Optimal generation of single-qubit operation from an always-on interaction by algebraic decoupling

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We present a direct algebraic decoupling approach to generate arbitrary single-qubit operations in the presence of a constant interaction by application of local control signals. To overcome the difficulty of undesirable entanglement generated by the untunable interaction, we use an algebraic approach to decouple the two-qubit Hamiltonian into two single-qubit Hamiltonians and the desired single-qubit operations are then generated by steering on the single-qubit operation spaces. Specifically, we derive local control fields that are designed to drive the qubit systems back to unentangled states at the end of the time interval over which the desired single-qubit operation is completed. As a result of the decoupling, optimal control strategies may be carried out on single qubit subspaces rather than on the full coupled qubit Hilbert space. This approach is seen to be particularly relevant for the physical implementation of solid-state quantum computation.

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Most schemes for implementation of quantum computation require achieving both single- and two-qubit operations in order to realize the speedup associated with quantum algorithms [1]. Typically, single-qubit operations are implemented by external local control fields applied to individual qubits, whereas two-qubit operations are generated by interplay of the couplings between qubits and local fields [2]. To simplify engineering design and reduce decoherence channels, many physical proposals of quantum computation have "always-on" and fixed couplings between qubits. This is often the case in arrays of solid-state qubits, which constitute a very attractive research direction because of the inherent scalability of the required microfabrication techniques. For example, in superconducting systems the interaction between qubits is often coupled by a capacitor or inductor, whose value is fixed by the fabrication and generally cannot be tuned during the computations [3,4]. Several variable coupling schemes have been suggested [5–9], but it is generally agreed that none of these is completely satisfactory. In contrast, proposals for using electron spins in quantum dots do in principle allow for electrical gating of the exchange interaction between dots [10,11], but engineering such control in practice still remains extremely challenging [12]. Other spin-coupled implementations of current interest include endohedral fullerenes for which nontunable magnetic dipole coupling between electron spins of neighboring endohedral species provide the required qubit coupling [13,14].

Coupling between qubits is essential for the implementation of two-qubit operations. An always-on and untunable coupling leads to additional complications in implementation of single-qubit operations. However, because the qubits may become entangled as a result of the coupling, causing errors in the target state, it is desirable to eliminate the effect of this coupling during single-qubit operations. This general issue of suppressing an always-on interaction is also encountered in nuclear magnetic resonance, where the nuclear spins are coupled by dipolar interactions and broaden the spectral resonances. A great deal of work has focused on decoupling of spins in NMR in order to achieve high-resolution spectra [15–19]. The use of refocusing pulse sequences designed to cancel out the effects of interactions in successive time intervals and to generate precise quantum evolutions has been extensively explored in NMR implementations of quantum information processing [20–24]. This approach includes numerical solutions based on extensive search methods that allow for short and strong pulses to minimize decoherence [21], as well as optimization in the limit of zero time local control pulses [24]. However, for low-power pulses such as are often used in homonuclear spin systems, the radio frequency signals can be of the same order of magnitude as the coupling strengths [22,25]. In such a "soft" pulse situation, single-qubit rotations cannot be assumed to be implemented instantaneously as is often the case with hard pulses, and consequently the interactions may strongly affect the intended operations. This situation arises in many prototypical coupled qubit systems in the solid state. An additional factor here is the requirement of low temperature operation which means that refocusing pulses should be as low power as possible in order to minimize heating [26,27].

While numerical construction of refocusing pulse sequences is always an option, several systematic attempts to overcome this problem more generally have been also been made in recent years in the context of quantum information processing. Reference [28] proposed to employ an encoding of logical qubits and to perform logic operations using an analog of the NMR selective recoupling method. Reference [29] presented another encoding scheme to realize universal quantum computation on carefully designed interaction free subspaces. Recently, Ref. [30] showed that one can also avoid this undesirable entanglement by tuning the transition energies of individual qubits. More complex schemes involving auxiliary degrees of freedom have also been proposed [13,14]. In this paper we present a direct approach for the design of local control signals enacting single-qubit operations in the presence of an always-on interaction, that is based on an exact algebraic decoupling of the two-qubit

Hamiltonian. To eliminate the accompanying entanglement generated by this untunable interaction, we derive local control fields that drive the qubit systems back to unentangled states at the end of the time interval over which the desired single-qubit operation is completed. The algebraic approach provides a significant improvement over proposals involving encoding of qubits, since it avoids the additional overheads and potential for decoherence incurred by encoding and decoding. The approach also has the benefit of leading naturally to optimization strategies that involve steering only on single-qubit Hilbert spaces, SU(2), rather than on higher dimensional spaces. It thereby presents an attractive route for implementation of optimal control of the single qubit operations. We derive an approximation solution to the control problem that can be readily optimized to arbitrary numerical accuracy of gate fidelity, and compare this with exact results obtained from minimal time and minimal energy control strategies based on Pontryagin's maximal principle. For the example of single-qubit operations on two identical spins that is studied here, we find that the fidelity optimal solution is very close to the minimum-energy solution. This is encouraging for applications to solid-state implementations where low temperatures and minimal-energy costs are essential [26,27].

We consider a two-qubit system with the following Hamiltonian:

$$H = \frac{\omega_1}{2}(\cos\phi_1\sigma_x^1 + \sin\phi_1\sigma_y^1) + \frac{\omega_2}{2}(\cos\phi_2\sigma_x^2 + \sin\phi_2\sigma_y^2) + \frac{J}{2}\sigma_z^1\sigma_z^2, \tag{1}$$

where σ_x, σ_y, and σ_z are the Pauli matrices, J the always-on and untunable coupling strength, ω_j and ϕ_j the amplitude and phase of the external control fields, respectively. This Hamiltonian describes a wide range of two-qubit systems, e.g., solid-state quantum computation with superconducting circuits as proposed in Ref. [6], as well as NMR double-resonance J cross polarization with two rf fields in the XY plane of the doubly rotating frame [31]. Note that the Hamiltonian in Eq. (1) can be transformed by local unitary operations into a Hamiltonian with YY coupling and σ_x, σ_z local terms, or into one with XX coupling and σ_y, σ_z local terms. Therefore the results in this paper are also applicable to these two types of Hamiltonians. The spin coupling J in Eq. (1) can be neglected only for short and high-power pulses, since for low-power pulses $\omega_1$and ω_2 can be of the same order as J. We will show below how to design amplitude-modulated pulses that can generate an arbitrary single-qubit operation for such a system in an optimal fashion. We first show that the desired quantum operation can be generated directly from the two-qubit Hamiltonian, Eq. (1), by algebraically decoupling this into two unentangled single-qubit Hamiltonians. The problem then reduces to generation of two local unitaries which can further be readily implemented using optimal control methods, either to minimize an imposed cost function (e.g., minimal time or energy) or to maximize the fidelity of the desired quantum operation.

An arbitrary local unitary operation k_1 on two qubits, the target operation here, can be written using Euler's XYX decomposition as

$$k_1 = (e^{-i\alpha_1\sigma_x/2} \otimes e^{-i\alpha_2\sigma_x/2})(e^{-i\beta_1\sigma_y/2} \otimes e^{-i\beta_2\sigma_y/2}) \times (e^{-i\gamma_1\sigma_x/2} \otimes e^{-i\gamma_2\sigma_x/2}), \tag{2}$$

where α_j, β_j, and γ_j are the Euler angles. In order to generate k_1, we need to generate arbitrary σ_x and σ_y rotations on each qubit. However, we can simplify this problem to the generation of only σ_x rotations $k_2 = e^{-i\gamma_1\sigma_x/2} \otimes e^{-i\gamma_2\sigma_x/2}$ from the following Hamiltonian:

$$H_1 = \frac{\omega_1}{2}\sigma_x^1 + \frac{\omega_2}{2}\sigma_x^2 + \frac{J}{2}\sigma_z^1\sigma_z^2, \tag{3}$$

where H_1 is obtained from Eq. (1) by setting the phases $\phi_1 = \phi_2 = 0$ for external control pulses. This leads immediately to the implementations of the first and third operations in Eq. (2). For the second operation in Eq. (2), we can set $\phi_1 = \phi_2 = \pi/2$ in Eq. (1) to obtain a Hamiltonian

$$H_2 = \frac{\omega_1}{2}\sigma_y^1 + \frac{\omega_2}{2}\sigma_y^2 + \frac{J}{2}\sigma_z^1\sigma_z^2 = V^\dagger H_1 V, \tag{4}$$

where $V = e^{i\pi/2\sigma_z/2} \otimes e^{i\pi/2\sigma_z/2}$. Now if H_1 generates a quantum operation $e^{-i\beta_1\sigma_x/2} \otimes e^{-i\beta_2\sigma_x/2}$, H_2 will generate the second operation in Eq. (2), since

$$e^{-i\beta_1\sigma_y/2} \otimes e^{-i\beta_2\sigma_y/2} = V^\dagger(e^{-i\beta_1\sigma_x/2} \otimes e^{-i\beta_2\sigma_x/2})V.$$

Our task has therefore been simplified to the generation of an arbitrary local unitary operation $e^{-i\gamma_1\sigma_x/2} \otimes e^{-i\gamma_2\sigma_x/2}$ from the Hamiltonian H_1 in Eq. (3). We now observe that the terms $i\sigma_x^1/2$, $i\sigma_x^2/2$, and $i\sigma_z^1\sigma_z^2/2$ appearing in H_1 generate the following Lie algebra:

$$\mathfrak{k}_1 = \frac{i}{2}\{\sigma_x^1, \sigma_x^2, \sigma_z^1\sigma_y^2, \sigma_y^1\sigma_z^2, \sigma_y^1\sigma_y^2, \sigma_z^1\sigma_z^2\}. \tag{5}$$

It is straightforward to show that $\mathfrak{k}_1$ satisfies the same commutation relations as so(4), where so(4) denotes the Lie algebra formed by all the 4×4 real skew symmetric matrices. Therefore $\mathfrak{k}_1$ is isomorphic to so(4). We also know that so(4) is isomorphic to $\mathrm{su}(2)\otimes\mathrm{su}(2)$ [32]. To realize this fact, let

$$\epsilon_x^1 = \frac{\sigma_x^1 - \sigma_x^2}{4}, \quad \epsilon_y^1 = \frac{\sigma_y^1\sigma_y^2 + \sigma_z^1\sigma_z^2}{4}, \quad \epsilon_z^1 = \frac{\sigma_z^1\sigma_y^2 - \sigma_y^1\sigma_z^2}{4},$$

$$\epsilon_x^2 = \frac{\sigma_x^1 + \sigma_x^2}{4}, \quad \epsilon_y^2 = \frac{\sigma_y^1\sigma_y^2 - \sigma_z^1\sigma_z^2}{4}, \quad \epsilon_z^2 = \frac{\sigma_z^1\sigma_y^2 + \sigma_y^1\sigma_z^2}{4}, \tag{6}$$

and use $\mathfrak{k}_2$ to denote the Lie algebra generated by $\{i\epsilon_x^1, i\epsilon_y^1, i\epsilon_z^1, i\epsilon_x^2, i\epsilon_y^2, i\epsilon_z^2\}$. We have the following commutation relations for $\mathfrak{k}_2$:

$[\cdot,\cdot]$	$i\epsilon_x^1$	$i\epsilon_y^1$	$i\epsilon_z^1$	$i\epsilon_x^2$	$i\epsilon_y^2$	$i\epsilon_z^2$
$i\epsilon_x^1$	0	$-i\epsilon_z^1$	$i\epsilon_y^1$	0	0	0
$i\epsilon_y^1$	$i\epsilon_z^1$	0	$-i\epsilon_x^1$	0	0	0
$i\epsilon_z^1$	$-i\epsilon_y^1$	$i\epsilon_x^1$	0	0	0	0
$i\epsilon_x^2$	0	0	0	0	$-i\epsilon_z^2$	$i\epsilon_y^2$
$i\epsilon_y^2$	0	0	0	$i\epsilon_z^2$	0	$-i\epsilon_x^2$
$i\epsilon_z^2$	0	0	0	$-i\epsilon_y^2$	$i\epsilon_x^2$	0.

It is clear that the Lie algebra $\mathfrak{k}_2$ satisfies the same commutation relations as $i/2\{\sigma_x^1, \sigma_y^1, \sigma_z^1, \sigma_x^2, \sigma_y^2, \sigma_z^2\}$, and therefore it is isomorphic to $\mathrm{su}(2)\otimes\mathrm{su}(2)$. This isomorphism allows great simplification for the generation of single-qubit operation from Hamiltonian (3), because it provides an algebraic way to decouple the entangling Hamiltonian into two unentangled single-qubit Hamiltonians. To our knowledge, this fact has not been recognized, although a transformation similar to Eq. (6) was presented in Ref. [31].

We can now rewrite H_1 as

$$H_1 = (\omega_1 - \omega_2)\epsilon_x^1 + J\epsilon_y^1 + (\omega_1 + \omega_2)\epsilon_x^2 - J\epsilon_y^2, \tag{7}$$

and the desired operation k_2 as

$$k_2 = e^{-i\gamma_1\sigma_x/2} \otimes e^{-i\gamma_2\sigma_x/2} = e^{-i[(\gamma_1-\gamma_2)\epsilon_x^1 + (\gamma_1+\gamma_2)\epsilon_x^2]}. \tag{8}$$

We now transform the parameters in k_2 and H_1 to reformulate the problem as generation of the local unitary,

$$e^{-i[(\gamma_1-\gamma_2)\sigma_x^1/2 + (\gamma_1+\gamma_2)\sigma_x^2/2]}, \tag{9}$$

from the Hamiltonian

$$\frac{\omega_1-\omega_2}{2}\sigma_x^1 + \frac{J}{2}\sigma_y^1 + \frac{\omega_1+\omega_2}{2}\sigma_x^2 - \frac{J}{2}\sigma_y^2. \tag{10}$$

To obtain Eqs. (9) and (10) we simply replaced ϵ_α^j in Eqs. (7) and (8) by $\sigma_\alpha^j/2$, which is warranted by the fact that $\{i\epsilon_x^1, i\epsilon_y^1, i\epsilon_z^1, i\epsilon_x^2, i\epsilon_y^2, i\epsilon_z^2\}$ is isomorphic to the Lie algebra $\mathrm{su}(2)\otimes\mathrm{su}(2)$. Taking advantage of the commutation of σ_α^1 and σ_β^2, the problem then naturally decomposes into two well-defined problems of generating single-qubit rotations:

(i) generate $e^{-i(\gamma_1-\gamma_2)\sigma_x^1/2}$ from the Hamiltonian $(\omega_1-\omega_2)\sigma_x^1/2 + J\sigma_y^1/2$; and

(ii) generate $e^{-i(\gamma_1+\gamma_2)\sigma_x^2/2}$ from the Hamiltonian $(\omega_1+\omega_2)\sigma_x^2/2 - J\sigma_y^2/2$.

By making the transformation from $\mathfrak{k}_1$ to $\mathrm{su}(2)\otimes\mathrm{su}(2)$, we have therefore arrived at two decoupled single-qubit quantum systems, solutions of which both reduce to a general steering problem on the Lie group SU(2) with dynamics determined by the Schrödinger equation:

$$i\dot{U} = \left(\frac{\omega(t)}{2}\sigma_x + \frac{J}{2}\sigma_y\right)U, \quad U(0) = I. \tag{11}$$

In general, $\omega(t)$ is a time-dependent external control field. The minimum energy control on the Lie group SU(2) has been studied in Ref. [33]. Here we will use Lie-Poisson reduction to derive both the minimum energy and time optimal control. We will also give a good approximate solution to this problem that can be further fidelity optimized.

Pontryagin's maximal principle provides an important mathematical tool for solving the optimal steering problem on Lie groups [34]. We solve for a control field ω that drives the system from the initial operation $U(0)=I$ to a prescribed target operation $U(T)=e^{-i\gamma/2\sigma_x}$, which also minimizes the cost function:

$$J = \int_0^T L(\omega(t))dt, \tag{12}$$

where $L(\omega(t))$ is a general functional of the control field $\omega(t)$ and is often referred to as the running cost. The first step is to construct the control Hamiltonian:

$$\mathcal{H}(t) = L(\omega(t)) + \langle M, -iU(t)^\dagger\left(\frac{\omega(t)}{2}\sigma_x + \frac{J}{2}\sigma_y\right)U(t)\rangle, \tag{13}$$

where M is a constant matrix in su(2), and $\langle X, Y\rangle = \mathrm{Tr}(XY^\dagger)$ is an inner product defined on su(2). For the ease of notation, we will suppress the time parameter unless otherwise specified. Proceeding further, we can write Eq. (13) as

$$\mathcal{H} = L(\omega) - \tfrac{1}{2}\langle M, iU^\dagger\sigma_x U\rangle\omega - \tfrac{1}{2}\langle M, iU^\dagger\sigma_y U\rangle J. \tag{14}$$

We then define three parameters p_1, p_2, and p_3 in terms of U and the matrix M by $p_1 = \langle M, iU^\dagger\sigma_x U\rangle/2$, $p_2 = \langle M, iU^\dagger\sigma_y U\rangle/2$, and $p_3 = \langle M, iU^\dagger\sigma_z U\rangle/2$, so that the control Hamiltonian can be written in terms of the parameters p_i as

$$\mathcal{H} = L(\omega) - p_1\omega - p_2 J. \tag{15}$$

Taking the derivative of p_1, we obtain

$$\dot{p}_1 = \tfrac{1}{2}\langle M, i\dot{U}^\dagger\sigma_x U\rangle + \tfrac{1}{2}\langle M, iU^\dagger\sigma_x\dot{U}\rangle = Jp_3. \tag{16}$$

By similar means, we can get the dynamics for p_2 and p_3. Combining these together, we have the dynamics for p_j as

$$\dot{p}_1 = Jp_3,$$

$$\dot{p}_2 = -\omega p_3,$$

$$\dot{p}_3 = \omega p_2 - Jp_1. \tag{17}$$

Equation (17) is indeed the Lie-Poisson equation on SU(2) [35]. Using this to solve for the parameters p_i as a function of time then allows explicit construction of the control Hamiltonian in Eq. (15) for a given control field ω. It is easy to verify that the functions $C_1 = p_1^2 + p_2^2 + p_3^2$ and $C_2 = p_1^2 + 2Jp_2$ are both invariant along the system trajectory. For a general optimal control problem on Lie group SU(2), one usually needs to solve a set of six differential equations. However, here we can obtain the reduced dynamics of three differential equations in Eq. (17) by using the Lie-Poisson reduction theorem [35]. The two conditions for this theorem are the vector field is right invariant and the cost function being independent of the quantum states, and they are both satisfied in this case. This reduces the number of the differ-

ential equations to be solved by half. This approach is a general technique applicable also to analysis of optimal control on multiqubit systems.

Now we derive the time optimal control, that is, the form of control field ω that achieves the target operation in the minimum time possible. In this case, the cost function can be written as

$$\min J = \int_0^T 1 dt,$$

and the running cost $L(\omega)=1$ is independent of control field ω. The corresponding control Hamiltonian is

$$\mathcal{H} = 1 - \omega p_1 - J p_2. \tag{18}$$

Let us assume that the control field ω is restricted to an interval $[\omega_m, \omega_M]$ due to physical bounds on the available frequencies. From Pontryagin's maximum principle, the optimal control field $\bar{\omega}(t)$ will minimize the control Hamiltonian (18) pointwise. Therefore $\bar{\omega}(t)$ can take only extremal values:

$$\bar{\omega}(t) = \begin{cases} \omega_m, & \text{if } p_1(t) \geqslant 0, \\ \omega_M, & \text{if } p_1(t) < 0. \end{cases}$$

This means that the time optimal control will switch back and forth between two extremal control values. This procedure is usually called bang-bang control in the control theory literature. (Note that the term "bang-bang control" has recently been adopted with a somewhat different meaning in the study of dynamical coupling of open quantum systems [36–39], where it is referred to as performing a set of instantaneously or as fast as physically possible hard pulses.) An example of this is given in Ref. [2] in the context of derivation of a constructive approach for steering on the Bloch sphere under general control fields. There we gave an explicit solution for achieving an arbitrary single-qubit target quantum operation by switching between two constant control fields and showed that this had the minimum number of such switchings. From the arguments above, we conclude now that this bang-bang control is also a time optimal control strategy and that the explicit solution presented in Ref. [2] is indeed the time optimal solution.

Next we consider the minimum-energy control which is encoded by the following cost function:

$$\min J = \frac{1}{2}\int_0^T \omega^2(t) dt.$$

The control Hamiltonian is now

$$\mathcal{H} = \tfrac{1}{2}\omega^2 - \omega p_1 - J p_2,$$

and thus the minimum-energy control is $\bar{\omega}(t)=p_1(t)$. Taking the derivative of $\dot{p}_1$ in Eq. (17), we have

$$\ddot{\bar{\omega}} = \left(\frac{C_2}{2} - J\right)\bar{\omega} - \tfrac{1}{2}\bar{\omega}^3, \tag{19}$$

where $C_2 = p_1^2 + 2Jp_2$ is constant along the optimal trajectory. The solution of this differential equation is given by the Jacobi elliptic function Cn [33]:

$$\bar{\omega}(t) = 2bk\,\mathrm{Cn}(bt + f, k), \tag{20}$$

where b, f, and k are real numbers. We can numerically determine the values of these parameters such that the control function (20) steers the Hamiltonian (3) from the initial operator $U(0)=I$ to the target operation $U(T)=e^{-i\gamma/2\sigma_x}$.

Finally we give an approximate solution to the control problem in terms of a sinusoidal control function $\omega = A\cos(\upsilon t)$, and show that this can be further fidelity optimized. Letting $U_1 = e^{i\upsilon/2\sigma_y t}U$, we transform the system (11) into the following form:

$$i\dot{U}_1 = \left(\frac{A}{2}(1+\cos 2\upsilon t)\frac{\sigma_x}{2} + (J-\upsilon)\frac{\sigma_y}{2} + \frac{A}{2}\sin 2\upsilon t\frac{\sigma_z}{2}\right)U_1. \tag{21}$$

The usual technique to solve this differential equation in the context of NMR is to drop the oscillating terms to get a time-independent Hamiltonian (rotating wave approximation). In order to get a more accurate solution, we use the Wei-Norman formula [40] to transform Eq. (21) to a dynamical system on $\mathbb{R}^3$. From Euler's *ZXZ* decomposition, a general solution to Eq. (21) can be written as

$$U_1(t) = e^{-i\alpha_1(t)\sigma_z/2}e^{-i\alpha_2(t)\sigma_x/2}e^{-i\alpha_3(t)\sigma_z/2}. \tag{22}$$

Taking the time derivative of U_1, we have

$$i\dot{U}_1 = \Big((\dot{\alpha}_2\cos\alpha_1 + \dot{\alpha}_3\sin\alpha_1\sin\alpha_2)\frac{\sigma_x}{2} + (\dot{\alpha}_2\sin\alpha_1 - \dot{\alpha}_3\cos\alpha_1\sin\alpha_2)\frac{\sigma_y}{2} + (\dot{\alpha}_1 + \dot{\alpha}_3\cos\alpha_2)\frac{\sigma_z}{2}\Big)U_1. \tag{23}$$

Comparing Eqs. (21) and (23), we get

$$\begin{bmatrix} A/2(1+\cos 2\upsilon t) \\ J-\upsilon \\ A/2\sin 2\upsilon t \end{bmatrix} = \begin{bmatrix} 0 & \cos\alpha_1 & \sin\alpha_1\sin\alpha_2 \\ 0 & \sin\alpha_1 & -\cos\alpha_1\sin\alpha_2 \\ 1 & 0 & \cos\alpha_2 \end{bmatrix}\begin{bmatrix} \dot{\alpha}_1 \\ \dot{\alpha}_2 \\ \dot{\alpha}_3 \end{bmatrix}.$$

Therefore we obtain a set of differential equations of the parameters α_j in $\mathbb{R}^3$:

$$\begin{bmatrix} \dot{\alpha}_1 \\ \dot{\alpha}_2 \\ \dot{\alpha}_3 \end{bmatrix} = \begin{bmatrix} -\dfrac{\sin\alpha_1}{\tan\alpha_2} & \dfrac{\cos\alpha_1}{\tan\alpha_2} & 1 \\ \cos\alpha_1 & \sin\alpha_1 & 0 \\ \dfrac{\sin\alpha_1}{\sin\alpha_2} & -\dfrac{\cos\alpha_1}{\sin\alpha_2} & 0 \end{bmatrix}\begin{bmatrix} A/2(1+\cos 2\upsilon t) \\ J-\upsilon \\ A/2\sin 2\upsilon t \end{bmatrix}. \tag{24}$$

Rigorous solution of Eq. (24) cannot be given in terms of elementary functions. However, when υ is close to J, a very good approximate solution can be found as

$$\alpha_1(t) = \frac{A}{2\upsilon}\sin^2\upsilon t,$$

$$\alpha_2(t) = \frac{A}{2}t + \frac{A}{4J}\sin 2\upsilon t,$$

$$\alpha_3(t) = 0.$$

Hence a sinusoidal control function $\omega = A\cos(\upsilon t)$ can achieve the following unitary operation at a final time T:

$$U(T) = e^{i\upsilon T\sigma_y/2} e^{-i\alpha_1(T)\sigma_z/2} e^{-i\alpha_2(T)\sigma_x/2}. \tag{25}$$

To generate an operation $e^{-i\gamma/2\sigma_x}$ with $\gamma \in [0, 2\pi]$, we only need that $\upsilon = J$, $AT/2 = \gamma$, and $JT = 2n\pi$, where n is an integer. This leads to the conditions

$$\upsilon = J, \quad A = \frac{\gamma J}{n\pi}, \quad T = \frac{2n\pi}{J}. \tag{26}$$

From Eq. (8), to implement a two-qubit local unitary operation $e^{-i\gamma_1\sigma_x/2} \otimes e^{-i\gamma_2\sigma_x/2}$, we require that

$$\omega_1 = \frac{\gamma_1 J}{n\pi}\cos Jt, \quad \omega_2 = \frac{\gamma_2 J}{n\pi}\cos Jt, \tag{27}$$

with a time duration $2n\pi/J$. Note that this is an approximate solution. Numerical simulations reveal that the greater the value of n, the better the approximation. To improve the accuracy, we can numerically search for the parameter values that maximize the fidelity of the actual achieved operation $U(T)$ to the desired target operation U_F as follows:

$$F(U(T), U_F) = \mathrm{Re}\,\mathrm{Tr}\{U(T)U_F^\dagger\}. \tag{28}$$

The values given by Eq. (26) can be used as a starting guess for the numerical optimization. This gives rise to a fidelity optimized control that can be made arbitrarily accurate.

We illustrate the control strategies aforementioned with a numerical example. Let $J = 200$ Hz in Eq. (1), and our target the generation of a 90° rotation about the x axis on the first qubit, that is, the operation $e^{-i\pi/4\sigma_x^1}$. Choosing $\phi_1 = \phi_2 = 0$, $n = 1$, the analytic approximation Eq. (26) yields

$$\upsilon = 200\ \mathrm{Hz}, \quad A = 100\ \mathrm{Hz}, \quad T = 10\pi\ \mathrm{ms}, \tag{29}$$

which leads to an approximate solution:

$$\omega_1 = 100\cos 200t, \quad \omega_2 = 0. \tag{30}$$

Numerical optimization via the maximization of the fidelity of actual achieved operation and the desired target operation, using the parameters in Eq. (29) as an initial guess, leads to the following fidelity optimized control function:

$$\omega_1 = 98.062\cos 196.900t, \quad \omega_2 = 0, \tag{31}$$

with a final time $T = 31.911$ ms. The corresponding fidelity error is 4.104×10^{-11} and can be further minimized to arbitrary accuracy (within machine precision). These two control functions, the analytic approximation and the fidelity optimized function, are shown in Fig. 1(A). The alternative minimum energy control function is determined numerically, resulting in parameters $b = 210.744$, $f = -0.00549$, and $k = 0.00236$, in Eq. (20), and the minimum energy control:

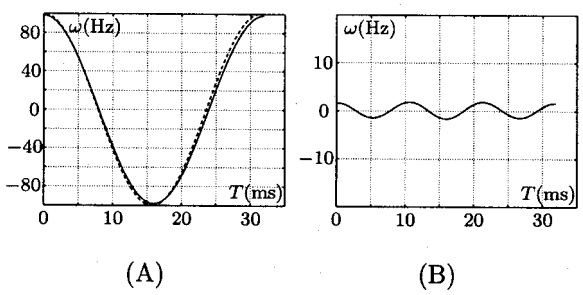

FIG. 1. Control functions that generate the single spin operation $e^{-i\pi/4\sigma_x^1}$ when $J = 200$ Hz. (A) Dashed line: approximate control in Eq. (30); solid line: fidelity optimized control in Eq. (31); (B) the difference between fidelity optimized control and minimum-energy control in Eq. (32).

$$\omega_1 = 99.678\mathrm{Cn}(210.744t - 0.005\,49, 0.002\,36). \tag{32}$$

This minimum-energy control solution is seen to be very close to the fidelity optimized control function of Eq. (31). The difference between these two control functions is plotted in Fig. 1(B).

In summary, we have presented a direct design of control pulses for an interacting two-qubit system that can implement any arbitrary single-qubit operations in a quantum system possessing an always-on interaction. This is crucial for the physical implementation of precise quantum operations in solid-state quantum computation where one needs to be able to generate all SU(2) operations on all individual spins. We derived here continuous control fields that can implement this in optimal fashion, by making use of an algebraic decoupling of the two-qubit Hamiltonian and combining this with Lie-Poisson reduction techniques. The generality of this algebraic decoupling approach, namely, its validity for all ratios of single-qubit frequencies ω_i to two-qubit interaction J, renders it useful for the design of low-power pulses in many situations, including low-temperature solid-state implementations of quantum information processing as well as broad band excitation in NMR. For generation of precise single-qubit operations, after the two-qubit system has been algebraically decoupled, we employ local control fields to drive the qubit systems to unentangled states at the end of the time interval over which the desired single-qubit operation is completed. The procedure thereby removes any undesirable entanglement generated by the untunable interaction. Furthermore, the local control fields may be steered with optimal control methods on SU(2) spaces, avoiding expensive numerical searches in higher-dimensional coupled qubit Hilbert spaces.

We have derived three explicit control strategies to generate arbitrary target quantum operations using this approach, namely, minimum time, minimum energy, and a third approximate analytic solution. The first two optimal strategies implement a desired target quantum operation exactly, whereas the approximate control strategy can be further optimized to perfect fidelity. Explicit solution for an example two-spin problem indicate that this fidelity optimized control strategy gives results very close to that obtained from the

minimum-energy control strategy. This is very encouraging for use of this technique to decouple qubits with always-on interactions in solid-state implementations of quantum computation that require low-temperature (mK) operation [26,27]. The fidelity optimized control strategy based on the approximate solution to the control equations possesses the attractive feature that we can easily determine the control parameters and we expect that it will consequently be very useful for applications to all systems of coupled spins and qubits characterized by always-on interactions.

The direct algebraic decoupling approach presented here can be extended to larger numbers of qubits. In its current form, the method allows straightforward implementation of optimal control strategies to find arbitrary quantum operations for any two-spin system with an always-on interaction, regardless of pulse durations and relative amplitude of single- and two-qubit terms in the Hamiltonian. Because of the decoupling, the optimization can be carried out as a steering problem on SU(2) and does not require numerical searches in higher-dimensional spaces. It also removes the need for expensive encoding steps, and the associated overhead and possible additional decoherence that this might introduce. In general the algebraic decoupling method thus provides an efficient, high-fidelity, and readily implementable approach to manipulation of individual spins in any coupled spin or qubit system with an always-on interaction.

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