

Elliptic functions and efficient control of Ising spin chains with unequal couplings

Haidong Yuan,^{1,*} Robert Zeier,^{2,†} and Navin Khaneja^{2,‡}

¹*Department of Mechanical Engineering, Massachusetts Institute of Technology,
77 Massachusetts Avenue, Cambridge, Massachusetts 02139, USA*

²*Harvard School of Engineering and Applied Sciences, 33 Oxford Street, Cambridge, Massachusetts 02138, USA*

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In this article, we study optimal control of dynamics of a linear chain of three spin 1/2, weakly coupled with unequal Ising couplings. We address the problem of time-optimal synthesis of multiple spin quantum coherences. We derive time-optimal pulse sequences for creating desired spin order by computing geodesics on a sphere under a special metric. The solution to the geodesic equation is related to the nonlinear oscillator equation and the minimum time to create multiple spin order can be expressed in terms of an elliptic integral. These techniques are used for efficient creation of multiple spin coherences in Ising spin chains with unequal couplings.

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I. INTRODUCTION

In the absence of relaxation, experiments in coherent spectroscopy and quantum information processing consist of a sequence of unitary transformations on the quantum system of interest. Pulse sequences that create a desired unitary transformation in the minimum possible time are of particular interest in experimental realizations as they can reduce losses due to relaxation. This poses the problem of time optimal control of quantum systems, which is of both theoretical and practical interest in the broad area of coherent control of quantum systems.

In addition to the application in spectroscopy, synthesizing unitary transformations in a time-optimal way using available physical resources is also a problem in quantum information processing. It has received significant attention, and time-optimal control of two coupled qubits [1–9] is now well understood. Recently, this problem has also been studied in the context of linearly coupled three-qubit topologies [10–12], where significant savings in the implementation time of trilinear Hamiltonians and logic gates between indirectly coupled qubits were demonstrated over conventional methods. Many of these ideas have found applications in efficient ways to propagate coherences along Ising spin chains [13,14]. However, the complexity of the general problem of time-optimal control of multiple qubit topologies is only beginning to be appreciated.

In this article, we study the problem of finding the shortest pulse sequences for creating desired coherences in a linear chain of spins (of spin 1/2) weakly coupled with unequal Ising couplings. In particular, we start by considering the case of three linearly coupled spins and generalize our methods to linear spin chains. This study has immediate applications to multidimensional nuclear magnetic resonance (NMR) spectroscopy [15]. In multidimensional NMR experiments [15], starting from the thermal state of the spins, a

multiple quantum coherence between spins is synthesized, which helps to correlate the frequencies of various spins. Efficient pulse sequences for creating such coherences help to improve the sensitivity of the experiments.

One approach for solving these problems reduces the efficient synthesis of multiple spin order to the geometrical question of finding shortest paths on the sphere under a special metric [1,8,12,16]. The metric enforces the constraints on the quantum dynamics that arise because only limited Hamiltonians can be realized [17–19]. Such analogies between optimization problems related to steering dynamical systems with constraints and geometry have been well explored in areas of control theory [20,21] and sub-Riemannian geometry [22]. In this paper, we study in detail the metric and the geodesics that arise from the problem of efficient synthesis of multiple spin coherences between qubits (spin 1/2) that are indirectly coupled via unequal couplings to a third qubit. This problem has been addressed in Refs. [1,8,12], under the special case where all couplings between the spins are equal. In this special case, it was shown that the geodesic equations can be explicitly integrated. The constraint of equal couplings limits the range of practical applications. In this paper, we show that for unequal couplings, the solution to the geodesic equations can be analytically characterized in terms of elliptic functions. The general solution with unequal couplings makes many practical applications possible.

II. OPTIMAL CONTROL OF A LINEAR THREE-SPIN SYSTEM WITH UNEQUAL COUPLINGS

We consider a linear chain of three spins placed in a static external magnetic field in the z direction with Ising type couplings between next neighbors [23,24]. In a suitably chosen (multiple) rotating frame which rotates with each spin at its resonant frequency, the Hamiltonian that governs the free evolution of the spin system is given by the coupling Hamiltonian

$$H_c = 2J_{12}I_{1z}I_{2z} + 2J_{23}I_{2z}I_{3z}.$$

*haidong@mit.edu

†zeier@eecs.harvard.edu

‡navin@hrl.harvard.edu

We use the notation $I_{lv} = \otimes_j I_{a_j}$, where $a_j = v$ for $j=l$ and $a_j = 0$ otherwise (see Ref. [15]). The matrices $I_x := (\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix})/2$, $I_y := (\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix})/2$, and $I_z := (\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix})/2$ are the Pauli spin matrices and $I_0 := (\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix})$ is the (2×2) -dimensional identity matrix.

We assume that the Larmor frequencies of the spins are well separated (compared to the strength of couplings between them), such that each spin can be selectively excited. The goal of the pulse designer is to derive explicit control variables comprising the frequency, amplitude, and phase of the external rf field to effect a net unitary evolution $U(t)$ most efficiently.

We begin with the problem of finding the shortest pulse sequence that transforms the initial polarization I_{1z} on the first spin to a multiple quantum coherence, i.e.,

$$I_{1x} \rightarrow 4I_{1z}I_{2z}I_{3z}.$$

Example 1. The conventional strategy for achieving this transfer is given by the following stages:

$$I_{1x} \xrightarrow{(H_c)\tau_1} 2I_{1y}I_{2z} \xrightarrow{I_{2y}} 2I_{1y}I_{2x} \xrightarrow{(H_c)\tau_2} 4I_{1y}I_{2y}I_{3z}.$$

In the first stage of the transfer, the operator I_{1x} evolves to $2I_{1y}I_{2z}$ under the natural coupling Hamiltonian H_c in $\tau_1 = \pi/(2J_{12})$ units of time. This operator is then rotated to $2I_{1y}I_{2x}$ by applying a hard $(\pi/2)_y$ pulse on the second spin, which evolves to $4I_{1y}I_{2y}I_{3z}$ under the natural coupling, in $\tau_2 = \pi/(2J_{13})$ units of time. Finally, hard $(\pi/2)_x$ pulses on the first and second spin prepare the desired final state. The total evolution time is then simply $\tau_1 + \tau_2 = \pi/(2J_{12}) + \pi/(2J_{13})$.

We now study time-optimal designs for achieving this (and more general) transfers. To simplify notation, we introduce the following symbols $\langle O \rangle := \text{Tr}(O\rho)$, where Tr denotes the trace, for the expectation values of operators O . Let $x_1 = \langle I_{1x} \rangle$, $x_2 = \langle 2I_{1y}I_{2z} \rangle$, $x_3 = \langle 2I_{1y}I_{2x} \rangle$, and $x_4 = \langle 4I_{1y}I_{2y}I_{3z} \rangle$ and $X = (x_1, x_2, x_3, x_4)^T$. By expressing the time t , in units of $1/J_{12}$, the evolution of the vector X is given by

$$\frac{dX}{dt} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & -u & 0 \\ 0 & u & 0 & -k \\ 0 & 0 & k & 0 \end{pmatrix} X = B(u, k)X, \quad (1)$$

where $k = J_{23}/J_{12}$ and $u = u(t)$ is the control parameter representing the amplitude of the y pulse on the second spin. Now, the problem of optimal transfer is to find the optimal $u(t)$ for steering the system from $(1, 0, 0, 0)^T$ to $(0, 0, 0, 1)^T$ in minimum time. We consider also the more general case of transferring the system from the vector $(\cos \alpha, \sin \alpha, 0, 0)^T$ to $(0, 0, \cos \beta, \sin \beta)^T$, where we consider different $\alpha, \beta \in [0, \pi/2]$.

Example 1 (continued). In this picture, the conventional method to transfer $(1, 0, 0, 0)^T$ to $(0, 0, 0, 1)^T$ is described by setting $u(t) = 0$ for τ_1 units of time, transferring $(1, 0, 0, 0)^T$ to $(0, 1, 0, 0)^T$. Using the control u , we rotate $(0, 1, 0, 0)^T$ to $(0, 0, 1, 0)^T$ in arbitrary small time, as the control can be performed much faster as compared to the evolution of couplings. Then, we set $u(t) = 0$ and evolve τ_2 units of time under the coupling Hamiltonian, transferring the vector $(0, 0, 1, 0)^T$

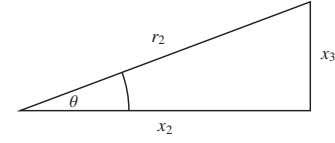


FIG. 1. Auxiliary variables r_2 and θ .

to $(0, 0, 0, 1)^T$. The total time for the transfer is $\tau_1 + \tau_2$.

We now show how significantly shorter transfer times are achievable, if we relax the constraint that the selective rotations on the second spin are only hard pulses. We show that if we let the selective operations be carried out by soft shaped pulses, along with evolution of the coupling Hamiltonian, then we can achieve shorter transfer times. The pulse shapes can be numerically computed by formulating the problem as a derivation of geodesics on a sphere under a special metric as detailed below.

We first make a change of variables (see Fig. 1). Let

$$r_1 = x_1, r_2 = \sqrt{x_2^2 + x_3^2}, r_3 = x_4, \quad \text{and} \quad \tan \theta = \frac{x_3}{x_2}.$$

Using $u(t)$, we can control the angle θ , so we can think of θ as a control variable. Expressing the time in units of $1/J_{12}$, the evolution of the system with respect to the coordinates r_i is given by

$$\frac{d}{dt} \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix} = \begin{pmatrix} 0 & -\cos \theta(t) & 0 \\ \cos \theta(t) & 0 & -k \sin \theta(t) \\ 0 & k \sin \theta(t) & 0 \end{pmatrix} \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix}. \quad (2)$$

The problem of transferring the system in Eq. (1) from $(\cos \alpha, \sin \alpha, 0, 0)^T$ to $(0, 0, \cos \beta, \sin \beta)^T$, reduces to finding $\theta(t)$, for steering the system from $(\cos \alpha, \sin \alpha, 0)^T$ to $(0, \cos \beta, \sin \beta)^T$ in minimum time in Eq. (2). We show that this is equivalent to finding the corresponding geodesic on the sphere, under the metric

$$g = \frac{k^2 dr_1^2 + dr_3^2}{k^2 r_2^2}. \quad (3)$$

By substituting for $\sin \theta(t)$ and $\cos \theta(t)$ from Eq. (2), the transfer time $\tau = \int_0^\tau \sqrt{[\sin \theta(t)]^2 + [\cos \theta(t)]^2} dt$ reduces to

$$\tau = \frac{1}{k} \int_0^\tau \sqrt{[k^2(\dot{r}_1)^2 + (\dot{r}_3)^2]} / r_2^2 dt = \frac{1}{k} \int_0^\tau L dt.$$

Thus, minimizing τ , amounts to computing the geodesic under the metric g . The Euler-Lagrange equations for the geodesic take the form

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{r}_1} \right) = \left(\frac{\partial L}{\partial r_1} \right) \quad \text{and} \quad \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{r}_3} \right) = \left(\frac{\partial L}{\partial r_3} \right).$$

Note, $r_2^2 = 1 - r_1^2 - r_3^2$ and along the geodesic, $L = k$ is constant. We get

$$\frac{d}{dt} \left(\frac{k^2 \dot{r}_1}{r_2^2} \right) = L^2 \frac{r_1}{r_2^2} \quad \text{and} \quad \frac{d}{dt} \left(\frac{\dot{r}_3}{r_2^2} \right) = L^2 \frac{r_3}{r_2^2}, \quad (4)$$

which implies that

$$\frac{d}{dt} \left(\frac{k^2 \dot{r}_1 r_3 - \dot{r}_3 r_1}{r_2^2} \right) = (k^2 - 1) \frac{\dot{r}_1 \dot{r}_3}{r_2^2}. \quad (5)$$

Let $f = (k^2 \dot{r}_1 r_3 - \dot{r}_3 r_1) / r_2^2$. From Eq. (4), we get

$$\frac{d}{dt} \left(\frac{k^2 \dot{r}_1}{r_2} \right) = -f \frac{\dot{r}_3}{r_2}.$$

Substitute with $\dot{r}_1 / r_2 = -\cos \theta(t)$ and $\dot{r}_3 / r_2 = k \sin \theta(t)$, and get

$$\frac{d}{dt} [-k^2 \cos \theta(t)] = -fk \sin \theta(t),$$

so $\dot{\theta} = -f/k$. Differentiating again, we obtain from Eq. (5), that

$$\ddot{\theta} = -\frac{1}{k} \frac{d}{dt} f = -\frac{k^2 - 1}{k} \frac{\dot{r}_1 \dot{r}_3}{r_2^2} = (k^2 - 1) \cos \theta \sin \theta.$$

Using $a = k^2 - 1$, we rewrite this as

$$\ddot{\theta} = \frac{a}{2} \sin 2\theta(t). \quad (6)$$

The solution to Eq. (6), can be given in terms of an elliptic integral. Note that by multiplying both sides of Eq. (6), with $\dot{\theta}$, we get the equation of an ellipse in terms of the coordinates $\dot{\theta}(0)$, and $\cos[\theta(0)]$ as

$$c = \dot{\theta}^2(t) + a \cos^2 \theta(t), \quad (7)$$

where c is a constant. Thus, we obtain, $\dot{\theta} = \pm \sqrt{c - a \cos^2 \theta(t)}$ and

$$\int_{\theta(0)}^{\theta(t)} \frac{d\sigma}{\sqrt{c - a \cos^2 \sigma}} = \pm t. \quad (8)$$

The left-hand side of Eq. (8) is an elliptic integral [25,26]. Equation (6), can be integrated if $\theta(0)$ and $\dot{\theta}(0)$ are both known explicitly. In transfers considered subsequently, only $\theta(0)$ is known and therefore one has to numerically search over the possible values of $\dot{\theta}(0)$, such that the resulting trajectory $X(t)$ achieves the desired transfer. Note, guessing an initial value of $\dot{\theta}(0)$ is the same as searching for the correct value of c in Eq. (7).

III. COMPUTATION OF OPTIMAL CONTROL LAWS

Now, consider the problem of steering the system of Eq. (2), from the initial state $(r_1, r_2, r_3)^T = (1, 0, 0)^T$ to the target state $(0, \cos \beta, \sin \beta)^T$. For $\beta = \pi/2$, we get the target state $(0, 0, 1)^T$. Recall that

$$-k \dot{\theta} = f = -k^2 \frac{r_3}{r_2} \cos \theta - k \frac{r_1}{r_2} \sin \theta. \quad (9)$$

At $t=0$, $r_1(0)=1$ and $r_2(0)=r_3(0)=0$. Therefore, in Eq. (9), at $t=0$, the term $\frac{r_1}{r_2} \sin \theta$ is infinite, unless we have $\sin \theta(0)=0$. This implies that in Eq. (6), the initial condition is $\theta(0)=0$. To solve Eq. (6), we only need to know the initial value of

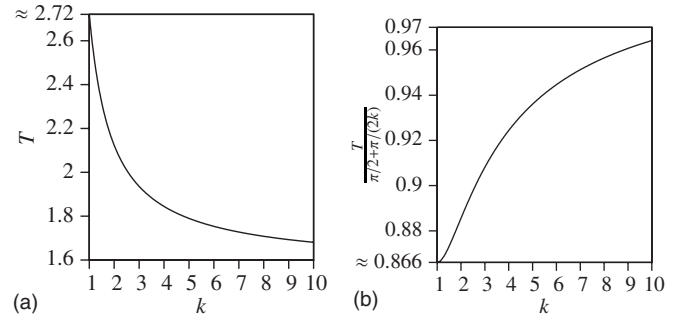


FIG. 2. For different k , we plot (a) the minimum time T in units of $1/J_{12}$ and (b) the corresponding ratio $T/[\pi/2 + \pi/(2k)]$.

$\dot{\theta}(0)$, which is the same as knowing the constant c in Eq. (7). Given $\theta(0)=0$ and the value of $\dot{\theta}(0)$, we can numerically solve first Eq. (6) and then Eq. (2). Consequently, we can determine for each value of $\dot{\theta}(0)$, the smallest time s such that $r_1(s)=0$ by using a one-dimensional search, e.g., using the bisection method (see pp. 46–51 of Ref. [27]). Thus, we can determine the value of $\dot{\theta}(0)$ such that $r_2(s)=\cos(\beta)$, again by using a one-dimensional search. In summary, we have reduced the original optimization problem to (combined) one-dimensional search problems.

For different values of k , we plot the minimum time $T = T(k)$ to transfer $(r_1, r_2, r_3)^T = (1, 0, 0)^T$ to $(0, 0, 1)^T$ in Fig. 2(a) in units of $1/J_{12}$. For example, when $k=1$, i.e., $J_{12} = J_{23} = J$, it takes $2.72/J$ amount of time, which is about 86.6% of π/J , the time needed using the conventional method. Figure 2(b), shows the ratio of the minimum time $T(k)$ to the time $\pi/2 + \pi/(2k)$ obtained using the conventional strategy. We define this ratio $\eta(k)$. In both the plots $k \geq 1$ is considered, as the case for $k < 1$ can be derived from this. Figure 3, shows the optimal control $u(t)$ in Eq. (1) for different values of k .

Observe that $T(1/k) = kT(k)$. Let $u(t, k)$ be the time optimal control for steering the system of Eq. (1) from

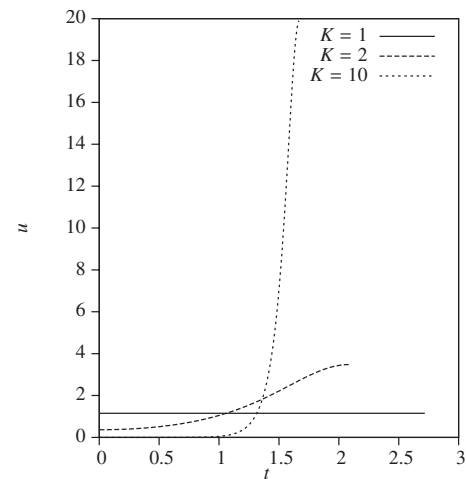


FIG. 3. The figure shows the shape of the optimal control $u(t)$ in Eq. (1) for $k=1, 2, 10$. The time is in units of $\frac{1}{J_{12}}$. The control amplitude is in units of J_{12} .

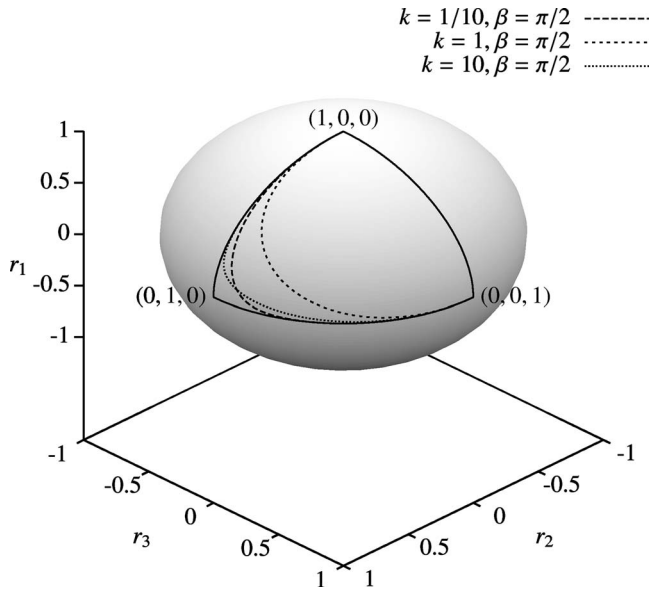


FIG. 4. Geodesics to transfer from $(r_1, r_2, r_3)^T = (1, 0, 0)^T$ to $(0, 0, 1)^T$, where $k = 1/10$, $k = 1$, and $k = 10$.

$(1, 0, 0, 0)^T$ to $(0, 0, 0, 1)^T$. Then the control $v(t) = u(T-t, k)$ will steer the same system from $(0, 0, 0, 1)^T$ to $(1, 0, 0, 0)^T$ using the same time, which is also minimum for this transfer. Let $Y = (x_4, x_3, x_2, x_1)^T$ and consider the control $v(t) = u(T-t, k)$. Then, we have

$$\frac{dY}{d\tau} = kB(1/k, v)Y.$$

However, we have just remarked that the minimum time to steer Y from $(1, 0, 0, 0)^T$ to $(0, 0, 0, 1)^T$ is $T(k)$, and it follows that $T(1/k)/k = T(k)$. It also follows that the optimal control is given by $u(t, 1/k) = u[T(k) - t/k, k]$, where $t \in [0, kT(k)]$. Note that $\eta(k) = \eta(1/k)$.

Remark 1. In Fig. 4, we present the geodesics of the metric of Eq. (3) for $\beta = \pi/2$ and $k \in \{1/10, 1, 10\}$, where $\beta = \tan^{-1}[r_3(T)/r_2(T)]$, i.e., $r_1(T) = r_2(T) = 0$ and $r_3(T) = 1$. Observe that the geodesics for the case $k > 1$, bend more towards the point $(r_1, r_2, r_3) = (0, 1, 0)$, before approaching the final point $(0, 0, 1)$. An intuitive way to understand this is to first consider the limit $k \gg 1$. In this limit, the minimum time to steer the system (2) from $(1, 0, 0)$ to $(0, 0, 1)$ is essentially the time required to steer the system (2) to the equator. This is achieved fastest by moving from $(1, 0, 0)$, directly to $(0, 1, 0)$ and keeping $\theta(0) = 0$. As k is decreased to 1, the geodesics gradually move away from $(0, 1, 0)$, implying that $\dot{\theta}(0)$ is smaller for $k > 1$ as compared to the case of $k = 1$. In the special case of $k = 1$, Eq. (6) reduces to $\dot{\theta} = C$, a constant. This case was been studied in detail in Refs. [12, 14]. Therefore, in the numerical computation of the optimal control, the search for true $\dot{\theta}(0)$ can be restricted to $[0, C]$.

In Fig. 5, we plot the minimum time $T = T(k, \beta)$ to transfer $(r_1, r_2, r_3)^T = (1, 0, 0)^T$ to $(0, \cos \beta, \sin \beta)^T$, for different values of k and $\beta = \tan^{-1}[r_3(T)/r_2(T)]$. Figure 6 shows the geo-

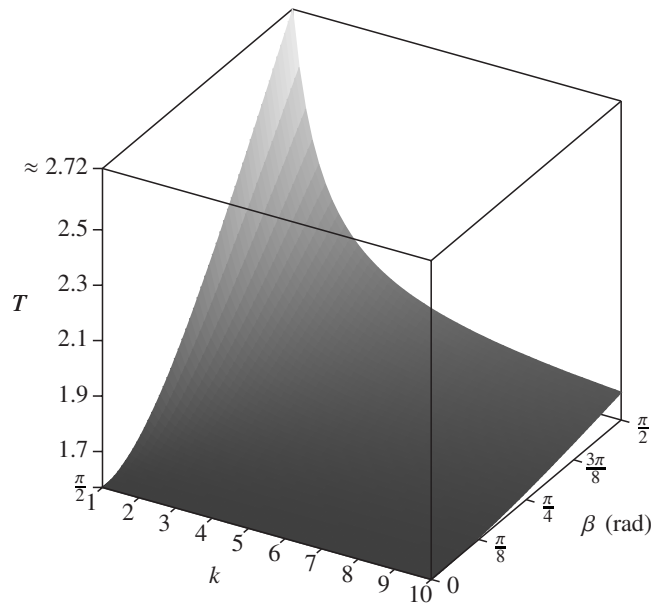


FIG. 5. For different k and $\beta = \tan^{-1}[r_3(T)/r_2(T)]$, we plot the minimum time T in units of $1/J_{12}$.

desics of the metric of Eq. (3) for $k = 2$, for two different values of $\beta \in \{\pi/4, \pi/2\}$ specifying the terminal point $(0, \cos \beta, \sin \beta)^T$.

If we transfer the system from $(x_1, x_2, x_3, x_4)^T = (\cos \alpha, \sin \alpha, 0, 0)^T$ to $(0, 0, \cos \beta, \sin \beta)^T$, where $\alpha > 0$, we do not know the value of $\theta(0)$. However, from Eq. (9), we have the relationship $\dot{\theta}(0) = \sin[\theta(0)] \cot(\alpha)$ between $\dot{\theta}(0)$ and $\theta(0)$. Thus, we can apply similar search methods for the right initial conditions as in the case of $\alpha = 0$. For $k = 2$ and different values of α and β , we plot in Fig. 7 the minimum time $T = T(\alpha, \beta)$ to transfer $(r_1, r_2, r_3)^T = (\cos \alpha, \sin \alpha, 0)^T$ to $(0, \cos \beta, \sin \beta)^T$.

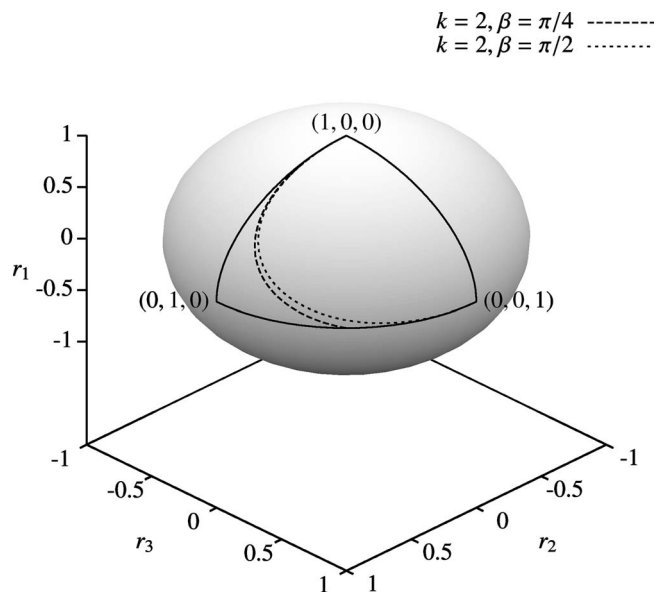


FIG. 6. Geodesics to transfer from $(r_1, r_2, r_3)^T = (1, 0, 0)^T$ to $(0, \cos \beta, \sin \beta)^T$, where $k = 2$ and $\beta \in \{\pi/4, \pi/2\}$.

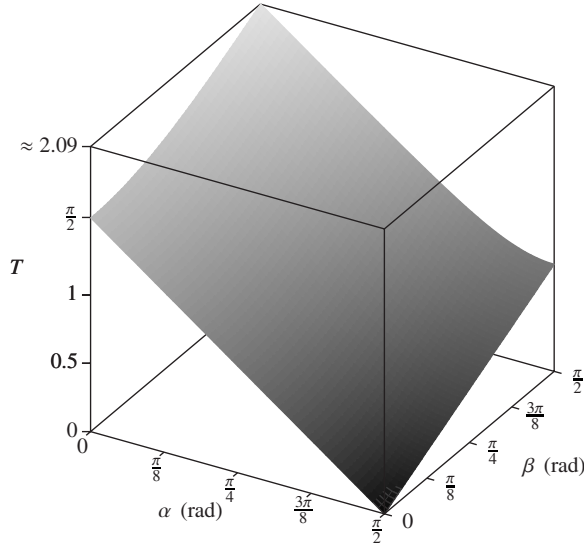


FIG. 7. For $k=2$ and different values of α and β , we plot the minimum time T in units of $1/J_{12}$.

IV. EFFICIENT CREATION OF COHERENCES IN ISING SPIN CHAINS WITH UNEQUAL COUPLINGS

We now consider a generalization of the problem treated above. We consider a linear chain of n spins, placed in a static external magnetic field in the z direction, with unequal Ising type couplings between next neighbors [23,24]. In a suitably chosen (multiple) rotating frame, which rotates with each spin at its resonant frequency, the free evolution of the spin system is given by the coupling Hamiltonian

$$H_c = 2 \sum_{l=1}^{n-1} J_{l,l+1} I_{lz} I_{(l+1)z}.$$

As before, we assume that the Larmor frequency of the spins are well separated compared to the coupling constant $J_{l,l+1}$, so that we can selectively rotate each spin at a rate much faster than the evolution of the couplings.

We first consider the problem of synthesizing a unitary U , which efficiently transfers a single spin coherence represented by the initial operator I_{1x} to a multiple spin order represented by the operator $2^{n-1} \prod_{l=1}^n I_{lz}$.

The conventional strategy for achieving this transfer is achieved through the following stages:

$$\begin{aligned} & I_{1x} \xrightarrow{H_c} 2I_{1y}I_{2z} \xrightarrow{I_{2y}} 2I_{1y}I_{2x} \xrightarrow{H_c} 4I_{1y}I_{2y}I_{3z} \\ & \xrightarrow{I_{3y}} 4I_{1y}I_{2y}I_{3x} \rightarrow \dots \rightarrow 2^{n-1} \left(\prod_{l=1}^{n-1} I_{ly} \right) I_{nz}, \end{aligned}$$

where each evolution represents an appropriate evolution by rotation angle $\pi/2$. The final state $2^{n-1} (\prod_{l=1}^{n-1} I_{ly}) I_{nz}$, is locally equivalent to $2^{n-1} \prod_{l=1}^n I_{lz}$. The whole transfer involves $n-1$ evolution steps under the natural Hamiltonian, where step 1 takes only $\pi/(2J_{l,l+1})$ units of time, resulting in a total time of $\sum_{l=1}^{n-1} \pi/(2J_{l,l+1})$. We now formulate the problem of this

transfer as a problem of optimal control and derive time efficient strategies for achieving this transfer.

To simplify notation, we introduce the following symbols for the expectation values of operators that play a key part in the transfer:

$$\begin{aligned} x_1 &= \langle I_{1x} \rangle, & x_2 &= \langle 2I_{1y}I_{2z} \rangle, \\ x_3 &= \langle 2I_{1y}I_{2x} \rangle, & x_4 &= \langle 4I_{1y}I_{2y}I_{3z} \rangle, \dots, \\ x_{2n-3} &= \langle 2^{n-1} I_{1y}I_{2y}I_{3y} \dots I_{(n-1)x} \rangle, \\ \text{and } x_{2n-2} &= \langle 2^n I_{1y}I_{2y}I_{3y} \dots I_{(n-1)y}I_{nz} \rangle. \end{aligned}$$

Let $X = (x_1, x_2, x_3, \dots, x_{2n-2})^T$. Expressing the time in units of $1/J_{12}$, the evolution of the system is given by

$$\frac{dX}{dt} = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 & \dots \\ 1 & 0 & -u_1 & 0 & 0 & 0 & \dots \\ 0 & u_1 & 0 & -k_3 & 0 & 0 & \dots \\ 0 & 0 & k_3 & 0 & -u_2 & 0 & \dots \\ 0 & 0 & 0 & u_2 & 0 & -k_5 & \dots \\ 0 & 0 & 0 & 0 & k_5 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} X, \quad (10)$$

where u_l are the control parameters representing the amplitude of the y pulse on spin $l+1$ and $k_l = J_{l,l+1}/J_{12}$. The problem now is to find the optimal $u_l(t)$, steering the system from $(1, 0, 0, \dots, 0)^T$ to $(0, 0, \dots, 0, 1)^T$ in the minimum time.

We divide the optimal transfer problem into multiple steps. Consider the step that steers $(x_{l-1}, x_l, x_{l+1}, x_{l+2})^T$ from the initial state $(\cos \beta_l, \sin \beta_l, 0, 0)^T$ to the target state $(0, 0, \cos \beta_{l+1}, \sin \beta_{l+1})^T$, by optimal choice of u_l :

$$\frac{d}{dt} \begin{pmatrix} x_{l-1} \\ x_l \\ x_{l+1} \\ x_{l+2} \end{pmatrix} = \begin{pmatrix} 0 & -k_l & 0 & 0 \\ k_l & 0 & -u_l & 0 \\ 0 & u_l & 0 & -k_{l+1} \\ 0 & 0 & k_{l+1} & 0 \end{pmatrix} \begin{pmatrix} x_{l-1} \\ x_l \\ x_{l+1} \\ x_{l+2} \end{pmatrix}. \quad (11)$$

We denote the minimum time for this transfer as $T(\beta_l, \beta_{l+1}, k_l, k_{l+1})$, as it depends on the parameters $(\beta_l, \beta_{l+1}, k_l, k_{l+1})$. Note that

$$k_l T(\beta_l, \beta_{l+1}, k_l, k_{l+1}) = T(\beta_l, \beta_{l+1}, 1, k_{l+1}/k_l).$$

We can then break the original transfer in Eq. (10), into subtransfers denoted by

$$\beta_1 \rightarrow \beta_2 \dots \rightarrow \beta_l \dots \rightarrow \beta_{n-1},$$

where both $\beta_1=0$ and $\beta_{n-1}=\pi/2$. The control u_l in Eq. (11) should be so chosen that the time to transfer β_l to β_{l+1} is minimized. Furthermore, the choice of intermediate β_l should be made to minimize the total time of transfer

$$J_1(0) = \sum_{l=1}^{n-2} T(\beta_l, \beta_{l+1}, k_l, k_{l+1}).$$

The notation for $J_1(0)$ denotes that the index l in the above summation begins with $l=1$ with initial angle $\beta_1=0$.

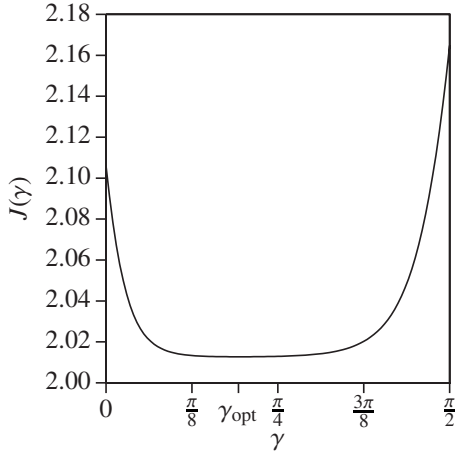


FIG. 8. The figure shows the plot of function $J(\gamma)$ in Eq. (13), as a function of γ .

Now suppose we have computed $J_{l+1}(\xi)$ for all $\xi \in [0, \pi/2]$. Then we can compute $J_l(\beta_l)$ from the equation below as

$$J_l(\beta_l) = \min_{\eta} \{J_{l+1}(\eta) + T(\beta_l, \eta, k_l, k_{l+1})\}. \quad (12)$$

We can solve Eq. (12) iteratively starting from $l=n-2$ and proceeding backwards and remembering that

$$J_{n-2}(\beta_{n-2}) = T(\beta_{n-2}, \pi/2, k_{n-2}, k_{n-1}).$$

Note that $T(\beta_l, \eta, k_l, k_{l+1})$ in Eq. (12) can be explicitly computed, as we showed in the previous section. Therefore Eq. (12) helps us to compute the optimal η and the corresponding optimal control u_l . Now, the problem is reduced to a simple dynamic programming problem, which can be solved efficiently.

Example 2. We consider as an example, an Ising spin chain with four spins with $\frac{J_{12}}{2\pi} = 91$ Hz, $\frac{J_{23}}{2\pi} = 15$ Hz, and $\frac{J_{34}}{2\pi} = 55$ Hz. This system represents the popular [28] HNCACO experiment in multidimensional NMR, where spin 1 is the proton, 2 represent ^{15}N , 3 and 4 are ^{13}C . For the transfer in Eq. (10), the dynamic programming equations for the minimum time in the units of $\frac{1}{J_{23}}$, can be written as $\min_{\gamma} J(\gamma)$, where

$$J(\gamma) = \left\{ T(0, \gamma, k_1, 1) + T\left(\gamma, \frac{\pi}{2}, 1, k_2\right) \right\}, \quad (13)$$

where $k_1 = \frac{J_{12}}{J_{23}}$ and $k_2 = \frac{J_{34}}{J_{23}}$. The value γ represents the intermediate angle, such that the transfer from the initial state $(x_1, x_2, x_3, x_4, x_5, x_6) = (1, 0, 0, 0, 0, 0)$ to the target state $(0, 0, 0, 0, 0, 1)$ is carried out through the intermediate state $[0, 0, \cos(\gamma), \sin(\gamma), 0, 0]$ as described before. The symbols x_i are as defined in Sec. IV. Figure 8 shows the plot of $J(\gamma)$. The minimum is achieved at $\gamma \approx 0.192\pi$ and the corresponding minimum value of $J(\gamma)$ is approximately 2.01. The conventional transfer strategy will take $(1 + 1/k_1 + 1/k_2) \frac{\pi}{2}$

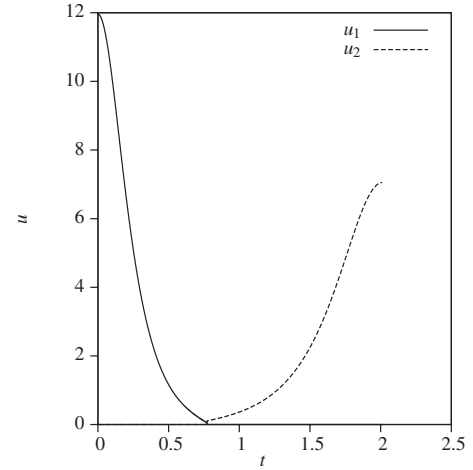


FIG. 9. The figure shows the shape of the optimal control $u_1(t)$ and $u_2(t)$ for example 2, where $n=6$ in Eq. (10). The time is given in units of $\frac{1}{J_{12}}$. The control amplitude is given in units of J_{12} .

≈ 2.26 , units of time, which is approximately 12.2% longer than the proposed efficient methodology. Figure 9 shows the corresponding control.

Remark 2. Note, in computing the time for conventional transfers we have assumed rf pulses to be delta pulses. This is a very good approximation as couplings between the spins are 2–3 orders of magnitude smaller than the strength of the rf field and therefore determine the time of transfer. Our analysis in this paper has been limited to a chain of heteronuclear spins. A problem of both theoretical and practical interest is to carry out the above analysis for a chain of coupled homonuclear spins, where selective excitation of individual spins may take significantly longer time. We plan to address this problem in our future work.

V. CONCLUSION

In this article, we studied the problem of efficient creation of multiple spin order in an Ising spin chain with unequal couplings. We first analyzed in detail the system of three linearly coupled spins. We showed that the time optimal pulse sequences for creating multiple spin order in this system can be obtained by computing geodesics on a sphere under a special metric and that the solution to the resulting Euler-Lagrange equation is related to the solution of a nonlinear oscillator equation $\ddot{\theta} = A \sin \theta$. We showed that the minimum times and optimal control laws for the studied problem can be explicitly computed and provide significant gains over conventional methods. The methods developed in the three spin case were then exploited to find efficient strategies for manipulating the dynamics of Ising spin chains with unequal couplings. It is expected that these methods will find immediate applications in coherent spectroscopy and quantum information processing.

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