Optimal control of Gmon qubits using Pontryagin’s minimum principle: preparing a maximally entangled state with singular bang-bang protocols

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We apply the theory of optimal control to the dynamics of two “Gmon” qubits, with the goal of preparing a desired entangled ground state from an initial unentangled one. Given an initial state, a target state, and a Hamiltonian with a set of permissible controls, can we reach the target state with coherent quantum evolution and, in that case, what is the minimum time required? The adiabatic theorem provides a far from optimal solution in the presence of a spectral gap. Optimal control yields the fastest possible way of reaching the target state and helps identify unreachable states. In the context of a simple quantum system, we provide examples of both reachable and unreachable target ground states, and show that the unreachability is due to a symmetry. We find the optimal protocol in the reachable case using three different approaches: (i) a brute-force numerical minimization (ii) an efficient numerical minimization using the bang-bang ansatz expected from the Pontryagin minimum principle, and (iii) direct solution of the Pontryagin boundary value problem, which yields an analytical understanding of the numerically obtained optimal protocols. Interestingly, our system provides an example of singular control, where the Pontryagin theorem does not guarantee bang-bang protocols. Nevertheless, all three approaches give the same bang-bang protocol.

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I. INTRODUCTION

The coherence times of quantum devices are rapidly increasing [1, 2], promising novel quantum machines and technologies [see, e.g., Refs. ([3–6])]. Optimal control plays a crucial role in driving machines governed by classical laws of physics, enhancing their performance and efficiency. Given the finite coherence times of quantum devices, optimal control may be even more important for quantum technologies, as slow performance may make certain coherent processes altogether impossible. How can we optimally manipulate systems and devices governed by coherent quantum dynamics? What are the characteristics of optimal quantum control protocols?

Despite a long history, specially in the few-body context [7, 8] (see also Ref. [9, 10]), several practical and fundamental questions remain unanswered [11]. With numerous novel applications to many-body dynamics [12–14], cold atoms [15, 16], and quantum information processing (e.g., topological quantum computing [17–19] and variational quantum algorithms [20–26]), quantum optimal control has emerged as an exciting frontier in nonequilibrium quantum dynamics. The objectives of quantum optimal control are diverse. We may want to steer the quantum states to a desired target state from a fixed initial state, prepare states with certain figures of merit (e.g., squeezed states) [27, 28], cool down the quantum systems [29–33], or generate a unitary evolution operator (e.g., a quantum gate) independently of the initial state [34–40].

One particular application of optimal control is finding shortcuts [41] to the adiabatic evolution without any modification to the form of the Hamiltonian: starting from the ground of a Hamiltonian (for certain values of the coupling constants), how should we change these tunable coupling constants, within a permissible range, to reach another ground state (corresponding to different values of the coupling constants) as fast as possible? Constraining the range of the coupling constants is one (not unique but experimentally motivated) way of fixing the energy scale of the Hamiltonian, which is important for making the problem well defined (an unphysical arbitrary increase of the energy scale can make all processes arbitrarily fast). Even in this simplest case, many questions remain unanswered. Of particular interest is the shortest possible time to reach the target state from a given initial state. This time scale sets a permissible-Hamiltonian-dependent distance between the initial and the target state, whose properties are relatively unexplored.

Focusing on a simple highly tunable two-qubit system [42] relevant to new superconducting devices, here we explore the properties of optimal control for transforming the quantum state from a given initial state. We consider, as an example, the creation of an entangled singlet state. Due to the purely quantum nature of these states and their sensitivity to environmental perturbations, it is difficult to prepare them directly. Thus, using quantum dynamics provides a promising approach. A simple method is based on the quantum adiabatic theorem: Using a tunable device whose Hamiltonian (for different parameters) supports both trivial and entangled ground states, we can reach the entangled state by slowly changing the device parameters.

According to the adiabatic theorem, this is achieved once the process takes much longer than a characteristic time scale set by the energy gap between the ground state and the first excited state. The long time scales required by the adiabatic theorem are undesirable. As only the final state is of interest, we do not need to constrain the system to remain in the instantaneous ground state, making these time scales unnecessary. This is the essence of the optimal-control approach to finding shortcuts to adiabaticity. In the absence of this constraint, can we reach the target ground state exactly in a finite time? In that case, what is the best way of changing the Hamiltonian

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**Notes:**

1. The coherence times of quantum devices are rapidly increasing, promising novel quantum machines and technologies.
2. The adiabatic theorem provides a far from optimal solution in the presence of a spectral gap.
3. Optimal control yields the fastest possible way of reaching the target state and helps identify unreachable states.
4. The coherence times of quantum devices are rapidly increasing, promising novel quantum machines and technologies.
5. The objectives of quantum optimal control are diverse.
6. We may want to steer the quantum states to a desired target state from a fixed initial state.
7. Preparing states with certain figures of merit (e.g., squeezed states) is also possible.
8. Cooling down the quantum systems is another application of optimal control.
9. Generating a unitary evolution operator (e.g., a quantum gate) independently of the initial state is a further application.
10. The shortest possible time to reach the target state from a given initial state is determined by this time scale.
parameters, i.e., the optimal protocol. What is the shortest time required?

Here we address these questions using a two-step approach. We choose a measure of distance (based on the wavefunction overlap) between the final and the target states. For a given total time, we find the protocol which minimizes this distance. We then keep increasing the total time until the optimal distance vanishes. Our permissible Hamiltonians are characterized by two bounded control knobs. A priori, our scheme is not concerned with a trajectory on the ground-state manifold and the system can be arbitrarily excited with respect to the instantaneous ground state. Interestingly, we find that in a case where the adiabatic transformation fails due to a level crossing, controlled nonadiabatic dynamics is also incapable of preparing the target state. While optimal control relies on nonadiabatic dynamics and should be naively insensitive to the properties of an adiabatic trajectory between the initial and target states, the same symmetry that protects a level crossing and prevents an adiabatic passage, forbids the more general transformation by nonadiabatic evolution.

In another case where the two ground states are not separated by a level crossing, we find that our optimal nonadiabatic protocol prepares the target state exactly with a sequence of square pulses, known as a bang-bang protocol. The general problem of finding such protocols is of considerable interest (particularly in the many-body context) and as we see in this simple model the knowledge of the bang-bang form of the protocol may significantly reduce the computational complexity of the problem. While, generically, bang-bang protocols are expected from the Pontryagin theorem, we can have singular controls that may not be bang-bang. Interestingly, in our model, we do find a singular interval. Nevertheless, the optimal solution turns out to be bang-bang.

II. MODEL AND SETUP

Consider a system described by a Hamiltonian with tunable parameters and an initial state that is the ground state of this Hamiltonian for certain values of these parameters. When attempting to transform this state by Hamiltonian evolution, the desired final state may be reachable or unreachable. In the special case where the initial and final states are both ground states of a gapped Hamiltonian, the adiabatic theorem implies that the desired state can be reached at least in the infinite time limit.

Consider as an example the case of preparing the maximally entangled singlet state of two qubits:

\[ |\psi_{\text{target}}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \]

from an unentangled initial ground state. The up and down spins are eigenstates of \( \sigma^z \) \( |\uparrow\rangle = |\uparrow\rangle \) and \( |\downarrow\rangle = |\downarrow\rangle \), where \( \sigma^{x,y,z,c} \) denote the Pauli matrices. The form of the Hamiltonian is set by the architecture of the device. Motivated by the coupling between powerful Gmon qubits developed in the Martinis group \[42\], we choose

\[ H = B_1 \sigma_1^z + B_2 \sigma_2^z + J \left( \sigma_1^+ \sigma_2^- + \sigma_1^- \sigma_2^+ \right). \]

The above Hamiltonian has three parameters. For simplicity, we focus on two cases with only two tunable parameters \( B \) and \( J \) with \( \pm B_1 = B_2 = B \). We assume that both of these parameters can be tuned as a function of time in the following range:

\[ 0 \leq B(t), J(t) \leq \Lambda, \]

where we set \( \Lambda = 1 \) for simplicity (we have also set \( \hbar \) to unity).

Note that the target state (1) is the ground state of the Hamiltonian (2) for \( J = 1 \) and \( B = 0 \). For \( J = 0 \), the two qubits are decoupled and the ground states for the two cases \( \pm B_1 = B_2 = B \) are unentangled direct products

\[ |\psi^+(0)\rangle = \frac{1}{2}(|\uparrow\uparrow\rangle - |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle), \]

\[ |\psi^-(0)\rangle = \frac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle - |\downarrow\downarrow\rangle). \]

To transform the initial states into the final target state, we need to turn off \( B \) and turn on \( J \). If this is done slowly enough and there is a gap to the excitations, the adiabatic theorem guarantees that the target state can be reached. Therefore, we first check the presence of a gap along a trajectory that connects the initial and final Hamiltonians. Factoring out the \( B \) coefficient from the Hamiltonian, we observe that the spectrum behaves as \( E(J/B)B \). To explore all ratios \( J/B \), we fix \( J = 1 - B \) and plot the energy gap as a function of \( B \) in the range \( 0 < B < 1 \). As seen in Fig. 1, the gap never closes for \( B_1 = -B_2 \) but closes at some intermediate value of \( B \) for \( B_1 = B_2 \).

In the \( B_1 = B_2 = B \) case, the level crossing occurs at \( J/B = 1/\sqrt{2} \), implying \( B = \sqrt{2}/(1 + \sqrt{2}) \) for \( J = 1 - B \) at the gap closure as seen in Fig. 1. The level crossing is exact and protected by the symmetry \( |\uparrow\downarrow\rangle \leftrightarrow |\downarrow\uparrow\rangle \). In other words, the permutation operator

\[ Q = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \]

in the \( (|\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle) \) basis, commutes with the Hamiltonian. All eigenstates of \( H \) are also eigenstates of \( Q \) with eigenvalues \( q = \pm 1 \). These two symmetry sectors are decoupled making the exact level crossing exact. This same symmetry forbids the transformation of \( |\psi^+(0)\rangle \) to the target state (1) by any coherent nonequilibrium evolution generated by \( H \). In fact, the singlet (1) is the only eigenstate of the Hamiltonian with \( q = -1 \) for arbitrary \( B \) and \( J \) (not necessarily the ground state) and cannot be reached from any other eigenstate.

To see this explicitly, notice that the time dependent wave function can be written as \( |\psi(t)\rangle = c_1(t)|\uparrow\uparrow\rangle + c_2(t)|\uparrow\downarrow\rangle + c_3(t)|\downarrow\uparrow\rangle + c_4(t)|\downarrow\downarrow\rangle \), with the amplitudes \( c_j \) evolving
according to
\[
\frac{d}{dt} c_1(t) = -i \{ B_2(t)c_2(t) + B_1(t)c_3(t) \},
\]
\[
\frac{d}{dt} c_2(t) = -i \{ B_2(t)c_1(t) + 2J(t)c_3(t) + B_1(t)c_4(t) \},
\]
\[
\frac{d}{dt} c_3(t) = -i \{ B_1(t)c_1(t) + 2J(t)c_2(t) + B_2(t)c_4(t) \},
\]
\[
\frac{d}{dt} c_4(t) = -i \{ B_1(t)c_2(t) + B_2(t)c_3(t) \}.
\]

We see that in the \( B_1 = B_2 \) case, the equations are symmetric under the \( c_2 \leftrightarrow c_3 \) exchange. As the initial state also has \( c_2 = c_3 \), this equality hold at arbitrary times under all possible dynamics generated by arbitrary \( B(t) \) and \( J(t) \) so the target state, which has \( c_2 = -c_3 \), cannot be reached by any protocol. Hereafter, we focus on the \( B_1 = -B_2 \) case, where the preparation of the target state is not forbidden.

### III. BRUTE-FORCE OPTIMIZATION: OPTIMAL VS LINEAR PERFORMANCE

Our goal is to reach the target ground state (1) from the initial state (5) in the shortest amount of time possible by adjusting the Hamiltonian parameters as a function of time. In real-world applications, we may have a shorter total time than the minimum time needed to reach the state exactly. Therefore, it is useful to be able to quantify the performance of different protocols in a fixed total time \( \tau \). This will also provide a practical approach for finding the minimum \( \tau \) for which exact preparation is possible. Using the overlap between the final state \( |\psi(\tau)\rangle \) and the target state (1), we define the error as
\[
E = 1 - |\langle \psi_{\text{target}} | \psi(\tau) \rangle|^2.
\]

The error above is always nonnegative and vanishes if the two states are the same.

The error (11) is a functional of the controllable time-dependent parameters \( B(t) \) and \( J(t) \) in the range defined in Eq. (3). To apply standard numerical optimization algorithms, we need to transform the functional to a multivariable function. There are multiple ways to do this, e.g., using truncated coefficients of a Taylor or Fourier expansion. For our bounded parameters, it is convenient to discretize time, i.e., divide \( T \) into \( N \) intervals of length \( T/N \), as seen in Fig. 2, creating piece-wise constant functions for \( B(t) \) and \( J(t) \), where

\[ B(t) = \tilde{B}_j \text{ for } (j-1)\tau/N < t < j\tau/N \text{ and similarly for } J(t). \]

Then, we can minimize \( E \) as a multivariable function of \( \tilde{B}_j \) and \( \tilde{J}_j \) (with \( 2N \) bounded variables). To avoid an artificial bias, we increase \( N \) until the results converge. In our simulations, using the interior-point minimization algorithm, we used \( N = 5 \) and 10 and found that the protocols and the associated errors were almost identical.

As seen in Fig. 3(a), we find that our optimal protocols beat the linear protocol shown in Fig. 3(b) significantly. Two examples of the optimal protocols for different values of \( \tau \) are shown in Fig. 3(c) and Fig. 3(d). At \( \tau = 0 \), both protocols give an error \( E = 0.5 \) (from the finite overlap of the initial and target states). Upon increasing \( \tau \), the error corresponding to the linear protocol decreases, approaching \( E = 0 \) only at \( \tau \rightarrow \infty \), while the error corresponding to the optimal one decreases more rapidly, reaching \( E = 0 \) at a finite time \( \tau \approx 0.9 \), indicating an exact preparation of the desired state.
IV. BANG-BANG OPTIMIZATION: CHARACTERIZING THE PROTOCOLS

From our brute-force optimization in Sec. III, we observe that the optimal \( B(t) \) and \( J(t) \) have discontinuous jumps between their minimum and maximum allowed values of 0 and 1. Such protocols are referred to as bang-bang protocols. As discussed in the next section, they are indeed expected to generically occur in linear optimal control problems. Knowing the bang-bang form of the protocol (and making an educated guess about the maximum number of bangs), we can perform a secondary optimization, which determines the optimal protocol very accurately. The new results are in agreement with the approximate (due to the finite discretization) results from the brute-force computations. Since we have a much smaller number of variational parameters, i.e., the times of the jumps, this optimization is much more efficient.

We performed this secondary optimization with two parameters (although one parameter would have been sufficient). As shown in Fig. 4, these parameters are \( t_B \) and \( t_J \). \( B(t) \) jumps from 0 to 1 at \( t_B \), \( J(t) \) jumps from 1 to 0 at \( t_J \). We find that \( t_J \) is always equal to \( \tau \), so there is no jump in \( J(t) \) in the middle of the evolution. As seen in the figure, for \( \tau \) larger than \( \tau^* \sim 0.9 \), the numerically obtained \( t_J \) is no longer equal to \( \tau \). This is precisely the total time \( \tau \) for which the optimal protocol prepares the state exactly (see Fig. 3). Therefore, for times longer than \( \tau^* \), many protocols can achieve this exact preparation and the optimal protocols are not unique. For \( \tau < \tau^* \), we find two distinct behaviors for \( t_B \). If \( \tau \) is smaller than a critical value \( \tau_0 \sim 0.4 \), we have \( t_B = 0 \). On the other hand, for \( \tau_0 < \tau < \tau^* \), we find the following linear relationship:

\[
t_B = \tau - \tau_0. \tag{12}
\]

At this point the results above are purely numerical findings, but we will explain them in Sec. V using the Pontryagin theorem.

V. CONNECTION WITH PONTRYAGIN’S MINIMUM PRINCIPLE: SINGULARITY OF THE CONTROL

The Pontryagin’s minimum principle explains the bang-bang nature of the protocol above and provides an alternative approach for determining the switching time \( t_B \). We first briefly review the formalism. For dynamical variables \( \mathbf{x} \) evolving with the equation of motion \( \mathbf{x} = \mathbf{f}(\mathbf{x}, \mathbf{b}) \) with controls \( \mathbf{b} \), we can write an optimal-control Hamiltonian \( \mathcal{H} \) in terms of conjugate momenta \( \mathbf{p} \) as

\[
\mathcal{H} = \mathbf{p}^T \mathbf{f}(\mathbf{x}, \mathbf{b}), \tag{13}
\]

where the superscript \( ^T \) indicates transpose. The dynamics of \( \mathbf{x} \) and \( \mathbf{p} \) are governed by the Hamilton equations

\[
\dot{\mathbf{x}} = \partial_\mathbf{p} \mathcal{H}, \quad \dot{\mathbf{p}} = -\partial_\mathbf{x} \mathcal{H}. \tag{14}
\]

Assuming we want to minimize a cost function \( \mathcal{E}[\mathbf{x}(\tau)] \) at the final time \( \tau \), the boundary conditions for the conjugate momenta are given by

\[
\mathbf{p}(\tau) = \partial_\mathbf{x} \mathcal{E}[\mathbf{x}(\tau)], \tag{15}
\]

and the key condition of optimal control is

\[
\mathcal{H}(\mathbf{x}^{\text{opt}}, \mathbf{p}^{\text{opt}}, \mathbf{b}^{\text{opt}}) = \min_{\mathbf{b}} \mathcal{H}(\mathbf{x}^{\text{opt}}, \mathbf{p}^{\text{opt}}, \mathbf{b}), \tag{16}
\]

where the superscript indicates the optimal protocol and the corresponding trajectories for the dynamical variables and their conjugates. A consequence of the above expression is that if the equations of motion and consequently \( \mathcal{H} \) are linear in the controls, the optimal protocol is generically bang-bang (unless the coefficient of a control identically vanishes over a finite interval, which is referred to as singular control).

In the context of quantum evolution, the equations of motion \( \frac{d}{dt} |\Psi\rangle = -i\mathcal{H}(t)|\Psi\rangle \) can be written as

\[
\frac{d}{dt} \mathcal{R} = \mathcal{H}(t) \mathcal{I}, \quad \frac{d}{dt} \mathcal{I} = -\mathcal{H}(t)^T \mathcal{R}, \tag{17}
\]

for a real Hamiltonian \( \mathcal{H}(t) \) (in this case a \( 4 \times 4 \) matrix), where the dynamical variables \( \mathcal{R} \) and \( \mathcal{I} \) contain the real and imaginary parts of the wavefunction. Let us denote the conjugate momenta by vectors \( \mathcal{P}_R \) and \( \mathcal{P}_I \), respectively for \( \mathcal{R} \) and \( \mathcal{I} \). The optimal-control Hamiltonian \( \mathcal{H} \) is then constructed as

\[
\mathcal{H} = \mathcal{P}_R^T \mathcal{H}(t) \mathcal{I} - \mathcal{P}_I^T \mathcal{H}(t) \mathcal{R}. \tag{18}
\]

We now observe that since \( \mathcal{H}(t) \) in linear in the controls \( \mathcal{B} \) and \( \mathcal{J} \), the optimal-control Hamiltonian \( \mathcal{H} \) is also linear in them. Eq. (16) then implies that, at any point in time, the controls \( \mathcal{B} \) and \( \mathcal{J} \) must be set to either their minimum or their maximum allowed values depending on the sign of their corresponding coefficient in the linear function \( \mathcal{H} \) (for optimal values of \( \mathcal{R} \), \( \mathcal{I} \), \( \mathcal{P}_R \), and \( \mathcal{P}_I \)). Thus, a bang-bang solution, as found in our numerical studies, is indeed expected, unless one of the aforementioned coefficients identically vanishes over a finite time interval.
The equations of motion for the conjugate momenta are obtained by differentiating $\mathcal{H}$ with respect to the corresponding dynamical variables and are given by

$$\frac{d}{dt}P_R = H(t)P_I, \quad \frac{d}{dt}P_I = -H(t)P_R. \quad (19)$$

Combining the conjugate momenta into $|\Pi\rangle = P_R + iP_I$, we can then write

$$\frac{d}{dt}|\Pi\rangle = -iH(t)|\Pi\rangle. \quad (20)$$

To proceed, we write the cost function (11) [see also Eq. (1)] in terms of the dynamical variables at time $\tau$ as

$$E = 1 - \frac{1}{2} \left[ (\mathcal{R}_2 - \mathcal{R}_3)^2 + (J_2 - J_3)^2 \right], \quad (21)$$

which using Eq. (15) leads to

$$|\Pi(\tau)\rangle = M|\Psi(\tau)\rangle, \quad (22)$$

with the matrix $M$ given by

$$M = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & -1 & 1 & 0 \\
0 & 1 & -1 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}. \quad (23)$$

It is illuminating to use the Pontyagin equations with an ansatz characterized by one parameter $t_B$ and $t_f = \tau$ to find the protocol shown in Fig. 4. Using Eq. (18), we find the coefficient of $B$ in $\mathcal{H}$ (a linear function of $B$) as

$$\frac{\partial B}{\partial H} = P_R^T \mathcal{K} T - P_I^T \mathcal{K} R = \text{Im}(\Pi(\tau)|\mathcal{K}|\psi(\tau)), \quad (24)$$

where

$$\mathcal{K} = \partial B H(B, J) = \begin{pmatrix}
0 & 1 & -1 & 0 \\
1 & 0 & 0 & -1 \\
-1 & 0 & 0 & 1 \\
0 & -1 & 1 & 0
\end{pmatrix}. \quad (25)$$

Thus, the minimum of $\mathcal{H}$ is achieved by choosing

$$B(t) = 1, \quad -\text{Im}(\Pi(\tau)|\mathcal{K}|\psi(\tau)) > 0, \quad (26)$$

$$B(t) = 0, \quad -\text{Im}(\Pi(\tau)|\mathcal{K}|\psi(\tau)) < 0, \quad (27)$$

The time-dependent evolution operator can be written in a convenient form by defining

$$U_1(t) = \exp[-i\mathcal{H}(B = 0, J = 1)] \equiv \exp(-iH_1), \quad (28)$$

$$U_2(t) = \exp[-i\mathcal{H}(B = 1, J = 1)] \equiv \exp(-iH_2), \quad (29)$$

which leads to

$$|\psi(t)\rangle = U_1(t)|\psi(0)\rangle, \quad t < t_B,$$

$$|\psi(t)\rangle = U_2(t - t_B)U_1(t_B)|\psi(0)\rangle, \quad t > t_B,$$

$$|\Pi(t)\rangle = U_2^\dagger(\tau - t_B)MU_2(\tau - t_B)U_1(t_B)|\psi(0)\rangle, \quad t > t_B,$$

$$|\Pi(t)\rangle = U_1(t_B - t)U_2^\dagger(\tau - t_B)MU_2(\tau - t_B)U_1(t_B)|\psi(0)\rangle, \quad t < t_B,$$

where we have used the boundary condition (22) and the equations of motion (20) for the conjugate momenta. Fixing $t$ and $t_B$, the four equations above uniquely determine $-\text{Im}(\Pi(\tau)|\mathcal{K}|\psi(\tau))$ as a function of $t$. For a fixed $\tau$, we can then scan over $t_B$ and see if we can find solutions where $-\text{Im}(\Pi(\tau)|\mathcal{K}|\psi(\tau))$ switches sign from negative to positive precisely at $t_B$. Indeed as seen in Fig. 5 as an example for $\tau = 0.75$ (a similar behavior was observed for other values of $\tau$), we find that for long $t_B$, $-\text{Im}(\Pi(\tau)|\mathcal{K}|\psi(\tau))$ is positive for all finite $t$. For shorter $t_B$ there is one sign switch from negative to positive at an intermediate time. We want this switch to occur precisely at the corresponding $t_B$. Starting from the short $t_B$ limit and searching for $t_B$ for which the crossing occurs precisely at $t_B$ gives $t_B \approx 0.3423 \pm 0.075$ and several values of $\tau$.

An unexpected result is that the control becomes singular for all $t < t_B$ for our solution. This simple system thus provides an example of singular control, in which the application of the Pontryagin theorem is rather subtle. While the sign of the coefficient of $B$ determines the value of $B$, if this coefficient vanishes over a finite interval as seen in Fig. 5 for $t_B \approx 0.3423$, the control is singular and the theorem does not directly yield the optimal protocol. In case of singular control, there is no reason to expect a bang-bang protocol in intervals with a vanishing $\text{Im}(\Pi(\tau)|\mathcal{K}|\psi(\tau))$. However, our brute-force numerical results indicate that the protocol is still bang-bang.

The numerically found relationship between $t_B$ and $\tau$ [see Fig. 4 and Eq. (12)] in the range of $\tau$ for which the optimal control is unique and $t_B$ is finite, can be understood in terms of the Pontryagin theorem. The singularity of the control for $t < t_B$ implies $\text{Im}(C) = 0$ with

$$C = \langle \psi(0)|U_1^\dagger(t_B)U_2^\dagger(\tau_0)MU_2(\tau_0)U_1(t_B)U_1^\dagger(\tau_0)\mathcal{K}U_1(\tau_0)|\psi(0)\rangle \quad (30)$$

independently of $t$ and $t_B$ as long as we have the correct $\tau_0$. Our particular value of $\tau_0$ has the property that

$$U_2^\dagger(\tau_0)MU_2(\tau_0) = \frac{1}{2} \begin{pmatrix}
-1 & e^{-i\pi/3} & -e^{-i\pi/3} & 1 \\
e^{i\pi/3} & -1 & 1 & -e^{i\pi/3} \\
e^{-i\pi/3} & 1 & -1 & e^{i\pi/3} \\
1 & e^{-i\pi/3} & e^{i\pi/3} & -1
\end{pmatrix}. \quad (31)$$
Using the above matrix, Eq. (29) can be explicitly computed as a function of $t$ and $t_B$:
\[
C = 2 \cos(2t) + \cos(2(t - t_B)) - \sqrt{3} \sin(2(t - t_B)),
\]
which is a real number. Therefore, for this particular $t_B$, we have $\text{Im}(C) = 0$ for all $t$ and $t_B$, demonstrating the validity of Eq. (12).

VI. CONCLUSIONS

In summary, we used optimal control to generate a maximally entangled quantum state from an unentangled state using quantum dynamics in a simple two-qubit system. The quantum dynamics was generated by a 2-parameter Hamiltonian relevant to the gmon architecture of superconducting qubits. We found that when the adiabatic theorem fails due to a level crossing, the symmetry responsible for the crossing also forbids state transformations by using a more general nonadiabatic optimal protocol, making the target state unreachable. In the case of a reachable target, for various total of times, we numerically found the optimal protocols that maximized the overlap of the final states with the target state. We found optimal protocols that substantially outperform a linear adiabatic optimal protocol, despite the presence of singular segments in the control. Our results provide a scheme for the fastest possible generation of quantum entanglement between gmon qubits, shed light on the conditions for reachability, and fully characterize both qualitative and quantitative characteristics of the optimal pulses.

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