Implementing High-fidelity Two-Qubit Gates in Superconducting Coupler Architecture with Novel Parameter Regions

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Superconducting circuits with coupler architecture receive considerable attention due to their advantages in tunability and scalability. Although single-qubit gates with low error have been achieved, high-fidelity two-qubit gates in coupler architecture are still challenging. This paper pays special attention to examining the gate error sources and primarily concentrates on the related physical mechanism of ZZ parasitic couplings using a systematic effective Hamiltonian approach. Benefiting from the effective Hamiltonian, we provide simple and straightforward insight into the ZZ parasitic couplings that were investigated previously from numerical and experimental perspectives. The analytical results obtained provide exact quantitative conditions for eliminating ZZ parasitic couplings, and trigger four novel realizable parameter regions in which higher fidelity two-qubit gates are expected. Beyond the numerical simulation, we also successfully drive a simple analytical result of the two-qubit gate error from which the trade-off effect between qubit energy relaxation effects and ZZ parasitic couplings is understood, and the resulting two-qubit gate error can be estimated straightforwardly. Our study opens up new opportunities to implement high-fidelity two-qubit gates in superconducting coupler architecture.

I. BACKGROUND AND MOTIVATION

Benefiting from the development of nano-technology and mature complementary metal-oxide-semiconductor technology, superconducting circuits become a promising hardware candidate for quantum computing [1–3]. In the past few years, significant progress has been achieved in this field, including not only the remarkable improvements of qubits’ quantity and quality [4–7], but also the realizations of some meaningful noisy intermediate-scale quantum applications [8–12].

To execute various and complex quantum tasks, quantum hardware with many superconducting qubits has to be developed. In addition to qubits’ quality, a natural problem followed is qubit architecture, namely the way of connecting different qubits. According to different purposes, various types of qubit architecture were designed and studied. The simplest one is to connect two adjacent qubits directly via either a capacitor [13] or an inductor [14, 15]. The corresponding qubits’ topological structure can be one dimensional or two-dimensional grid [16, 17]. Such kinds of architectures were used frequently to explore various exciting problems, e.g., demonstration of Greenberger–Horne–Zeilinger state using the full set of gates [16], verification of surface codes for quantum error correction [17], and so on. An alternative way to connect qubits is to couple different qubits via a common resonator (named as a “quantum bus”) [18–22]. In such indirect coupling architecture, multicomponent atomic Schrödinger cat states were realized [20], and intriguing physics of quantum many-body systems were simulated [21, 22].

In the typical architectures mentioned above, the unavoidable problem is that the neighboring qubits will suffer from crosstalk. Moreover, even if the qubit’s frequency is tuned away from others (so that the crosstalk can be suppressed), we will still encounter the frequency crowing problem. To overcome this difficulty, some novel qubit architectures were designed and studied. In 2014, Gmon was firstly proposed in Ref. [23]. It overcomes the challenge of incorporating tunable coupling with high coherence devices [24]. Very recently, one simple and generic architecture with an additional qubit (named as “coupler”) attract wide attention and become the research forefront of superconducting circuits [25–38]. The impressive achievement is that such architecture made great success in Google’s quantum supremacy experiment [4]. In the quantum processor, each qubit is connected to its neighboring qubits using an adjustable coupler. Tunable coupling and relatively higher fidelity quantum gates were realized. In particular, the coupling strengths were able to be tuned continuously from −40 MHz to 5 MHz, and the average single-qubit gate error can be reached as lower as 0.15%. However, realizing fault-tolerant quantum computing [39] with coupler architecture is still out of reach because of the overhead needed for error-correction with state-of-the-art two-qubit gate performance. One of the main reasons for the slow progress in improving two-qubit gate fidelity could be an incomplete understanding of the gate error mechanism. While some previous work mainly concentrates on the tunable coupling effects and ZZ coupling characteristics between computational qubits [25–28, 33–35], other essential problems are less explored. For instance, what are the error sources of two-qubit gates and the corresponding physical mechanism behind? How does the higher energy level of the coupler affect the resulting gate fidelity? What is the optimized gate fidelity using this architecture? Could we find some alternative parameter regions or schemes whose gate performances are better than the traditional ones? To better understand

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and solve these problems, we focus on studying ZZ parasitic coupling mechanism and exploring novel parameter regions, which may advance the technology of large-scale coupler architecture.

This paper concentrates on exploring the physical mechanism of two-qubit gate error sources from the effective Hamiltonian perspective. As the primary error source for the targeted gate, we pay special attention to the characteristics and physical mechanisms of ZZ parasitic couplings [26, 28, 30, 31, 40, 41]. Interestingly and surprisingly, we find some novel parameter regions in which high-fidelity two-qubit gates are expected. The main contributions and findings of this work are summarized as follows: i) we provide clear and straightforward understandings to the physical mechanism of ZZ parasitic coupling in coupler architecture. Using the effective Hamiltonian derived, the physical processes that describe different parametric coupling can be explained clearly. To the author’s knowledge, this is the first time to find the physical mechanism of ZZ parasitic couplings from the effective Hamiltonian perspective which usually contains richer physics than other methods; ii) using the analytical results obtained in this paper, some impressive results of previous work [27, 28, 34, 42] can be explained and the related physical mechanism can be understood. More importantly, four unexplored parameter regions are inspired for eliminating ZZ parasitic coupling. The physical mechanism for ZZ coupling elimination is: the coupler’s high energy level can be used to neutralize the energy shift induced by computational qubits’ high energy level; iii) we demonstrate high-fidelity two-qubit gates are realizable using our suggested parameter regions. Beyond numerical simulations, an analytical expression is derived for the two-qubit gate error. As applications, it can be applied to estimate the average gate error of superconducting quantum processor with coupler architecture conveniently.

The remainder of this paper is organized as follows. We start from the system Hamiltonian in lab frame and derive the effective Hamiltonian using Schrieffer-Wolf transformation (SWT) [43] in Sec. II. With the help of the resulting effective Hamiltonian, the physical mechanisms of ZZ parasitic couplings are discussed and analyzed in Sec. III. In Sec. IV, inspired by the analytical results, we propose four novel parameter regions in which ZZ parasitic couplings are expected to be eliminated. As a further step, we also suggest some possible experimental realization to achieve high-fidelity two-qubit gates. Involving different types of noises, we study the gate error characteristics using the suggested parameter regions in Sec. V; moreover, the tradeoff effects between energy relaxation effect and parasitic couplings are discussed as well. We conclude in Sec. VI and give some technical details in Appendices.

II. COUPLER ARCHITECTURE AND EFFECTIVE HAMILTONIAN

As shown in Fig. 1, our studied architecture consists of two computational qubits (q1 and q2, solid circles), which has a direct coupling g_{12}. An auxiliary qubit is introduced as a coupler (c, dashed circle) to interact with each computational qubit, which will generate an effective indirect coupling. Both computational qubits and coupler are modelled by Duffing oscillators [44], the Hamiltonian in lab frame describes the coupler architecture consists of three parts:

\[
\hat{H}_{\text{Lab}} = \hat{H}_0 + \hat{H}_{qq} + \hat{H}_{qc}
\]  

with

\[
\hat{H}_0 = \sum_{\lambda=q_1,q_2,c} \omega_{\lambda} \hat{a}_\lambda^\dagger \hat{a}_\lambda + \frac{\alpha_{\lambda}}{2} \hat{a}_\lambda^\dagger \hat{a}_\lambda^\dagger \hat{a}_\lambda \hat{a}_\lambda,
\]

\[
\hat{H}_{qq} = g_{12} \left( \hat{a}_{q_1}^\dagger \hat{a}_{q_2} + \hat{a}_{q_1} \hat{a}_{q_2}^\dagger - \hat{a}_{q_1}^\dagger \hat{a}_{q_2} - \hat{a}_{q_1} \hat{a}_{q_2}^\dagger \right),
\]

\[
\hat{H}_{qc} = \sum_{k=1,2} g_k \left( \hat{a}_{q_k}^\dagger \hat{a}_c + \hat{a}_{q_k} \hat{a}_c^\dagger - \hat{a}_{q_k}^\dagger \hat{a}_c - \hat{a}_{q_k} \hat{a}_c^\dagger \right),
\]

where \(\hat{H}_0\) describes the free energy of these three subsystems, \(\omega_{\lambda}\) and \(\alpha_{\lambda}\) (\(\lambda = q_1, q_2, c\)) are the frequency and anharmonicity of the subsystem \(\lambda\), respectively. The operators \(\hat{a}_\lambda\), \(\hat{a}_\lambda^\dagger\) are annihilation and creation operators for each qubit. \(\hat{H}_{qq}\) represents the direct coupling between two computational qubits, and \(g_{12}\) is the coupling strength. \(\hat{H}_{qc}\) means the couplings between computational qubits and coupler, and \(g_1\), \(g_2\) is the corresponding coupling strength. It is noticeable that we keep not only the usual Jaynes-Cummings interaction terms but also the counter-rotating terms in \(\hat{H}_{\text{Lab}}\). This is because the couplings among the three subsystems are usually charge-charge couplings; all of these terms should be involved when one expends the charge operators in terms of annihilation and creation operators.

![Fig. 1. Two computational qubits (q1 and q2, solid circles) are connected directly with a coupling strength g_{12}. Besides, a coupler (c, dashed circle), usually realized with a qubit, is introduced to connect the two qubits indirectly. Benefiting from the interference effect between these two different coupling paths, the effective coupling g_{eff} between two computational qubits becomes tunable. More importantly, g_{eff} is allowed to be tuned off if necessary.](image-url)
terference between the direct and indirect coupling of two computational qubits, so the first and foremost task is to derive the effective indirect coupling. Since we mainly concentrate on two-qubit gates realized between $q_1$ and $q_2$, an approach to decouple the coupler from the whole system is required. As a perturbed method, SWT is applied to adiabatically eliminate qubit-coupler couplings and work out the indirect coupling. In particular, the system Hamiltonian in lab frame is transformed to, 

$$
\hat{H}_{\text{eff}} = e^{\hat{s}_1} \hat{H}_{\text{lab}} e^{-\hat{s}_1}, \quad \hat{H}_2^{\text{eff}} = e^{\hat{s}_2} \hat{H}_2 e^{-\hat{s}_2}
$$

with choosing

$$
\hat{s}_1 = \sum_{k=1,2} \frac{g_k}{\Delta_k} \left( \hat{a}_{qk}^{\dagger} \hat{a}_{c} - \hat{a}_{qk} \hat{a}_{c}^{\dagger} \right) - \sum_{k} \frac{g_k}{\Delta_k} \left( \hat{a}_{qk}^{\dagger} \hat{a}_{c}^{\dagger} - \hat{a}_{qk} \hat{a}_{c} \right),
$$

(5)

$$
\hat{s}_2 = \sum_{k=1,2} \frac{g_k \alpha_{qk}}{\Delta_k} \left( \hat{a}_{qk}^{\dagger} \hat{a}_{qk} \hat{a}_{c}^{\dagger} - \hat{a}_{qk} \hat{a}_{qk}^{\dagger} \hat{a}_{c} \right) + \sum_{k=1,2} \frac{g_k \alpha_c}{\Delta_k} \left( \hat{a}_{qk} \hat{a}_{c}^{\dagger} \hat{a}_{c}^{\dagger} - \hat{a}_{qk}^{\dagger} \hat{a}_{c} \hat{a}_{c} \right),
$$

(6)

where the detunings $\Delta_k = \omega_{qk} - \omega_c$ with $k = 1, 2$, $\Sigma_k = \omega_{qk} + \omega_c$, and $\Delta_k = \omega_{qk} - \omega_c$. Here, the shifted qubits frequencies $\tilde{\omega}_{qk}$, $\tilde{\omega}_c$ and the shifted anharmonicities $\tilde{\alpha}_{qk}$ will be given in Eqs. (8) and (9).

Applying two times SWT to the fourth order, and considering dispersive regimes, i.e., $g_k \ll |\Delta_k|$, the Hamiltonian in new representation $\hat{H}_{\text{eff}}^{2}$ is obtained as follows. More details concerning the cumbersome derivation are given in Appendix A. This effective Hamiltonian will be the cornerstone of the following analysis and discussions. In addition, it maybe also helpful in exploring other problems in coupler architecture.

$$
\hat{H}_{\text{eff}}^{2} \approx \sum_{\lambda=q_1,q_2,c} \tilde{\omega}_{\lambda} \hat{a}_{\lambda}^{\dagger} \hat{a}_{\lambda} + \frac{\tilde{\alpha}_{\lambda}}{2} \hat{a}_{\lambda}^{\dagger} \hat{a}_{\lambda}^{\dagger} \hat{a}_{\lambda} \hat{a}_{\lambda} + g_{\text{eff}} \left( \hat{a}_{q1}^{\dagger} \hat{a}_{q2} - \hat{a}_{q1} \hat{a}_{q2}^{\dagger} + H.c. \right) - \frac{g_{g_{12}} \alpha_{q1}}{\Delta_1 \Delta_2} \left( \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} + H.c. \right) - \frac{g_{g_{12}} \alpha_{q2}}{\Delta_1 \Delta_2} \left( \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} + H.c. \right) + \frac{g_{g_{12}} \alpha_c}{\Delta_1 \Delta_2} \left( \hat{a}_{q1} \hat{a}_{q2}^{\dagger} \hat{a}_{c}^{\dagger} \hat{a}_{c} + H.c. \right) + \frac{1}{2} \left( \frac{g_{g_{12}}}{\Delta_1 \Delta_2} \right)^2 (\alpha_{q1} + \alpha_{q2} + 4 \alpha_c) \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q2}^{\dagger} \hat{a}_{q2},
$$

(7)

where the shifted qubit frequencies and anharmonicities are obtained as

$$
\tilde{\omega}_{qk} = \omega_{qk} + \frac{g_{k}^2}{\Delta_k} - \frac{g_{k}^2}{\Sigma_k}, \quad k = 1, 2,
$$

$$
\tilde{\omega}_c = \omega_c - \sum_{k=1}^2 \left( \frac{g_{k}^2}{\Delta_k} + \frac{g_{k}^2}{\Sigma_k} \right),
$$

(8)

$$
\tilde{\alpha}_{qk} = \alpha_{qk} \left[ 1 - \frac{2g_{k}^2}{\Delta_k (\Delta_k + \alpha_{qk})} \right], \quad k = 1, 2,
$$

(9)

respectively, and the effective coupling between two computational qubits is obtained as $g_{\text{eff}} = g_{12} + \tilde{g}_{12}$ with

$$
\tilde{g}_{12} = \frac{g_{g_{12}}^2}{2} \sum_{k=1}^2 \left( \frac{1}{\Delta_k} - \frac{1}{\Sigma_k} \right).
$$

(10)

As seen obviously from the Hamiltonian $\hat{H}_{\text{eff}}^{2}$, the effective coupling $g_{\text{eff}}$ becomes tunable through simply varying the coupler frequency $\omega_c$. Moreover, this coupling can be switched off, i.e., $g_{\text{eff}} = 0$, if necessary. Comparing with previous work [25] which only give the effective coupling between computational qubits, we check carefully the additional second and fourth-order perturbative contributions, which contain more fruitful physics. In particular, we will see later that these terms induced by the nonlinear terms exactly correspond to gate error sources. Apart from these, we apply a second SWT to extend the analytical results to a more general regime, i.e., $\alpha_{\lambda} \sim |\Delta_{k}|$ (in Ref. [25], it was restricted to $\alpha_{\lambda} \ll |\Delta_{k}|$). Particularly, the second SWT results in the modification of qubits’ anharmonicity. We will see that the second SWT becomes very important when the coupler architecture is studied in certain regimes.

As we know, the original idea for coupler architecture is to make the coupling between computational qubits tunable, and more importantly to isolate one qubit from the neighboring qubits if necessary. As a further step, we specify the explicit parameter regions and conditions for realizing a switch. The first condition is $g_k \ll |\Delta_k|$ (dispersive couplings), meanwhile we have to take $\Delta_k < 0$ which is used to generate negative indirect couplings between computational qubits. As obtained approximately from Eq. (10), the required coupler frequency for $g_{\text{eff}} = 0$ is estimated roughly as

$$
\omega_{\text{eff}}^c \approx \omega_{q1} + \frac{g_{g_{12}}}{g_{12}},
$$

(11)

where we assumed $\omega_{q1} \approx \omega_{q2} = \omega_{q}$ and $\sum_{k} \gg |\Delta_{k}|$, $k = 1, 2$. To meet the dispersive conditions $g_k/(\omega_{\text{eff}} - \omega_{qk}) \ll 1$, and zero effective coupling condition Eq. (11) simultaneously, it requires the direct coupling $g_{12} \ll g_{12}$, which is exactly the usual parameter regimes in realistic coupler type experiments.

Once achieving $g_{\text{eff}} = 0$, one may think qubits $q1$ and $q2$ become completely isolated from each other. As a consequence, high-fidelity single-qubit gates are expected. Furthermore, if we consider the coupler architecture with many qubits (e.g., [4]), two-qubit gates can also avoid the crosstalk from other neighboring qubits, resulting in high-fidelity gates. Some previous work [27] indeed held similar arguments. However, our findings indicate it is not the case. As seen clearly from the effective Hamiltonian $\hat{H}_{\text{eff}}^{2}$ [Eq. (7)], even with $g_{\text{eff}} = 0$, the parasitic
couplings between computational qubits could still introduce unavoidable crosstalk. This will be discussed in the following sections.

III. CHARACTERISTICS AND PHYSICAL MECHANISMS OF PARASITIC COUPLINGS

To realize two-qubit native gates in superconducting quantum computing, for instance iSWAP gate, the XY type of coupling (i.e., $\hat{\sigma}^x_1$ and $\hat{\sigma}^x_2$) between computational qubits is required [45]. Except for it, other couplings with different forms are counted as parasitic couplings, which will induce gate errors. In this section, we study the characteristics and physical mechanisms of these parasitic couplings from the effective Hamiltonian perspective.

First of all, the effective Hamiltonian $\hat{H}''_{\text{eff}}$ reduces approximately to $\sum_{\alpha=a,b,c} \hat{\omega}_\alpha \hat{a}^\dagger_\alpha \hat{a}_\alpha + (\hat{\alpha}_x/2) \hat{a}^\dagger_1 \hat{a}^\dagger_2 \hat{a}_1 \hat{a}_2 + g_{\text{eff}} (\hat{a}_1 \hat{a}_2 - \hat{a}^\dagger_1 \hat{a}^\dagger_2 + H.c.)$ and high-order contributions are neglected when we consider the regime $|\alpha_\lambda| \ll |\Delta_k|, \Sigma_k$ [25]. Next, tuning the two computational qubits to be resonant, i.e., $\hat{\omega}_q = \hat{\omega}_c$, and reducing to computational basis (i.e., using Pauli representation), moreover transforming the resulting Hamiltonian into rotating representation with qubit frequency $\hat{\omega}_1$ and $\hat{\omega}_2$, we ultimately get an effective Hamiltonian

$$H_{\text{eff}}'' = \hat{\omega}_1 |100\rangle \langle 100| + \hat{\omega}_2 |001\rangle \langle 001| + (\hat{\omega}_1 + \hat{\omega}_2) |101\rangle \langle 101| + (2\hat{\omega}_1 + \hat{\alpha}_x) |200\rangle \langle 200| + (2\hat{\omega}_2 + \hat{\alpha}_x) |002\rangle \langle 002|
$$

where the coupling strengths for different physical processes are computed as

$$g_{200} = \sqrt{2} \left( g_{\text{eff}} - \frac{1}{2} \frac{g_1 g_2}{\Delta_1 \Delta_2} \alpha_1 \right), \quad g_{002} = \sqrt{2} \left( g_{\text{eff}} - \frac{1}{2} \frac{g_1 g_2}{\Delta_1 \Delta_2} \alpha_2 \right), \quad g_{202} = \sqrt{2} \frac{g_1 g_2}{\Delta_1 \Delta_2} \alpha_c, \quad g_{\text{cross-Kerr}} = \frac{1}{2} \left( \frac{g_1 g_2}{\Delta_1 \Delta_2} \right)^2. \quad (13)$$

It is noticeable that we consider only those states with excitation not more than two (neglect the states with larger excitation) and those coupling with the state $|101\rangle$ of computational space. Since the key goal is to realize an iSWAP gate, the transition between $|100\rangle$ and $|001\rangle$ is used to realize the target gate exactly. Therefore, the last four terms of Eq. (12), describing the coupling processes between $|101\rangle$ and high-energy states $|200\rangle$, $|020\rangle$, $|002\rangle$, are counted as parasitic couplings. Specifically, when the driven pulses are applied adiabatically, these couplings will lead to the additional phase, which results in a parasitic control phase gate. Such interaction is often called ZZ crosstalk which becomes a performance-limiting factor for gate fidelity [40, 46–49] and quantum error correction [50]. Unlike classical crosstalk, which can be removed through careful characterization and control optimization [51], ZZ parasitic crosstalk is hard to be mitigated [33].

Next, reducing to the basis which consists of the lowest two energy levels of computational qubits, the effective Hamiltonian is expressed as

$$H''_{\text{eff}} \approx \frac{\hat{\omega}_1}{2} \hat{\sigma}_z^1 + \frac{\hat{\omega}_2}{2} \hat{\sigma}_z^2 + \hat{H}_{\text{int}}^{XY} + \hat{H}_{\text{int}}^{ZZ}, \quad (14)$$

with two different types of coupling reading

$$\hat{H}_{\text{int}}^{XY} = \frac{g_{\text{eff}}}{2} (\hat{\sigma}_x^1 \hat{\sigma}_x^2 + \hat{\sigma}_y^1 \hat{\sigma}_y^2), \quad (15)$$

$$\hat{H}_{\text{int}}^{ZZ} = \zeta_{zz} \hat{\sigma}_z^1 \hat{\sigma}_z^2, \quad (16)$$

where both XY and ZZ coupling strengths, namely $g_{\text{eff}}$ and $\zeta_{zz}$, can be derived analytically from Hamiltonian...
\[ \hat{H}_{\text{eff}} \] within the regimes of interest. Moreover, the correctness of the analytical results can be further verified via numerically diagonalizing the system Hamiltonian \[ \hat{H}_{\text{Lab}} \] in Eq. (1). In particular, \( 2g_{\text{eff}} \) is evaluated as the energy difference between \( |\omega_{100} - \omega_{001} \rangle \), and \( \zeta_{zz} = \omega_{101} - \omega_{100} - \omega_{001} \). Here, \( \omega_{1,0,2} \) denotes the eigenenergy of the system Hamiltonian, and \( \omega_{100} \) is set to zero for simplification.

As seen clearly from Eq. (12) that the parasitic ZZ coupling \( \zeta_{zz} \) originate from various couplings between the states \(|101\rangle \) and \(|200\rangle, |020\rangle, |002\rangle, |101\rangle \). In addition to the numerical results which can be solved trivially, previous investigations \([26, 28, 31, 34]\) calculated \( \zeta_{zz} \) via diagonalizing the system Hamiltonian perturbatively. Apart from the extremely cumbersome calculations, one cannot obtain clear physical mechanisms. As a contrast, the effective Hamiltonian as well as the analytical results obtained in this paper have simple forms, and can be interpreted as the physical processes of parasitic couplings. For different parameter regime, we find that different coupling term dominates. Here, we concentrate on three different regimes representing three typical physical processes. The first one is to consider the resonant process between \(|101\rangle \) and \(|200\rangle \) (or \(|002\rangle \)), which will be discussed in subsection III A. The second one is to consider the resonant process between \(|101\rangle \) and \(|020\rangle \), the high energy level of the coupler will play an important role; this will be discussed in subsection III B. The third one is to consider the dispersive regime, namely the effective coupling strengths are much smaller than the energy difference between \(|101\rangle \) and \(|200\rangle \) (or \(|002\rangle \), \(|020\rangle \)), which will be discussed in subsection III C.

### A. Parasitic couplings due to high energy levels of computational qubits

In actual superconducting circuits experiments, in addition to computational space consisting of \(|000\rangle, |001\rangle, |100\rangle, |101\rangle \), the effect of computational qubits’ higher energy levels has to be considered as well. Even if without the coupler (namely two computational qubits couple directly \([16, 17]\)), the usual Jaynes-Cummings interaction between two computational qubits, i.e., \( \hat{a}_q \dagger \hat{a}_q + \hat{a}_g \dagger \hat{a}_g \), will couple the states \(|11\rangle \) and \(|20\rangle \) (or \(|02\rangle \)). Besides, the terms \( \hat{a}_q \dagger \hat{a}_q \hat{a}_g \hat{a}_g + \hat{a}_g \dagger \hat{a}_g \hat{a}_q \hat{a}_q + \hat{H}.c. \) of effective Hamiltonian \( \hat{H}_{\text{eff}} \) in Eq. (7), contribute to parasitic coupling as well. In particular, it describes the transition between the states \(|101\rangle \) and \(|200\rangle \) (or \(|002\rangle \) exactly, because the term has the relations: \( \hat{a}_q \dagger \hat{a}_q \hat{a}_q \hat{a}_q \hat{q}_2|200\rangle = \sqrt{2}|101\rangle \) and \( \hat{a}_g \dagger \hat{a}_g \hat{a}_g \hat{a}_g \hat{q}_1|002\rangle = \sqrt{2}|101\rangle \). Specially, in the parameter regime with \( \omega_{1q} + \omega_{gq} \approx 2\omega_{q1} + \omega_{q2} \) or \( \omega_{1q} + \omega_{gq} \approx 2\omega_{g2} + \omega_{gq} \), namely the states \(|101\rangle \) and \(|200\rangle \) (or \(|002\rangle \)) are in resonant nearly, the resulting ZZ coupling \( \zeta_{zz} \) will originate from this resonant process while the contributions from other disperse couplings can be neglected. Using Eq. (12), \( \zeta_{zz} \) can be derived analytically. In particular, we obtain

\[
|\zeta_{zz}| = \frac{1}{2} \left( (\Delta_{12} + \tilde{\alpha}_{q1})^2 + 4\tilde{g}_{200}^2 - |\Delta_{12} + \tilde{\alpha}_{q1}| \right) \left( \frac{1}{2} (\sqrt{(\Delta_{12} - \tilde{\alpha}_{q2})^2 + 4\tilde{g}_{002}^2} - |\Delta_{12} - \tilde{\alpha}_{q2}|) \right),
\]

where \( \Delta_{12} = \omega_{q1} - \omega_{q2} \) is the frequency detuning of two computational qubits in new representation, and the corresponding coupling strength \( \tilde{g}_{200}, \tilde{g}_{002} \) was given in Eq. (13). The first (last) two terms in the bracket of Eq. (17) corresponds to the resonant process between \(|101\rangle \) and \(|200\rangle \) (or \(|002\rangle \)). The derivation of Eq. (17) is presented in Appendix B.

With the regime of interest, we evaluate and plot ZZ coupling strength \( |\zeta_{zz}| \) with varying \( \Delta_{12} \) (\( \Delta_{12} = \omega_{q1} - \omega_{q2} \)) in Fig. 2. As expected, ZZ parasitic coupling becomes pronounced when the state \(|101\rangle \) is on resonance with the states \(|200\rangle \) (or \(|002\rangle \). Specially, when \( \Delta_{12} = -\tilde{\alpha}_{q1}(\tilde{\alpha}_{q2} \) the ZZ coupling strength is evaluated as \( |\zeta_{zz}| \approx |\tilde{g}_{200}|(|\tilde{g}_{002}|) \) at the resonant point. Besides, ZZ coupling is largely suppressed once it is tuned away from the resonant processes. A similar result was also obtained in Ref. [28] using numerical methods. The correctness of our analytical result (blue solid), plotted using Eq. (17), is verified through numerically diagonalizing the system Hamiltonian \( \hat{H}_{\text{Lab}} \) (orange dotted). It is obvious that the analytical result matches very well with the numerical one. Another thing we want to point out is that the second SWT is very important in the regime considered. As shown in the inset of Fig. 2, the ZZ coupling strengths \( |\zeta_{zz}| \) are evaluated using three different Hamiltonian, namely \( \hat{H}_{\text{Lab}} \) [Eq. (1)] in lab frame, \( \hat{H}_{\text{eff}} \) [Eq. (A15)] with 1 time SWT, and \( \hat{H}_{\text{eff}} \) with 2 times SWT [Eq. (7)]. In absence of 2nd SWT, the result solved from \( \hat{H}_{\text{eff}} \) does not match very well with that of the original Hamiltonian \( \hat{H}_{\text{Lab}} \), which implies the effective Hamiltonian method with two time SWT gives an accurate result.

### B. Parasitic couplings due to high energy levels of coupler

As an auxiliary qubit, the coupler’s main purpose is to generate tunable coupling between two computational qubits and serve as a switch if necessary. Another advantage is that the external driven noise induced through the coupler can be suppressed largely in dispersive regimes, comparing with directly driving computational qubits. However, due to the existence of the coupler’s high energy levels, we may have to pay the price of additional parasitic coupling. Using the effective Hamiltonian \( \hat{H}_{\text{eff}} \), the generation of parasitic coupling can be explained. In particular, the term \( \hat{a}_q \dagger \hat{a}_g \dagger \hat{a}_q \hat{a}_g + \hat{H}.c. \) of \( \hat{H}_{\text{eff}} \), i.e., Eq. (7), exactly describes this process. It reflects the transition between the states \(|101\rangle \) and \(|020\rangle \), because the term has the relations: \( \hat{a}_q \dagger \hat{a}_g \dagger \hat{a}_q \hat{a}_g |101\rangle = \sqrt{2}|020\rangle \).
processes can be neglected. As a further step, the ana-

FIG. 2. ZZ coupling strength $|\zeta_{zz}|$ characteristics in the regime that $|101\rangle$ is closely in resonance with $|200\rangle$ or $|002\rangle$. The analytical result (blue solid) is computed using Eq. (17), while the numerical result (orange dotted) is evaluated through diagonalizing the system Hamiltonian $\hat{H}_{\text{Lab}}[\text{Eq. (1)}]$. (inset) ZZ coupling strength $|\zeta_{zz}|$ are evaluated numerically using three different Hamiltonian, including $\hat{H}_{\text{Lab}}$ [Eq. (1)] in lab frame, $\hat{H}^{\text{eff}}_\text{Lab}$ [Eq. (15)] with 1 time SWT, $\hat{H}^{\text{eff}}_\text{Lab}$ with 2 times SWT [Eq. (7)]. Our results indicates the importance of the 2nd SWT in effective Hamiltonian approach. The used parameters are: $\omega_{q1}/(2\pi) = 5$ GHz, $\omega_{c}/(2\pi) = 6$ GHz, $\alpha_{q1}/(2\pi) = 0.2$ GHz, $g_{1}/(2\pi) = 0.05$ GHz, $g_{12} = 0$. and $\hat{a}_{q1}\hat{a}_{q2}|020\rangle = \sqrt{2}|101\rangle$. Furthermore, when we consider the parameter regime with $\tilde{\omega}_{q1} + \tilde{\omega}_{q2} \approx 2\tilde{\omega}_{c} + \tilde{\alpha}_{c}$, the states $|101\rangle$ and $|020\rangle$ are in resonant nearly. Under this regime, the ZZ parasitic coupling $\zeta_{zz}$ mainly originate from this resonant process and other non-resonant processes can be neglected. As a further step, the analytical results of $\zeta_{zz}$ can be derived. We obtain

$$|\zeta_{zz}| = \left\{\frac{1}{2}\left((\tilde{\omega}_{c} - \tilde{\omega}_{c}^*)^2 + \tilde{g}_{020}^2 - |\tilde{\omega}_{c} - \tilde{\omega}_{c}^*|^2\right)\right\}^{1/2},$$

(18)

where the central frequency $\tilde{\omega}_{c}^*$ is given as $\tilde{\omega}_{c}^* = (\tilde{\omega}_{q1} + \tilde{\omega}_{q2} - \tilde{\alpha}_{c})/2$, and the corresponding coupling strength $|\tilde{g}_{020}|$ was given in Eq. (13). The derivation of Eq. (18) is presented in Appendix B.

With the parameter regime of interest, we evaluate and plot ZZ coupling strengths $|\zeta_{zz}|$ as a function of coupler frequency $\tilde{\omega}_{c}$ in Fig. 3. The analytical result (blue solid) is plotted using Eq. (18). To verify the correctness of analytical result, we also compute numerically $\zeta_{zz}$ using three different system Hamiltonian, including $\hat{H}_{\text{Lab}}$ [Eq. (1)] in lab frame, $\hat{H}^{\text{eff}}_\text{Lab}$ [Eq. (15)] with 1 time SWT, and $\hat{H}^{\text{eff}}_\text{Lab}$ with 2 times SWT [Eq. (7)]. It is shown that the analytical result matches very well with the numerical result. Apart from that, we verify again that the necessity of 2nd SWT in the resonant regimes. It is noticeable that the central frequency for larger ZZ coupling is $\tilde{\omega}_{c}^*$, which corresponds to the resonant process between the states $|101\rangle$ and $|020\rangle$. The maximum ZZ coupling strength is evaluated as $\zeta_{zz}(\tilde{\omega}_{c} = \tilde{\omega}_{c}^*) = \tilde{g}_{020}$. Once the coupler frequency is tuned away from $\tilde{\omega}_{c}^*$, ZZ couplings are suppressed gradually.

As the effects of computational qubits’ higher energy levels were discussed before, it is quite natural to think about the consequence of possible resonant process between the states $|101\rangle$ and $|020\rangle$. If it happens, a larger ZZ parasitic coupling $\zeta_{zz}$ may appear. To explore the physical mechanism of resonant parasitic coupling induced by the coupler, we study it from the perspective of energy level diagrams. Initially, the coupler is prepared in ground state $|0\rangle$. Firstly, the question we want to ask is, is it possible to excite the coupler from the ground state to the first excited state, i.e., $|0\rangle \rightarrow |1\rangle$? To make it happen, an external energy $\tilde{\omega}_{c}$ is required. However, we realize this is almost impossible under the dispersive conditions $g_{c} \ll |\Delta_{k}|, k = 1, 2$. Secondly, is it possible to excite the coupler from the ground state to the second excited state, i.e., $|0\rangle \rightarrow |2\rangle$? To make it happen, it requires an energy $2\tilde{\omega}_{c} + \tilde{\alpha}_{c}$ ($\tilde{\alpha}_{c} < 0$ for transmon qubit). This becomes possible if both qubit 1 and qubit 2 drop from $|1\rangle$ to $|0\rangle$. As seen from the effective Hamiltonian $\hat{H}^{\text{eff}}_\text{Lab}$ [Eq. (7)], the term with $\hat{a}_{q1}^{\dagger}\hat{a}_{q2}^{\dagger} \hat{a}_{q2} + \text{H.c.}$ describes exactly this process. The physical picture for this resonant process is explained using energy levels diagrams.

FIG. 3. (upper) ZZ coupling strength $|\zeta_{zz}|$ characteristics in the regime that the state $|101\rangle$ is closely in resonance with $|020\rangle$. The analytical result (blue solid) is plotted using Eq. (18). To verify the correctness of the analytical result, we compute numerically using the Hamiltonian $\hat{H}_{\text{Lab}}$. Besides, we also show the numerical results with the Hamiltonian $\hat{H}^{\text{eff}}_{\text{Lab}}$ and $\hat{H}^{\text{eff}}_{\text{Lab}}$ with 2 times SWT, $\hat{H}^{\text{eff}}_{\text{Lab}}$ with 2 times SWT [Eq. (7)]. The used parameters are: $\omega_{q1}/(2\pi) = 5$ GHz, $\omega_{q2}/(2\pi) = 3$ GHz, $\alpha_{q1}/(2\pi) = -0.2$ GHz, $g_{1}/(2\pi) = g_{2}/(2\pi) = 0.05$ GHz, $g_{12} = 0$. (lower) Energy level diagrams corresponds to the resonant process between the states $|101\rangle$ and $|020\rangle$. It can be used to explain the physical mechanism of parasitic coupling due to the coupler’s second excite state. The initial state of the system is prepared with $|101\rangle$, one is able to create the resonant process between $|101\rangle$ and $|020\rangle$ (governed by the term $\hat{a}_{q1}^{\dagger}\hat{a}_{q2}^{\dagger} \hat{a}_{q2} + \text{H.c.}$ of $\hat{H}^{\text{eff}}_{\text{Lab}}$) when the system parameters satisfy the condition $\tilde{\omega}_{q1} + \tilde{\omega}_{q2} \approx 2\tilde{\omega}_{c} + \tilde{\alpha}_{c}$. The maximum ZZ coupling is $\tilde{g}_{020}$. Once the coupler frequency is tuned away from $\tilde{\omega}_{c}^*$, ZZ couplings are suppressed gradually.
in the lower one of Fig. 3. To focus on the effect of the coupler, we restrict the computational qubits as two-level systems (for simplicity and no loss of generality) and regard the coupler as a qutrit. The transition between the states $|010\rangle$ and $|020\rangle$ may occur when we consider the parameter regime $\tilde{\omega}_{q1} + \tilde{\omega}_{q2} \approx 2\tilde{\omega}_c + \tilde{\alpha}_c$. In particular, the initial state of the system is prepared with $|101\rangle$ (black dots), after applying the operation $\hat{a}_{q1}^\dagger \hat{a}_{q2}^\dagger$, it transforms to the state $|020\rangle$ (orange dots). As seen from the upper plot, the more close to this resonant condition, the larger $|\zeta_{zz}|$ obtained. In current experiments with coupler architecture, a larger detuning between qubits and coupler frequency and a relatively small negative $\alpha_c$ are frequently used [4, 27], hence the resonant condition does not hold. Consequently, the parasitic coupling raised due to the coupler’s higher energy levels is largely suppressed and thus can be ignored. Very recently, novel parameter regimes (beyond dispersive approximation) of coupler architecture were proposed and experimentally realized [29, 52]. In this new regime, the resonant process between $|101\rangle$ and $|020\rangle$ may occur, and therefore the coupler’s higher energy plays an essential role in the resulting ZZ parasitic coupling.

### C. Parasitic couplings in dispersive regime

In addition to the two special resonant regimes discussed above, we turn to explore a different parameter regions: dispersive regime, i.e., $g_{200} \ll |(\tilde{\omega}_{q1} + \tilde{\omega}_{q2}) - (2\tilde{\omega}_c + \tilde{\alpha}_c)|$, $g_{020} \ll |(\tilde{\omega}_{q1} + \tilde{\omega}_{q2}) - (2\tilde{\omega}_c + \tilde{\alpha}_c)|$, and $g_{002} \ll |(\tilde{\omega}_{q1} + \tilde{\omega}_{q2}) - (2\tilde{\omega}_c + \tilde{\alpha}_c)|$. Comparing with the two resonant regimes in which only one specific term dominates, all the terms of the effective Hamiltonian $\hat{H}_{\text{eff}}$, [Eq. (7)] contribute in dispersive regime. Summation up all different kinds of contributions, we arrive at a quite concise and meaningful analytical result for $|\zeta_{zz}|$, expressing as

$$|\zeta_{zz}| \approx 2g_{12}^2 \left| \frac{1}{\alpha_{q1}} + \frac{1}{\alpha_{q2}} + \frac{4}{\alpha_c - 2\Delta} \right|,$$

where for simplification we set $g_{12} = 0$ and $\Delta_{12} = 0$ ($\Delta_{12} = \omega_{q1} - \omega_{q2}$). As for the general cases with finite coupling $g_{12}$ and finite detunings $\Delta_{12}$, we also derive the corresponding analytical expression for $\zeta_{zz}$ [see Eq. (B5)]. Besides, $g_{12}$ is the effective coupling between computational qubits given in Eq. (10), and the three terms correspond to the contribution from the coupling between the states $|101\rangle$ and $|200\rangle, |002\rangle, |020\rangle$, respectively. The derivation of Eq. (19) is presented in Appendix B.

In Fig. 4, the ZZ parasitic coupling dependent on coupling frequency is evaluated and plotted. First and foremost, our analytical result (blue solid), namely Eq. (19), is verified via numerically diagonalizing the Hamiltonian $\hat{H}_{\text{Lab}}$ (orange dotted). It is shown clearly that the analytical result matches very well with the numerical one. As a further step, it is also interesting to study the contribution for each of the coupling processes, named as $\zeta_{zz}^{(200)}$, $\zeta_{zz}^{(002)}$, $\zeta_{zz}^{(020)}$, and $\zeta_{zz}^{\text{cross-Kerr}}$. To do so, we evaluate and plot the resulting $|\zeta_{zz}|$ in absence of one of them. As seen from the plots, the result cannot match well with the exact one without involving any one of them. This implies that all the coupling terms matter to the resulting ZZ parasitic coupling. In our specific case with chosen parameters specified in Fig. 4, the contribution of $\zeta_{zz}^{(200)}$ is the largest one while that of $\zeta_{zz}^{(020)}$ is relatively smaller. Another characteristic is that the strength for $\zeta_{zz}$ is suppressed apparently in dispersive regimes comparing with the resonant regimes discussed before. In the next section, we will mainly focus on the dispersive regime and further explore the elimination of ZZ parasitic couplings.

### IV. NOVEL PARAMETER REGIONS FOR ELIMINATING ZZ PARASITIC COUPLINGS

In this section, we further explore ZZ parasitic coupling characteristics. Especially, we pay attention to those parameter regions in which ZZ parasitic couplings can be suppressed or even eliminated. We first examine ZZ coupling characteristics with current existing experimental parameters in subsection IV A, and further figure out the optimized parameter regions for minimizing ZZ couplings. In addition to the general numerical results, we provide a clear physical understanding benefiting from the analytical result obtained. More importantly, inspired by the analytical results, we also propose four novel parameter regions and the related experimental realizations in which ZZ couplings are expected to be eliminated; this will be discussed in subsection IV B.
A. ZZ coupling characteristics in existing experimental parameter regions

Concentrating on dispersive regime and using current experimental parameters, e.g., \( \omega_{q1}/(2\pi) = \omega_{q2}/(2\pi) = 5 \) GHz, \( \omega_c/(2\pi) = 6 \) GHz, \( \alpha_c/(2\pi) = -0.25 \) GHz, \( g_1/(2\pi) = g_2/(2\pi) = 0.08 \) GHz, \( g_{12} = 0 \), we evaluate and plot the ZZ coupling strength in Fig. 5. In particular, we study ZZ coupling characteristics with varying qubits anharmonicities \( \alpha_{q1} \) and \( \alpha_{q2} \).

Let us first consider the general case that the computational qubits’ anharmonicities have the same sign, e.g., \( \zeta \) ferent signs, band). The used parameters are: \( \omega_{q1}/(2\pi) = \omega_{q2}/(2\pi) = 5 \) GHz, \( \omega_c/(2\pi) = 6 \) GHz, \( \alpha_c/(2\pi) = -0.25 \) GHz, \( g_1/(2\pi) = g_2/(2\pi) = 0.08 \) GHz, \( g_{12} = 0 \). We find that ZZ couplings are suppressed through increasing the order of \( |\zeta_{zz}| \). The larger anharmonicities chosen, the weaker ZZ parasitic coupling we will obtain. Unfortunately, larger anharmonicities are restricted by current technology and qubit anharmonicities are usually small (around \(-100 \) to \(-300 \) MHz) for the frequently used transmon qubits.

Interestingly, \(|\zeta_{zz}|\) can be suppressed when the two qubits’ anharmonicities have different signs; for instance, one is transmon qubit \([53]\) with \( \alpha_{q1} < 0 \) and the other one is capacitively shunted flux qubit (CSFQ) \([54–56]\) with \( \alpha_{q2} > 0 \). In this regime, it is seen from the lower figure that ZZ coupling characteristics are quite different from the traditional one (the upper figure). In particular, we find that the resulting \(|\zeta_{zz}|\) are suppressed evidently for arbitrary negative \( \alpha_{q1} \) and positive \( \alpha_{q2} \); more interestingly, ZZ couplings could be eliminated at specific regions. Actually, such parameters regime was studied and discussed in Ref.[28, 30] and the ZZ coupling suppressing effects were also verified in a very recent experiment [42]. Although high-fidelity two-qubit gates were realized in such parameter regime, a couple of essential questions were not explored. For instance, are we able to figure out the specific parameter region (i.e., red band in the lower figure) for \( \zeta_{zz} \rightarrow 0^+ \)? Furthermore, what is the physical mechanism for ZZ coupling elimination? To solve these critical issues, we drive the explicit expression for \( \zeta_{zz} \) with the effective Hamiltonian approach introduced before.

Considering the regime of our interest, i.e., \( \Delta_1 = \Delta_2 = \Delta \) (i.e., \( \Delta_{12} = 0 \)), we obtain the explicit form of \( \zeta_{zz} \) (see detailed derivation in Appendix B):

\[
\zeta_{zz} = -2g_{eff} \left[ g_{eff} \left( \frac{1}{\alpha_{q1}} + \frac{1}{\alpha_{q2}} \right) + \frac{4g_{12}g_{12}\alpha_c}{\Delta(\alpha_c - 2\Delta)} \right].
\]

As for the more general case, i.e., \( \Delta_1 \neq \Delta_2 \), the result is given in Eq. (BS) of Appendix B, which can be used to explore the regime with finite detuning between qubits’ frequencies. When the effective coupling between qubits \( q_1 \) and \( q_2 \) is tuned off (i.e., \( g_{eff} = 0 \), the above equation (20) reduces to a simple form, i.e., \( 4g_{12}g_{12}\alpha_c/\Delta(\alpha_c - 2\Delta) \). This is normally a small value which implies that the parasitic ZZ coupling is extremely weak. This conclusion is indeed verified by the very recent experiment [27]. Beyond the commonly accepted view that ZZ parasitic coupling is suppressed by tuning off \( g_{eff} \), we find an alternative means to mitigate ZZ couplings: adjusting system parameters to make \( g_{eff} = 0 \), \( 1/\alpha_{q1} + 1/\alpha_{q2} + 4g_{12}/(\alpha_c - 2\Delta) \rightarrow 0 \). One advantage of this new means is that XY coupling \( g_{xy} \) can be maintained while mitigating ZZ crosstalk. The physical mechanism behind is that the coupler’s high-energy state plays a vital role, it can neutralize the energy shift induced by high-energy states of computational qubits. Actually, our findings can be used to explain the key results of Ref. [34]: two separated branches for mitigating ZZ coupling are obtained. More importantly, we can even figure out the explicit condition for the two branch using Eq. (20). Choosing \( \alpha_c = 0 \) and \( \alpha_{q1} = \alpha_{q2} = \alpha_\xi \), the upper branch corresponds to \( g_{12} = -g_{12}/\Delta \) [i.e., Eq. (11)], and the lower branch can also be solved easily as \( g_{12} = -(g_{12}/\Delta)(1 - \alpha_\xi/\Delta) \). It is obvious the lower branch will get close to the upper branch with larger detuning \( |\Delta| \) (which is normally the case for current ex-
In the remainder of this paper, we concentrate on the regime \( g_{12} \ll |\tilde{g}_{12}| \) (the regime beyond this will be studied in future work), then Eq. (20) reduces approximately to a simple form: \( |\zeta_{zz}| \approx 2\tilde{g}_{12}^2/[\alpha_{q1} + 1/\alpha_{q2} + 4/(\alpha_c - 2\Delta)] \) [namely Eq. (19)]. Next, we use this analytical result to explain the above numerical results shown in Fig. 5. If all of the three elements are transmon qubits, moreover \( |\Delta| \gg \alpha_\lambda \), \( \lambda = q1, q2, c \), \( |\zeta_{zz}| \) is estimated as \( \tilde{g}_{12}^2/|\alpha_\lambda| \). It is obvious that ZZ coupling strength is proportional to the effective XY coupling \( g_{12} \), implying stronger XY coupling has to pay the price of larger ZZ parasitic couplings. Moreover, ZZ coupling strength is inversely proportional to qubit anharmonicities. As the anharmonicities for transmon qubits are usually small, ZZ coupling becomes one of the leading gate error sources for coupler architecture with traditional parameter region. Then, we turn to the case that qubit anharmonicities have different signs. Apparently, \( \zeta_{zz} \) becomes weaker compared with the general case with using transmon qubits. To suppress largely ZZ coupling, the choice of \( \alpha_{q1} \) and \( \alpha_{q2} \) should satisfy some specific condition. If one simplify choose \( \alpha_{q1} = -\alpha_{q2} \), the ZZ coupling can not be eliminated completely. To further eliminate ZZ coupling, we need to let \( 1/\alpha_{q1} + 1/\alpha_{q2} + 4/(\alpha_c - 2\Delta) = 0 \), from which we solve the explicit analytical condition for zero ZZ coupling, namely

\[
\alpha_{q1} = \left[ \frac{4}{2\Delta - \alpha_c} - \frac{1}{\alpha_{q2}} \right]^{-1},
\]

which corresponds exactly to the red band in the lower one of Fig. 5. This tells us that one has to design proper superconducting circuit parameters to realize lower ZZ coupling. In this paper, we provide an explicit condition which could be applied to real experiments.

With choosing fixed \( \alpha_{q2} \) (either negative or positive), we plot \( |\zeta_{zz}| \) dependent of \( \alpha_{q1} \) in Fig. 6. Here, \( \zeta_{zz} \) is computed numerically and analytically, respectively. In particular, the numerical results (orange dotted) are computed via numerically diagonalizing the Hamiltonian \( \hat{H}_{\text{Lab}} \) [Eq. (1)], while the analytical results (blue solid) are plotted using Eq. (19). As expected, the ZZ coupling strength decreases with larger \( |\alpha_{q1}| \) for negative \( \alpha_{q2} \) (the upper one). As for positive \( \alpha_{q2} \) (the lower one), the ZZ coupling strength can be eliminated at certain \( \alpha_{q1} \). Using Eq. (21) it is estimated as \( \alpha_{q1}/(2\pi) \approx -178 \) MHz with the parameters used. Moreover, we verify that our derived analytical expression, i.e., Eq. (19), matches well with the numerical results.

### B. Novel parameter regions for eliminating ZZ couplings

Although the regime for qubit anharmonicity with different signs could reduce ZZ parasitic couplings, in practice the qubits with positive anharmonicity are usually unstable and own relatively short coherence time. As a consequence, the resulting gate error would suffer from the decoherence of computational qubits. Inspired by the analytical expression [i.e., Eq. (19)] obtained, we may ask a question: are there other parameter regions existing for mitigating ZZ coupling? Actually, beyond the regimes discussed above, we find four novel parameter regions (unexplored yet), in which ZZ coupling elimination may be expected. The four types of parameter regions are introduced as follows. Some typical system parameters for different type are listed in Table I.

**Type I:** the first parameter regions we suggest are, both the computational qubits and coupler have negative anharmonicity and could be typical transmon qubits, but the frequency detunings between qubits and coupler as well as the coupling strengths \( g_1, g_2 \) are relatively small comparing with the general case. It is noted that the dispersive couplings \( g_0/|\Delta_k| \ll 1, k = 1, 2 \) always hold.

**Type II:** the second parameter regions we suggest are, both computational qubits are transmon with negative anharmonicity; moreover the frequency detunings between qubits and coupler are similar to the general case, but the coupler is realized with a strong negative anhar-
monicity [26].

Type III: the third parameter regions we suggested are, both computational qubits are transmon with negative anharmonicity, while the coupler is chosen with a positive anharmonicity (namely $\alpha_c > 0$), which could be realized with CSFQ.

Type IV: the fourth parameter regions we suggested are, both computational qubits and coupler have positive anharmonicities, i.e., $\alpha_{q1}, \alpha_{q2}, \alpha_c > 0$, all of them may be realized with CSFQ.

Using the superconducting circuit parameters given in Table I, we evaluate and plot ZZ coupling strengths $|\zeta_{zz}|$ dependent of qubit anharmonicities $\alpha_{q1}$ and $\alpha_{q2}$ with different type of parameter regions in Fig. 7 (a)-(d). $\zeta_{zz}$ are computed through numerically diagonalizing the lab frame Hamiltonian $H_{lab}$. Comparing with the result with traditional parameter regions (i.e., the top one of Fig. 5), ZZ couplings are largely suppressed with the novel system parameters suggested. As seen from Fig. 7 (a)-(d), ZZ coupling characteristics for different parameter regions are slightly different. However, they share a similar property: to achieve lower ZZ couplings, qubit anharmonicities have to be chosen properly to satisfy specific conditions (the red band), which can be figured out using the analytical expression, i.e., Eq. (21). Once the superconducting circuit parameters are tuned away from the red band, the resulting gate fidelity will be affected unavoidably by ZZ parasitic couplings.

According to ZZ coupling characteristics in our suggested parameter regions, it seems that the superconducting circuit parameters have to be designed carefully for suppressing ZZ couplings. Moreover, the parameter regions for $\zeta_{zz} \rightarrow 0$ are relatively narrow, which implies that it might not be easy to reach these specific parameter regions. Fortunately, we can still tune off ZZ coupling even if the parameters are not optimized perfectly. This is true because ZZ coupling strength $\zeta_{zz}$ can also be controlled by tuning the coupler frequency $\omega_c$ [26]. In Fig. 8, using the same parameters as in parameter region I, and choosing qubit anharmonicities randomly with $\alpha_{q1}/(2\pi) = -0.2$ GHz and $\alpha_{q2}/(2\pi) = -0.3$ GHz, we get a finite $\zeta_{zz}$. However, through further tuning the coupler frequency $\omega_c$, ZZ coupling $\zeta_{zz}$ can be tuned continuously from negative to positive. This means that one can always eliminate ZZ coupling by further adjusting coupler frequency.

To further understand the resulting ZZ coupling characteristics and the mechanisms of ZZ coupling elimination, we use the language of energy level diagrams to explain. As discussed before, the origin of ZZ coupling $\zeta_{zz}$ comes from the parasitic coupling between the state $|101\rangle$ (in computational space) and other states $|200\rangle, |020\rangle, |002\rangle$ (out of computational space). In particular, with considering adiabatically external drive, these couplings will result in a shift of energy level $|101\rangle$. Depending on the specific energy level interacted with $|101\rangle$, the energy shift to $|101\rangle$ could be either positive or negative. Under dispersive regime, ZZ parasitic coupling contains the contribution from different energy levels, incl., $|200\rangle, |020\rangle, |002\rangle$. Once the positive energy shift equals exactly with the negative energy shift, the consequence of the overall effect will keep the energy level of $|101\rangle$ remain unchanged. This is indeed the physical mechanism of eliminating ZZ coupling. Our four suggested parameter regions I-IV and the case with considering two computational qubits’ anharmonicity with different signs share a similar mechanism. According to the derivations and analysis, we realize that the effect of $|020\rangle$ is vital for eliminating ZZ couplings, which was usually ignored in previous work. For general parameter regions, namely the traditional transmon qubits are used for both computational qubits and coupler, the usual large energy difference between $|101\rangle$ and $|020\rangle$ results in a very small energy shift, therefore cannot neutralize the energy level shift induced by $|200\rangle$ and $|002\rangle$. By contrast, the situation is quite different in the four parameter regions we proposed in this paper. Through choosing proper system parameters, the energy shifts induced by $|200\rangle$ and $|002\rangle$ are always able to be neutralized by that induced by $|020\rangle$.

Finally, the natural thing is to think about experimental realizations for these four novel parameter regions. The good thing is that every suggested parameter region can be realized within current experimental technology. As shown in Fig. 9, for different parameter regions I-IV, the superconducting circuit architecture is the same and the main difference is the qubit type for computational qubits and coupler. Currently, for most of the existing experiments with coupler architecture [4, 26, 27, 29, 31, 32, 35], both computational qubits and coupler are transmon qubits, as shown in Fig. 9 (a). Our suggested parameter regions I, II are realized with such superconducting circuit as well, but the specific parameter regimes are different from those of the general

| $\omega_{q1}/2\pi$ | $\omega_{q2}/2\pi$ | $\omega_c/2\pi$ | $\alpha_c/2\pi$ | $g_1/2\pi$ | $g_2/2\pi$ | $\zeta_{zz}$ characteristics | SC realization |
|------------------|------------------|-----------------|----------------|----------|----------|------------------------|----------------|
| I 5              | 5                | 5.4             | -0.3           | 0.04     | 0.04     | Fig. 7 (a)             | Fig. 9 (a)     |
| II 5             | 5                | 5.6             | -0.8           | 0.06     | 0.06     | Fig. 7 (b)             | Fig. 9 (a)     |
| III 5.8          | 5.8              | 5.4             | 1.2            | 0.04     | 0.04     | Fig. 7 (c)             | Fig. 9 (c)     |
| IV 5.8           | 5.8              | 5               | 0.6            | 0.06     | 0.06     | Fig. 7 (d)             | Fig. 9 (d)     |
FIG. 7. ZZ coupling $\zeta_{zz}$ characteristics with our suggested parameter regions I, II, III, IV. $\zeta_{zz}$ are computed numerically via diagonalizing the system Hamiltonian $\hat{H}_{Lab}$. The superconducting circuit parameters used for the four different parameter regions are listed in Table I, respectively. Our results indicate that ZZ couplings can be eliminated at certain region (red bands).

FIG. 8. ZZ coupling $\zeta_{zz}$ dependent of coupler frequency $\omega_c$. With varying $\omega_c$, $\zeta_{zz}$ changes continually from negative to positive, which implies that zero $\zeta_{zz}$ (red dot) can be achieved via adjusting the coupler frequency. The parameter used are: $\omega_q1/(2\pi) = \omega_q2/(2\pi) = 5$ GHz, $\alpha_q1/(2\pi) = -0.2$ GHz, $\alpha_q2/(2\pi) = \alpha_c/(2\pi) = -0.3$ GHz, $g1/(2\pi) = g2/(2\pi) = 0.04$ GHz.

ones. For Fig. 9 (b), two computational qubits are realized with different types of qubits which correspond to the anharmonicities with different signs. As discussed before, lower ZZ couplings and high-fidelity two-qubit gate were investigated [28] and realized in such hybrid systems [42]. Our suggested parameter region III is realized with the superconducting circuit shown in Fig. 9 (c), i.e., two transmon qubits are sandwiched by a CSFQ. Comparing with the superconducting circuit of Fig. 9 (b), CSFQ is changed from the computational qubit to the coupler. Benefited from this change, higher two-qubit gate fidelity may be expected and realized. As for the parameter region IV, it can be realized with the same type of qubit, as shown in Fig. 9 (d). Comparing with the general superconducting circuit in Fig. 9 (a), all the transmon qubits are replaced by positive-anharmonicity qubits, i.e., CSFQ. We expect these superconducting circuits with novel parameter regions could be fabricated and studied in future experiments.

V. IMPLEMENTING LOW-ERROR TWO-QUBIT GATES WITH SUGGESTED PARAMETER REGIONS

In this section, we further study two-qubit gate errors in coupler architecture, especially focus on the novel parameter regions proposed in this paper. There exist several different kinds of noises which may affect the desired two-qubit gate fidelity. In particular, the first one could be some noises induced by external driven pulses on computational qubits, e.g., pulse amplitude fluctuations [45], classical crosstalk [51], etc. The second one could be quasistatic flux noise induced by flux fluctuations of the coupler. Benefiting from the dispersive couplings between computational qubits and coupler, such kind of noise would be largely suppressed. The third one is energy relaxation of computational qubits and coupler. The
Involving different kinds of noises, the dynamics of the density matrix $\rho(t)$ is governed by the well-known Lindblad equation [57]:
$$\frac{\partial}{\partial t}\rho(t) = -i[H_{\text{Lab}}, \rho(t)] + \sum_{i=q_1, c, q_2} \gamma_i [\hat{a}_i, \rho(t)] \hat{a}_i^\dagger - \{\hat{a}_i^\dagger, \hat{a}_i, \rho(t)\}/2.$$ Here, $H_{\text{Lab}}$ is the system Hamiltonian given in Eq. (1), the Lindblad operators $\hat{a}_i$ ($\hat{a}_i^\dagger$) is annihilation (creation) operator for computational qubits and coupler, and $\gamma_i$ represents the energy relaxation rate of computational qubits or coupler (it often relates to the qubit energy relaxation time $T_1^i = 1/\gamma_i$). Besides, $\{A, B\} = AB + BA$ denotes the anti-commutator of two elements A and B. Using the new representation introduced in this paper, we transform the Lindblad equation to a new form. To distinguish the new representation from the origin lab frame, we add a symbol “tilde” to every quantity in the Lindblad equation:
$$\frac{\partial}{\partial t}\tilde{\rho}(t) = -i[H_{\text{Lab}}, \tilde{\rho}(t)] + \sum_{i=q_1, c, q_2} \tilde{\gamma}_i [\tilde{\hat{a}}_i, \tilde{\rho}(t)] \tilde{\hat{a}}_i^\dagger - \{\tilde{\hat{a}}_i^\dagger, \tilde{\hat{a}}_i, \tilde{\rho}(t)\}/2.$$ In particular, with the help of SW transformations specified in Sec. II, $H_{\text{Lab}}$ is transformed to $\tilde{H} \approx \tilde{H}_{\text{eff}}$, and the Lindblad operators are transformed to $\tilde{\hat{a}}_k \approx \hat{a}_k - (g_k/\Delta_k) \hat{a}_c$, $\tilde{\hat{a}}_c \approx \hat{a}_c + \sum_{k=1,2} (g_k/\Delta_k) \hat{a}_c$, $k = 1, 2$. Considering all of these and reducing to computational space, we ultimately obtain the dynamical equation for the density matrix $\tilde{\rho}(t)$ in Eq. (22). The validation of Eq. (22) is verified numerically through comparing with the corresponding results solved from the lab frame Hamiltonian.

$$\frac{\partial}{\partial t}\tilde{\rho}(t) \simeq -i \left[ \tilde{H}_{\text{int}}^\text{XY}, \tilde{\rho}(t) \right] - i \left[ \tilde{H}_{\text{int}}^\text{ZZ}, \tilde{\rho}(t) \right] + \sum_{i,j=q_1, q_2} \tilde{\gamma}_{i,j} \left( \tilde{\sigma}_i^\dagger, \tilde{\rho}(t), \tilde{\sigma}_j \right) + \frac{1}{2} \left( \tilde{\sigma}_i^\dagger, \tilde{\sigma}_j^\dagger, \tilde{\rho}(t) \right),$$

where $\tilde{H}_{\text{int}}^\text{XY}$ and $\tilde{H}_{\text{int}}^\text{ZZ}$ were given in Eqs. (15) and (16), the operators $\tilde{\sigma}_i^\dagger$ ($\tilde{\sigma}_i^\dagger$) are annihilation (creation) operators for computational qubits, and the effective energy relaxation rates of computational qubits are affected by the coupler, obtaining as

$$\tilde{\gamma}_{qk, qk} = \gamma_{qk} + \left( \frac{g_k}{\Delta_k} \right)^2 \gamma_c, \quad k = 1, 2,$n
$$\tilde{\gamma}_{q1, q2} = \tilde{\gamma}_{q2, q1} = \frac{g_1 g_2}{\Delta_1 \Delta_2} \gamma_c.$$

In the equation above, $\gamma_{q1}$, $\gamma_{q2}$, $\gamma_c$ are the energy relaxation rates of qubit 1, qubit 2, and the coupler, respectively. It is interesting to see that the effective energy relaxation rates for computational qubits are still dominant by their own energy relaxation rate, while the influence induced by the coupler is suppressed by a prefactor $(g_k/\Delta_k)^2$ (which is a smaller value in dispersive regime). Benefiting from the robustness to the noise induced by the coupler, high-fidelity two-qubit gates are still realizable even with a noised coupler. In addition to realize tunable coupling, this can be seen as another advantage for coupler architecture. Beyond qualitative analysis, we further obtain a quantitative result to clarify how strong does the coupler noise affects the resulting gate error. Using the above analytical result [i.e., Eq. (23)], we can obtain approximately the critical point at which the noise from the coupler matters. In particular, the critical point
is estimated roughly as $T_1^c \approx \frac{g_{\text{ef}}}{\pi} T_1^i$ ($i = q1, q2$). Using current experimental parameters (e.g., taking from Ref. [27]), we find that the resulting two-qubit gate errors are almost independent of the coupler's energy relaxation once $T_1^c \gg 1 \mu s$. Normally this is the case with current superconducting circuits technology. Besides, we notice that an additional effective bath induced by the coupler appears in Eq. (22). Apart from the independent local baths for each computational qubit, the non-negligible term with $i \neq j$ in Eq. (22) can be interpreted as a global bath for the composed system qubit 1 and qubit 2.

Next, we use the idea of process tomography [57] to compute gate fidelity. In particular, setting randomly $N$ initial input states $\tilde{\rho}_0^k(0)$ in computational space with $k = 1, 2, 3, \ldots , N$ indicating the $k$-th initial state, and then let the state evolve in noise and noise-free cases, respectively. After a certain time (e.g., gate time $t_g$), the final states $\tilde{\rho}^k(t_g)$ (noise case) and $\tilde{\rho}_0^k(t_g)$ (noise-free case) are solved from the above Lindblad equation. In this particular case, it is reasonable to define the average gate fidelity as [58, 59]

$$\mathcal{F} = \frac{1}{N} \sum_{k=1}^{N} \text{tr} \left( \tilde{\rho}^k(t_g) \tilde{\rho}_0^k(t_g) \right).$$

(24)

Choosing proper system parameters and numerically solving the Lindblad equations (22), we can ultimately obtain the average gate error $\varepsilon = 1 - \mathcal{F}$.

Let us first consider the general case with frequently used parameters of coupler architecture [4], namely both computational qubits and coupler are realized with transmon qubits. In this regime, the qubits’ anharmonicities are negative and the strengths are usually designed to be around $0.1 - 0.3$ GHz. Moreover, the frequency detunings between computational qubits and coupler are usually large, e.g., $\sim 1$ GHz. Using the experimental parameter regimes, we evaluate and plot the gate error $\varepsilon$ dependent of gate time $t_g$ with different energy relaxation time $T_1$ in Fig. 10. Without loss of generality, the relaxation time for computational qubits and coupler is identical for simplicity. The specific definitions for these novel parameter regions were explained in Sec. IV and the typical system parameters can be found in Table I. Although these four suggested regions correspond to very different parameter regimes, they share a common physical mechanism and exhibit similar gate error characteristics. To concentrate on gate error characteristics induced by ZZ parasitic effects, we choose a longer energy relaxation time, e.g., $T_1 = 100 \mu s$. Obviously, the gate errors obtained in these novel parameter regions are much lower than those in the general case (e.g., Fig. 10). Moreover, the gate error reaches a minimum value at certain gate time. It is clearly seen that these novel realizable parameter regions provide a new way to reach lower error two-qubit gates without changing circuit architecture. Here, the gate errors $\varepsilon$ are evaluated with various methods that correspond to different lines of each figure. The dotted orange lines (labelled as “Analytic”) are plotted using Eq. (32) which will be derived in next subsection. The good agreement between the analytical and numerical results indicates
that Eq. (32) would be a good approximated expression to estimate the gate errors as well as explore the gate error’s physical mechanism in coupler architecture. To further analyze the gate error components, we also evaluate and plot the gate error in absence of ZZ couplings, i.e., taking $|\zeta_{zz}| = 0$. The results (black dashed lines, labelled as “$\zeta_{zz} = 0$”), containing only qubits’ energy relaxation contributions, behave linear approximately as expected. Specially, we find that gate error reaches a minimum value at a specific gate time $t_g^\ast$. This critical point $t_g^\ast$ corresponds to a minimum $|\zeta_{zz}|$. At this point, the gate error is limited mainly by the energy relaxation of computational qubits and coupler. Therefore, the coupler architecture with our suggested parameter regions is viable in the long term as superconducting qubits’ coherence time continues to improve [60].

Finally, we add some remarks to gate error characteristics with the four suggested parameter regions discussed above. For parameter regions I, II, III, the computational qubits $q_1, q_2$ are realized with transmon-type qubits that are stable and own longer coherent time. The main difference among these three regions is the specific character of the coupler. For region I, the coupler is realized with transmon qubit as well. Besides, it requires a relatively small detuning between computational qubits and coupler. Restricting by dispersive relations, one also has to choose weaker qubit-coupler couplings $g_1$, $g_2$. As a consequence, it results in longer gate time $t_g$. This might be a disadvantage, especially when qubits’ energy relaxation time is shorter. By contrast, the couplers in regions II and III are realized by either large-anharmonicity transmon qubit or CSFQ, whose energy relaxation time is usually shorter than mature transmon-type qubits. Thus, one may worry that this will lead to larger gate errors. However, this is not the case. In coupler architecture, we find that the noises (of course, including the qubits’ energy relaxation) induced by the coupler are suppressed largely by the dispersive couplings between the computational qubits and coupler. This is very different from the case of choosing two qubits’ anharmonicity with different signs [28, 30, 42]. Therefore, we expect that our suggested parameter regions may exhibit higher gate fidelity. As for region IV, the situation is different from the other three regions. Since all the elements are positive-anharmonicity qubits realized with CSFQ, one may worry about the ultimate performance (e.g., gate fidelity) because the stability and coherence of CSFQ cannot be comparable with mature transmon qubits. However, the situation may be improved rapidly in the future with mature CSFQ technology. Indeed, some promising progress has already been made very recently that the coherent time of CSFQ achieved in the range of 50 µs to 100 µs [56, 61]. Therefore, high-fidelity two-qubit gates may be realized in the parameter region IV as well.

![FIG. 11. Average gate error characteristics with our suggested parameter regions I-IV. The numerical results (orange dotted) are solved via diagonalizing the system Hamiltonian $\hat{H}_{\text{Lab}}$ while the analytical results (blue solid) are plotted using Eq. (32). The black dashed lines corresponds to the cases in absence of ZZ couplings. The used parameters are identical to Table I and the anharmonicity of two computational qubits are chosen as: (a) regions I: $\alpha_{q_1}/(2\pi) = \alpha_{q_2}/(2\pi) = -0.3$ GHz; (b) regions II: $\alpha_{q_1}/(2\pi) = \alpha_{q_2}/(2\pi) = -0.25$ GHz; (c) regions III: $\alpha_{q_1}/(2\pi) = \alpha_{q_2}/(2\pi) = -0.15$ GHz; (d) regions IV: $\alpha_{q_1}/(2\pi) = \alpha_{q_2}/(2\pi) = 0.4$ GHz; the number of random initial states $N = 10^5$, and the energy relaxation time $T_1 = 100$ µs for both computational qubits and coupler.]


B. Analytical results and Discussion

In addition to numerical results, we are also interested in deriving the corresponding analytical results using the method “vectorization of the Lindblad equation” [62, 63]. In particular, the density matrix \( \hat{\rho}(t) \) is vectorized as a column vector \( |\hat{\rho}(t)\rangle \). It is noted that the double bracket notation serves to remind us that this is not the standard Hilbert space of state vectors. Using the vectorization property \( |A\hat{\rho}(t)B\rangle \rightarrow B^T \otimes |A\hat{\rho}(t)| \) (\( A, B \) are matrices, \( B^T \) denotes the transpose of matrix \( B \)), the Lindblad equation \((22)\) is rewritten as

\[
\frac{\partial}{\partial t}|\hat{\rho}(t)\rangle = \hat{L}|\hat{\rho}(t)\rangle,
\]

where \( \hat{L} = \hat{L}_0 + \hat{L}_{\text{noise}}^{ZZ} + \hat{L}_{\text{decay}} \) consists of three parts: \( \hat{L}_0 \) corresponds to the noise-free case while \( \hat{L}_{\text{noise}}^{ZZ}, \hat{L}_{\text{noise}}^{\text{decay}} \) represents the noise contribution induced by ZZ parasitic coupling and qubits decay effect, respectively. The specific expressions are obtained as

\[
\hat{L}_0 = -i\hat{I} \otimes \hat{H}_{\text{XY}}^{\text{int}} + i \left( \hat{H}_{\text{ZZ}}^{\text{int}} \right)^T \otimes \hat{I},
\]

\[
\hat{L}_{\text{noise}}^{ZZ} = -i\hat{I} \otimes \hat{H}_{\text{ZZ}}^{\text{int}} + i(\hat{H}_{\text{ZZ}}^{\text{int}})^T \otimes \hat{I},
\]

\[
\hat{L}_{\text{noise}}^{\text{decay}} = \sum_{i,j=1,2} \tilde{\gamma}_{ij} \left[ (\hat{\sigma}_+^i)^T \otimes \hat{\sigma}_-^j - \frac{1}{2} \hat{\sigma}_+^i \hat{\sigma}_-^j - \frac{1}{2} (\hat{\sigma}_+^i \hat{\sigma}_-^j)^T \otimes \hat{I} \right],
\]

where the expressions for Hamiltonian \( \hat{H}_{\text{XY}}^{\text{int}} \) and \( \hat{H}_{\text{ZZ}}^{\text{int}} \) were given in Eqs. (15) and (16) respectively, \( \hat{I} \) is identity operator, and the effective decay rates \( \tilde{\gamma}_{ij} \) were given in Eq. (23).

With the new notations, it is very natural to make a connection using the relation \( \text{tr}(\hat{\rho}_0(t_g)|\hat{\rho}(t_g)|) = \langle \langle \hat{\rho}_0^*|\hat{\rho}(t_g)|\rangle \rangle \), where the trace of two density matrix can be evaluated by computing the inner product of the two corresponding “vectorization states” \( |\hat{\rho}_0(t_g)\rangle \) and \( |\hat{\rho}(t_g)\rangle \). With considering these and using Eqs. (24) and (25), we obtain

\[
\mathcal{F} = \frac{1}{N} \sum_{k=1}^{N} \langle \langle \hat{\rho}_0^*(0)|e^{-\hat{L}_{\text{dec}}e^{\hat{L}_{\text{ts}}}}|\hat{\rho}_0(0)\rangle \rangle,
\]

where we used \( |\hat{\rho}_0(k)\rangle = |\hat{\rho}_0(0)\rangle \) because the initial states for the noise and noise-free cases are identical. Next, the task becomes to compute the quantity \( e^{-\hat{L}_{\text{dec}}e^{\hat{L}_{\text{ts}}}} \). In particular, this calculation can be simplified through making representation transformation upon \( \hat{L} \) with choosing \( V(t) = e^{\hat{L}_{\text{dec}}t/2} \), obtaining \( \hat{L} = V^{-1}(t)\hat{L}_0V(t) + V^{-1}(t)(\hat{L}_{\text{noise}}^{ZZ} + \hat{L}_{\text{noise}}^{\text{decay}})V(t) - 2V^{-1}(t)\partial V(t) \). Here, the prefactor of the last term is “2” (instead of “1”) because we perform representation transformation on two independent operators. Under the new representation, we obtain

\[
\hat{L} = \hat{L}_{\text{noise}}^{ZZ} + e^{-\hat{L}_{\text{dec}}t/2}\hat{L}_{\text{noise}}^{\text{decay}} e^{\hat{L}_{\text{dec}}t/2},
\]

where the commute relation \( [\hat{\sigma}_+^1, \hat{\sigma}_+^2] = \hat{\sigma}_+^1 \hat{\sigma}_+^2 + \hat{\sigma}_+^2 \hat{\sigma}_+^1 = \hat{\sigma}_+^2 \hat{\sigma}_+^1 = 0 \) was used. Consequently, the key quality in new representation is computed as

\[
e^{-\hat{L}_{\text{dec}}t_g e^{\hat{L}_{\text{ts}}}} \rightarrow \exp \left( \hat{L}_{\text{noise}}^{ZZ} t_g + e^{-\hat{L}_{\text{dec}}t_g/2}\hat{L}_{\text{noise}}^{\text{decay}} t_g e^{\hat{L}_{\text{dec}}t_g/2} \right) \\
\approx i + e^{-\hat{L}_{\text{dec}}t_g/2}\hat{L}_{\text{noise}}^{\text{decay}} t_g e^{\hat{L}_{\text{dec}}t_g/2} + \frac{(\hat{L}_{\text{noise}}^{ZZ})^2 t_g^2}{2},
\]

where in the last step we used the approximations that gate time is much smaller than the decay time, i.e., \( t_g \ll T_1 \), and the ZZ coupling strength is much smaller than the XY coupling strength, i.e., \( |\tilde{\gamma}_z| \ll |\tilde{\gamma}_x| \). Ultimately, substituting Eq. (31) back into Eq. (29), the average gate error arrives as a simple form

\[
\varepsilon(t_g) \approx \frac{\lambda_{\text{decay}}}{T_1} \varepsilon_{t_g} + \frac{1}{N} \sum_{k=1}^{N} \langle \langle \hat{\rho}_0^*(0)|e^{-\hat{L}_{\text{dec}}t_g e^{\hat{L}_{\text{ts}}}}|\hat{\rho}_0(0)\rangle \rangle
\]

(32)}

where \( \text{sgn} \) is signum function; \( \lambda_{zz} \) and \( \lambda_{\text{decay}} \) can be evaluated with randomized initial states, namely \( \lambda_{\text{decay}} = -\frac{1}{N} \sum_{k=1}^{N} \langle \langle \hat{\rho}_0^*(0)|e^{-\hat{L}_{\text{dec}}t_g e^{\hat{L}_{\text{ts}}}}|\hat{\rho}_0(0)\rangle \rangle \approx 0.81 \) and \( \lambda_{zz} = -\frac{1}{N} \sum_{k=1}^{N} \langle \langle \hat{\rho}_0^*(0)|\hat{L}_{\text{noise}}^{ZZ}(\hat{\rho}_0(0)) \rangle \rangle \approx 18.55 \). The correctness of the analytical result is verified using numerical results with different parameter regimes (see Fig. 11). We find it gives a good result whose behaviors are very close to the accurate numerical results. Therefore, with the help of Eq. (32), one is able to estimate the average two-qubit gate errors of coupler architecture conveniently with given superconducting circuit parameters. This would be very helpful to experimental scientists when they design superconducting circuits.

Furthermore, more interesting physics can be reflected from this analytical result. As seen clearly from Eq. (32), the first term represents the gate error induced by qubits’ energy relaxation while the second term corresponds to the error induced by ZZ parasitic couplings. The characteristics are different for different parameter regime. When the energy relaxation effect dominates, the average gate errors are proportional to gate time \( t_g \) and inversely proportional to qubits’ energy relaxation time \( T_1 \). This is why short pulses are usually favorable. When ZZ parasitic coupling dominates, the average gate errors are inversely proportional to the gate time’s square; hence lower gate errors favor longer gate time. This is understandable because longer gate time corresponds to weaker ZZ parasitic couplings, the price we have to pay is larger parasitic couplings. This would be very helpful to experimental scientists when they design superconducting circuits.
\[ t_g^* = \frac{2\lambda_{zz}T_1 (1/\alpha_{q1} + 1/\alpha_{q2})^2/\lambda_{\text{decay}}^{1/3}}{\lambda_{\text{coeff}}} \] and the corresponding minimum gate error is estimated as \( \varepsilon(t_g^*) \).

VI. SUMMARY AND PERSPECTIVES

In summary, we studied systematically the physical mechanisms of ZZ parasitic coupling and the resulting two-qubit gate error characteristics in coupler architecture using effective Hamiltonian approach. Through applying two times Schrieffer-Wolf transformation, we obtained an effective Hamiltonian containing some intriguing terms (unexplored yet) which can be interpreted as parasitic couplings between the state \( |101\rangle \) in computational space and high-energy states \( |200\rangle, |002\rangle, \) and \( |020\rangle \) out of computational space. These parasitic couplings are counted as noise source for realizing iSWAP gates. Benefiting from the effective Hamiltonian, we successfully derived the analytical result for ZZ coupling strength \( \zeta_{zz} \) for different regime; using it, some previous impressive research \([28, 34, 42]\) can be thoroughly explained and understood. Beyond it, we also provided an explicit quantitative condition for eliminating ZZ parasitic couplings. As applications, this can be used to fix the proper parameters in designing superconducting quantum processor. Last but not least, we proposed four novel parameter regions in which minimum ZZ couplings and high-fidelity gates are expected. Using the novel parameter regions, we found that the coupler’s high energy lev-els play a vital role (ignored in previous research), which can neutralize the energy shift induced by computational qubits’ high energy levels. We hope the coupler architecture with these suggested parameter regions and the predicted characteristics could be realized and verified in future experiments.

Numerically solving the Lindblad equation containing both energy relaxation effects and ZZ parasitic couplings, we verified that high-fidelity two-qubit gates are realizable with our suggested parameter regions. In particular, ZZ parasitic coupling can be eliminated with proper system parameters and the resulting gate errors are limited mainly by qubits’ energy relaxation. Apart from the numerical results, we also successfully derived an analytical expression \([\text{Eq. (32)}]\) of the average gate error via vectorizing the Lindblad equation. We found the trade-off effect between the error induced by qubit energy relaxation and ZZ parasitic couplings with different gate time. Moreover, this can be applied to estimate the average gate error in coupler architecture with given system parameters conveniently.

Beyond the architecture and dispersive regime discussed in this paper, new coupler architecture connecting fixed-frequency floating qubits and new regime were also studied and high-fidelity gates were realized very recently \([31, 64, 65]\). Therefore, it would be also interesting to study the interesting physical mechanism behind and explore more possibility.

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Appendix A: Derivation of the Effective Hamiltonian

In this appendix, we show the detailed derivation of Eq. (7) (which is the cornerstone of this paper) using Schrieffer–Wolff transformation (SWT). In particular, we apply two times SWT and consider the fourth-order contribution. Comparing with previous work \([25]\) in which only 1 time SWT was applied and only the first-order contribution was involved, our results are more accurate and contain richer physics. Benefiting from the substantial derivation, the irrelevant terms will be got rid from the lab Hamiltonian eventually. More importantly, the physical mechanisms can be understood clearly using the resulting effective Hamiltonian.

1. 1st SWT

In order to obtain the indirect coupling between computational qubits, the first and foremost task is to decouple the coupler using SWT. In particular, we need to find a suitable \( \hat{s}_1 \) and compute \( e^{\hat{s}_1} \hat{H}_{\text{lab}} e^{-\hat{s}_1} \). The explicit form for \( \hat{s}_1 \) is given by

\[ \hat{s}_1 = \sum_{k=1,2} \frac{g_k}{\Delta_k} \left( \hat{a}_{qk}^\dagger \hat{a}_c - \hat{a}_{qk} \hat{a}_c^\dagger \right) - \frac{g_k}{\sum_k} \left( \hat{a}_{qk}^\dagger \hat{a}_c^\dagger - \hat{a}_{qk} \hat{a}_c \right), \quad (A1) \]

where \( \Delta_k = \omega_{qk} - \omega_c \) and \( \sum_k = \omega_{qk} + \omega_c \). For easy reference, we write down again the lab frame Hamiltonian.

\[ \hat{H}_{\text{lab}} = \sum_{\lambda=q1,q2,c} \omega_{\lambda} \hat{a}_\lambda^\dagger \hat{a}_\lambda + \frac{\alpha_{q1}}{2} \hat{a}_{q1}^\dagger \hat{a}_{q1} \hat{a}_\lambda \hat{a}_\lambda + g_{12} \left( \hat{a}_{q1}^\dagger \hat{a}_{q2} - \hat{a}_{q1} \hat{a}_{q2}^\dagger \right) + H.c. \] + \sum_{k=1,2} g_k \left( \hat{a}_{qk}^\dagger \hat{a}_c - \hat{a}_{qk} \hat{a}_c^\dagger \right) + H.c. \]. \quad (A2)
Next, the task becomes to compute \( e^{\hat{s}_1 \hat{H}_{\text{Lab}} e^{-\hat{s}_1}} = \hat{H}_{\text{Lab}} + [\hat{s}_1, \hat{H}_{\text{Lab}}] + [\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]/2! + \cdots \). First of all, the zero-order contribution is \( \hat{H}_{\text{Lab}} \) itself. Since the calculation for the higher order contributions always rely on the results of lower orders, we compute it order by order respectively.

The first-order contribution

As a starting point, let us compute the first-order contribution \([\hat{s}_1, \hat{H}_{\text{Lab}}]\). Since \( \hat{s}_1 \) contains four terms, they can be computed separately. Here, we show only the first term calculation, i.e., \([\hat{a}_{q1} \hat{a}_c - \hat{a}_q \hat{a}_c^\dagger, \hat{H}_{\text{Lab}}]\), as an example. Besides, it is noticeable there are nine terms in Hamiltonian \( \hat{H}_{\text{Lab}} \), we compute them independently and then combine. At the end, we obtain

\[
\left[ \hat{a}_{q1}^\dagger \hat{a}_c - \hat{a}_{q1} \hat{a}_c^\dagger, \hat{H}_{\text{Lab}} \right] = -\Delta_1 \left( \hat{a}_{q1}^\dagger \hat{a}_c + \hat{a}_{q1} \hat{a}_c^\dagger \right) + 2g_1 \left( \hat{a}_{q1}^\dagger \hat{a}_{q1} - \hat{a}_{q1} \hat{a}_{q1}^\dagger \right) + g_2 \left( \hat{a}_{q1}^\dagger \hat{a}_{q2} + \hat{a}_{q1} \hat{a}_{q2}^\dagger - \hat{a}_{q1} \hat{a}_{q2}^\dagger - \hat{a}_{q1} \hat{a}_{q2}^\dagger \right) \\
\quad - g_1 \left( \hat{a}_{q1}^\dagger \hat{a}_{q1} + \hat{a}_{q1} \hat{a}_{q1}^\dagger \right) + g_1 \left( \hat{a}_{q1} \hat{a}_{q1}^\dagger + \hat{a}_{q1} \hat{a}_{q1}^\dagger \right) - g_1 \left( \hat{a}_{q2} \hat{a}_c + \hat{a}_{q2} \hat{a}_c^\dagger - \hat{a}_{q2} \hat{a}_c^\dagger - \hat{a}_{q2} \hat{a}_c^\dagger \right) \\
\quad - a_{q1} \left( \hat{a}_{q1}^\dagger \hat{a}_{q1} \hat{a}_c + \hat{a}_{q1} \hat{a}_{q1} \hat{a}_c^\dagger \right) + a_c \left( \hat{a}_{q1} \hat{a}_{q1}^\dagger \hat{a}_c + \hat{a}_{q1}^\dagger \hat{a}_{q1} \hat{a}_c \right). \quad (A3)
\]

Using the same procedure, we obtain

\[
\left[ \hat{a}_{q1}^\dagger \hat{a}_c - \hat{a}_{q1} \hat{a}_c^\dagger, \hat{H}_{\text{Lab}} \right] = -\Sigma_1 \left( \hat{a}_{q1}^\dagger \hat{a}_c + \hat{a}_{q1} \hat{a}_c^\dagger \right) + 2g_1 \left( \hat{a}_{q1} \hat{a}_{q1} + \hat{a}_{q1} \hat{a}_{q1}^\dagger \right) + g_2 \left( \hat{a}_{q1} \hat{a}_{q2} + \hat{a}_{q1} \hat{a}_{q2}^\dagger - \hat{a}_{q1} \hat{a}_{q2}^\dagger - \hat{a}_{q1} \hat{a}_{q2}^\dagger \right) \\
\quad - g_1 \left( \hat{a}_{q1}^\dagger \hat{a}_{q1} + \hat{a}_{q1} \hat{a}_{q1}^\dagger \right) - g_1 \left( \hat{a}_{q1} \hat{a}_{q1}^\dagger + \hat{a}_{q1} \hat{a}_{q1}^\dagger \right) + g_1 \left( \hat{a}_{q2} \hat{a}_c + \hat{a}_{q2} \hat{a}_c^\dagger - \hat{a}_{q2} \hat{a}_c^\dagger - \hat{a}_{q2} \hat{a}_c^\dagger \right) \\
\quad - a_{q1} \left( \hat{a}_{q1}^\dagger \hat{a}_{q1} \hat{a}_c + \hat{a}_{q1} \hat{a}_{q1} \hat{a}_c^\dagger \right) - \alpha_c \left( \hat{a}_{q1} \hat{a}_{q1}^\dagger \hat{a}_c + \hat{a}_{q1}^\dagger \hat{a}_{q1} \hat{a}_c \right). \quad (A4)
\]

Similarly, through simply exchanging the subscripts “q1” and “q2”, the other two terms \([\hat{a}_{q2}^\dagger \hat{a}_c - \hat{a}_{q2} \hat{a}_c^\dagger, \hat{H}_{\text{Lab}}]\) and \([\hat{a}_{q2}^\dagger \hat{a}_c^\dagger - \hat{a}_{q2} \hat{a}_c^\dagger, \hat{H}_{\text{Lab}}]\) are computed as well. Finally, using the equations above and considering the related prefactors, we are able to obtain the first-order contribution. It reads

\[
\left[ \hat{s}_1, \hat{H}_{\text{Lab}} \right] = -\sum_{k=1,2} g_k \left( \hat{a}_{qk}^\dagger \hat{a}_c - \hat{a}_{qk} \hat{a}_c^\dagger + H.c. \right) + \sum_{k=1,2} \left[ \left( \frac{2g_k^2}{\Delta_k} - \frac{2\Sigma_k}{\Delta_k} \right) \hat{a}_{qk}^\dagger \hat{a}_{qk} - \left( \frac{2g_k^2}{\Delta_k} + \frac{2\Sigma_k}{\Delta_k} \right) \hat{a}_c^\dagger \hat{a}_c \right] \\
+ g_1 g_2 \left( \frac{1}{\Delta_1} + \frac{1}{\Delta_2} - \frac{1}{\Sigma_1} - \frac{1}{\Sigma_2} \right) \left( \hat{a}_{q1} \hat{a}_{q2} - \hat{a}_{q2}^\dagger \hat{a}_{q1}^\dagger + H.c. \right) - \sum_{k=1,2} \left( \frac{g_k \alpha_k}{\Delta_k} \hat{a}_{qk}^\dagger \hat{a}_{qk} \hat{a}_{qk}^\dagger + \frac{g_k \alpha_k}{\Sigma_k} \hat{a}_{qk} \hat{a}_{qk}^\dagger \hat{a}_{qk} \hat{a}_{qk}^\dagger \right) \\
+ \sum_{k=1,2} \left( \frac{g_k^2}{\Sigma_k} \hat{a}_{qk}^\dagger \hat{a}_{qk}^\dagger + \frac{g_k^2}{\Sigma_k} \hat{a}_{qk} \hat{a}_{qk} \hat{a}_{qk} \hat{a}_{qk}^\dagger + H.c. \right) \right] \\
- \sum_{k=1,2} \left( \frac{g_k \Sigma_k}{\Delta_k} \left( \hat{a}_{qk}^\dagger \hat{a}_c + \hat{a}_{qk} \hat{a}_c^\dagger - \hat{a}_{qk}^\dagger \hat{a}_c^\dagger - \hat{a}_{qk} \hat{a}_c \right) + \frac{g_k g_{12}}{\Sigma_k} \left( \hat{a}_{qk}^\dagger \hat{a}_c + \hat{a}_{qk} \hat{a}_c - \hat{a}_{qk} \hat{a}_c^\dagger - \hat{a}_{qk}^\dagger \hat{a}_c \right) \right), \quad (A5)
\]

where for simplification we defined \( \tilde{k} \): \( \tilde{1} = 2 \) and \( \tilde{2} = 1 \).

It is necessary to point out that the above equation is the exact result without any approximations. In particular, the first term of the equation’s right side is used to cancel \( H_{qc} \), i.e., Eq. (4). The second term implies the frequency shift of the qubits induced by the couplings. The third term represents the effective indirect coupling between two computational qubits due to the coupler. It is exactly this term that made the coupling between computational qubits tunable. For the fourth term, it originates from the three nonlinear Kerr interaction terms of \( \hat{H}_0 \), i.e., Eq. (2). Since they describe higher energy levels of superconducting qubits, we will see very fruitful physics originated from these nonlinear terms. The contribution of the fourth term was usually ignored in previous research [25], but we find they are indeed very important especially when the condition \( \alpha_\lambda \ll \Delta_{1,2} \), \( \lambda = q1, q2 \) violates (for instance when the qubits are not transmon type). In the following, we keep only the first four terms and neglect the last two terms. The reason is as follows: firstly, the fifth term is high-frequency rotating and thus can be ignored; meanwhile, even if the second-order contribution of the fifth term produces some terms describing the coupling between computational qubits and coupler but with a small prefactor \( (g_k/\Delta_k)^2 \) or \( (g_k/\Sigma_k)^2 \), \( k = 1, 2 \), thus the strength goes to zero under dispersive regime; secondly, the last term can also be ignored with further considering \( g_{12} \ll \Delta_k, \Sigma_k \), namely assuming
the direct coupling between the computational qubits are rather weak. Comparing the last term and the first term, it is obvious the last term can be ignored. Meanwhile, for the corresponding second-order contribution, all of the terms are along with small prefactors \((g_k/\Delta_k)^2\) or \((g_k/\Sigma_k)^2\); therefore, we can safely neglect them as well.

### The second-order contribution

Using the same procedure, we continue to compute the second-order contribution. Although there are many terms in \([\hat{s}_1, \hat{H}_{\text{Lab}}]\), i.e., Eq. (A5), we will see most of them can be neglected under dispersive regime. To present the calculation in a simple way, the contribution from each term of \([\hat{s}_1, \hat{H}_{\text{Lab}}]\) is labelled as \([\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]](k)\) \((k\) indicates the \(k\)-th term of Eq. (A5)). In the following, they are computed one by one. First of all, we consider

\[
[\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]^{(1)} = \sum_{k=1,2} \left[ \left( \frac{2g_k^2}{\Sigma_k} - \frac{2g_k^2}{\Delta_k} \right) \hat{a}_q^\dagger \hat{a}_{qk} + \left( \frac{2g_k^2}{\Delta_k} + \frac{2g_k^2}{\Sigma_k} \right) \hat{a}_q^\dagger \hat{a}_c - g_1 g_2 \left( \frac{1}{\Delta_k} - \frac{1}{\Sigma_k} \right) \left( \hat{a}_q^\dagger \hat{a}_{q2} - \hat{a}_q^\dagger \hat{a}_{q2} + H.c. \right) \right].
\]

For the second and third terms of \([\hat{s}_1, \hat{H}_{\text{Lab}}]\), namely \([\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]^{(2)}\) and \([\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]^{(3)}\), we can straightforward compute them using the previous results. However, they do not generate new terms (comparing with the first-order result, i.e., Eq. (A5)) but with small prefactors \((g_k/\Delta_k)^2\), \((g_k/\Sigma_k)^2\), or \((g_k/\Delta_k)(g_k/\Sigma_k)\), \(k = 1, 2\), hence can be neglected under the regime of interest, namely \(g_k \ll |\Delta_k|, \Sigma_k\).

Next, we turn to look into the nonlinear terms, namely \([\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]^{(4)}\). We obtain

\[
[\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]^{(4)} \approx \sum_{k=1,2} \left( \frac{2g_k^2}{\Delta_k} \right) \hat{a}_q^\dagger \hat{a}_{qk} \hat{a}_q \hat{a}_k - \frac{2g_k^2}{\Delta_k} \hat{a}_q^\dagger \hat{a}_{qk} \hat{a}_q \hat{a}_k - \frac{g_1 g_2}{\Delta_k} \hat{a}_q^\dagger \hat{a}_{qk} \hat{a}_q \hat{a}_k + \frac{g_1 g_2}{\Delta_k} \hat{a}_q^\dagger \hat{a}_{qk} \hat{a}_q \hat{a}_k + H.c.,
\]

for simplification we defined \(\tilde{k}: 1 = 2 \text{ and } 2 = 1\). Moreover, we neglected those high rotating terms, e.g., \(\hat{a}_q^\dagger \hat{a}_{qk} \hat{a}_q \hat{a}_c + H.c.\) in the equation above. The same rule will be applied in the following calculations.

As discussed before, the last two terms of Eq. (A5) does not generate new term and along with some small prefactors, and hence can be ignored in first and second contributions.

Combining all of these terms, the second-order contribution arrives as

\[
[\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]] = - \sum_{k=1,2} \left( \left( \frac{2g_k^2}{\Delta_k} - \frac{2g_k^2}{\Sigma_k} \right) \hat{a}_q^\dagger \hat{a}_{qk} + \left( \frac{2g_k^2}{\Delta_k} + \frac{2g_k^2}{\Sigma_k} \right) \hat{a}_q^\dagger \hat{a}_c - \frac{2g_k^2}{\Delta_k} \hat{a}_q^\dagger \hat{a}_{qk} \hat{a}_q \hat{a}_k - \frac{2g_k^2}{\Delta_k} \hat{a}_q^\dagger \hat{a}_{qk} \hat{a}_q \hat{a}_k + \frac{2g_k^2}{\Delta_k} \hat{a}_q^\dagger \hat{a}_{qk} \hat{a}_q \hat{a}_k \right),
\]

As seen from the equation above, both the qubits’ frequency and anharmonicity are shifted; this would be vital for some specific parameters regime. Besides, the resulting effective couplings between the computational qubits are generated as expected. More importantly, some interesting interacting terms (e.g., the last two terms) arise. We will see they describe very fruitful and clear physics when we study ZZ parasitic couplings and two-qubit gate error sources.

### The third-order contribution

Due to the existence of Kerr terms in lab frame Hamiltonian, we expect the cross-Kerr interaction (which is related to ZZ crosstalk) term, i.e., \(\hat{a}_q^\dagger \hat{a}_{q1}^\dagger \hat{a}_{q2} \hat{a}_q\), will appear when the fourth-order contribution is involved.

The same procedure is used to compute the third order contribution \([\hat{s}_1, [\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]\]). As we keep in mind that the goal is to derive the cross-Kerr interaction \(\hat{a}_q^\dagger \hat{a}_{q1}^\dagger \hat{a}_{q2} \hat{a}_q\), only the terms related to \(\hat{a}_q^\dagger \hat{a}_{q1}^\dagger \hat{a}_{q2} \hat{a}_q\) are kept, while other irrelevant terms will be neglected. It is not hard to recognize that only the last three terms of Eq. (A8)
contribute effectively. Hence, we compute \( [\hat{s}_1, [\hat{s}_1, \hat{s}_1, \hat{H}_{\text{Lab}}]]^{(k)} \) \((k\) represents the \(k\)-th term of Eq. (A8)\) one by one independently. The 3rd, 4th, and 5th terms are obtained as follows, respectively.

\[
[\hat{s}_1, [\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]]^{(3)} = \frac{4g_1g_2}{\Delta_1 \Delta_2} \sum_{k=1,2} g_k (\alpha_{qk} + \alpha_c) \left( \hat{a}_{qk}^{\dagger} \hat{a}_{qk}^{\dagger} \hat{a}_c + H.c. \right), \quad (A9)
\]

\[
[\hat{s}_1, [\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]]^{(4)} = \frac{2g_1g_2}{\Delta_1 \Delta_2} \sum_{k=1,2} g_k \alpha_{qk} \left( \hat{a}_{qk}^{\dagger} \hat{a}_{qk}^{\dagger} \hat{a}_c + H.c. \right), \quad (A10)
\]

\[
[\hat{s}_1, [\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]]^{(5)} = \frac{8g_1g_2 \alpha_c}{\Delta_1 \Delta_2} \sum_{k=1,2} g_k \left( \hat{a}_{qk}^{\dagger} \hat{a}_{qk}^{\dagger} \hat{a}_c + H.c. \right). \quad (A11)
\]

During the derivation, we used the approximated condition \( g_k/\Sigma_k \ll g_k/|\Delta_k| \), \( k = 1, 2 \), so those terms containing \((g_k/\Sigma_k)^2\) were neglected for simplification. Collecting these contributed terms, the third order contribution arrives as

\[
\[\hat{s}_1, [\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]\] = \frac{6g_1g_2}{\Delta_1 \Delta_2} \sum_{k=1,2} g_k (\alpha_{qk} + 2\alpha_c) \left( \hat{a}_{qk}^{\dagger} \hat{a}_{qk}^{\dagger} \hat{a}_c + H.c. \right). \quad (A12)
\]

**The forth-order contribution**

Using the result of third-order contribution, we continue compute the fourth-order contribution. There are two terms in Eq. (A12). We compute \([\hat{s}_1, [\hat{s}_1, [\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]]]^{(k)} \) \((k\) represents the \(k\)-th term) independently.

\[
[\hat{s}_1, [\hat{s}_1, [\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]]]^{(12)} = 12 \left( \frac{g_1g_2}{\Delta_1 \Delta_2} \right)^2 (\alpha_{qk} + 2\alpha_c) \hat{a}_{q1}^{\dagger} \hat{a}_{q1}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}, \quad k = 1, 2. \quad (A13)
\]

Summing up the two contributed terms, we finally obtain

\[
[\hat{s}_1, [\hat{s}_1, [\hat{s}_1, [\hat{s}_1, \hat{H}_{\text{Lab}}]]]] = 12 \left( \frac{g_1g_2}{\Delta_1 \Delta_2} \right)^2 (\alpha_{q1} + \alpha_{q2} + 4\alpha_c) \hat{a}_{q1}^{\dagger} \hat{a}_{q1}^{\dagger} \hat{a}_{q2}. \quad (A14)
\]

As expected, the strength for the cross-Kerr interaction is expressed in the fourth-order. Besides, the amplitude is related to the anharmonicity of both computational qubits and coupler.

**The effective Hamiltonian after 1st SWT**

Using the results we obtained above, including Eqs. (A2), (A5), (A8), (A12), (A14), and considering the prefactors, the Hamiltonian after 1st SWT is obtained as

\[
\hat{H}_{\text{eff}} \approx \sum_{\lambda=q1,q2,c} \omega_{\lambda} \hat{a}_{\lambda}^{\dagger} \hat{a}_{\lambda} + \frac{\alpha_{q1}^{\prime} \alpha_{q2}^{\prime}}{\Delta_1} \hat{a}_{q1}^{\dagger} \hat{a}_{q2}^{\dagger} \hat{a}_c + \frac{\alpha_{q1}^{\prime} \alpha_{q2}^{\prime}}{\Delta_2} \hat{a}_{q1}^{\dagger} \hat{a}_{q2}^{\dagger} \hat{a}_c + g_{\text{eff}} \left( \hat{a}_{q1}^{\dagger} \hat{a}_{q2} + \hat{a}_{q1} \hat{a}_{q2}^{\dagger} - \hat{a}_{q1}^{\dagger} \hat{a}_{q2}^{\dagger} - \hat{a}_{q1} \hat{a}_{q2} \right) + \sum_{k=1,2} \frac{2g_k^2 (\alpha_{qk} + \alpha_c)}{\Delta_k} \hat{a}_{qk}^{\dagger} \hat{a}_{qk} \hat{a}_c + \frac{g_1g_2}{\Delta_1 \Delta_2} \sum_{k=1,2} \alpha_{qk} \left( \hat{a}_{qk}^{\dagger} \hat{a}_{qk}^{\dagger} \hat{a}_c + H.c. \right) + \frac{1}{2} \left( \frac{g_1g_2}{\Delta_1 \Delta_2} \right)^2 (\alpha_{q1} + \alpha_{q2} + 4\alpha_c) \hat{a}_{q1}^{\dagger} \hat{a}_{q1}^{\dagger} \hat{a}_{q2} \hat{a}_{q2} \right) - \sum_{k=1,2} \left( \frac{g_k \alpha_{qk}}{\Delta_k} \hat{a}_{qk}^{\dagger} \hat{a}_{qk} \hat{a}_c + H.c. \right) + \frac{g_1 \alpha_{q1} \alpha_{q2}}{\Delta_k} \hat{a}_{q1}^{\dagger} \hat{a}_{q1}^{\dagger} \hat{a}_c + H.c. \right) \right] \right. \quad (A15)
\]

where the shifted qubit frequencies are

\[
\omega_{qk} = \omega_{qk} + \frac{g_k^2}{\Delta_k} - \frac{g_k^2}{\Sigma_k}, \quad \omega_c = \omega_c - \sum_{k=1,2} \left( \frac{g_k^2}{\Delta_k} + \frac{g_k^2}{\Sigma_k} \right) \quad \text{.} \quad (A16)
\]

and the shifted anharmonicity are

\[
\alpha_{qk}^{\prime} = \alpha_{qk} \left( 1 - 2 \frac{g_k^2}{\Delta_k^2} \right), \quad \alpha_c^{\prime} = \alpha_c \left[ 1 - 2 \left( \frac{g_1^2}{\Delta_1^2} + \frac{g_2^2}{\Delta_2^2} \right) \right]. \quad (A17)
\]
Moreover, the effective coupling between the two computational qubits are

\[ g_{\text{eff}} = g_{12} + \frac{g_1 g_2}{2} \left( \frac{1}{\Delta_1} + \frac{1}{\Delta_2} - \frac{1}{\Sigma_1} - \frac{1}{\Sigma_2} \right). \] (A18)

Next, let us add some remarks to these new interaction terms of Eq. (A8). First of all, the resonant terms \( \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1}, \) \( \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2}, \) and \( \hat{a}_{q1}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q1}, \) do not contribute at the end, because the coupler stays in ground states all the time. Secondly, the last non-resonant terms generated from the first-order contributions indeed can be ignored with considering \( \alpha_k \ll |\Delta_k|, \) \( \lambda = q_1, q_2, c, \) and \( k = 1, 2. \) However, they should be kept when the condition does not hold, e.g., \( \alpha_\lambda \sim |\Delta_\lambda| \). Later, we will see they will bring additional energy level shifts. Thirdly, apart from these terms discussed, other interacting terms can be interpreted as parasitic couplings, which are discussed in the main text. Finally, noted that during the whole derivation, the only approximated conditions we used are: \( g_k/|\Delta_k| \ll 1 \) and \( (g_k/\sum k)^2 \ll (g_k/|\Delta_k|)^2. \)

2. 2nd SWT

The effective Hamiltonian after 1st SWT can be further simplified via performing a second SWT. The goal is to eliminate the last non-resonant term of Eq. (A15). Introducing \( \hat{s}_2 \) with

\[
\hat{s}_2 = -\frac{g_1 \alpha_{q1}}{\Delta_1} \left( \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} - \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \right) - \frac{g_2 \alpha_{q2}}{\Delta_2} \left( \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} - \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \right) - \frac{g_2 \alpha_{q2}}{\Delta_2} \left( \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} - \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \right)
\]

\[ -\frac{g_1 \alpha_{q1}}{\Delta_1} \left( \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} - \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \right) - \frac{g_2 \alpha_{q2}}{\Delta_2} \left( \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} - \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \right)
\]

\[ -\frac{g_2 \alpha_{q2}}{\Delta_2} \left( \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} - \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \right)
\]

where \( \Delta'_k = \omega'_k - \omega'_c, k = 1, 2. \) Applying the 2nd SWT, i.e., the Hamiltonian is transformed to \( \hat{H}_{\text{eff}}^2 = e^{i \hat{s}_2} \hat{H}_{\text{eff}}^1 e^{-i \hat{s}_2} = \hat{H}_{\text{eff}}^1 + [\hat{s}_2, \hat{H}_{\text{eff}}^1]/\Delta_2 + [\hat{s}_2, \hat{H}_{\text{eff}}^1][\hat{s}_2, \hat{H}_{\text{eff}}^1]/2! + \cdots \) where the 1st SWT result \( \hat{H}_{\text{eff}}^1 \) was given in Eq. (A15). As did in 1st SWT, we have to compute the first-order contribution and the-second contribution, respectively.

Let us first compute the first-order contribution \([\hat{s}_2, \hat{H}_{\text{eff}}^1]/\Delta_2 + \cdots \]. Although \( \hat{H}_{\text{eff}}^1 \) contains many terms, most of them can be neglected due to the smallness prefactors and only few of them contributes. Besides, \( \hat{s}_2 \) contains four terms, we compute them separately. At the end, we obtain

\[ [\hat{s}_2, \hat{H}_{\text{eff}}^1] \simeq \frac{g_1 \alpha_{q1}}{\Delta_1} \left( \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} - \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \right) + \frac{g_2 \alpha_{q2}}{\Delta_2} \left( \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} - \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \right) + \frac{g_2 \alpha_{q2}}{\Delta_2} \left( \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} - \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \right)
\]

Similarly, the second order contribution is computed as

\[ [\hat{s}_2, [\hat{s}_2, \hat{H}_{\text{eff}}^1]] \simeq -\frac{g_1^2 \alpha_{q1}^2}{\Delta_1^2} \left( \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} - 2 \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \right) + \frac{g_2^2 \alpha_{q2}^2}{\Delta_2^2} \left( \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} - 2 \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \right)
\]

On top of the first SWT result, summing up all of these contributions, we ultimately obtain

\[ \hat{H}_{\text{eff}}^2 \approx \sum_{\lambda=q_1,q_2,c} \hat{\omega}_\lambda \hat{a}_{\lambda}^{\dagger} \hat{a}_{\lambda} + \hat{\alpha}_\lambda^{\dagger} \hat{a}_{\lambda}^{\dagger} \hat{a}_{\lambda} \hat{a}_{\lambda} + g_{\text{eff}} \left( \hat{a}_{q1}^{\dagger} \hat{a}_{q2} - \hat{a}_{q2}^{\dagger} \hat{a}_{q1} + H.c. \right), \]

\[ -\frac{1}{2} \frac{g_1 \alpha_{q2}}{\Delta_1} \left( \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} + \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q1}^{\dagger} \hat{a}_{q1} + \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} + \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q2} \right)\]

\[ + \frac{g_1 \alpha_{q2}}{\Delta_2} \left( \hat{a}_{q1}^{\dagger} \hat{a}_{q2} \hat{a}_{q2}^{\dagger} \hat{a}_{q1} + \hat{a}_{q1} \hat{a}_{q2}^{\dagger} \hat{a}_{q1}^{\dagger} \hat{a}_{q2} \right) + \frac{1}{2} \left( \frac{g_1 g_2}{\Delta_1^2} \right)^2 \left( \alpha_{q1} + \alpha_{q2} + 4 \alpha_{c} \right) \hat{a}_{q1}^{\dagger} \hat{a}_{q1} \hat{a}_{q2}^{\dagger} \hat{a}_{q2}, \] (A22)
where the qubits' frequency are unchanged, namely \( \tilde{\omega}_\lambda = \omega_\lambda \), and shifted anharmonicity become

\[
\tilde{\alpha}_{qk} = \alpha_{qk} \left( 1 - 2 \frac{g_k^2}{\Delta_k} + 2 \frac{g_k^2}{\Delta'_k} \frac{\alpha_{qk}}{\Delta_k + \alpha_{qk}} \right) \approx \alpha_{qk} \left[ 1 - 2 \frac{g_k^2}{\Delta_k (\Delta_k + \alpha_{qk})} \right], \tag{A23}
\]

\[
\tilde{\alpha}_c = \alpha_c \left[ 1 - \sum_{k=1,2} \left( 2 \frac{g_k^2}{\Delta_k} + 2 \frac{g_k^2 \alpha_c}{\Delta_k (\Delta_k - \alpha_c)} \right) \right] \approx \alpha_c \left[ 1 - 2 \sum_{k=1,2} \frac{g_k^2}{\Delta_k (\Delta_k - \alpha_c)} \right]. \tag{A24}
\]

Note that the additional approximate condition we used are: \(|\alpha_{qk}/(\Delta_k + \alpha_{qk})| \leq 1\) and \(|\alpha_c/(\Delta_k - \alpha_c)| \leq 1, k = 1, 2\). Till now, we ultimately obtain the effective Hamiltonian, which was given in Eq. (7) of the main text.

### Appendix B: Analytical expressions of ZZ coupling for different regime

In this Appendix, we show the derivation of the analytical ZZ coupling expressions \( \zeta_{zz} \) for different regime discussed in Sec. III. For easy reference, the system Hamiltonian [i.e., Eq. (12) in the main text] containing only the terms related to ZZ couplings is written down as follows.

\[
\hat{H}^{\text{eff}} = (\tilde{\omega}_q + \tilde{\omega}_q) |101\rangle \langle 101| + (2\tilde{\omega}_q + \tilde{\alpha}_q) |200\rangle \langle 200| + (2\tilde{\omega}_q + \tilde{\alpha}_q) |002\rangle \langle 002| + (2\tilde{\omega}_c + \tilde{\alpha}_c) |020\rangle \langle 020| + \tilde{g}_{200} (|200\rangle \langle 101| + |101\rangle \langle 200|) + \tilde{g}_{002} (|002\rangle \langle 101| + |101\rangle \langle 002|) + \tilde{g}_{020} (|020\rangle \langle 101| + |101\rangle \langle 020|) + \tilde{g}_{\text{cross-Kerr}} (\alpha_1 + \alpha_2 + 4\alpha_c) |101\rangle \langle 101|, \tag{B1}
\]

where those irrelevant terms with ZZ coupling were neglected. The explicit expressions of the coupling strengths \( \tilde{g}_{200}, \tilde{g}_{002}, \tilde{g}_{020}, \) and \( \tilde{g}_{\text{cross-Kerr}} \) were given in Eq. (13). With the help of this effective Hamiltonian, we are able to derive the analytical expression of ZZ couplings for different parameter regime.

#### 1. Parasitic couplings due to high energy levels of computational qubits

When we pay specific attention to the effects of computational qubits' high energy levels, namely concentrating on the regime either \( \tilde{\omega}_q + \tilde{\omega}_q \approx 2\tilde{\omega}_q + \tilde{\alpha}_q \) or \( \tilde{\omega}_q + \tilde{\omega}_q \approx 2\tilde{\omega}_q + \tilde{\alpha}_q \), the resonant couplings between \(|101\rangle \) and \(|200\rangle \) or \(|002\rangle \) play a vital role. As a consequence, the effective Hamiltonian in matrix form reduces to

\[
\hat{H}^{200/002} = \begin{pmatrix}
|101\rangle & |200\rangle & |002\rangle \\
\tilde{g}_{200} & \tilde{g}_{002} & \tilde{g}_{020} \\
\tilde{g}_{002} & 0 & 2\tilde{\omega}_q + \tilde{\alpha}_q \\
\end{pmatrix}. \tag{B2}
\]

To compute the ZZ coupling strength \( \zeta_{zz} = \tilde{\omega}_{101} - \tilde{\omega}_{100} - \tilde{\omega}_{001} \) (\( \tilde{\omega}_{101,c,q} \) denotes the eigenenergy of the effective Hamiltonian), the key step is figuring out \( \tilde{\omega}_{101} \) which are affected by the nearly resonant couplings with the states \(|200\rangle \) or \(|002\rangle \). In particular, the energy shift of \( \tilde{\omega}_{101} \) is calculated by diagonalizing the matrix above. Ultimately, we obtain the resulting ZZ coupling expression, which is present in Eq. (17) of the main text.

#### 2. Parasitic couplings due to high energy levels of the coupler

Next, we turn to consider the effects of the coupler's high energy levels, namely concentrating on the regime \( \tilde{\omega}_q + \tilde{\omega}_q \approx 2\tilde{\omega}_c + \tilde{\alpha}_c \). Under this regime, we mainly concentrate on the resonant coupling between \(|101\rangle \) and \(|020\rangle \). As a consequence, the effective Hamiltonian becomes

\[
\hat{H}^{020} = \begin{pmatrix}
|101\rangle & |020\rangle \\
\tilde{\omega}_q + \tilde{\omega}_q & \tilde{g}_{020} \\
\tilde{g}_{020} & 2\tilde{\omega}_c + \tilde{\alpha}_c \\
\end{pmatrix}. \tag{B3}
\]

As before, the critical step is to calculate the frequency shift of \( \tilde{\omega}_{101} \). In particular, we figure it out via diagonalizing the equation above. Ultimately, we obtain the resulting ZZ coupling expression, which is present in Eq. (18) of the main text.
3. Parasitic couplings in dispersive regime

In dispersive regime, we have to consider the couplings between $|101\rangle$ and those states out of the computational space, including $|200\rangle$, $|002\rangle$, $|020\rangle$. As a consequence, the effective Hamiltonian in matrix form is given by

$$\hat{H}_{\text{disp}}^{\text{eff}} \approx \begin{pmatrix} |101\rangle & |200\rangle & |002\rangle & |020\rangle \\ \tilde{\omega}_{q1} + \tilde{\omega}_{q2} & \tilde{g}_{200} & \tilde{g}_{002} & \tilde{g}_{020} \\ \tilde{g}_{200} & 2\tilde{\omega}_{q1} + \tilde{\alpha}_{q1} & 0 & 0 \\ \tilde{g}_{002} & 0 & 2\tilde{\omega}_{q2} + \tilde{\alpha}_{q2} & 0 \\ \tilde{g}_{020} & 0 & 0 & 2\tilde{\omega}_{c} + \tilde{\alpha}_{c} \end{pmatrix}. \quad (B4)$$

In the equation above, the coupling strengths satisfy: $\tilde{g}_{200} \ll |(\tilde{\omega}_{q1} + \tilde{\omega}_{q2}) - (2\tilde{\omega}_{q1} + \tilde{\alpha}_{q1})|$, $\tilde{g}_{002} \ll |(\tilde{\omega}_{q1} + \tilde{\omega}_{q2}) - (2\tilde{\omega}_{q2} + \tilde{\alpha}_{q2})|$, ZZ coupling contributed from each type of coupling can be solved independently via diagonalizing analytically the couplings between $|101\rangle$ and $|200\rangle$, $|101\rangle$ and $|002\rangle$, and $|101\rangle$ and $|020\rangle$, respectively. Ultimately, summing up different contributions, we obtain approximately

$$\zeta_{zz} \approx \frac{\tilde{g}_{200}^2}{(\tilde{\omega}_{q1} + \tilde{\omega}_{q2}) - (2\tilde{\omega}_{q1} + \tilde{\alpha}_{q1})} + \frac{\tilde{g}_{002}^2}{(\tilde{\omega}_{q1} + \tilde{\omega}_{q2}) - (2\tilde{\omega}_{q2} + \tilde{\alpha}_{q2})} + \frac{\tilde{g}_{020}^2}{(\tilde{\omega}_{q1} + \tilde{\omega}_{q2}) - (2\tilde{\omega}_{c} + \tilde{\alpha}_{c})} + \zeta_{\text{cross}-\text{Kerr}}$$

$$\approx -2 \left( \frac{(g_{12} + g_{12}/\Delta_2)^2}{\alpha_{q1} + \Delta_1} + \frac{(g_{12} + g_{12}/\Delta_2)^2}{\alpha_{q2} - \Delta_2} + \frac{(g_{12} + g_{12}/\Delta_2)^2}{\alpha_{c} - \Delta_1 - \Delta_2} - \frac{2g_{12}g_{12}}{\Delta_1\Delta_2} \right), \quad (B5)$$

where we used the approximated conditions $\tilde{\alpha}_{x} \approx \alpha_{x}$ ($x = q1, c, q2$), $\Delta_{k} \approx \Delta_{k}$ ($k = 1, 2$), and $\Delta_{12} = \Delta_1 - \Delta_2$ is the frequency detuning between computational qubits. This result would be useful for exploring ZZ coupling characteristics. Considering $\Delta_1 = \Delta_2$ and rewriting the expression in terms of $g_{\text{eff}}$ and $g_{12}$, the analytical result above reduces to Eq. (20) of the main text. Note that the analytical result of ZZ parasitic coupling valid for more general regimes comparing with previous investigations [25–28, 30].

In absence of the direct coupling $g_{12}$, the result above can be simplified. It becomes

$$\zeta_{zz} = -2g_{12}^2 \left[ \frac{1}{\Delta_2^2} \frac{1}{\alpha_{q1} + \Delta_1} + \frac{1}{\Delta_2^2} \frac{1}{\alpha_{q2} - \Delta_2} + \left( \frac{1}{\Delta_1} + \frac{1}{\Delta_2} \right)^2 \frac{1}{\alpha_{c} - \Delta_1 - \Delta_2} \right]. \quad (B6)$$

Actually, a similar result was also referred in previous work [28, 34] which was obtained using perturbation analysis. Comparing with the previous method used, we give not only the origin for each term but also the clear physical mechanisms.

As a further step, if we focus on the resonant case with $\omega_{q1} = \omega_{q2}$, namely $\Delta_{12} = 0$, then the analytical expression reduces to a simple form [Eq. (19) of the main text]:

$$\zeta_{zz} = -2g_{12}^2 \left( \frac{1}{\alpha_{q1}} + \frac{1}{\alpha_{q2}} + \frac{4}{\alpha_{c} - 2\Delta} \right), \quad (B7)$$

where we take $\Delta_1 = \Delta_2 = \Delta$. This results can be used to explain the physical mechanism for the elimination of ZZ parasitic couplings, and more importantly trigger some novel parameter regions in which high-fidelity two-qubit gates are expected.

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