the single spin operations can be done in negligible time.

In [12], time optimal generation of unitary propagators of the form

$$U_F(\theta) = e^{-i\theta\, I_{1z} I_{2z} I_{3z}}$$

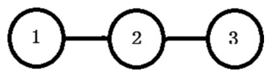

FIG. 1. Three linearly coupled spins.

was studied. These propagators are hard to produce as they involve trilinear terms in the effective Hamiltonian. The optimal sequence can be related to a geodesic on a sub-Riemannian geometry and involves both hard and soft pulses on the intermediate spin [12]. The minimum time $t^*(\theta)$ required to produce the propagator $U_F(\theta)$ is given by

$$t^*(\theta) = \frac{\sqrt{8\pi\theta - \theta^2}}{4\pi J}, \tag{2}$$

where $\theta \in [0,4\pi]$. The pulse sequence that produces the propagator U_F is as follows:

$$U_F(\theta) = e^{-i(\pi/2)I_{2y}} e^{-i[\pi+\beta/2]I_{2x}} \times e^{T[-i2\pi J(I_{1z}I_{2z}+I_{2z}I_{3z})+i(\beta/T)I_{2x}]} e^{i(\pi/2)I_{2y}}, \tag{3}$$

where $\beta = 2\pi - \frac{\theta}{2}$ and $T = t^*(\theta)$. Interested readers are referred to [12] for the details of the derivation.

III. QUANTUM GATES BETWEEN INDIRECTLY COUPLED SPINS

A. Time optimal sequences

In this article, we are going to extend the previous results, studying efficient constructions of unitary propagators on a three-spin system beyond the form of $U_F(\theta) = \exp(-i\theta\ I_{1z}I_{2z}I_{3z})$. We are going to first consider generating unitary propagators with two trilinear coupling terms,

$$U = e^{-4i\theta[I_{1x}I_{2z}I_{3y}+I_{1y}I_{2z}I_{3x}]};$$

such unitary operators will then be used to simulate couplings between indirectly coupled spins as we will show in the following section.

One way to generate U is to make use of the sequence in Eq. (3) that generates $U_F(\theta)$. Since the two trilinear terms in U commute with each, we can write $U = U_1U_2$, where

$$\begin{aligned} U_1 &= e^{-4i\theta I_{1x}I_{2z}I_{3y}} \\ &= e^{-(\pi/2)i(I_{1y}-I_{3x})} e^{-4i\theta\ I_{1z}I_{2z}I_{3z}} e^{(\pi/2)i(I_{1y}-I_{3x})}, \\ U_2 &= e^{-4i\theta I_{1y}I_{2z}I_{3x}} \\ &= e^{(\pi/2)i(I_{1x}-I_{3y})} e^{-4i\theta\ I_{1z}I_{2z}I_{3z}} e^{-(\pi/2)i(I_{1x}-I_{3y})}, \end{aligned} \tag{4}$$

they are both locally equivalent to $U_F(4\theta)$ and can be generated separately, thus the total time to generate U in this way is

$$T_C = 2t^*(4\theta) = 2\frac{\sqrt{2\pi\theta - \theta^2}}{\pi J}. \tag{5}$$

Note that in this way although U_1 and U_2 are generated optimally, to simply concatenate them is not necessary optimal. The optimal pulse sequence actually takes a shorter time as we are going to show.

We are going to use optimal control technique to derive the optimal sequence. First let

$$\begin{aligned} S_1 &= -4i[I_{1x}I_{2z}I_{3y} + I_{1y}I_{2z}I_{3x}], \\ S_2 &= -2i[I_{1x}I_{2x} + I_{2x}I_{3x}], \\ S_3 &= -2i[I_{1y}I_{2y} + I_{2y}I_{3y}]; \end{aligned} \tag{6}$$

here S_2,S_3 are locally equivalent to the coupling Hamiltonian H_d (up to a rescaling of time, from now on we are going to assume the time unit is $\frac{1}{\pi J}$), i.e., they can be obtained by applying local controls on the system,

$$\begin{aligned} S_2 &= e^{-(\pi/2)i(I_{1y}+I_{2y}+I_{3y})}(-iH_d)e^{(\pi/2)i(I_{1y}+I_{2y}+I_{3y})}, \\ S_3 &= e^{(\pi/2)i(I_{1x}+I_{2x}+I_{3x})}(-iH_d)e^{-(\pi/2)i(I_{1x}+I_{2x}+I_{3x})}. \end{aligned}$$

Note that

$$[S_1,S_2] = S_3, \quad [S_2,S_3] = S_1, \quad [S_3,S_1] = S_2,$$

thus S_1,S_2,S_3 form an so(3) algebra. We will map S_1,S_2,S_3 to $\Omega_x,\Omega_y,\Omega_z$, where

$$\Omega_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\Omega_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix},$$

$$\Omega_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The problem can now be reformulated as an optimal control problem on SO(3),

$$\frac{d}{dt}\Omega = A\Omega, \quad A = u(t)\Omega_z + v(t)\Omega_y; \tag{7}$$

here $u(t),v(t)$ can be $\{\pm 1,0\}$ as we can change the sign of the Hamiltonian by local controls, and it is 0 when it is not switched on. Since at each instant of time, only one Hamiltonian can be switched on, so $\forall t, |u(t)| + |v(t)| = 1$. The goal is to generate $\Omega(T) = e^{\alpha\Omega_x}$ in minimum time starting from $\Omega(0) = I$, which is equivalent to find the optimal sequence

$$\exp(\pm\Omega_y t_1)\exp(\pm\Omega_z t_2)\exp(\pm\Omega_y t_3)\exp(\pm\Omega_z t_4)\ldots$$

to generate $\exp(\alpha\Omega_x)$, such that $T = \sum_i t_i$ is minimized.

The conventional method is to use the Baker-Campbell-Hausdorff (BCH) formula [20]

$$e^{\alpha\Omega_x} = e^{(\pi/2)\Omega_y} e^{\alpha\Omega_z} e^{-(\pi/2)\Omega_y}, \tag{8}$$

which corresponds to set $u(t) = 0, v(t) = -1$ when $t \in [0,\frac{\pi}{2}]$, $u(t) = 1, v(t) = 0$ when $t \in [\frac{\pi}{2},\frac{\pi}{2}+\alpha]$ and $u(t) = 0, v(t) = 1$ when $t \in [\frac{\pi}{2}+\alpha,\pi+\alpha]$, the total time cost is $\pi+\alpha$ units of time. While this is optimal when α is larger than $\frac{\pi}{2}$, for small α, it is far from optimal since there is always an offset π for the total time.

The minimum time can actually be achieved by adding one switch. For $\alpha \in [0,\frac{\pi}{2}]$, the time optimal sequence takes the form

$$e^{\alpha\Omega_x} = e^{t_2\Omega_z} e^{-\delta t\Omega_y} e^{-\delta t\Omega_z} e^{t_1\Omega_y}, \tag{9}$$

while

$$\begin{aligned} t_2 = t_1 &= \arccos\frac{1}{\sin\frac{\alpha}{2} + \cos\frac{\alpha}{2}}, \\ \delta t &= \arccos\left(\cos\frac{\alpha}{2} - \sin\frac{\alpha}{2}\right). \end{aligned} \tag{10}$$

The total time to generate $e^{\alpha\Omega_x}$ is

$$\begin{aligned} f(\alpha) = 2\Bigg[&\arccos\frac{1}{\sin\frac{\alpha}{2} + \cos\frac{\alpha}{2}} \\ &+ \arccos\left(\cos\frac{\alpha}{2} - \sin\frac{\alpha}{2}\right)\Bigg]. \end{aligned} \tag{11}$$

Symmetrically when $\alpha \in [-\frac{\pi}{2},0]$,

$$f(\alpha) = f(-\alpha).$$

So for $\alpha \in [-\frac{\pi}{2},\frac{\pi}{2}]$,

$$\begin{aligned} f(\alpha) = 2\Bigg[&\arccos\frac{1}{\sin\frac{|\alpha|}{2} + \cos\frac{|\alpha|}{2}} \\ &+ \arccos\left(\cos\frac{|\alpha|}{2} - \sin\frac{|\alpha|}{2}\right)\Bigg]. \end{aligned}$$

The details of the derivation of this optimal sequence can be found in the Appendix; here we just give an intuitive picture of how the sequence works. Geometrically $\{e^{\alpha\Omega_x}\}$ corresponds to a rotation on a sphere which moves the point $a = (0, \sin\alpha, \cos\alpha)$ to $(0,0,1)$ while keeping the x axis fixed. The conventional method using the BCH formula as in Eq. (8) corresponds to first rotate $\frac{\pi}{2}$ around the (y) axis which moves the point a to the XY plane, then rotate the α angle around the z axis which moves the point to $(1,0,0)$, then apply another $\frac{\pi}{2}$ rotation around the y axis, and move the point to $(0,0,1)$. Such a sequence always applies $\frac{\pi}{2}$ rotations around the y axis in the first and third steps, thus there is always an offset π for the total time. The optimal sequence in Eq. (9) corresponds to four steps which avoids such offset. As shown in Fig. 2, the sequence first rotates the point around the y axis for time t_1, which moves the point $a = (0, \sin\alpha, \cos\alpha)$ to $b = (\cos\alpha\sin t_1, \sin\alpha, \cos\alpha\cos t_1)$; then rotate around the (z) axis for time δt, which rotates point b to the point $c = (\sqrt{\cos^2\alpha\sin^2 t_1 + \sin^2\alpha}, 0, \cos\alpha\cos t_1)$ which is on the XZ plane; after that it rotates around the (y) axis for time δt to the point $d = (0,0,1)$; since the x axis is orthogonal to $\overrightarrow{oa}$ and rotations do not change the angles, after these rotations, the x axis has moved to somewhere which is orthogonal to $\overrightarrow{od}$, i.e., somewhere on the XY plane, so one needs to make another rotation around the z axis for time t_2, that moves the x axis back to the original position.

In concluding this section, we note that a similar construction of the time-optimal sequences was also given by Mittenhuber [21].

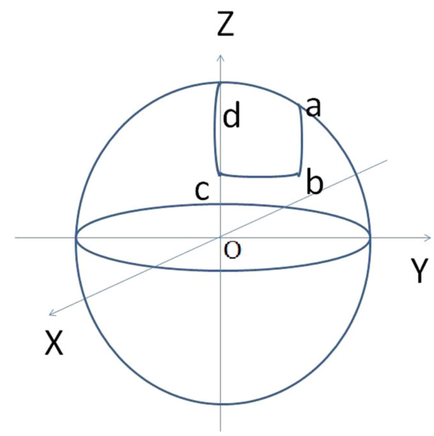

FIG. 2. (Color online) Rotation corresponds to $e^{\alpha\Omega_x}$ that moves $a = (0, \sin\alpha, \cos\alpha)$ to $d = (0,0,1)$ via the point $b = (\cos\alpha\sin t_1, \sin\alpha, \cos\alpha\cos t_1)$ and $c = (\sqrt{\cos^2\alpha\sin^2 t_1 + \sin^2\alpha}, 0, \cos\alpha\cos t_1)$.

B. Quantum gates on indirectly coupled spins

The sequence can be directly used to simulate

$$U = e^{\theta S_1} = e^{-4i\theta[I_{1x}I_{2z}I_{3y} + I_{1y}I_{2z}I_{3x}]}$$

on the linearly coupled three-spin system; from Fig. 3, we can see that the total time cost of the optimal sequence is not only smaller than the conventional method using the BCH formula as in Eq. (8), but is also smaller than T_C of Eq. (5).

Various gates between indirectly coupled spins 1 and 3 can be constructed by concatenating the optimal sequence. For example, operators of the form $e^{-2i\theta[I_{1x}I_{3x} + I_{1y}I_{3y}]}, \theta \in [0,\frac{\pi}{2}]$ can be constructed as follows: First let

$$\begin{aligned} S_1 &= -4i[I_{1x}I_{2z}I_{3y} + I_{1y}I_{2z}I_{3x}], \\ S_4 &= -2i[I_{1z}I_{2z} + I_{2z}I_{3z}], \\ S_5 &= -2i[I_{1x}I_{3x} - I_{1y}I_{3y}]; \end{aligned} \tag{12}$$

they form an so(3) algebra, thus by the optimal sequence

$$e^{\theta S_5} = e^{-t_2 S_1} e^{-\delta t S_4} e^{\delta t S_1} e^{t_1 S_4}, \tag{13}$$

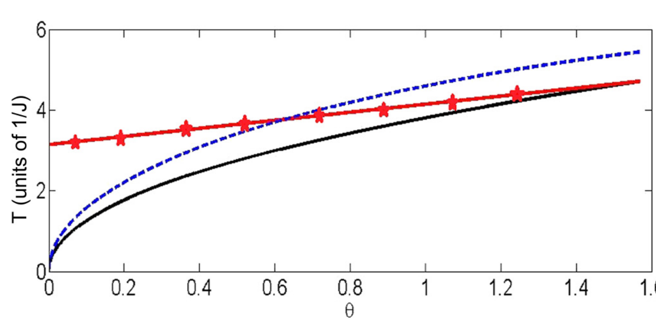

FIG. 3. (Color online) The solid black line represents the time cost of generating $e^{-i4\theta[I_{1x}I_{2z}I_{3y} + I_{1y}I_{2z}I_{3x}]}$ using the optimal sequence; the star red line represents T_C of Eq. (5), the total time cost by concatenating the sequence described in Sec. II; the dotted blue line represents the total time cost using BCH formula as in Eq. (8).

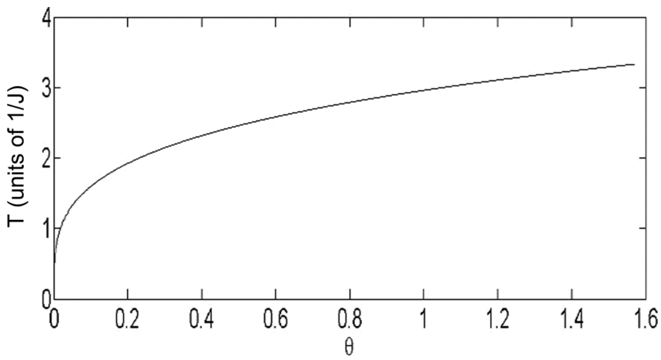

FIG. 4. Time needed to generate $e^{-2i\theta[I_{1x}I_{3x}+I_{1y}I_{3y}]}$.

where

$$t_1 = t_2 = \arccos\frac{1}{\sin\frac{\theta}{2} + \cos\frac{\theta}{2}},$$
$$\delta t = \arccos\left(\cos\frac{\theta}{2} - \sin\frac{\theta}{2}\right); \tag{14}$$

here $e^{-t_2 S_1}$ and $e^{\delta t S_1}$ can again be decomposed into four pulses, thus $e^{\theta S_5} = e^{-2i\theta[I_{1x}I_{3x}-I_{1y}I_{3y}]}$ can be generated within the time $g(\theta) = t_1 + \delta t + f(t_1) + f(\delta t)$(plotted in Fig. 4), where f is the function given by Eq. (11). This operator is locally equivalent to $e^{-2i\theta[I_{1x}I_{3x}+I_{1y}I_{3y}]}$ as

$$e^{-2i\theta[I_{1x}I_{3x}+I_{1y}I_{3y}]} = e^{i\pi I_{3x}} e^{\theta S_5} e^{-i\pi I_{3x}}.$$

Similarly we can efficiently generate the operators $e^{-2i\theta[I_{1x}I_{3x}+I_{1z}I_{3z}]}$ and $e^{-2i\theta[I_{1y}I_{3y}+I_{1z}I_{3z}]}$. These operators can be combined together to efficiently simulate the Heisenberg coupling $e^{-2i\theta[I_{1x}I_{3x}+I_{1y}I_{3y}+I_{1z}I_{3z}]}$ between the indirectly coupled spins.

C. Simulation of multibody interactions

The application of the time optimal sequence in Eq. (9) is not restricted to the linearly coupled three-spin system, but can be applied to various physical systems wherever an so(3) algebra can be identified. For example it can be used to simulate the couplings required for topological quantum computing on a spin lattice. Topological quantum computing on a spin lattice requires multibody interaction Hamiltonians; for example, the toric code model on a square lattice requires four-body interaction, and the honeycomb lattice model requires six-body interaction. Most physical Hamiltonians only contain two-body interaction. The pulse sequence can be used to simulate a multibody Hamiltonian on physical systems, which promises faster execution.

Let us consider the toric code on a square lattice; the desired Hamiltonian is given by

$$H_T = -J_e \sum_s A_s - J_m \sum_p B_p,$$

where s runs over vertices (stars) of the lattice and p runs over the plaquette (see Fig. 5).

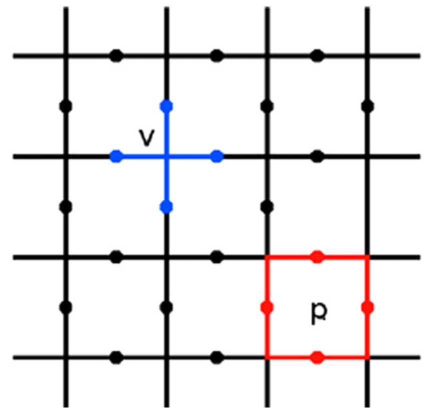

FIG. 5. (Color online) The spins live on the edges of the square lattice. The spins adjacent to a star operator A_s and a plaquette operator B_p are shown.

The star operator acts on the four spins surrounding a vertex s,

$$A_s = \prod_{j\in \mathrm{star}(s)} \sigma_j^x,$$

while the plaquette operator acts on the four spins surrounding a plaquette,

$$B_p = \prod_{j\in\partial p} \sigma_j^z,$$

where $\sigma_x := \left(\begin{smallmatrix} 0 & 1\\ 1 & 0\end{smallmatrix}\right)$, $\sigma_y := \left(\begin{smallmatrix} 0 & -i\\ i & 0\end{smallmatrix}\right)$, and $\sigma_z := \left(\begin{smallmatrix} 1 & 0\\ 0 & -1\end{smallmatrix}\right)$. Assume we have two-body Ising coupling between nearest-neighbor and selective fast single spin operations, i.e., we have $\sigma_z \otimes \sigma_z$ couplings between two neighboring spins. We show how to use this to simulate the toric code model. We just show how to generate $\exp(-i\theta B_p)$, i.e., simulate one B_p term; as all the terms commute with each other, they can be simulated in a similar way independently.

Let us first index the four spins that B_p act on with numbers 1,2,3,4, and assume they have couplings to the nearest neighbor: $\sigma_{1z}\sigma_{2z}$, $\sigma_{2z}\sigma_{3z}$, $\sigma_{3z}\sigma_{4z}$, $\sigma_{4z}\sigma_{1z}$, where $\sigma_{1z}\sigma_{2z}$ denote an operator acting σ_z on spins 1 and 2 and identity on other spins. These couplings can be effectively turned on and off by decoupling techniques. To simulate $\exp(-i\theta B_p)$, we

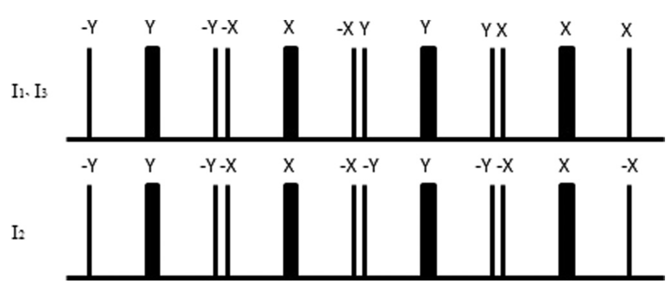

FIG. 6. Pulse sequence diagram for the unitary transformation $e^{2\pi i(I_{1x}I_{2z}I_{3y}+I_{1y}I_{2z}I_{3x})}$: the pulses of the first line are on spins 1 and 3, pulses of the second line are in spin 2; thin vertical lines denote 90° pulses and wide vertical lines denote 180° pulses which are inserted for refocusing of frequency offset effects; the durations t_1, t_2, and δt can be calculated according to the above theory, which is $t_1 = t_2 = \arccos\frac{1}{\sin\frac{\theta}{2}+\cos\frac{\theta}{2}}, \delta t = \arccos(\cos\frac{\theta}{2} - \sin\frac{\theta}{2})$.

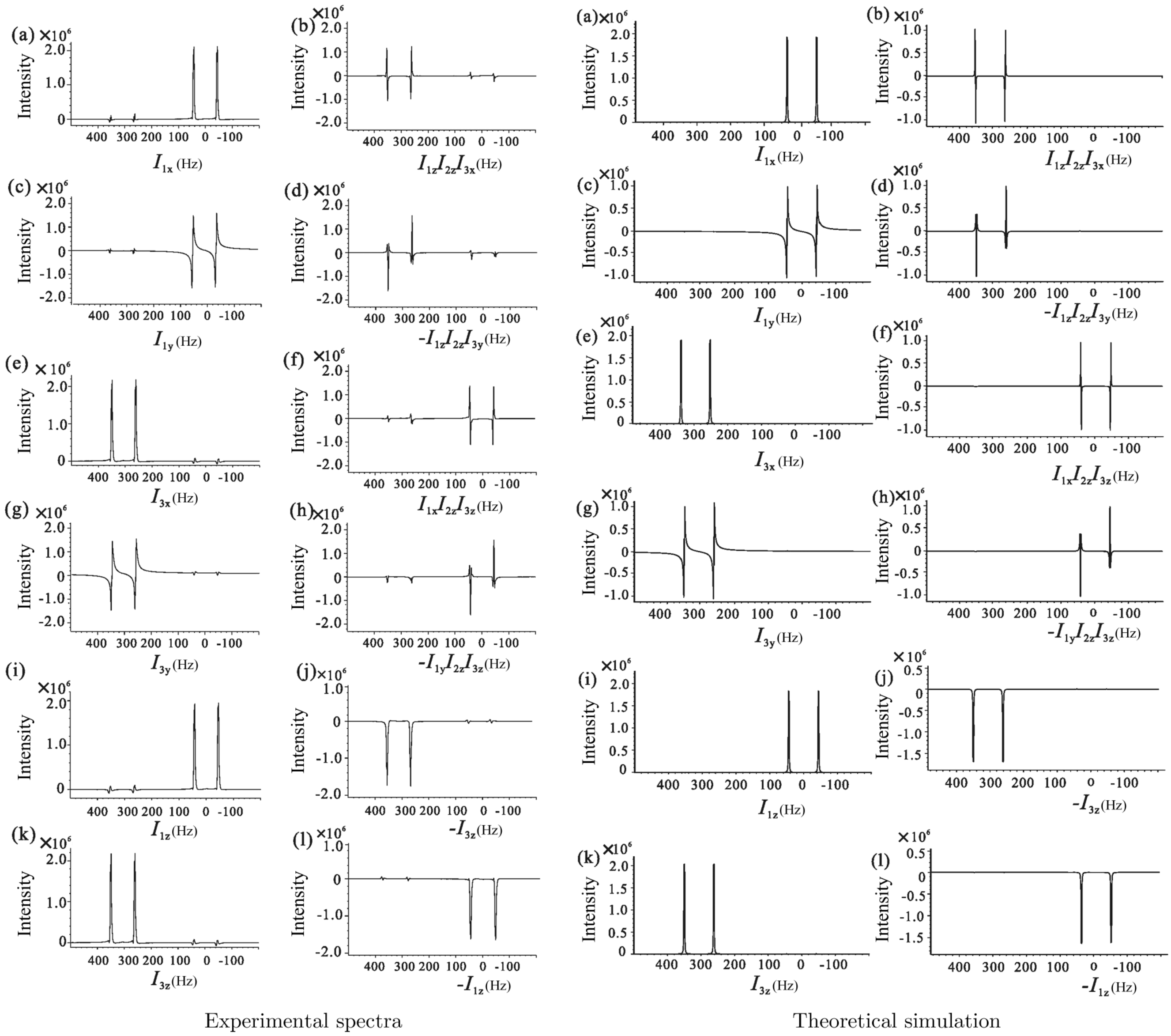

FIG. 7. (a), (c), (e), (g), (i), and (k) correspond to the spectra of six different initial states I_{1x}, I_{1y}, I_{3x}, I_{3y}, I_{1z}, I_{3z}; (b), (d), (f), (h), (j), and (l) correspond to the spectra of respective final states $I_{1z}I_{2z}I_{3x}$, $-I_{1z}I_{2z}I_{3y}$, $I_{1x}I_{2z}I_{3z}$, $-I_{1y}I_{2z}I_{3z}$, $-I_{3z}$, and $-I_{1z}$.

can implement the time optimal sequence as follows:

$$\exp(-i\theta B_p) = \exp(-it_1\sigma_{1z}\sigma_{2z}\sigma_{3y})\exp(it_2\sigma_{3x}\sigma_{4z}) \times \exp(it_2\sigma_{1z}\sigma_{2z}\sigma_{3y})\exp(-it_1\sigma_{3x}\sigma_{4z}), \quad (15)$$

where

$$t_1 = \arccos\frac{1}{\sin\frac{\theta}{2}+\cos\frac{\theta}{2}}, \quad t_2 = \arccos\left(\cos\frac{\theta}{2}-\sin\frac{\theta}{2}\right). \quad (16)$$

Here $\exp(-it_1\sigma_{1z}\sigma_{2z}\sigma_{3y})$ can again be generated by the sequence

$$\exp(-it_1\sigma_{1z}\sigma_{2z}\sigma_{3y}) = \exp(-it_1'\sigma_{1z}\sigma_{2y})\exp(it_2'\sigma_{2x}\sigma_{3y}) \times \exp(it_2'\sigma_{1z}\sigma_{2y})\exp(-it_1'\sigma_{2x}\sigma_{3y}), \quad (17)$$

where

$$t_1' = \arccos\frac{1}{\sin\frac{t_1}{2}+\cos\frac{t_1}{2}}, \quad t_2' = \arccos\left(\cos\frac{t_1}{2}-\sin\frac{t_1}{2}\right); \quad (18)$$

here terms containing σ_x and σ_y can be obtained from Ising coupling by applying single spin operations. Thus by repeatedly using the four-pulses sequence, one can efficiently simulate B_p. Note that the concatenation of the optimal sequence may not be optimal, nevertheless it is much more efficient than the conventional method using the BCH formula.

IV. EXPERIMENT

We experimentally demonstrated the implementation of the unitary transformation $e^{2\pi i(I_{1x}I_{2z}I_{3y}+I_{1y}I_{2z}I_{3x})}$ on a BRUKER

AVANCE 500M NMR spectrometer; this corresponds to the case $\theta = -\frac{\pi}{2}$ in $e^{-4i\theta[I_{1x}I_{2z}I_{3y}+I_{1y}I_{2z}I_{3x}]}$. The sample is the amino moiety of 15N acetamide (NH_2COCH_3). Two protons in the spin system $-NH_2$ present spins 1 and 3. The chemical shift difference between the two protons is 306 Hz. Nuclear 15N denotes spin 2. The J-coupling constants among the three spins are $J_{12} = J_{23} = 88$ Hz, $J_{13} = 2.6$ Hz. The pulse sequence used in the experiment is shown in Fig. 6.

In this experiment $t_1 = t_2 = 2.84$ ms, $\delta t = 5.68$ ms. The whole duration of this pulse is 17 ms. We choose six different initial states to observe the final states after the pulses are applied. For the six different initial states I_{1x}, I_{1y}, I_{3x}, I_{3y}, I_{1z}, I_{3z}, the corresponding final states should be $I_{1z}I_{2z}I_{3x}$, $-I_{1z}I_{2z}I_{3y}$, $I_{1x}I_{2z}I_{3z}$, $-I_{1y}I_{2z}I_{3z}$, $-I_{3z}$, and $-I_{1z}$, respectively. Figure 7 shows the experimental spectra [for the state I_{iz} ($i = 1,3$), a 90° reading pulse along the y axis has been applied before acquisition] and the theoretical simulations. The experimental spectra are almost identical to the theoretical spectra except for some little peaks in addition to the expected peaks, which is mainly due to experimental imperfections, such as rf inhomogeneity, imperfect calibrations, and incomplete field drift compensation. The consistency between experimental and theoretical spectra indicates that the pulse sequence works accurately and the unitary transformation has been experimentally implemented.

V. CONCLUSION

In many applications of quantum information processing, one needs to perform quantum gates efficiently on indirectly coupled spins. The most simple but nontrivial case is the linearly coupled three-spin system. We studied the time optimal constructions of various quantum gates on such a three-spin system, which boils down to solving an optimal control problem on an so(3) algebra. Although there is no systematical way to identify an so(3) algebra in general physical systems, so(3) algebra is ubiquitous and often easy to spot for a given physical system. We demonstrate such identification with another example of simulating multibody coupling for topological quantum computing on spin lattice. Possible future work is on time optimal constructions of quantum gates on a linear spin system with more than three spins and a spin system with various other topologies.

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APPENDIX: TIME OPTIMAL PULSE SEQUENCES

In this Appendix, we derive the solution of the optimal control problem for

$$\frac{d}{dt}\Omega(t) = A(t)\Omega(t), \tag{A1}$$

where

$$A(t) = u(t)\Omega_z + v(t)\Omega_y, \tag{A2}$$

$u(t),v(t) \in \{1,-1,0\}$, and $\forall t, |u(t)| + |v(t)| = 1$. We would like to generate $\Omega(T) = e^{\alpha\Omega_z}$ in minimum time with the initial condition $\Omega(0) = I$. For ease of notation we will omit t for the rest of the derivation when it does not cause confusion.

We first apply the maximum principle [22]. It is known that there is no singular extremal for such a system [23]. The control Hamiltonian then can be written as

$$H = -1 + \mathrm{tr}(\lambda^T A\Omega),$$

where λ is an auxiliary three-dimensional vector variable and $\dot{\lambda} = A\lambda$, the optimal control u,v should maximize the control Hamiltonian, i.e., $u,v = \mathrm{argmax}\{H\}$,

$$\begin{aligned} H &= -1 + \mathrm{tr}(\lambda^T A\Omega) = -1 + \mathrm{tr}(A\Omega\lambda^T) \\ &= -1 + \mathrm{tr}\left(A\frac{\Omega\lambda^T - \lambda\Omega^T}{2} + A\frac{\Omega\lambda^T + \lambda\Omega^T}{2}\right), \\ &= -1 + \mathrm{tr}\left(A\frac{\Omega\lambda^T - \lambda\Omega^T}{2}\right), \end{aligned} \tag{A3}$$

where the last step holds because A is skew symmetric and $S = \frac{\Omega\lambda^T + \lambda\Omega^T}{2}$ is symmetric, as

$$\mathrm{tr}(AS) = \mathrm{tr}[(AS)^T] = \mathrm{tr}(-SA) = -\mathrm{tr}(AS),$$

thus $\mathrm{tr}(AS) = 0$. Now let

$$M = \frac{\Omega\lambda^T - \lambda\Omega^T}{2} = m_x\Omega_x + m_y\Omega_y + m_z\Omega_z, \tag{A4}$$

then

$$\begin{aligned} H &= -1 + \mathrm{tr}\big(um_z\Omega_z^2\big) + \mathrm{tr}\big(vm_y\Omega_y^2\big) \\ &= -1 - 2um_z - 2vm_y. \end{aligned} \tag{A5}$$

From the definition of M and the dynamics of Ω and λ, we get

$$\dot{M} = [A,M],$$

substituting M and A with Eqs. (A2) and (A4) respectively,

$$\begin{aligned} &\dot{m}_x\Omega_x + \dot{m}_y\Omega_y + \dot{m}_z\Omega_z \\ &\quad = [u\Omega_z + v\Omega_y, m_x\Omega_x + m_y\Omega_y + m_z\Omega_z], \end{aligned}$$

which gives

$$\dot{m}_x = -um_y + vm_z, \quad \dot{m}_y = um_x, \quad \dot{m}_z = -vm_x. \tag{A6}$$

As $u,v = \mathrm{argmax}\{H\}$, we get

$$\begin{aligned} u &= -\mathrm{sgn}(m_z), \quad v = 0 \quad \text{if} \quad |m_z| > |m_y|, \\ u &= 0, \quad v = -\mathrm{sgn}(m_y) \quad \text{if} \quad |m_z| < |m_y|; \end{aligned}$$

if $|m_z| = |m_y|$, then u,v can be either.

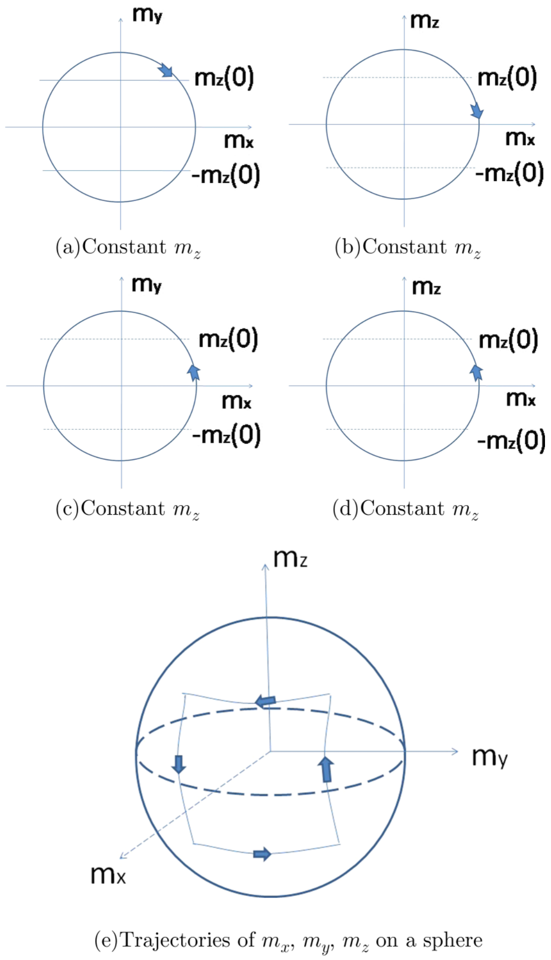
Assume that initially $m_z(0) > m_y(0) > 0, m_x(0) > 0$ (solutions under other initial conditions can be similarly worked out), then initially

$$u = -\mathrm{sgn}[m_z(0)] = -1, \quad v = 0.$$

From Eq. (A6) we get

$$\dot{m}_x = m_y, \quad \dot{m}_y = -m_x, \quad \dot{m}_z = 0. \tag{A7}$$

It evolves as in Fig. 8(a).



(a)Constant m_z (b)Constant m_z (c)Constant m_z (d)Constant m_z (e)Trajectories of m_x, m_y, m_z on a sphere

FIG. 8. (Color online) The evolution trajectory of m_x,m_y,m_z.

Case I: If $m_x^2(0)+m_y^2(0)<m_z^2(0)$, then the controls are constant, $u=-\text{sgn}[m_z(0)]=-1, v=0$ throughout.

Case II: If $m_x^2(0)+m_y^2(0)>m_z^2(0)$, then after evolving for some time, $|m_y|$ will exceed $|m_z|$, so we need to switch the controls at t_1, where $m_y(t_1)=-m_z(0)$—to $v=-\text{sgn}(m_y)=1, u=0$, then from Eq. (A6) we get

$$\dot{m_x}=m_z,\quad \dot{m_y}=0,\quad \dot{m_z}=-m_x, \tag{A8}$$

which evolves as in Fig. 8(b) until $m_z(t_2)=-m_z(0)$ at some point t_2, where we shall switch the controls to $u=-\text{sgn}(m_z)=1, v=0$ and the dynamics changes to

$$\dot{m_x}=-m_y,\quad \dot{m_y}=m_x,\quad \dot{m_z}=0, \tag{A9}$$

which evolves as in Fig. 8(c) until $m_y(t_3)=m_z(0)$ where we shall switch the controls to $v=-\text{sgn}(m_y)=-1, u=0$ and the dynamics becomes

$$\dot{m_x}=-m_z,\quad \dot{m_y}=0,\quad \dot{m_z}=m_x, \tag{A10}$$

which evolves until $m_z(t_4)=m_z(0)$ at some time point t_4, then we switch back to Eq. (A7) and the process repeats. Other initial conditions of m_x,m_y,m_z give similar periodical controls. Thus the optimal sequences in this case display the following patterns:

	1	2	3	4	5	...	n
	t_1	δt	δt	δt	δt	...	t_2
u,v	1,0	0,−1	−1,0	0,1	1,0	...	
u,v	1,0	0,1	−1,0	0,−1	1,0	...	
u,v	−1,0	0,−1	1,0	0,1	−1,0	...	
u,v	−1,0	0,1	1,0	0,−1	−1,0	...	

and also the sequences with u,v switched. Here $t_1,t_2\leqslant \delta t<\pi$, are the evolving time of the dynamics with the corresponding controls; the evolving time for intermediate steps are all equal.

Case III: If $m_x^2(0)+m_y^2(0)=m_z^2(0)$, the process starts similarly; first $u=-\text{sgn}[m_z(0)]=-1, v=0$,

$$\dot{m_x}=m_y,\quad \dot{m_y}=-m_x,\quad \dot{m_z}=0. \tag{A11}$$

It evolves until $m_y(t_1)=-m_z(0)$ at time t_1. In this case since $m_x^2(0)+m_y^2(0)=m_z^2(0)$, at time t_1, $m_x(t_1)=0$. From Eq. (A6), at time t_1

$$\begin{aligned}\dot{m_x}&=-um_y+vm_z,\quad \dot{m_y}=um_x=0,\\ \dot{m_z}&=-vm_x=0.\end{aligned} \tag{A12}$$

This is a singular point and we can choose u,v such that $\dot{m_x}=-um_y+vm_z=0$, which can be achieved by rapidly changing between $u=-1$, $v=0$, and $u=0, v=1$ (equivalent to rotate around $\Omega_y-\Omega_z$), and the dynamics can stay at this point for an arbitrarily long time. After that, one can either continue with $u=-1, v=0$ or switch to $u=0, v=1$. If it continues with $u=-1, v=0$, then it will evolves until t_2 such that $m_y(t_2)=m_z(0)$ and reach another singular point, where we can switch rapidly between $u=-1, v=0$ and $u=0, v=-1$, which is equivalent to evolve along $-(\Omega_y+\Omega_z)$. If it continues with $u=0, v=1$, then it follows the dynamics

$$\dot{m_x}=m_z,\quad \dot{m_y}=0,\quad \dot{m_z}=-m_x, \tag{A13}$$

until t_2 such that $m_z(t_2)=-m_z(0)=m_y(t_2)$, where it can switch rapidly between $u=1, v=0$ and $u=0, v=1$, which is equivalent to evolve along $\Omega_y+\Omega_z$. So in this case we have the following possible sequences:

$$\begin{aligned}&e^{-\delta t_1\Omega_z}\; e^{\delta t_2(\Omega_y-\Omega_z)}e^{-\pi\Omega_z}e^{-\delta t_3(\Omega_y+\Omega_z)}\cdots e^{\delta t_n\Omega_{z/y}},\\ &e^{-\delta t_1\Omega_z}\; e^{\delta t_2(\Omega_y-\Omega_z)}e^{\pi\Omega_y}e^{\delta t_3(\Omega_y+\Omega_z)}\cdots e^{\delta t_n\Omega_{z/y}}\\ &\qquad\vdots\end{aligned} \tag{A14}$$

Here $\Omega_{z/y}$ means it can be either Ω_z or Ω_y. The sequence is switching between regular points ($\Omega_{z/y}$) and singular points ($\Omega_z\pm\Omega_y$) and the regular points in the middle of sequence have to evolve for π units of time each. For the optimal sequence, we can just consider the sequences with at most one singular point, as if it appears twice, for example if the optimal sequence contains $e^{\delta t_2(\Omega_y-\Omega_z)}e^{\pi\Omega_y}e^{\delta t_3(\Omega_y+\Omega_z)}$, then we can replace it by

$$\begin{aligned}&e^{\delta t_2(\Omega_y-\Omega_z)}e^{\pi\Omega_y}e^{\delta t_3(\Omega_y+\Omega_z)}e^{-\pi\Omega_y}e^{\pi\Omega_y}\\ &\quad=e^{(\delta t_2+\delta t_3)(\Omega_y-\Omega_z)}e^{\pi\Omega_y},\end{aligned} \tag{A15}$$

which is a sequence that has the same time cost but has only one singular point.

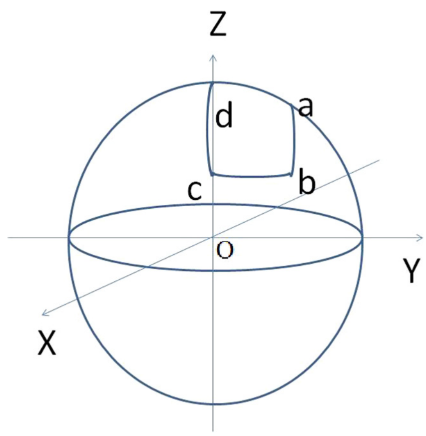


FIG. 9. (Color online) Rotations that move $a = (0, \sin\alpha, \cos\alpha)$ to $d = (0,0,1)$ via the point $b = (\cos\alpha \sin t_1, \sin\alpha, \cos\alpha \cos t_1)$ and $c = (\sqrt{\cos^2\alpha \sin^2 t_1 + \sin^2\alpha}, 0, \cos\alpha \cos t_1)$.

With this information, we can determine the optimal sequence to generate $e^{\alpha\Omega_x}, \alpha \in [0,\pi/2]$. The element $\{e^{\alpha\Omega_x}\}$ has a one-to-one correspondence to the action on the sphere of rotating the point $(0, \sin\alpha, \cos\alpha)$ to $(0,0,1)$ while keeping the x axis fixed. We now study the time optimal way to generate such actions.

Clearly the constant controls cannot rotate the point $(0, \sin\alpha, \cos\alpha)$ to $(0,0,1)$ and using two rotations we cannot rotate the point $(0, \sin\alpha, \cos\alpha)$ to $(0,0,1)$ while keeping the x axis fixed. There are a few ways to generate $e^{\alpha\Omega_x}$ using three rotations; they are all essentially equivalent to

$$e^{\alpha\Omega_z} e^{\beta(\Omega_z+\Omega_y)} e^{\gamma\Omega_z}, \quad e^{\alpha\Omega_z} e^{\beta(\Omega_z+\Omega_y)} e^{\gamma\Omega_y},$$

or

$$e^{\alpha\Omega_z} e^{\beta\Omega_y} e^{\gamma\Omega_z}.$$

All these pulses turn out to take a longer time than the four rotations presented below, so we will not present the details of the calculation on these pulses.

We now give the strategy with four rotations that moves $(0, \sin\alpha, \cos\alpha)$ to $(0,0,1)$ and keeps the x axis fixed. As shown in Fig. 9, it is first rotated around the y axis for time t_1, which rotates the point $a = (0, \sin\alpha, \cos\alpha)$ to $b = (\cos\alpha \sin t_1, \sin\alpha, \cos\alpha \cos t_1)$; then it is rotated around the (z) axis for time δt, which rotates point b to point $c = (\sqrt{\cos^2\alpha \sin^2 t_1 + \sin^2\alpha}, 0, \cos\alpha \cos t_1)$ which is on the XZ plane; after that it is rotated around the (y) axis for time δt to the point $d = (0,0,1)$; since the x axis is orthogonal to $\overrightarrow{oa}$ and rotations do not change the angles, so after these rotations, the x axis has moved to somewhere which is orthogonal to $\overrightarrow{od}$, i.e., somewhere on the XY plane, so we need to make another rotation around the z axis for time t_2, which moves the x axis back to the original position. After combining these rotations, we get

$$e^{\alpha\Omega_x} = e^{t_2\Omega_z} e^{-\delta t\Omega_y} e^{-\delta t\Omega_z} e^{t_1\Omega_y}. \tag{A16}$$

From the second and third rotations, we get two equations on δt and t_1,

$$\tan(\delta t) = \frac{\sin\alpha}{\cos\alpha \sin t_1}, \qquad \tan(\delta t) = \frac{\sqrt{\cos^2\alpha \sin^2 t_1 + \sin^2\alpha}}{\cos\alpha \cos t_1}, \tag{A17}$$

which we can solve to get the value of t_1 and δt:

$$t_1 = \arccos\frac{1}{\sin\frac{\alpha}{2} + \cos\frac{\alpha}{2}}, \qquad \delta t = \arccos\left(\cos\frac{\alpha}{2} - \sin\frac{\alpha}{2}\right). \tag{A18}$$

To calculate the value of t_2, we need to figure out the trajectory of the x axis: it is first rotated from $(1,0,0)$ to $(\cos t_1, 0, -\sin t_1)$, then it is rotated to $(\cos t_1 \cos\delta t, -\cos t_1 \sin\delta t, -\sin t_1)$, then to $(\sqrt{\cos^2 t_1 \cos^2\delta t + \sin^2 t_1}, -\cos t_1 \sin\delta t, 0)$. The last rotation around the z axis should rotate $(\sqrt{\cos^2 t_1 \cos^2\delta t + \sin^2 t_1}, -\cos t_1 \sin\delta t, 0)$ back to $(1,0,0)$, i.e.,

$$\cos t_2 = \sqrt{\cos^2 t_1 \cos^2\delta t + \sin^2 t_1} = \frac{1}{\sin\frac{\alpha}{2} + \cos\frac{\alpha}{2}},$$

so

$$t_2 = t_1 = \arccos\frac{1}{\sin\frac{\alpha}{2} + \cos\frac{\alpha}{2}},$$

so the total time to generate $e^{\alpha\Omega_x}$ is

$$f(\alpha) = 2\left[\arccos\frac{1}{\sin\frac{\alpha}{2} + \cos\frac{\alpha}{2}} + \arccos\left(\cos\frac{\alpha}{2} - \sin\frac{\alpha}{2}\right)\right]. \tag{A19}$$

Symmetrically when $\alpha \in [-\frac{\pi}{2}, 0]$,

$$f(\alpha) = f(-\alpha).$$

So for $\alpha \in [-\frac{\pi}{2}, \frac{\pi}{2}]$,

$$f(\alpha) = 2\left[\arccos\frac{1}{\sin\frac{|\alpha|}{2} + \cos\frac{|\alpha|}{2}} + \arccos\left(\cos\frac{|\alpha|}{2} - \sin\frac{|\alpha|}{2}\right)\right]. \tag{A20}$$

This is actually the optimal sequences; adding more switches would not help [21]. For completeness, we sketch the proof in [21] showing that if a pulse sequence contains more than four pulses, then it can be replaced by a pulse sequence with a shorter duration, thus it cannot be optimal.

From the periodic pattern of optimal pulses, we know that for an optimal pulse sequence with more than four pulses, it will contain some typical sequence such as $e^{t\Omega_y} e^{s\Omega_z} e^{-s\Omega_y} e^{-s\Omega_z} e^{t\Omega_y}$; we will show that such a pulse sequence cannot be part of an optimal sequence. First note that

$$e^{s\Omega_z} e^{-s\Omega_y} e^{-s\Omega_z} = e^{-(\pi-s)\Omega_z} e^{s\Omega_y} e^{(\pi-s)\Omega_z};$$

note that when $s > \frac{\pi}{2}$, $3s > 2\pi - s$, thus when $s > \frac{\pi}{2}$, the pulse sequence is not optimal.

For $s = \frac{\pi}{2}$,

$$\begin{aligned} e^{t\Omega_y} e^{(\pi/2)\Omega_z} e^{-(\pi/2)\Omega_y} e^{-(\pi/2)\Omega_z} &= e^{t\Omega_y} e^{-(\pi/2)\Omega_x} \\ &= e^{t\Omega_y} e^{-(\pi/2)\Omega_y} e^{(\pi/2)\Omega_z} e^{(\pi/2)\Omega_y} \\ &= e^{(t-\pi/2)\Omega_y} e^{(\pi/2)\Omega_z} e^{(\pi/2)\Omega_y}, \end{aligned} \tag{A21}$$

as $\frac{\pi}{2} - t + \frac{\pi}{2} + \frac{\pi}{2} < t + \frac{3\pi}{2}$, thus when $s = \frac{\pi}{2}$ the sequence is also not optimal.

For $s \in (0,\frac{\pi}{2})$, let

$$\gamma_s(t) = e^{t\Omega_y} e^{s\Omega_z} e^{-s\Omega_y} e^{-s\Omega_z} e^{t\Omega_y}.$$

Consider a map $F : \mathbb{R}^3 \to \mathrm{SO}(3)$,

$$F(r_1,r_2,r_3) = e^{r_1\Omega_y} e^{r_2\Omega_z} e^{-r_2\Omega_y} e^{-r_3\Omega_z}. \quad \text{(A22)}$$

It is easy to see that $\gamma_s(0) = F(0,s,s)$. Since the differential $dF(0,s,s)$ is invertible, by implicit function theorem, we know that there exists $\epsilon > 0$, such that for $t \in (-\epsilon,\epsilon)$, there exists a smooth curve $r(t)$ such that $r(0) = (0,s,s)$, and $\gamma_s(t) = F(r(t))$. Thus $F(r(t))$ provides an alternate factorization of $\gamma_s(t)$ with the total time $r_1(t) + 2r_2(t) + r_3(t)$. Now let us look at the difference between the total time of $\gamma_s(t)$ and $F(r(t))$,

$$\delta(t) = 3s + 2t - [r_1(t) + 2r_2(t) + r_3(t)],$$

since $\delta(0) = \delta'(0) = 0$, and

$$\delta''(0) = \tfrac{1}{2}[\sin(s) + 3\tan(s)] > 0$$

when $s \in (0,\frac{\pi}{2})$, thus $\delta(t) > 0$ for small $t \neq 0$, which implies that $F(r(t))$ provides a better factorization. Hence an optimal pulse sequence never contains more than four rotations.

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