Efficient synthesis of quantum gates on a three-spin system with triangle topology

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Experiments in coherent nuclear and electron magnetic resonance and optical spectroscopy correspond to control of quantum-mechanical ensembles, guiding them from initial states to 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 give an efficient synthesis of a class of unitary transformations on a three coupled spin-$\frac{1}{2}$ system with equal Ising coupling strengths. We show a significant time saving compared with conventional methods.

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I. INTRODUCTION

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), electron spin resonance (ESR) spectroscopy [1,2], laser coherent control [3], and quantum computing [4,5]. Developing a specific set of control laws (pulse sequences) that produce a desired unitary evolution of the state has been a major thrust in NMR spectroscopy [1]. For example, in the NMR spectroscopy of proteins [6], the transfer of coherence along spin chains is an essential step in a large number of key experiments. Spin-chain topologies have also been proposed as architectures for quantum information processing [7,8]. In practice, the transfer time should be as short as possible in order to reduce the loss due to relaxation or decoherence.

The time-optimal synthesis of unitary operators is now well understood for coupled two-spin systems [9–15]. This problem has also been studied recently in the context of linear three-spin topology [16–21], where significant savings in the implementation time of trilinear Hamiltonians and synthesis of couplings between indirectly coupled spins were demonstrated compared with conventional methods. In [16,18–21], it was shown that the time-optimal synthesis of indirect couplings and of trilinear Hamiltonians from linear Ising couplings can be reduced to the problem of computing geodesics on a sphere under a special metric. In this paper, we extend these methods to three-spin system with equal Ising couplings, and we study the efficient synthesis of the unitary transformations on the system, which constitutes an important step in understanding control of multiple-spin dynamics. Synthesizing quantum gates on more than two qubits is appealing because, although single- and two-qubit operations form a universal set for quantum computing, it scales unfavorably with the complexity of implemented algorithms. Multiqubit gates can replace complex sequences of two-qubit gates, thus promising faster execution and higher fidelity.

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II. TIME-OPTIMAL CONTROL FOR THREE LINEARLY COUPLED SPINS

In this section, we give a brief introduction of previous results on efficient synthesis of unitary transformations on three linearly coupled spins [16], upon which our present results are based.

Consider a chain of three spins coupled by scalar couplings ($J_{13} = 0$), Fig. 1(a). Furthermore, assume that it is possible to selectively excite each spin (perform one-qubit operations in the context of quantum computing). The goal is to produce a desired unitary transformation, $U \in SU(8)$, from the specified couplings and single-spin operations in the shortest possible time. The dynamics of 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 $I_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}/2$, $I_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}/2$, and $I_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}/2$ are the Pauli spin matrices, and we denote by $I_{\ell\nu}$ the operator that acts as I_ν on the ℓth spin, for example, $I_{1x} = I_x \otimes I_0 \otimes I_0$, where $I_0 := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is the (2×2)-dimensional identity matrix. The symbols 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 ($J_{12} = J_{23} = J$). We will be most interested in unitary propagators of the form

$$U = \exp(-i2\pi\kappa\, I_{1z} I_{2z} I_{3z}).$$

These propagators are hard to produce as they involve trilinear terms in the effective Hamiltonian. We will refer to such propagators as *trilinear propagators*.

We assume that we can selectively rotate each spin at a rate much faster than the evolution caused by the couplings, i.e., the single-spin operations can be done in a negligible amount of time.

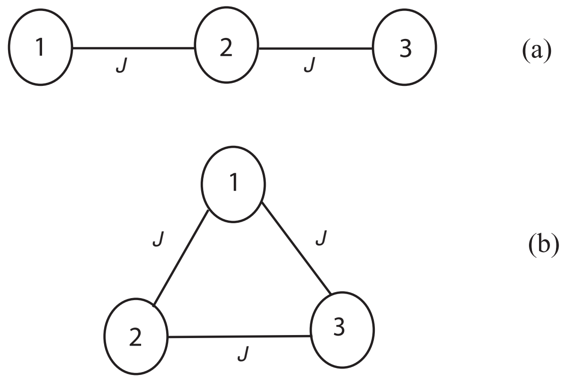

FIG. 1. Spins in linear (a) and triangle (b) topology.

Theorem 1 [16]. Given the spin system in (1), with $J_{12} = J_{23} = J$ and $J_{13} = 0$, the minimum time required to produce a propagator of the form $U_F = \exp(-i2\pi\kappa I_{1z}I_{2z}I_{3z})$, $\kappa \in [0,2]$, by using an effective Hamiltonian $H_{\rm eff}(t)$ equal to

$$2\pi J\{(I_{1z}I_{2x} + I_{2x}I_{3z})\cos\theta(t) + (I_{1z}I_{2y} + I_{2y}I_{3z})\sin\theta(t)\},$$

is

$$T(\kappa) = \frac{\sqrt{\kappa(4-\kappa)}}{2J}.$$

The sequence of unitary transformations that produces the propagator U_F is as follows:

$$\begin{aligned} U_F = &\exp\left(-i\frac{\pi}{2}I_{2y}\right)\exp\left(-i\left[\pi + \frac{\beta}{2}\right]I_{2x}\right) \\ &\times \exp\left(T(\kappa)\left[-i2\pi J(I_{1z}I_{2z} + I_{2z}I_{3z}) + i\frac{\beta}{T(\kappa)}I_{2x}\right]\right) \\ &\times \exp\left(i\frac{\pi}{2}I_{2y}\right), \end{aligned} \tag{2}$$

where $\beta = (2-\kappa)\pi$ and $T(\kappa) = \frac{\sqrt{\kappa(4-\kappa)}}{2J}$.

Some properties of the function $T(\kappa) = \frac{\sqrt{\kappa(4-\kappa)}}{2J}$ are in order.

Theorem 2. The function

$$T(\kappa) = \frac{\sqrt{\kappa(4-\kappa)}}{2J}, \quad \kappa \in [0,2],$$

is a concave function satisfying

$$T(\kappa_1 + \kappa_2) \leqslant T(\kappa_1) + T(\kappa_2).$$

To prove concavity, we just have to show that $\frac{d^2T}{d\kappa^2} < 0$. The computation is simplified by substituting $\kappa = 2 - \gamma$, and then $\frac{d^2T}{d\kappa^2} = \frac{d^2T(2-\gamma)}{d\gamma^2}$. A direct computation shows that for $\gamma \in [0,2)$,

$$\frac{d^2T(2-\gamma)}{d\gamma^2} = \frac{-(4+2\gamma^2)}{(4-\gamma^2)^{\frac{3}{2}}} < 0.$$

Thus T is a concave function, which implies

$$T(\alpha\delta_1 + (1-\alpha)\delta_2) \geqslant \alpha T(\delta_1) + (1-\alpha)T(\delta_2). \tag{3}$$

Proposition 1. If

$$(\kappa_1,\kappa_2), \quad \text{where} \quad \kappa_2 \leqslant \kappa_1$$

and

$$(\kappa_1',\kappa_2'), \quad \text{where} \quad \kappa_2' \leqslant \kappa_1'$$

are two divisions of κ, i.e., $\kappa = \kappa_1 + \kappa_2 = \kappa_1' + \kappa_2'$, and furthermore if $\kappa_1 \geqslant \kappa_1'$, then

$$T(\kappa_1) + T(\kappa_2) \leqslant T(\kappa_1') + T(\kappa_2').$$

To see this, first note that $\kappa_1' \in [\kappa_2,\kappa_1]$, so $\kappa_1' = \alpha\kappa_1 + (1-\alpha)\kappa_2$ for $\alpha \in [0,1]$. Then using $\kappa_1 + \kappa_2 = \kappa_1' + \kappa_2'$, one gets $\kappa_2' = (1-\alpha)\kappa_1 + \alpha\kappa_2$. Using concavity,

$$\begin{aligned} T(\kappa_1') &\geqslant \alpha T(\kappa_1) + (1-\alpha)T(\kappa_2), \\ T(\kappa_2') &\geqslant (1-\alpha)T(\kappa_1) + \alpha T(\kappa_2). \end{aligned}$$

Adding the two equations, we get

$$T(\kappa_1') + T(\kappa_2') \geqslant T(\kappa_1) + T(\kappa_2).$$

In particular, this implies

$$T(\kappa_1) + T(\kappa_2) \geqslant T(\kappa_1 + \kappa_2) + T(0) = T(\kappa_1 + \kappa_2).$$

III. EFFICIENT CONTROL ON THREE COUPLED SPINS WITH A TRIANGLE TOPOLOGY

Now consider three spins coupled to each other with equal Ising couplings, Fig. 1(b). The dynamics of the unitary propagator U, which describes the evolution of the system in a suitable rotating frame, is well approximated by

$$\dot{U} = -i\left(H_d + \sum_{j=1}^{6} u_j H_j\right)U, \quad U(0) = I, \tag{4}$$

where

$$\begin{aligned} &H_d = 2\pi J I_{1z}I_{2z} + 2\pi J I_{2z}I_{3z} + 2\pi J I_{1z}I_{3z}, \quad H_1 = 2\pi I_{1x}, \\ &H_2 = 2\pi I_{1y}, \quad H_3 = 2\pi I_{2x}, \quad H_4 = 2\pi I_{2y}, \\ &H_5 = 2\pi I_{3x}, \quad H_6 = 2\pi I_{3y}. \end{aligned}$$

We will be most interested in synthesizing a Toffoli gate on this three-spin system. The quantum Toffoli gate is the archetype of a three-qubit gate that performs a controlled NOT operation on a target qubit depending on the state of two control qubits. It constitutes one of the basic building blocks for quantum computation and is widely used in quantum computation, for example in Shor's algorithm and quantum error correction.

The quantum Toffoli gate is a unitary propagator of the form

$$\begin{aligned} U_T &= \exp\left[-i\pi\left(\frac{1}{2}I - I_{1z}\right)\left(\frac{1}{2}I - I_{2z}\right)I_{3x}\right] \\ &= \exp\left[-i\frac{\pi}{2}I_{3y}\right] \\ &\quad \times \exp\left[-i\pi\left(\frac{1}{2}I - I_{1z}\right)\left(\frac{1}{2}I - I_{2z}\right)I_{3z}\right] \\ &\quad \times \exp\left[i\frac{\pi}{2}I_{3y}\right]. \end{aligned}$$

Since the single operations take a negligible amount of time, it is equivalent to synthesize the gate

$$U = \exp\left[-i\pi\left(\tfrac{1}{2}I - I_{1z}\right)\left(\tfrac{1}{2}I - I_{2z}\right)I_{3z}\right] = \exp\left[-i\pi\left(\tfrac{1}{4}I_{3z} - \tfrac{1}{2}I_{1z}I_{3z} - \tfrac{1}{2}I_{2z}I_{3z} + I_{1z}I_{2z}I_{3z}\right)\right], \quad (5)$$

which is again equivalent to synthesizing

$$\exp\left[-i\pi\left(-\tfrac{1}{2}I_{1z}I_{3z} - \tfrac{1}{2}I_{2z}I_{3z} + I_{1z}I_{2z}I_{3z}\right)\right]. \quad (6)$$

The rest of the paper will focus on how to efficiently synthesize this unitary operator. The conventional way is to synthesize terms in the Hamiltonian separately while using π pulses to decouple part of the coupling interactions. It takes $\frac{1}{4J}$ to generate $\exp[i\frac{\pi}{2}I_{1z}I_{3z}]$ by decoupling the second spin, which is obtained by using the Hamiltonian

$$H_1 = 2\pi J(I_{1z}I_{2z} + I_{2z}I_{3z} + I_{1z}I_{3z}) \quad (7)$$

and

$$H_2 = 2\pi J(-I_{1z}I_{2z} - I_{2z}I_{3z} + I_{1z}I_{3z}), \quad (8)$$

each for $\frac{1}{8J}$ units of time, and then applying a hard π pulse on spin 1 or spin 3. The Hamiltonian H_2 is synthesized by application of a hard π pulse on spin 2, i.e.,

$$\exp(-iH_2t) = \exp(-i\pi I_{2y})\exp(-iH_1t)\exp(i\pi I_{2y}). \quad (9)$$

It takes same amount of time to generate $\exp[i\frac{\pi}{2}I_{2z}I_{3z}]$. The term $\exp[-i\pi I_{1z}I_{2z}I_{3z}]$ can be obtained by the Baker-Campbell-Hausdorff formula

$$\exp(-i\pi I_{1z}I_{2x})\exp\left(-i\frac{\pi I_{2y}I_{3z}}{2}\right)\exp(i\pi I_{1z}I_{2x}) = \exp(-i\pi I_{1z}I_{2z}I_{3z}). \quad (10)$$

Therefore, the total time required to produce the unitary propagator is

$$2\frac{1}{4J} + \frac{1}{4J} + 2\frac{1}{2J} = \frac{7}{4J}.$$

We will show that this can be significantly shortened.

From the preceding section, we know that

$$\exp\left(-i\frac{\pi}{2}I_{2y}\right)\exp\left(-i\left[\pi + \frac{\beta}{2}\right]I_{2x}\right)\exp\left(T(\kappa)\left[-i2\pi J(I_{1z}I_{2z} + I_{2z}I_{3z}) + i\frac{\beta}{T(\kappa)}I_{2x}\right]\right)\exp\left(i\frac{\pi}{2}I_{2y}\right) = \exp(-i2\pi\kappa I_{1z}I_{2z}I_{3z}),$$

where $\beta = (2-\kappa)\pi$ and $T(\kappa) = \frac{\sqrt{\kappa(4-\kappa)}}{2J}$. Now, replace the linear-coupled Hamiltonian with the triangle-coupled Hamiltonian. As the new coupling term $I_{1z}I_{3z}$ commute with all other terms, we get

$$\exp\left(-i\frac{\pi}{2}I_{2y}\right)\exp\left(-i\left[\pi + \frac{\beta}{2}\right]I_{2x}\right)\exp\left(T(\kappa)\left[-i2\pi J(I_{1z}I_{2z} + I_{2z}I_{3z} + I_{1z}I_{3z}) + i\frac{\beta}{T(\kappa)}I_{2x}\right]\right)\exp\left(i\frac{\pi}{2}I_{2y}\right) = \exp\{-i[2\pi\kappa I_{1z}I_{2z}I_{3z} + 2\pi JT(\kappa)I_{1z}I_{3z}]\}.$$

Similarly, we can get

$$\exp\left(-i\frac{\pi}{2}I_{1y}\right)\exp\left(-i\left[\pi + \frac{\beta}{2}\right]I_{1x}\right)\exp\left(T(\kappa)\left[-i2\pi J(I_{1z}I_{2z} + I_{2z}I_{3z} + I_{1z}I_{3z}) + i\frac{\beta}{T(\kappa)}I_{1x}\right]\right)\exp\left(i\frac{\pi}{2}I_{1y}\right) = \exp\{-i[2\pi\kappa I_{1z}I_{2z}I_{3z} + 2\pi JT(\kappa)I_{2z}I_{3z}]\}.$$

All the terms we need have appeared but some signs are different, which can be reversed by applying π rotations on a single spin. From now on, we just show how to optimally combine the terms

$$\begin{aligned} &\exp\{-i[2\pi\kappa I_{1z}I_{2z}I_{3z} \pm 2\pi JT(\kappa)I_{1z}I_{3z}]\},\\ &\exp\{-i[2\pi\kappa I_{1z}I_{2z}I_{3z} \pm 2\pi JT(\kappa)I_{2z}I_{3z}]\}, \end{aligned} \quad (11)$$

with possible decoupling terms to get the desired gate, particularly the Toffoli gate.

We begin by considering how to generate

$$U_k = \exp\left[-i\left(2\pi\kappa I_{1z}I_{2z}I_{3z} - \frac{\pi}{2}I_{1z}I_{3z}\right)\right] \quad (12)$$

efficiently.

A. When $T(\kappa) \leqslant \frac{1}{4J}$

If $T(\kappa) \leqslant \frac{1}{4J}$, then the minimum time to synthesize the above propagator is simply $\frac{1}{4J}$. The first $T(\kappa)$ units can be used to synthesize $\exp\{-i[2\pi\kappa I_{1z}I_{2z}I_{3z} - 2\pi JT(\kappa)I_{1z}I_{3z}]\}$

and the remaining $\frac{1}{4J} - T(\kappa)$ to synthesize the remaining part of $I_{1z}I_{3z}$. Note that it takes at least $\frac{1}{4J}$ to synthesize the term $\frac{\pi}{2}I_{1z}I_{3z}$, so the minimum time is $\frac{1}{4J}$.

B. $T(\kappa) > \frac{1}{4J}$

If $T(\kappa) > \frac{1}{4J}$, then it is not a good strategy to sequentially synthesize Hamiltonians

$$\exp\{-i[2\pi\kappa_a I_{1z}I_{2z}I_{3z} - 2\pi J T(\kappa_a) I_{1z}I_{3z}]\} \tag{13}$$

and

$$\exp\{-i[2\pi\kappa_b I_{1z}I_{2z}I_{3z} - 2\pi J T(\kappa_b) I_{1z}I_{3z}]\}, \tag{14}$$

where $\kappa_a + \kappa_b = \kappa$. As by concavity $T(\kappa_a) + T(\kappa_b) \geqslant T(\kappa_a + \kappa_b) \geqslant \frac{1}{4J}$, so additional overhead in a time of $T(\kappa_a) + T(\kappa_b) - \frac{1}{4J}$ is needed to remove the extra buildup of the term $I_{1z}I_{3z}$. Therefore, in this way the total time would be

$$T(\kappa_a) + T(\kappa_b) - \frac{1}{4J} + T(\kappa_a) + T(\kappa_b) \geqslant T(\kappa) - \frac{1}{4J} + T(\kappa),$$

i.e., it takes more time than directly synthesizing $\exp[-i2\pi\kappa I_{1z}I_{2z}I_{3z} + 2\pi J I_{1z}I_{3z}T(\kappa)]$, which takes $T(\kappa)$ units of time, then removing the extra build up of the term $I_{1z}I_{3z}$ with $T(\kappa) - \frac{1}{4J}$ units of time.

But, if we flip one sign, we sequentially synthesize

$$\exp\{-i[2\pi\kappa_a I_{1z}I_{2z}I_{3z} - 2\pi J T(\kappa_a) I_{1z}I_{3z}]\} \tag{15}$$

and

$$\exp\{-i[2\pi\kappa_b I_{1z}I_{2z}I_{3z} + 2\pi J T(\kappa_b) I_{1z}I_{3z}]\}. \tag{16}$$

Combining these two terms,

$$\begin{aligned}
&\exp\{-i[2\pi\kappa_a I_{1z}I_{2z}I_{3z} - 2\pi J T(\kappa_a) I_{1z}I_{3z}]\} \\
&\quad\times \exp\{-i[2\pi\kappa_b 2I_{1z}I_{2z}I_{3z} + 2\pi J T(\kappa_b) I_{1z}I_{3z}]\} \\
&= \exp\{-i2\pi(\kappa_a + \kappa_b) I_{1z}I_{2z}I_{3z} + i2\pi J[T(\kappa_a) \\
&\quad - T(\kappa_b)] I_{1z}I_{3z}\},
\end{aligned} \tag{17}$$

where $\kappa_a + \kappa_b = \kappa$, then the total time for this strategy is $T(\kappa_a) + T(\kappa_b) + |\frac{1}{4J} - [T(\kappa_a) - T(\kappa_b)]|$, which can be shorter than direct synthesis. To find the minimum time with this strategy, we need to solve the following optimization problem:

$$S(\kappa) = \min \left| \frac{1}{4J} - [T(\kappa_a) - T(\kappa_b)] \right| + T(\kappa_a) + T(\kappa_b)$$
$$\text{such that } \kappa_a + \kappa_b = \kappa \leqslant 2. \tag{18}$$

Here $T(\kappa) = \frac{\sqrt{\kappa(4-\kappa)}}{2J}$.

It is worth observing that if $T(\kappa) > \frac{1}{4J}$, the minimum $S(\kappa)$ is achieved when

$$T(\kappa_a^*) - T(\kappa_b^*) - \frac{1}{4J} = 0. \tag{19}$$

As for other choices of κ_a, κ_b, where $\kappa_a + \kappa_b = \kappa$, if $\kappa_a > \kappa_a^*$, we will have $[T(\kappa_a) - T(\kappa_b)] > \frac{1}{4J}$. The cost then becomes $2T(\kappa_a) - \frac{1}{4J}$, which is an increasing function of κ_a. If $\kappa_a < \kappa_a^*$, then $[T(\kappa_a) - T(\kappa_b)] < \frac{1}{4J}$, and the cost becomes $2T(\kappa_b) + \frac{1}{4J}$, which is an increasing function of κ_b and hence a decreasing function of $\kappa_a = \kappa - \kappa_b$. Therefore, the minimum value is achieved at κ_a^*. With this observation, we find that when $T(\kappa) \geqslant \frac{1}{4J}$, the optimal (κ_a^*, κ_b^*) to the minimum problem described by Eq. (18) is the solution to the following joint equations:

$$\kappa_a + \kappa_b = \kappa,$$
$$T(\kappa_a) - T(\kappa_b) = \frac{1}{4J},$$

where $T(\kappa) = \frac{\sqrt{\kappa(4-\kappa)}}{2J}$.

Remark 1. We will denote κ_J as the solution to the equation $T(\kappa) = \frac{1}{4J}$, i.e., $T(\kappa_J) = \frac{1}{4J}$.

IV. EFFICIENT SYNTHESIS OF THE TOFFOLI GATE

We now use the results of the previous section to efficiently construct the Toffoli gate. The strategy is to generate

$$\begin{aligned}
&\exp\left[-i\left(2\pi\kappa_1 I_{1z}I_{2z}I_{3z} - \frac{\pi}{2}I_{1z}I_{3z}\right)\right], \\
&\exp\left[-i\left(2\pi\kappa_2 I_{1z}I_{2z}I_{3z} - \frac{\pi}{2}I_{2z}I_{3z}\right)\right],
\end{aligned} \tag{20}$$

separately, where $\kappa_1 + \kappa_2 = \kappa$ (for the Toffoli gate, $\kappa = \frac{1}{2}$) and each term is generated optimally as in the previous section.

Under this strategy, the goal is to find the optimal splitting, $\kappa = \kappa_1 + \kappa_2$, such that

$$G(\kappa) = \min\{S(\kappa_1) + S(\kappa_2)\}, \tag{21}$$

where $S(\kappa)$ is defined in Eq. (18).

A few observations are in order.

Proposition 2. For $T(\kappa) \geqslant \frac{1}{4J}$, the function $S(\kappa)$ is an increasing function of κ.

Note $S(\kappa) = 2T(\kappa_a^*) - \frac{1}{4J}$, where, κ_a^* solves Eq. (19). κ is an increasing function of κ_a^* as T is an increasing function of κ_a^*. Therefore, for $\kappa > \kappa_J$,

$$\frac{dS}{d\kappa} = 2\frac{dT(\kappa_a^*)}{d\kappa_a^*}\frac{d\kappa_a^*}{d\kappa} > 0.$$

Proposition 3. For $\kappa > \kappa_J$, the function $S(\kappa)$ is a concave function of κ.

To show this, we would like to evaluate $\frac{d^2S(\kappa)}{d\kappa^2}$. We express this in terms of the derivative of $T(\kappa_a^*)$ as

$$\frac{d^2S(\kappa)}{d\kappa^2} = -\frac{2}{\left(\frac{d\kappa}{d\kappa_a^*}\right)^2}\left\{\frac{dT(\kappa_a^*)}{d\kappa_a^*}\frac{d^2\kappa_b^*}{d\kappa_a^{*2}} - \frac{d^2T(\kappa_a^*)}{d\kappa_a^{*2}}\frac{d\kappa}{d\kappa_a^*}\right\},$$

$$\frac{d^2S(\kappa)}{d\kappa^2} = -\frac{2}{J\left(\frac{d\kappa}{d\kappa_a^*}\right)^2}\{F(\kappa)\}.$$

The function $F(\kappa)$ is plotted in Fig. 2, which is non-negative, thus $\frac{d^2S(\kappa)}{d\kappa^2}$ is nonpositive, so $S(\kappa)$ is a concave function of κ when $\kappa > \kappa_J$.

Proposition 4. If $\kappa = \kappa_1 + \kappa_2 = \kappa_3 + \kappa_4$ are two divisions such that $T(\kappa_i) \geqslant \frac{1}{4J}$, $k_2 \leqslant k_1$, and $k_4 \leqslant k_3$, then when $k_1 \geqslant k_3$ we will have

$$S(\kappa_1) + S(\kappa_2) \leqslant S(\kappa_3) + S(\kappa_4).$$

The result follows from concavity of $S(\kappa)$ over the range of $\kappa_1, \kappa_2, \kappa_3, \kappa_4$.

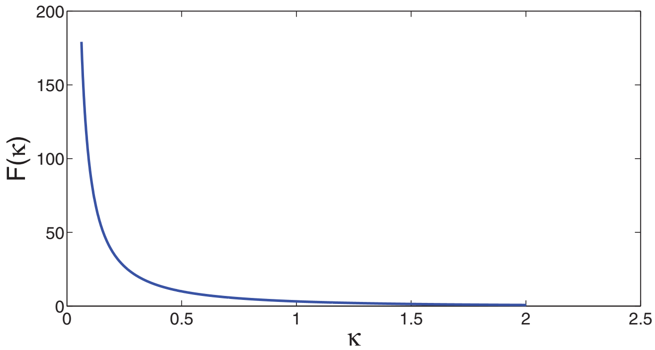

FIG. 2. (Color online) Plot of function $F(\kappa)$ vs κ, demonstrating concavity of $S(\kappa)$.

We are now ready to find the best division of κ in Eq. (21). It can be shown that for $T(\kappa) \geqslant \frac{1}{2J}$, the best division of κ in Eq. (21) is

$$\kappa = (\kappa - \kappa_J) + \kappa_J,$$

and the minimum time is

$$G(\kappa) = S(\kappa - \kappa_J) + \frac{1}{4J},$$

where $T(\kappa_J) = \frac{1}{4J}$.

To see this, consider a splitting of $\kappa = \kappa_1 + \kappa_2$ if $\kappa_2 < \kappa_J$. Then from Sec. III A, we know $S(\kappa_2) = \frac{1}{4J}$, therefore

$$S(\kappa_1) + S(\kappa_2) = S(\kappa - \kappa_2) + \frac{1}{4J} > S(\kappa - \kappa_J) + \frac{1}{4J}.$$

If $S(\kappa_1) > \frac{1}{4J}$ and $S(\kappa_2) > \frac{1}{4J}$, then using concavity of the function $S(\kappa)$, we will have

$$S(\kappa - \kappa_J) + S(\kappa_J) \leqslant S(\kappa_1) + S(\kappa_2).$$

So the best splitting of (κ_1,κ_2) in Eq. (20) to generate the Tofolli gate is $(0.5 - \kappa_J,\kappa_J)$, i.e., the best value of κ_2 in Eq. (20) should satisfy $T(\kappa_2) = \frac{1}{4J}$, that is,

$$\sqrt{\kappa_2(4 - \kappa_2)} = \tfrac{1}{2},$$

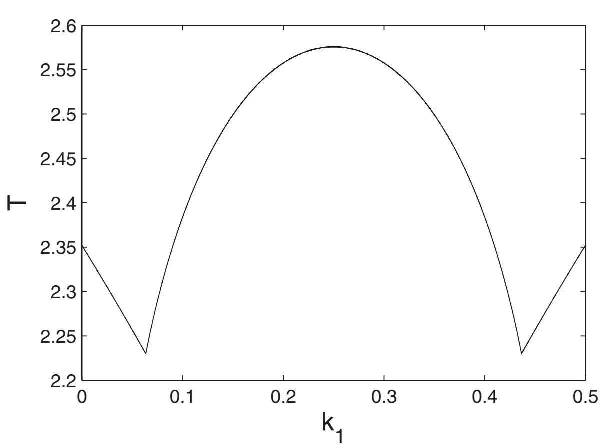

FIG. 3. The time T (in units of $\frac{1}{2J}$), spent to construct the Toffoli gate as a function of κ_1 (in units 2π) as in Eq. (21).

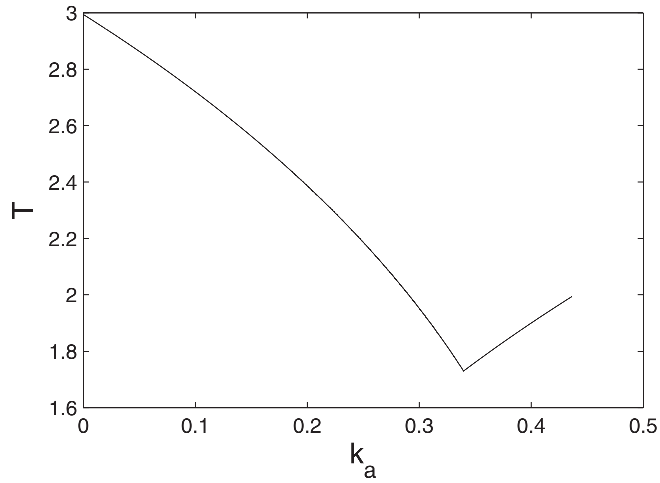

FIG. 4. The time T (in units of $\frac{1}{2J}$), spent to construct the first term in Eq. (20), as a function of κ_a as in Eq. (23).

hence $\kappa_2 = (2 - \frac{\sqrt{15}}{2}) \sim 0.0635$, and $\kappa_1 = 0.5 - \kappa_2 = (\frac{\sqrt{15}}{2} - 1.5) \sim 0.4365$, which again needs to be divided into two parts κ_a, κ_b as in the preceding section, i.e., to solve the following equations:

$$\frac{\sqrt{\kappa_a(4 - \kappa_a)}}{2J} - \frac{\sqrt{\kappa_b(4 - \kappa_b)}}{2J} = \frac{1}{4J}, \quad \kappa_a + \kappa_b = \kappa_1. \quad (22)$$

It is easy to find that the solution is $\kappa_a = 0.339\,607$, $\kappa_b = 0.096\,884\,7$.

Thus the total time to generate the Toffoli gate is

$$\frac{1}{4J} + T(\kappa_a) + T(\kappa_b) = \frac{2.229\,88}{2J},$$

which is 63.71% of the conventional method.

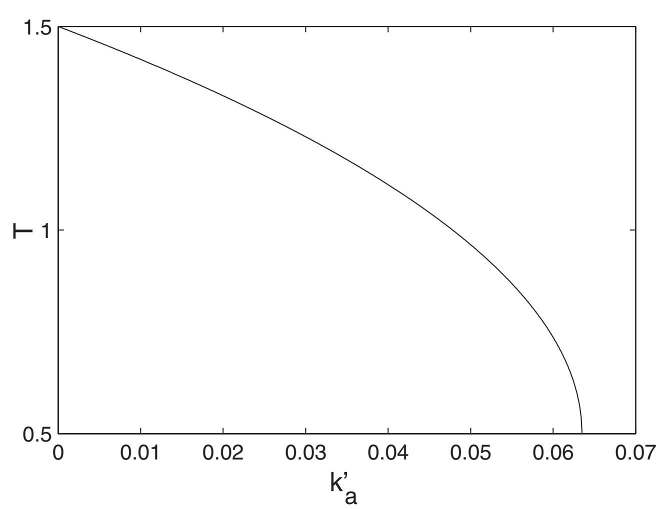

FIG. 5. The time T (in units of $\frac{1}{2J}$), spent to construct the second term in Eq. (20), as a function of κ'_a as in Eq. (24).

V. NUMERICAL RESULTS

We can also numerically search for the best choice of κ_1 and κ_2. For each such subdivision $\kappa_1 + \kappa_2 = 0.5$, we solve the following two optimal problems numerically:

$$\min \frac{\sqrt{\kappa_a(4-\kappa_a)}}{2J} + \frac{\sqrt{\kappa_b(4-\kappa_b)}}{2J} + \left|\frac{1}{4J} - \frac{\sqrt{\kappa_a(4-\kappa_a)}}{2J} + \frac{\sqrt{\kappa_b(4-\kappa_b)}}{2J}\right| \quad \text{such that } \kappa_a + \kappa_b = \kappa_1, \quad \text{and} \tag{23}$$

$$\min \frac{\sqrt{\kappa_a'(4-\kappa_a')}}{2J} + \frac{\sqrt{\kappa_b'(4-\kappa_b')}}{2J} + \left|\frac{1}{4J} - \frac{\sqrt{\kappa_a'(4-\kappa_a')}}{2J} + \frac{\sqrt{\kappa_b'(4-\kappa_b')}}{2J}\right| \quad \text{such that } \kappa_a' + \kappa_b' = 0.5 - \kappa_1. \tag{24}$$

We plot the time as a function of κ_1 as in Fig. 3. There are two minima, and we just work out one of them as the other is totally symmetric:

$$\kappa_1 = 0.4365, \quad \kappa_2 = 0.0635,$$

which agrees with the analytical results.

The corresponding best splitting for κ_1 and κ_2 is $\kappa_a = 0.3396$ and $\kappa_b = 0.0969$, as can be seen in Fig. 4, and $\kappa_a' = 0.0635$ and $\kappa_b' = 0$, as can be seen in Fig. 5, which again agrees with the analytical results. The time to generate the first term is $\frac{1.7299}{2J}$ with the following propagators:

$$\begin{aligned}
&\exp\left[-i\left(0.873\pi I_{1z}I_{2z}I_{3z} - \frac{\pi}{2}I_{1z}I_{3z}\right)\right] \\
&\quad = \exp[-i\pi I_{2y}]\exp[-i\pi I_{3x}]\exp\left(-i\frac{\pi}{2}I_{2y}\right)\exp(-i1.83\pi I_{2x})\exp\{1.115[-i\pi(I_{1z}I_{2z} + I_{2z}I_{3z} + I_{1z}I_{3z}) + i1.489\pi I_{2x}]\} \\
&\qquad \times \exp[i\pi I_{2y}]\exp[i\pi I_{3x}]\ \exp[-i(1.9515\pi)I_{2x}]\exp\{0.615[-i\pi(I_{1z}I_{2z} + I_{2z}I_{3z} + I_{1z}I_{3z}) + i3.09\pi I_{2x}]\}\exp\left(i\frac{\pi}{2}I_{2y}\right),
\end{aligned}$$

and the time to generate the second term is $\frac{0.5}{2J}$ with the following propagators:

$$\begin{aligned}
\exp\left[-i\left(0.127\pi I_{1z}I_{2z}I_{3z} - \frac{\pi}{2}I_{2z}I_{3z}\right)\right] &= \exp[-i\pi I_{1y}]\exp[-i\pi I_{3x}]\exp\left(-i\frac{\pi}{2}I_{1y}\right)\ \exp(-i1.968\pi I_{1x}) \\
&\quad \times \exp\{0.5[-i\pi(I_{1z}I_{2z} + I_{2z}I_{3z} + I_{1z}I_{3z}) + i3.873\pi I_{1x}]\}\exp[i\pi I_{1y}]\exp[i\pi I_{3x}].
\end{aligned}$$

Combining the two, we get the pulse sequences and the total time to generate the Toffoli gate, which is $\frac{2.2299}{2J}$, 63.71% of the conventional method, which again agrees with the analytical result.

VI. CONCLUSION

This paper demonstrated some novel pulse sequences for efficient synthesis of unitary transformations in a three triangle-coupled spin-$\frac{1}{2}$ system. In particular, unitary transformations that map onto Toffoli gates in the context of quantum computing were described, and a significantly better performance compared with state-of-the-art methods was demonstrated. Future work will involve extending to a broader class of unitary transformations, more general multiqubit topologies, and incorporating noise effects.

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