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Quantum control of tunable-coupling transmons using dynamical invariants of motion

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Abstract

We analyze the implementation of a fast nonadiabatic CZ gate between two transmon qubits with tunable coupling. The gate control method is based on a theory of dynamical invariants which leads to reduced leakage and robustness against decoherence. The gate is based on a description of the resonance between the $|11\rangle$ and $|20\rangle$ using an effective Hamiltonian with the six lowest energy states. A modification of the protocol allows us to take into account the higher-order perturbative corrections of this effective model. This enables a gate fidelity several orders of magnitude higher than other quasiadiabatic protocols, with gate times that approach the theoretical limit.

1. Introduction

Superconducting qubits are currently one of the most promising platforms to perform highly scalable quantum computations. In the last two decades, there has been great progress both in the quantity of qubits and the quality of their operations [1–4]. This progress has been largely made possible thanks to the transmon qubit [5], a relatively simple, easy to reproduce design, with competitive decoherence times [6, 7]. Recent progress in quantum gates with transmons have led to substantial speed-ups, surpassing coherence times by up to three orders of magnitude, with fidelities that approach the requirements for scalable quantum error correction [8–10] and fault-tolerant quantum computation [11–13]. The implementation of two-qubit gates with superconducting qubits is possible with many different strategies: gates assisted by microwave controls [14], parametrically modulated qubits [15] and couplers [16, 17], gates implemented with tunable-frequency qubit-qubit resonances [18] or tunable couplings [19–24]. These demonstrations have proved successful at performing CZ [2, 18, 19, 22, 24], CPHASE [23] and iSWAP [21] gates with fidelities over 99%.

Using a tunable coupling to implement quantum gates presents the advantage of requiring less control lines, and having better coherence in general [19]. The use of tunable couplers allows isolating the qubits and cancelling parasitic interactions during single-qubit gates and rest periods. Tunable couplings also eliminate the problem of frequency crowding that arises in other two-qubit gate strategies with always-on interactions [20]. In order to manipulate the qubits, most of the current protocols benefit from adiabatic controls [2, 19, 20, 22, 23]. Although adiabatic processes are robust against control imperfections, they are intrinsically slow, limiting the number of operations that can be performed within the lifespan of the qubits, and thus leaving the system more vulnerable to incoherent errors. This has motivated the development of nonadiabatic protocols [25, 26] using the frequency-tunable, fixed-coupling architecture [27–29]. The principle of these nonadiabatic designs is to allow transitions along the process that implements the gate, but suppress them once said process is finished. A common technique to achieve this is to drive the computational states using dynamical invariants of motion [30], such that the system’s Hamiltonian and the invariant share eigenstates at the beginning and at the end of the control [31].

In this work, we present a new method to implement universal CZ gates between transmon connected by a tunable coupler. The formalism is based on an exact technique that uses invariants of motion to...
inverse-engineer the gate protocol, and is made possible by a simpler formulation of the transmon dynamics in a reduced space. The derivation of an effective Hamiltonian, starting from the standard two-transmon Hamiltonian, is carried out in section 2. Using this simplified version, in section 3 we design faster-than-adiabatic protocols to perform the CZ gate. We compare two different approaches to engineer the turn-on and off processes of the coupling: fast quasidiabatic dynamics (FAQUAD) and invariant-based inverse engineering. In section 4, we numerically simulate the two-transmon system to evaluate the driving performance and identify possible sources of infidelity. With the aid of the effective description we introduce higher order energy corrections to rectify incoherent errors due to an energy Stark-shift, showing that the invariant-based method has a great resilience, bringing the gate infidelity below $10^{-5}$ in competitive operation times. Finally, section 5 contains the manuscript main conclusions.

2. Transmon model

2.1. Single transmon

A transmon is a charge-based superconducting qubit that is created by shunting a Josephson Junction with a large capacitor. The shunting capacitor reduces the sensitivity to charge fluctuations around the superconducting island, while preserving an anharmonicity that separates the qubit subspace from the rest of energy levels [5]. The Hamiltonian describing one ‘bare’ transmon, in the number-phase representation, reads [32, 33]

$$\hat{H}_{\text{transmon}} \equiv \hat{H}_T = 4E_C \hat{n}^2 - E_J \cos(\hat{\phi}),$$

with $\hat{n}$ and $\hat{\phi}$ satisfying the canonical commutation relation $[\hat{n}, \exp(i\hat{\phi})] = -\exp(i\hat{\phi})$. $E_C$ is the charging energy, related to the total capacitance $C$ of the transmon qubit as $E_C = 2e^2/C$, and $E_J$ is the Josephson energy. A transmon typically operates at a large $E_J/E_C$ ratio ($\gtrsim 50$), where the qubit dynamics are analogous to a massive particle in a weakly anharmonic potential,

$$\hat{H}_T = 4E_C \hat{n}^2 + \frac{E_J}{2} \hat{\phi}^2 - \frac{E_J}{4\hbar} \hat{\phi}^4 + \cdots.$$  

Identifying $\hat{\phi}^2/2m \sim 4E_C \hat{n}^2$ and $m\omega^2 \hat{x}^2 \sim E_J \hat{\phi}^2$, the quadratic part of the Hamiltonian can be diagonalized using the ladder operators of the harmonic oscillator, $\hat{a}$ and $\hat{a}^\dagger$, defined as,

$$\hat{n} = i \left( \frac{E_J}{8E_C} \right)^{1/4} \left( \frac{\hat{a} - \hat{a}^\dagger}{\sqrt{2}} \right), \quad \hat{\phi} = \left( \frac{8E_C}{E_J} \right)^{1/4} \left( \frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}} \right).$$

Notice how at large $E_J/E_C$ the fluctuations of $\hat{\phi}$ are reduced, and larger powers of $\hat{\phi}$ can be neglected in the expansion (2). Introducing equation (3) into this expansion, the transmon Hamiltonian reads

$$\hat{H}_T \simeq \omega_{01} \hat{a}^\dagger \hat{a} + \frac{\alpha}{2} \hat{a}^2 \hat{a}^\dagger + \frac{\alpha}{12} \left( \hat{a}^4 + \hat{a}^4 + 4\hat{a}^3 \hat{a} + 4\hat{a}^2 \hat{a}^2 + 6\hat{a}^2 \hat{a}^2 + 6\hat{a}^2 \hat{a}^2 \right),$$

where $\omega_{01} \simeq \sqrt{8E_CE_J} - E_C$ represents the splitting between the two lowest energy states, $|0\rangle$ and $|1\rangle$. The anharmonicity $\alpha \simeq -E_C$ is small but allows us to detune all higher energy states, $|2\rangle$, $|3\rangle$, $|4\rangle$, … from the qubit subspace.

The eigenstates of the transmon Hamiltonian, denoted by $|n\rangle$, differ from the eigenstates of the harmonic oscillator due to all the anharmonic terms in equation (4) that do not preserve the number of excitations, i.e. those with different number of $\hat{a}$ and $\hat{a}^\dagger$ operators. In fact, these counter-rotating terms can be treated as a perturbation to the reference Hamiltonian $\hat{H}_0 = \omega_{01} \hat{a}^\dagger \hat{a} + (\alpha/2) \hat{a}^2 \hat{a}^\dagger$, whose eigenstates are those of the harmonic oscillator. Using standard time-independent perturbation theory at first order in $\alpha/\omega_{01}$, we find for the lowest-energy states

$$|0\rangle \simeq |\Psi_0\rangle - \frac{\sqrt{2\alpha}}{3(2\omega_{01} + \alpha)} |\Psi_2\rangle - \frac{\sqrt{6\alpha}}{12(2\omega_{01} + 3\alpha)} |\Psi_4\rangle,$$

$$|1\rangle \simeq |\Psi_1\rangle - \frac{5\sqrt{6\alpha}}{6(2\omega_{01} + 3\alpha)} |\Psi_3\rangle - \frac{\sqrt{30\alpha}}{12(2\omega_{01} + 5\alpha)} |\Psi_5\rangle,$$

$$|2\rangle \simeq |\Psi_2\rangle + \frac{\sqrt{2\alpha}}{3(2\omega_{01} + \alpha)} |\Psi_0\rangle - \frac{8\sqrt{3\alpha}}{3(2\omega_{01} + 5\alpha)} |\Psi_4\rangle - \frac{\sqrt{10\alpha}}{2(4\omega_{01} + 15\alpha)} |\Psi_6\rangle,$$

where $|\Psi_i\rangle$ represents the $i$th eigenstate of the harmonic oscillator. The perturbative expansion reveals that, when an interaction term proportional to $\hat{n}$ is present, both $\hat{a}$ and $\hat{a}^\dagger$ produce a coupling between two adjacent states, in opposition to what happens in the harmonic oscillator. For instance, the operator $\hat{a}$ projects the state $|0\rangle$ into state $|1\rangle$ with an amplitude proportional to $\alpha/\omega_{01}$. 


2.2. Coupled transmons

In this work we consider two transmons with a tunable interaction between them using the design demonstrated in [19]. In this design, two superconducting Xmon qubits are coupled through a circuit that uses a single flux-biased Josephson junction and acts as a tunable current divider. The physics behind this tunable coupler is well explained using a simple linear model (see [34] for a full discussion),

\[ \hat{H}(t) = \hat{H}_{T,a} + \hat{H}_{T,b} + g_C(t) \hat{n}_a \hat{n}_b, \]

where \( g_C \) is the tunable coupling that embodies an interaction that can be varied continuously with nanosecond resolution from negative to positive, going smoothly through zero, where the transmons are isolated. \( \hat{H}_{T,i} \) is the Hamiltonian given by equation (1) of each 'bare' transmon \( i = a, b \) used to encode a qubit.

For typical experimental circuit parameters, the coupling takes values in the MHz range, while \( \omega_{01} \) is usually in the GHz range. Due to this energy mismatch, only close-to-degeneracy states will be able to interact and produce transitions from one state to another. Assuming that both transmons have similar frequencies, these close-to-degeneracy states are the ones that share the total number of excitations, for instance, states \(|01\rangle\) and \(|10\rangle\), or states \(|11\rangle, |02\rangle\) and \(|20\rangle\). In particular, denoting the ladder operators as \( \hat{a}, \hat{a}^\dagger \) for the first qubit, and \( \hat{b}, \hat{b}^\dagger \) for the second qubit, we can compute the non-zero matrix elements of the coupling between these states using the perturbative expansions from equation (5),

\[
\tilde{J}_1(t) \equiv \langle 01 | g_C(t) \hat{n}_a \hat{n}_b | 10 \rangle = J(t) \langle 01 | (-\hat{a}^\dagger \hat{b}^\dagger + \hat{a}^\dagger \hat{b} + \hat{a} \hat{b}^\dagger - \hat{a} \hat{b}) | 10 \rangle = J(t) \left[ 1 + \frac{2 \alpha_a}{3 (2 \omega_a + \alpha_a)} + \frac{2 \alpha_b}{3 (2 \omega_b + \alpha_b)} + O \left( \frac{\alpha^2_a, b}{\omega^2_a, b} \right) \right],
\]

\[
\tilde{J}_2(t) \equiv \langle 11 | g_C(t) \hat{n}_a \hat{n}_b | 02 \rangle = \sqrt{2} J(t) \left[ 1 + \frac{-\alpha_b}{2 \omega_a + \alpha_a} + \frac{5 \alpha_a}{2 (2 \omega_b + 3 \alpha_b)} + \frac{2 \alpha_a}{3 (2 \omega_a + \alpha_a)} + O \left( \frac{\alpha^2_a, b}{\omega^2_a, b} \right) \right],
\]

\[
\tilde{J}_3(t) \equiv \langle 11 | g_C(t) \hat{n}_a \hat{n}_b | 20 \rangle = \sqrt{2} J(t) \left[ 1 + \frac{-\alpha_a}{3 (2 \omega_a + \alpha_a)} + \frac{5 \alpha_a}{2 (2 \omega_b + 3 \alpha_b)} + \frac{2 \alpha_b}{3 (2 \omega_b + \alpha_b)} + O \left( \frac{\alpha^2_a, b}{\omega^2_a, b} \right) \right],
\]

where \( J(t) = (1/2) g_C(t) \left| E_{i,a} E_{i,b} / (64 E_C, a E_C, b) \right|^{1/4} \). For typical experimental values, the first order corrections represent 5%–10% of the total coupling, and they become smaller as the ratios \( \alpha_i / \omega_i \) decrease.

As we already mentioned, due to energy mismatch of 2-3 orders of magnitude between the frequency of the transmons \( \sim \text{GHz} \) and the coupling \( \sim \text{MHz} \), states with different number of excitations are well separated in energy and are not affected by the coupling term. For instance, the \( \hat{a}^\dagger \hat{b}^\dagger \) term that appears in Hamiltonian (6) couples states \(|00\rangle\) and \(|11\rangle\) with an amplitude \( \sim J(t) \). However, the energy separation between these two levels \( \Delta E = \omega_a + \omega_b \) is much greater than the coupling. Thus, the coupling term only leads to perturbations in the energy of said states of order \( \tilde{F}(t) / (\omega_a + \omega_b) \sim \text{KHz} \), and can be safely neglected when compared with the rest of energy scales. This is not the case when the energy levels involved are close to degeneracy, or with an energy separation comparable with the coupling term. Therefore, in the basis of eigenstates of the uncoupled problem, \{|00⟩, |01⟩, |10⟩, |02⟩, |11⟩, |20⟩\}, the Hamiltonian (6) is very well approximated by a block-diagonal matrix

\[
\hat{H}(t) = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & \omega_b & \tilde{J}_1(t) & 0 & 0 & 0 \\
0 & 0 & \omega_a & \tilde{J}_2(t) & 0 & 0 \\
0 & 0 & 0 & \omega_b + \alpha_b & \tilde{J}_3(t) & 0 \\
0 & 0 & 0 & 0 & \omega_a + \alpha_a & 0 \\
0 & 0 & 0 & 0 & 0 & \omega_a + \alpha_a
\end{pmatrix}.
\]

The structure of equation (10) evidences three subspaces \( S_0 := \{|00⟩\} \), \( S_1 := \{|01⟩, |10⟩\} \), and \( S_2 := \{|02⟩, |11⟩, |20⟩\} \), each of them with different number of excitations and uncoupled from each other. In order to perform a certain operation, the coupling \( g_C(t) \) can be engineered to produce the desired dynamics in each of these subspaces. Henceforth, we will design \( J(t) \) instead of \( g_C(t) \) for simplicity (they only differ in a scale factor).
Figure 1. (a) Numerically calculated lowest eigenenergies of Hamiltonians (6) (solid lines) and (10) (round markers) as a function of the coupling strength between the two transmons. The lower panel shows a zoom-in at the avoided crossing of levels $|11\rangle$ and $|20\rangle$, that are degenerate when there is no coupling ($J=0$) and split into two dressed states $|\pm\rangle$ as the coupling strength grows. (b) Energy difference between the effective Hamiltonian and the complete Hamiltonian levels.

In figure 1 we test the validity of the approximations made to find the Hamiltonian (10) by comparing its eigenenergies with the lowest six numerically calculated eigenenergies of the complete Hamiltonian (6) as a function of the coupling strength $J$, not taking into account its time dependence. As shown in figure 1(b), the effective Hamiltonian reproduces the lower energy levels of the two-transmon system with very little deviation, despite having neglected interactions between two-qubit states with a different number of excitations. In the following section, we will derive the different control protocols from (10) to construct a CZ gate, although the full Hamiltonian (6) will be simulated with the experimental parameters [19]:

$$\begin{align*}
\omega_a &= 2\pi \times 6.00\, \text{GHz}, \\
\omega_b &= 2\pi \times 5.67\, \text{GHz}, \\
\alpha_a &= \alpha_b = -2\pi \times 0.33\, \text{GHz}, \\
J_M &= 2\pi \times 16.0\, \text{MHz},
\end{align*}$$

with $J_M$ the maximum coupling. Thus, small deviations such as those shown in figure 1(b), shall be numerically corrected when designing the protocols to achieve maximum fidelity.

3. The CZ gate

The CZ gate is a universal two-qubit gate that is equivalent to other maximally entangling gates, such as the controlled-NOT operation, up to local transformations. Acting on the computational basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, the CZ operation only changes the phase of the last state $U_{\text{CZ}} = \text{diag}(1, 1, 1, -1)$ by a $\pi$-phase shift. This gate has been already experimentally demonstrated using tunable-frequency transmons qubits [2, 18, 35], and with transmons connected through a tunable coupler [19, 22, 24]. A recent work [29] showed that, among the different possible protocols that implement the gate, those inspired on invariants and variational methods lead to more experimentally friendly controls such as better properties of finite bandwidth and resilience to discretization, optimal control of leakage outside the computational basis, and a greater robustness against decoherence. Using quantum control, the performance of this gate can be improved independently of the control design by a proper optimization of the waiting time and destination frequency [29].

3.1. Design of the gate

We propose the use control techniques based on invariants to design a CZ gate with tunable-coupling transmons where $J(t)$ is the control. Within this approach, the entangling phase acting on the $|11\rangle$ state is achieved by the interaction with states outside of the computational basis—$|02\rangle$ and $|20\rangle$—in equation (10). Consequently, the designed protocols have to be particularly robust to avoid leakage.

The operation will be designed in three steps; (i) the coupling is switched on from the initial value $J(0) = 0$ to $J(T) = J_M$, (ii) the control remains constant during a waiting time $t_w$, (iii) the coupling is
switched off by reversing the ramp from step (i). The gate is implemented in a time $T_g = 2T + t_w$, see figure 2, and the shape of the ramps is determined by the quantum control method used to design the operation.

The design of the gate can be simplified by placing the transmons at different frequencies that ensure a quasi-resonance condition in the two-excitation subspace. If the two transmons are identical (same frequency and anharmonicity), the non-computational states $|02⟩$ and $|20⟩$ are degenerate, showing an avoided crossing behavior when the interaction is ‘on’. If instead, the frequency of the second qubit is set to $\omega_b = \omega_a + \alpha_a$, the $|11⟩$ and $|20⟩$ states are brought to degeneracy while the $|02⟩$ state is separated by an energy gap $|\alpha_a + \alpha_b|$. As result of such interaction, the $|11⟩$ computational state acquires an adjustable phase compatible with the implementation of a CZ gate [2, 35].

Under the resonant condition, the effective matrix Hamiltonian becomes block-diagonal:

$$
H(t) = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & \omega_a + \alpha_a & \tilde{J}_1(t) & 0 & 0 & 0 \\
0 & \tilde{J}_1(t) & \omega_a & 0 & 0 & 0 \\
0 & 0 & 0 & \Omega_2 & \tilde{J}_2(t) & 0 \\
0 & 0 & 0 & \tilde{J}_2(t) & \Omega_1 & \tilde{J}_3(t) \\
0 & 0 & 0 & 0 & \tilde{J}_3(t) & \Omega_1
\end{pmatrix},
$$

(12)

where $\Omega_1 = 2\omega_a + \alpha_a$ and $\Omega_2 = 2\omega_a + 2\alpha_a + \alpha_b$. The dynamics to implement a CZ gate can be studied separately in each subspace. We must require that the components of the state in $S_0$ and $S_1$ remain invariant, up to local phases, while the state $|11⟩ ∈ S_2$ is mapped back to itself with a $\pi$ shift.

The previous goal is achieved trivially in the $S_0$ subspace. Within $S_2$, provided there is an energy mismatch $\Delta E = |\alpha_a + \alpha_b| ≥ 20f_M$, the state $|02⟩$ decouples from the rest and the Hamiltonian becomes block-diagonal with $1 × 1$ and $2 × 2$ boxes:

$$
H(t) \approx \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & \tilde{J}_1(t) & 0 & 0 \\
0 & 0 & \Omega_2 & 0 \\
0 & 0 & 0 & \tilde{H}_2(t)
\end{pmatrix},
$$

(13)

The dynamics in the $\{|20⟩, |11⟩\}$ subsystem is now generated by a $2 × 2$ matrix

$$
\tilde{H}_2(t) = (2\omega_a + \alpha_a)I + \tilde{J}_3(t)\sigma_1,
$$

(14)

where $\sigma_1 = |20⟩⟨11| + |11⟩⟨20|$ represents the first Pauli matrix. The unitary transformation produced by Hamiltonian (14) along the path from figure 2 is

$$
\tilde{U}_3(T_g) = e^{-i(2\omega_a + \alpha_a)T_g} \exp \left[-i\tilde{J}_1(2\tilde{J}_3(T) + \tilde{J}_3(T)T_w)\right],
$$

(15)

with $\tilde{J}_3(t) = \int_0^T dt\tilde{J}_3(t)$. Regardless of the control shape $J(t)$, we need to adjust the waiting time to recover the desired final state (times a phase), i.e. $|11⟩ → e^{-i(2\omega_a + \alpha_b)T_g}(-|11⟩)$. The condition is

$$
t_w = (\pi - 2\tilde{J}_3(T))/\tilde{J}_3(T).
$$

(16)
Within the $S_1$ subspace, the dynamics is governed by

$$\dot{\hat{H}}_1(t) = \left( \omega_a + \frac{\alpha_a}{2} \right) I + \frac{\alpha_a}{2} \hat{\sigma}_3 + \tilde{J}_1(t) \hat{\sigma}_1,$$

(17)

where $\sigma_1 = |01\rangle \langle 10| + |10\rangle \langle 01|$ and $\sigma_3 = |01\rangle \langle 01| - |10\rangle \langle 10|$ represent the first and third Pauli matrices.

We discuss two strategies that preserve the state in $S_1$ by mapping the eigenstates $|01\rangle$ and $|10\rangle$ of $\hat{H}_1(0) = \hat{H}_1(T_0)$ back to themselves. The first strategy is based on the fast quasiadiabatic dynamics (FAQUAD) method [36], a technique to create adiabatic passages with short duration and low probability of unwanted excitations. The second strategy relies on the inverse-engineering of controls using invariants of motion [25, 26], a technique that achieves similar goals at a potentially faster speed.

### 3.2. FAQUAD passage

The fast quasiadiabatic dynamics method is a commonly used technique that aims at speeding up a given process while still making it as adiabatic as possible at all times. It relies on making the standard adiabaticity parameter constant such that the transition probability is equally delocalized during the whole process,

$$\mu(t) \equiv \left| \frac{\langle + (t) | \hat{H}_1 | - (t) \rangle}{E_+(t) - E_-(t)} \right|^2 = \mu,$$

(18)

where the dot represents the time derivative, $| + (t) \rangle$ and $| - (t) \rangle$ are the two instantaneous eigenstates of $\hat{H}_1(t)$ and $E_+(t)$ and $E_-(t)$ their respective eigenenergies. The process is considered to be adiabatic if $\mu \ll 1$. From equation (18) it follows (see appendix A)

$$\mu = \frac{\tilde{J}_1(t) \alpha_a}{\sqrt{4 \tilde{J}_1^2(t) + \alpha_a^2} \beta_a^2}.$$

(19)

Equation (19) can be integrated with the initial and final conditions $J(0) = 0$ and $J(T) = J_M$, which set a value for the integration constant and the adiabaticity parameter. The control is thus

$$\tilde{J}_1(t) = \frac{-\alpha_a \tilde{J}_1(T) t}{T \sqrt{\alpha_a^2 + 4 \tilde{J}_1^2(T) \left[ 1 - \left( \frac{t}{T} \right)^2 \right]}},$$

(20)

which has the same profile for every value of the ramp time $T$, since $\tilde{J}_1(t)$, as given by equation (20), is a function of $t/T$. However, it can be seen that the adiabaticity parameter obtained with this control is inversely proportional to $T$ (see appendix A) meaning that shorter times lead to ‘less adiabatic’ protocols and a corresponding loss of fidelity.

### 3.3. Invariants passage

We can obtain shorter operation times by inverse-engineering the control $\tilde{J}_1(t)$ with the invariants of motion [25, 26]. Associated with a Hamiltonian $\hat{H}_1(t)$, there are infinitely many time-dependent Hermitian invariants of motion $I(t)$ that satisfy [30]

$$\frac{d I(t)}{dt} = \frac{\partial I(t)}{\partial t} - \frac{i}{\hbar} [\hat{H}_1(t), I(t)] = 0.$$

(21)

A wave function $|\Psi(t)\rangle$ which evolves with $\hat{H}_1(t)$ can be expressed as a linear combination of invariant modes [30]

$$|\Psi(t)\rangle = \sum_n c_n e^{i \beta_n(t)} |\chi_n(t)\rangle$$

(22)

where the $c_n$ are constant, and the real phases $\beta_n$ fulfil

$$\hbar \dot{\beta}_n(t) = \langle \chi_n(t) | i \hbar \partial_t - \hat{H}_1(t) | \chi_n(t) \rangle,$$

(23)

and are explicitly computed in appendix C. The eigenvectors $|\chi_n(t)\rangle$ of the invariant are assumed to form a complete set and satisfy $I(t) |\chi_n(t)\rangle = \lambda_n |\chi_n(t)\rangle$, with $\lambda_n$ the corresponding constant eigenvalues.

The $\hat{H}_1$ Hamiltonian has SU(2) structure, $\hat{H}_1(t) = \sum_j \hat{h}_j(t) \hat{T}_j$ where $\hat{h}_j(t)$ are general controls of the Hamiltonian and $\hat{T}_j = \frac{1}{2} \hat{\sigma}_j$ are the Lie algebra generators satisfying $[\hat{T}_j, \hat{T}_k] = i \epsilon_{ijk} \hat{T}_l$, with $\epsilon_{ijk}$ the Levi-Civita
tensor. Assuming that the invariant is also a member of the dynamical algebra, it can be written as \( \hat{I}(t) = \sum_{j} f_j(t) \hat{T}_j \) where \( f_j(t) \) are real, time-dependent functions. A standard formalism [37] would lead to the requirement of a time-dependent anharmonicity \( \alpha_a(t) \). Instead, due to the structure of \( \hat{H}_I \), where \( (h_1, h_2, h_3) = (2f_1(t), 0, \alpha_a) \), we can make use of the dynamical algebra [38] to engineer the invariant of motion and, consequently, \( \hat{J}_I(t) \).

Replacing the closed forms of \( \hat{H}_I \) and \( \hat{I} \) into equation (21), the Hamiltonian controls \( h_j \) and the invariant’s time dependency \( f_j \) are related by a set of ordinary differential equation

\[
\dot{f}_j(t) - \frac{1}{R} \sum_{k} \sum_{l} \epsilon_{kl} h_k(t) f_l(t) = 0, \quad j = 1, 2, 3.
\]  

(24)

Usually, in these equations the functions \( f_j(t) \) are regarded as the unknown to be solved for a known set of controls \( h_j(t) \) [39–43]. We adopt here the opposite perspective, and focus on deriving the controls \( h_j(t) \) that engineer a particular evolution of the invariant \( f_j(t) \) [38].

For this approach to succeed, we need to complete equation (24) with an additional set of equations that express the relations between the invariant and the Hamiltonian at initial and final times. We know from equation (22) that the wave function is transitionless driven with respect to the instantaneous eigenstates of the invariant—i.e. the weights \( c_p \) are constant. This is an exact result, regardless of the duration of the drive \( T \), in contrast with a quasi-adiabatic driving, where shortening the controls leads to an increase in errors. We can use this property to ensure also a frictionless dynamics that maps the eigenstates of the Hamiltonian at initial time \( \hat{H}_I(0) \) to those at the end \( \hat{H}_I(T) \) [25, 26, 31]. This happens through an appropriate design of the invariant \( \hat{I}(t) \), imposing the so-called ‘frictionless conditions’, which ensure that \( \hat{I} \) and \( \hat{H}_I \) share a common basis of eigenstates at the boundary times [31]

\[ [\hat{H}_I(t_b), \hat{I}(t_b)] = 0, \quad t_b = 0, \quad T. \]  

(25)

As explained in appendix B, for our problem the inverse design and the frictionless conditions result in a suitable definition of just the \( f_1(t) \) function. As a first step, we realize that the system of equation (24) is compatible only if \( \sum_j f_j(t) = c^2 \), with arbitrary constant \( c^2 \). The choice \( c^2 = \sum_j h_j^2(0) = \alpha_a^2 \) leads to an invariant that trivially commutes at initial time \( \hat{I}(0) = \hat{H}_I(0) \). The resulting system (24) is now invertible and has infinite solutions reflecting the infinite invariants [44]. Given our control \( \hat{H}_I \), the coupling \( \hat{J}_I(t) \) is derived from the invariant \( f_1(t) \) (see appendix B) as

\[ J_I(t) = \frac{1}{2c^2 - f_1^2 - \left( \frac{\dot{f}_1}{\alpha_a} \right)^2} \left( \frac{\dot{f}_1}{\alpha_a} + \alpha_a f_1 \right). \]  

(26)

According to (25) and (26), \( f_1(t) \) must satisfy the frictionless boundary conditions

\[ f_1(t_b) = -2J_I(t_b) \sqrt{\frac{c^2}{4J_I(t_b) + \alpha_a^2}}, \quad \dot{f}_1(t_b) = J_I(t_b) = 0. \]  

(27)

Given a ramp-up control that starts as \( J_I(0) = 0 \) and grows up to its maximum value at \( J_I(T) \), we know the initial and final boundary conditions for \( f_1(t) \). In general, \( f_1(t) \) can adopt any dependency that preserves those conditions. For simplicity, we choose a polynomial ansatz \( f_1(t) = \sum_{m=0}^{M} a_m t^m \) which must contain at least \( M = 5 \) coefficients \( \{a_m\} \) to satisfy all six equation (27)—although additional constrains can be applied [45] with higher order polynomials. Note that once the ramp-up control is fixed, we immediately obtain controls in the waiting period \( J_I(\tau + T) = J_I(T), \tau \in [0, t_w] \), and also in the symmetric ramp-down, \( J_I(\tau + T + t_w) = J_I(T - \tau), \tau \in [0, T] \).

The resulting gate using either this method or the previous one is equivalent to a CZ gate up to local rotations in each individual qubit (see appendix D). However, as it will be shown in the following section, the control based on invariants of motions leads to a better driving of the states of the \( S_1 \) subspace, enabling higher fidelity gates.

4. Applications

Throughout this work, we have derived two types of controls for a CZ gate using an approximate model, in a reduced Hilbert space, neglecting higher-order corrections due to coupling to highly excited states. To gauge these approximations and appropriately judge the performance of those controls, we have simulated the
implementation of the CZ gates, using the full Hamiltonian given by (1) and (6), in a higher dimensional space with a cut-off controlled for convergence.

In doing the simulations, we expect three types of inaccuracies to arise as a result of using the whole system Hamiltonian instead of the reduced Hilbert space in which the derivations were made. The first type of errors is given by additional local phases that act on one qubit or the other, in such a way that they can be rectified by applying one qubit gates. We will neglect those correctable errors by extracting the effective dynamics $U_{\text{id}}$ from the full evolution $U(t)$. The second type of errors appears as deviations in the entangling phase

$$\phi^{12} = \frac{\phi_{00} - \phi_{01} - \phi_{10} + \phi_{11}}{4}. \quad (28)$$

This phase is computed from the individual phases $\phi_{ij}$ accumulated by the $|ij\rangle$ state, and should achieve the value $\pi/4$ for maximally entangling CZ gate, see appendix D. The third type of errors appears as changes in the populations of the computational states $|ij\rangle$, through excitations among them or, more likely, leakage outside the computational space.

As figure of merit that combines all errors and evaluates the performance of the gate, we use the average gate infidelity $1 - \mathcal{F}$. This quantity is obtained from the entanglement fidelity $\mathcal{F}_e$ as [46]

$$\mathcal{F} = \frac{N\mathcal{F}_e + 1}{N + 1}, \quad (29)$$

where N is the size of the Hilbert space ($N < \infty$ in a numerical simulation). The entanglement fidelity compares the final states resulting from the evolution $U(T_g)$ of each computational state with the ideal operation $U_{\text{id}}$ to be implemented. As explained above, we subtract the dynamics due to local phases $\hat{U}_{\text{loc}}^T$, leaving the entanglement fidelity as

$$\mathcal{F}_e[\hat{U}_{\text{id}}, \hat{U}(T_g)] = \frac{1}{4} \sum_{i=1}^{4} \langle s|\hat{U}_{\text{id}}^\dagger \hat{U}_{\text{loc}}^T \hat{U}(T_g) |s\rangle^2, \quad (30)$$

with $|s\rangle = 1, 2, 3, 4 := \{ |00\rangle, |01\rangle, |10\rangle, |11\rangle \}$.

4.1. Uncorrected gates

We now study the possibility of implementing the CZ gate and compare the performance of the gates obtained using the FAQUAD and invariants approaches. In figure 3(a) we show the average gate infidelity using both designs as a function of the total time taken by the operation. These curves are obtained by varying the ramp time $T$ from 1 to 8 nanoseconds and computing the waiting time $t_w$ using equation (16). Both FAQUAD and the invariant method achieve fidelities over 99.9%, with the invariant protocol giving slightly better results in general. The infidelity saturation at the same value, regardless of the applied control, is due to a common issue of both protocols: the driving of the $|11\rangle$ state is based on a coarse approximation, where a weak interaction with the $|02\rangle$ state has been ignored.

The infidelity is the result of (i) the phase $\phi^{12}$ deviating from its expected value, $\pi/4$, and (ii) the populations of states from the computational basis suffering from losses, such as undesired transfer to other states from the basis or even leakage outside of it, such that $\langle s|\hat{U}(T_g)|s\rangle < 1$. The phase deviation using the two kinds of control is shown in figure 3(b), while the population loss of each state is shown in figure 3(c). A common characteristic of controls based on shortcuts to adiabaticity, such as driving the states using dynamical invariants, is that they are minimally affected by leakage within the computational space. This characteristic can be observed in the minimal population loss suffered by the $|01\rangle$ and $|10\rangle$ states when using the invariants passage. By contrast, the population loss of these states when using the FAQUAD passage represents a limiting factor in the achieved fidelity. The results shown in these figures suggest that both the phase deviation from $\pi/4$ and the population losses are substantial sources of error that shall be mitigated. In particular, the population of the $|11\rangle$ state is saturating the infidelity curves. Since the driving of the $|11\rangle$ state does not depend on the shape of $J(t)$, only on its integral, the saturation value is the same regardless of the protocol. As we will see, this saturation of the infidelity does not correspond to a fundamental limitation and can be attributed to approximations in the reduced model and a Stark-shift produced in the $S_2$ subspace by the interaction between $|11\rangle$ and $|20\rangle$. We shall introduce higher energy corrections and adjust our protocols to increase the average fidelity.
Figure 3. Performance of the invariants (solid blue line) and FAQUAD (orange dashed line) controls producing a CZ gate as a function of the total duration, with a ramp time ranging from 1 to 8 ns. (a) Average infidelity of the CZ gate. (b) Deviation of the entangling phase $\varphi_{12}$ from its expected value, $\pi/4$. (c) Average population loss of the computational basis states.

4.2. Stark-shift corrected gates

With the argument $|\alpha_a + \alpha_b| \gtrsim 20 J_M$ to decouple the $|02\rangle$ state from the dynamics on the $S_2$ subspace, we found an analytical expression for the waiting time $t_w$, equation (16). This approximation may be reexamined to improve the performance of the protocols.

According to equation (12), the dynamics in the $S_2$ subspace is generated by a Hamiltonian that, up to a global shift of energy, reads

$$\hat{H}_2(t) = \begin{pmatrix} \alpha_a + \alpha_b & \tilde{J}_z(t) & 0 \\ \tilde{J}_z(t) & 0 & \tilde{J}_s(t) \\ 0 & \tilde{J}_s(t) & 0 \end{pmatrix}.$$  \hspace{1cm} (31)

The low-energy effective Hamiltonian within the lin $\{|11\rangle, |20\rangle\}$ subspace can be more accurately derived using a Schrieffer–Wolff transformation [47]. The derivation from appendix E leads to

$$\hat{H}_2^{SW} = \begin{pmatrix} \delta\Omega & \tilde{J}_s + \delta\tilde{J}_s \\ \tilde{J}_s + \delta\tilde{J}_s & 0 \end{pmatrix},$$  \hspace{1cm} (32)

where the time dependence has been dropped for simplicity, and

$$\delta\Omega = \tilde{J}_z \frac{\alpha_a + \alpha_b}{\tilde{J}_s - (\alpha_a + \alpha_b)^2},$$  \hspace{1cm} (33)

$$\delta\tilde{J}_s = -\frac{1}{2} \frac{\tilde{J}_z \tilde{J}_s}{\tilde{J}_s - (\alpha_a + \alpha_b)^2}.$$  \hspace{1cm} (34)
The interaction between the $|11\rangle$ and $|02\rangle$ states manifests as a Stark shift $\delta\Omega$ in the energy of $|11\rangle$. The effect of $H_\text{SW}^1$ acting on the $|11\rangle$ state can be visualized using the Bloch sphere with antipodal points corresponding to the pseudospin states $|11\rangle$ and $|20\rangle$. In this representation, the shift $\delta\Omega$ misaligns the rotation axis preventing a perfect $|11\rangle \leftrightarrow |20\rangle$ swap—this effect is magnified in the Bloch sphere from figure 4 for a clearer visualization. The Stark shift causes a reduction in the amplitude and the period of the Rabi oscillations. In terms of our reduced Hamiltonian model, this speed-up leads to a small deviation in the waiting time as compared to equation (16). This explains the relatively high leakage of the $|11\rangle$ state in figure 3(c), regardless of the control method. It also accounts for deviations in the $\phi_{11}$ phase and in the entangling phase $\varphi^{12} \neq \pi/4$.

Figure 3(b) shows that we cannot fix these errors by tuning the waiting time $t_w$, as this would lead to very slow CZ gates, because of the slow phase rate $\sim \mu$s. However, both the population loss of the state $|11\rangle$ and $\varphi^{12}$ can be simultaneously corrected by introducing a slight detuning in the second qubit, $\omega_b = \omega_x + \alpha_a + \Delta$, where $|\Delta| \ll J_2(T), J_3(T)$, which sets the $|11\rangle$ state to rotate along the time dependent axis $(J_3 + \delta J_3)\vec{u}_z + (\Delta + \delta\Omega)\vec{u}_z/2$, see appendix E. First, the symmetry of the protocols (see figure 2) allows us to always perfectly recover the $|11\rangle$ state with an appropriate waiting time, independently of $\Delta$. Second, adjusting numerically $t_w$ reduces the population loss caused by deviations of the effective model from the complete Hamiltonian. Third and equally important, the fine-tuning of $\Delta$ enables adjusting $\varphi^{12}$, even if $\delta\Omega$ is in fact time-dependent. It must be remarked that the detuning $\Delta$ also affects the $S_1$ subspace. In full rigor, the designed protocols must be corrected by substituting $\alpha_a \rightarrow \alpha_a + \Delta$ in equations (20) and (26). In practice, provided $|\Delta| \ll |\alpha_a|$, the controls barely change.

In figure 5 we show the results correcting the FAQUAD and invariant protocols, by numerically optimizing both the detuning $\Delta$ and the waiting time $t_w$ to minimize the gate infidelity. The simulation assumes ramp times $T$ between 1 and 8 ns, leading to fast gate times between 26 and 34 ns. Figure 5(a) shows a drastic improvement of the gate fidelity. This improvement is most remarkable in the protocol derived using invariants of motion, where the fidelity is not limited by the population loss of states $|01\rangle$ and $|10\rangle$. This figure shows the great potential of non-adiabatic protocols over adiabatic processes, in which $T \rightarrow \infty$ is required for a truly faultless transition between the eigenstates of the instantaneous Hamiltonian. In figure 5(b) we show the deviations in the entangling phase deviation are also corrected with this method, which leaves the population losses as the main source of errors.

Figure 5(c) shows the optimal detuning of both controls as a function of the gate time. Notice that, even though $\delta\Omega$ is positive for the chosen range of parameters, the detuning is also positive. Given equation (32), this may seem counter-intuitive, but it is actually compatible with all our derivations. The detuning not only affects the phase of the $|11\rangle$ state, $\phi_{11}$, but also $\phi_{01}$ and $\phi_{10}$ by approximately the same amount. Thus, a correction in the $\phi_{11}$ phase leads to approximately the same correction in $\varphi^{12}$ with opposite sign, see equation (28). The detuning is about the same order and sign as the mean value of $\delta\Omega$ over the whole process, which confirms our assumption $|\Delta| \ll |\alpha_a|$. Achieving such a high level of accuracy in the transmon frequencies (in the order of the MHz) would require improved fabrication techniques, using for instance laser-annealing [48] to reach scalability in fixed-frequency architectures.
5. Conclusions

To sum up, we demonstrate the possibility of implementing a CZ gate using a control protocol that exploits dynamical invariants of motion to drive the states frictionlessly in a system of two transmons and a tunable coupler. The designed control takes advantage of having the coupling strength at its maximum value during most of the gate time, accelerating the processes close to their speed limits. This method has been compared with the adiabatic process, showing that the method based on invariants leads to an overall better performance for any gate time. The protocol was found analytically using a simplified effective Hamiltonian that describes the lowest six energy levels of the two-transmon system. We then numerically adjusted the waiting time and the destination frequency of the qubits—slightly out of the avoided crossing between $|11\rangle$ and $|02\rangle$—to correct higher order errors coming from the Stark shift produced by the $|20\rangle$ state. With these corrections, the invariants method achieves infidelities 2 to 3 orders of magnitude lower than the adiabatic protocol.

The demonstration of such a high fidelity CZ gate shows the viability of the theory of dynamical invariants to construct fast diabatic gates in a tunable-coupling qubit architecture. Short gate times, low losses, and reported greater robustness to decoherence make control protocols designed using the theory of dynamical invariants superior candidates for implementing fast and high-fidelity quantum gates in existing setups.

**Data availability statement**

The data that support the findings of this study are available upon reasonable request from the authors.

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Appendix A. Design of FAQUAD passage

After shifting the zero of energy, Hamiltonian $\hat{H}_1(t)$ from equation (17) can be written in matrix form as

$$
\hat{H}_1(t) = \left( \begin{array}{cc} \frac{\alpha_a}{2} & \tilde{J}_1(t) \\ \tilde{J}_1(t) & -\frac{\alpha_a}{2} \end{array} \right). 
$$

(A.1)

The instantaneous eigenstates of this Hamiltonian are

$$
| + \rangle (t) = \begin{pmatrix} \cos \theta(t) \\ -\sin \theta(t) \end{pmatrix}, \quad | - \rangle (t) = \begin{pmatrix} \sin \theta(t) \\ \cos \theta(t) \end{pmatrix},
$$

(A.2)

where $\theta(t) = \arctan \left( \frac{\tilde{J}_1(t)}{\alpha_a} \right)$. Thus, we find

$$
\langle + | \dot{\hat{H}}_1 | - \rangle = \frac{\tilde{J}_1(t) \alpha_a}{2 \sqrt{\frac{\alpha_a^2}{4} + \tilde{J}_1^2(t)}}.
$$

(A.3)

The energy associated with each eigenstate is

$$
E_{\pm}(t) = \pm \sqrt{\left( \frac{\alpha_a}{2} \right)^2 + \tilde{J}_1^2(t)},
$$

(A.4)

and using equation (18), we get

$$
\mu = \frac{\tilde{J}_1(t) \alpha_a}{\sqrt{4\tilde{J}_1^2(t) + \alpha_a^2}}.
$$

(A.5)

Integrating both sides of the equation, we find

$$
\mu t + c_0 = \frac{\tilde{J}_1(t)}{\alpha_a \sqrt{4\tilde{J}_1^2(t) + \alpha_a^2}}^{1/2},
$$

(A.6)

where $c_0$ is an integration constant. The previous equation can be inverted into

$$
\tilde{J}_1(t) = -\alpha_a \sqrt{\frac{(\mu t + c_0)^2}{1 - 4\alpha^2 (\mu t + c_0)^2}}.
$$

(A.7)

Finally, using the boundary conditions on $\tilde{J}_1(t)$ at $t = 0$ and $t = T$, we find the value of $c_0$ and $\mu$

$$
c_0 = 0, \quad \mu = \frac{\tilde{J}_1(T)}{T \alpha_a} \frac{1}{\sqrt{4\tilde{J}_1^2(T) + \alpha_a^2}}.
$$

(A.8)

Putting it altogether leads to

$$
\tilde{J}_1(t) = \frac{-\alpha_a \tilde{J}_1(T) t}{T \sqrt{\alpha_a^2 + 4\tilde{J}_1^2(T) \left[ 1 - \left( \frac{t}{T} \right)^2 \right]}}.
$$

(A.9)
Appendix B. Inverse engineering of the controls

The set of equation (24) can be represented matricially

\[
\begin{pmatrix}
\dot{f}_1 \\
\dot{f}_2 \\
\dot{f}_3
\end{pmatrix} = \frac{1}{\hbar} \begin{pmatrix}
f_0 & -f_2 & h_f^2 \\
0 & f_3 & -f_2 \\
-f_2 & 0 & h_f^1
\end{pmatrix} \begin{pmatrix}
h_1 \\
h_2 \\
h_3
\end{pmatrix}.
\]  

(B.1)

As \(A = -A^\dagger\) is a real antisymmetric matrix and with odd dimensionality, the eigenvalues are conjugate pure imaginary pairs, and zero, \(a^{(0)} = 0, a^{(1)} = -i\sqrt{\gamma}/\hbar,\) and \(a^{(2)} = i\sqrt{\gamma}/\hbar\) with \(\gamma = f_1^2 + f_2^2 + f_3^2\). As \(a^{(0)} = 0\) then \(\det(A) = 0\), there is no inverse matrix \(A^{-1}\). However, we can still invert the system, for example using Gauss elimination, to reduce the system to an equivalent one with the same solutions applying elementary operations. These are the multiplication of a row by a non-zero scalar, the interchange of columns or rows, and the addition to a row of the multiple of a different one. The augmented matrix of (B.1) is

\[
\begin{pmatrix}
-f_3 & 0 & f_1 & h_f^2 \\
0 & f_3 & -f_2 & h_f^1 \\
-f_2 & 0 & 0 & h_f^3
\end{pmatrix}.
\]  

(B.2)

After some algebra the system can be written as a lower triangular matrix,

\[
\begin{pmatrix}
-f_3 & 0 & f_1 & h_f^2 \\
0 & f_3 & -f_2 & h_f^1 \\
0 & 0 & 0 & h_f^3
\end{pmatrix}.
\]  

(B.3)

This system is compatible and has infinite solutions if and only if \(f_1h_1 + f_2h_2 + f_3h_3 = 0\) or, equivalently, \(f_1^2 + f_2^2 + f_3^2 = c^2\). The solutions satisfy

\[h_f^1 = f_2h_2 - f_3h_1,\]

\[h_f^2 = -f_3h_1 + f_1h_3,\]

(B.4)

or in a compact form

\[h_i = -\hbar c_{ij} \frac{\dot{f}_j}{f_k} + \frac{\dot{f}_i}{f_k} h_k,\]

(B.5)

with all indices \(i, j, k\) different. \(h_k(t)\) is considered a free function chosen for convenience, for example, making it zero if we want to cancel the \(h_k\) control of the Hamiltonian.

Our aim is to find \(H_1(t) = \frac{2}{\hbar} \sigma_3 + \dot{f}_1(t) \sigma_1\) so that the ground and excited states of \(\hat{H}_1(0)\) become the ground and excited states of \(\hat{H}_1(T)\) in an arbitrary time \(T\), up to phase factors, in such a way that \(h_3(t) = 0, h_3(t) = \alpha_a \forall t\). Choosing \((i, j, k) = (3, 1, 2)\) in equation (B.5) and using \(\gamma = c^2\) we can express \(f_3\) and \(f_2\) in terms of \(f_1\),

\[f_2 = \frac{\dot{f}_1}{\alpha_3},\]

\[f_3 = \sqrt{c^2 - f_1^2 - \frac{\dot{f}_1^2}{\alpha_3^2}}.\]

(B.6)

Substituting this in the other equation of equation (B.5), with \((i, j, k) = (1, 3, 2)\),

\[h_1(t) = \frac{1}{\sqrt{c^2 - f_1^2 - \frac{\dot{f}_1^2}{\alpha_3^2}}} \left( \frac{\dot{f}_1}{\alpha_3} + \alpha_a f_1 \right),\]

(B.7)

leading to \(\dot{h}_1(t) = h_1(t)/2\).

The ‘frictionless conditions’ \([\hat{H}(t_0), \hat{I}(t_0)] = 0\) for a closed Lie algebra of \(\hat{H}\) and \(\hat{I}\) can be reformulated as

\[\sum_{j,k,l}^{N} \epsilon_{jkl} h_k(t_0) f_l(t_0) T_j = 0.\]

(B.8)
Since the $\hat{T}_j$ generators are independent, the coefficients must satisfy

$$\sum_{k,l}^3 \epsilon_{jkl} h_k(t_b) f_l(t_b) = 0, \quad j = 1, \ldots, 3, \quad t_b = 0, T. \quad (B.9)$$

For $\hat{H}_I(t)$, having $h_2(t) = 0$ and $h_3(t) = \alpha_{a_0}$ these conditions read $f_2(t_b) = 0$ and $\alpha_{a_0}/h_1(t_b) = f_3(t_b)/f_1(t_b)$ or, equivalently with the help of (B.6),

$$f_1(t_b) = -h_1(t_b) \sqrt{\frac{\epsilon^2}{h_1^2(t_b) + \alpha_{a_0}^2}}, \quad \hat{f}_I(t_b) = 0. \quad (B.10)$$

In addition, from equation (B.7) at the boundary times $t_b$,

$$\hat{f}_I(t_b) = 0. \quad (B.11)$$

We then interpolate $f_1(t)$ with a simple polynomial $f_1(t) = \sum_{\ell=0}^3 a_\ell t^\ell$ where the $a_\ell$ coefficients are determined from equations (B.10) and (B.11), or following some more sophisticated approach, e.g. to optimize some additional constraint, and construct the control $\hat{f}_I(t)$ using equation (B.7).

**Appendix C. The Lewis-Riesenfeld phase**

During the ramp-up and down the Lewis-Riesenfeld phase $\beta_n$ accumulated by the states, see equation (23) is fully determined by the ramp time $T$ and the particular election of the invariant auxiliary function $f_1(t)$. Since the ramp-up and down processes are symmetric, meaning that the control at $t_w + T + t$ is identical to itself at $T - t$, the term coming from the time derivative in the Lewis-Riesenfeld phase has the opposite sign at each ramp, meaning that this term gets cancelled when the whole operation is performed. Therefore,

$$\beta_n^{\text{tot}} = \beta_n^{\text{up}} + \beta_n^{\text{down}} = -2 \int_0^T dt \langle \chi_n(t) | \hat{H}(t) | \chi_n(t) \rangle. \quad (C.1)$$

The eigenvectors and eigenvalues of the invariant $\hat{I}(t) = \sum_{\ell=1}^3 f_\ell(t) \frac{\sigma_\ell}{2}$ with $\sum_{\ell=1}^3 f_\ell(t) = \epsilon^2$ acting on the $S_1 = |01\rangle, |10\rangle$ subspace are

$$|\chi_{\pm}\rangle = \frac{1}{\sqrt{2\epsilon \pm \epsilon}} \left[ (f_3 \pm \epsilon) |01\rangle + (f_1 + if_2) |10\rangle \right],$$

$$\lambda_{\pm} = \pm \frac{\epsilon}{2}, \quad (C.2)$$

with $|\chi_+\rangle = |\chi_{|10\rangle}\rangle$ and $|\chi_-\rangle = |\chi_{|01\rangle}\rangle$. Replacing (C.2) into equation (C.1) with $h_1(t) = 2\hat{I}_1(t)$, $h_2(t) = 0$ and $h_3(t) = \alpha_{a_0}$ we finally find

$$\beta_n^{\text{tot}} = \frac{2}{|\alpha_{a_0}|} \int_0^T dt \left( 2f_1\hat{I}_1 + f_3 \frac{\alpha_{a_0}}{2} \right). \quad (C.3)$$

**Appendix D. Effective gate**

In principle, due to different phases accumulated by each of the computational states, with the described procedure we do not get a CZ gate, but instead a transformation that, acting on the computational basis, is given by the unitary matrix

$$\hat{U} = \begin{pmatrix}
\phi_{00} & 0 & 0 & 0 \\
0 & \phi_{01} & 0 & 0 \\
0 & 0 & \phi_{10} & 0 \\
0 & 0 & 0 & \phi_{11}
\end{pmatrix}. \quad (D.1)$$

In fact, this would only correspond to a CZ gate if $\phi_{00} = \phi_{01} = \phi_{10} = 0$ and $\phi_{11} = \pi$. An alternative way of writing equation (D.1) is

$$\hat{U} = \exp[i(\phi^0 \sigma_0 \otimes I + \phi^1 \sigma_0 \otimes I \otimes \sigma_3 + \phi^{12} \sigma_3 \otimes \sigma_3)]. \quad (D.2)$$
ϕ^0 represents a global phase, while ϕ^1 and ϕ^2 are local phases that can be corrected at each qubit using one-qubit gates. ϕ^{12} is the entangling phase resulting from the interaction between the two qubits. Each of these phases can be written in terms of \{ϕ_q\}. In particular, the entangling phase,

ϕ^{12} = \frac{ϕ_{00} - ϕ_{01} - ϕ_{10} + ϕ_{11}}{4}. \hspace{1cm} (D.3)

Equations (D.2) and (28) reveal that the unitary transformation given by equation (D.1) can be turned into a CZ gate by applying additional one qubit gates only if ϕ^{12} = π/4.

Let us explicitly calculate the entangling phase. According to the Hamiltonian (12) the state |00⟩ is left completely unchanged (ϕ_{00} = 0). Independently of the type of passage, FAQUAD or invariants, the states |01⟩ and |10⟩ acquire the following phases

ϕ_{01} = -\left(\frac{\omega_a}{2} + \frac{\alpha_a}{2}\right) T_x - \Omega t_x - 2 \int_0^T dt \langle \hat{H}_1(t) \rangle_{|01⟩}, \hspace{1cm} (D.4)

ϕ_{10} = -\left(\frac{\omega_a}{2} + \frac{\alpha_a}{2}\right) T_x + \Omega t_x - 2 \int_0^T dt \langle \hat{H}_1(t) \rangle_{|10⟩}, \hspace{1cm} (D.5)

where Ω′ = \sqrt{\left(\alpha_a/2\right)^2 + \hat{J}_1(T)^2}, and \langle \hat{H}_1(t) \rangle_{|nm⟩} is the expectation value of the S₁ Hamiltonian at time t when the state is initially |nm⟩. This expectation value depends on the design of the control, since in the FAQUAD passage the states evolves approximately as the instantaneous eigenstates of \hat{H}_1(t), while in the invariants passage, they coincide with the eigenstates of \hat{I}(t). However, in both cases \langle \hat{H}_1(t) \rangle_{|01⟩} + \langle \hat{H}_1(t) \rangle_{|10⟩} = 0, cancelling their contribution to the entangling phase. Finally, from equation (15), the state |11⟩ acquires a phase

ϕ_{11} = -(2ω_a + α_a) T_x + π. \hspace{1cm} (D.6)

Thus, inserting these results into equation (28) we find that ϕ^{12} is precisely equal to π/4. Consequently, the designed protocols produce a transformation which, after local rotations on each of the qubits, is equivalent to a CZ gate.

Appendix E. Schrieffer–Wolff transformation

The Schrieffer–Wolff transformation is a unitary transformation used to diagonalize a given Hamiltonian to first perturbative order in the interaction. It is often used to project out the high (low) energy excitations of a given quantum many-body Hamiltonian in order to obtain an effective low (high) energy model. The transformation is conventionally written as

\hat{H}' = e^{\hat{S}}He^{-\hat{S}}, \hspace{1cm} (E.1)

where \hat{S} is the generator of the transformation and \hat{H} is a Hamiltonian that can be written as

\hat{H} = \hat{H}_0 + \hat{V}, \hspace{1cm} (E.2)

with \hat{H}_0 being block-diagonal and \hat{V} purely off-diagonal in the eigenbasis of \hat{H}_0. In our particular case, the starting point is the S₂ subspace Hamiltonian that corresponds to the block of equation (12)

\hat{H}_2(t) = \begin{pmatrix} \alpha_a + \alpha_b + 2\Delta & \tilde{J}_2(t) & 0 \\ \tilde{J}_2(t) & \Delta & \tilde{J}_3(t) \\ 0 & \tilde{J}_3(t) & 0 \end{pmatrix}, \hspace{1cm} (E.3)

where we have included the second qubit detuning \omega_b = \omega_a + \Delta and the zero energy has been shifted. We chose

\hat{H}_0 = \begin{pmatrix} \alpha_a + \alpha_b + 2\Delta & 0 & 0 \\ 0 & \Delta & \tilde{J}_3 \end{pmatrix}, \hspace{1cm} (E.4)

and

\hat{V} = \begin{pmatrix} 0 & \tilde{J}_2 & 0 \\ \tilde{J}_2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \hspace{1cm} (E.5)
with the time-dependence notation dropped for simplicity. The transformation can be expanded in \( \hat{S} \) using the Baker-Campbell-Haussdorf formula

\[
\hat{H}' = \hat{H}_0 + \hat{V} + \left[ \hat{S}, \hat{H}_0 \right] + \left[ \hat{S}, \hat{V} \right] + \frac{1}{2} \left[ \hat{S}, \left[ \hat{S}, \hat{H}_0 \right] \right] + \cdots.
\]

(E.6)

The Hamiltonian can then be made diagonal to first order in \( \hat{V} \) by choosing the generator \( \hat{S} \) such that

\[
\left[ \hat{S}, \hat{H}_0 \right] = -\hat{V},
\]

(E.7)

so that the off-diagonal terms are cancelled to the first order in the perturbation. The difficult step is the computation of the generator of the Schrieffer–Wolff transformation. The method presented in [49] to calculate the generator starts by calculating the commutator \( \left[ \hat{H}_0, \hat{V} \right] \) and replace every non-zero matrix element of the commutator by undetermined coefficients. Then, those coefficients are computed using equation (E.6). Using from the commutator of (E.4) and (E.5), the generator takes the form

\[
\hat{S} = \begin{pmatrix}
0 & a_1 & a_2 \\
-a_1 & 0 & 0 \\
-a_2 & 0 & 0
\end{pmatrix}.
\]

(E.8)

Using the condition (E.6), the coefficients are found to be

\[
a_1 = \frac{\tilde{J}_2 (\alpha_a + \alpha_b + 2\Delta)}{-\tilde{J}_3 + (\alpha_a + \alpha_b + \Delta)(\alpha_a + \alpha_b + 2\Delta)},
\]

(E.9)

\[
a_2 = \frac{\tilde{J}_2 \tilde{J}_3}{\tilde{J}_3 - (\alpha_a + \alpha_b + \Delta)(\alpha_a + \alpha_b + 2\Delta)}.
\]

(E.10)

Finally, the effective Hamiltonian is calculated using the first order of the BCH formula from the exponential expansion,

\[
\hat{H}' = \hat{H}_0 + \frac{1}{2} \left[ \hat{S}, \hat{V} \right],
\]

(E.11)

which gives

\[
\hat{H}' = \begin{pmatrix}
\alpha_a + \alpha_b + 2\Delta - \delta\Omega & 0 & 0 \\
0 & \Delta + \delta\Omega & \tilde{J}_3 + \delta\tilde{J}_3 \\
0 & \tilde{J}_3 + \delta\tilde{J}_3 & 0
\end{pmatrix},
\]

(E.12)

where

\[
\delta\Omega = \frac{\tilde{J}_2 (\alpha_a + \alpha_b + 2\Delta)}{\tilde{J}_3 - (\alpha_a + \alpha_b + \Delta)(\alpha_a + \alpha_b + 2\Delta)},
\]

(E.13)

\[
\tilde{\delta}\tilde{J}_3 = -\frac{1}{2} \frac{\tilde{J}_2 \tilde{J}_3}{\tilde{J}_3 - (\alpha_a + \alpha_b + \Delta)(\alpha_a + \alpha_b + 2\Delta)},
\]

(E.14)

and generalizes (32) in the presence of a detuning \( \Delta \).

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