Interqubit coupling mediated by a high-excitation-energy quantum object

S. Ashhab,[1,2] A. O. Niskanen,[3,4] K. Harrabi,[3] Y. Nakamura,[1,3,5] T. Picot,[6] P. C. de Groot,[6] C. J. P. M. Harmans,[6] J. E. Mooij,[6] and Franco Nori[1,2]

[1]*Frontier Research System, The Institute of Physical and Chemical Research (RIKEN), Wako-shi, Saitama 351-0198, Japan*

[2]*Physics Department and Michigan Center for Theoretical Physics, The University of Michigan, Ann Arbor, Michigan 48109-1040, USA*

[3]*CREST-JST, Kawaguchi, Saitama 332-0012, Japan*

[4]*VTT Technical Research Centre of Finland, Sensors, P.O. Box 1000, 02044 VTT, Finland*

[5]*NEC Nano Electronics Research Laboratories, Tsukuba, Ibaraki 305-8501, Japan*

[6]*Quantum Transport Group, Kavli Institute of NanoScience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands*

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We consider a system composed of two qubits and a high excitation energy quantum object used to mediate coupling between the qubits. We treat the entire system quantum mechanically and analyze the properties of the eigenvalues and eigenstates of the total Hamiltonian. After reproducing well-known results concerning the leading term in the mediated coupling, we obtain an expression for the residual coupling between the qubits in the off state. We also analyze the entanglement between the three objects, i.e., the two qubits and the coupler, in the eigenstates of the total Hamiltonian. Although we focus on the application of our results to the recently realized parametric-coupling scheme with two qubits, we also discuss extensions of our results to harmonic-oscillator couplers, couplers that are near resonance with the qubits and multiqubit systems. In particular, we find that certain errors that are absent for a two-qubit system arise when dealing with multiqubit systems.

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I. INTRODUCTION

Superconducting qubits are among the main candidates for the possible implementation of quantum-information-processing tasks.[1] Coherent dynamics of a single qubit has been achieved at various laboratories. Several interesting two-qubit experiments have also been performed.[2–20] The early experiments[2–12] were limited to fixed interqubit coupling. In order to scale up qubit circuits, however, it is highly desirable to be able to tune *in situ* the coupling strengths between the different qubits. The idea of coupling two qubits to a high excitation energy quantum object that would mediate coupling between the qubits[21–26] has lead to experimental demonstrations of tunable coupling.[13–15] However, Refs. 13 and 14 probed the magnetic properties of the circuit in its ground state; thus, the approach used there is not suited to implement the standard gate-based quantum computing, but possibly adiabatic quantum computing,[27] where the quantum register is ideally never excited. In Ref. 15, tunability of the coupling was demonstrated through spectroscopic measurements with the qubits biased away from their coherence optimal points. Generalizing the idea of mediated coupling[21–26] to parametric tunable coupling,[28–31] it was proposed that one can bias the qubits at their optimal points and also adjust the dc component of the mediated coupling to cancel the direct interqubit coupling throughout the experiment. Applying a microwave pulse to the coupler at the sum or difference frequency of the qubits' characteristic frequencies would then turn on the coupling, but only for the duration of the applied microwave pulse. This proposal, combining tunable coupling and long coherence times, was realized experimentally in Ref. 17.

Another related direction of growing research activity is the idea of using a harmonic-oscillator "cavity" as a data bus with the potential that a single cavity could mediate coupling between a large number of qubits.[19,20,32,33] If the harmonic oscillator mediates coupling via high-energy virtual excitations, it can be described similarly to other high excitation energy couplers. Couplers that are near resonance with the qubits, but sufficiently detuned such that they mediate coupling through virtual excitations, can also be treated using a similar approach. We shall show, however, that it would be rather difficult to achieve tunability in the coupling in the case of harmonic-oscillator couplers.

Early theoretical studies on tunable couplers have generally taken the semiclassical approach, which we shall explain below. The semiclassical treatment is sufficient to evaluate the leading term in the effective coupling mediated by the coupler. As qubit circuits that include couplers are becoming an experimental reality, however, there is an increasing need for a more careful analysis of these quantum couplers. Some recent studies[29,34] used a number of quantum-mechanical techniques and obtained results beyond the semiclassical calculations. For example, Ref. 34 derived an expression for the residual coupling term when the main coupling channel is turned off. Here, we take a fully quantum approach, where we analyze the properties of the eigenvalues and eigenstates of the total Hamiltonian. We obtain results that were not captured by previous studies, particularly results concerning the ideality of the off state in this coupling scheme.

The main questions of interest that the quantum treatment can be used to answer include the following. (1) Can we make the coupler's energy splitting very large but still maintain the mediated coupling between the qubits? (2) Can we turn the coupling off completely? In other words, will there be any residual coupling terms if the system is biased such that the main coupling channel is at its zero point? (3) How much entanglement is there between the qubits and the coupler, and how does this entanglement affect a realistic experi-

mental setup? These questions will be answered in the analysis below.

The paper is organized as follows. In Sec. II, we describe the system and its Hamiltonian. In Sec. III, we review the semiclassical approach and discuss what predictions we can expect from it regarding the ideality of the off state. In Sec. IV, we perform the fully quantum analysis of the problem: We derive expressions for the leading-order effective coupling strength mediated by the coupler, the residual coupling in the off state, and the amount of entanglement between the qubits and the coupler. We also discuss the extension of our results to the case of a harmonic-oscillator coupler and that of a coupler that is almost resonant with the qubits. We discuss in Sec. V the implications of the results obtained in Sec. IV with regard to present-day and future experiments. In this context, we also consider multiqubit systems. Section VI contains concluding remarks. Some details of the calculations are explained in the Appendix.

II. SYSTEM AND HAMILTONIAN

Let us take a system composed of two qubits and a third object that we would like to use as a coupler. Although tunability is considered the main advantage of this coupling scheme, for the purpose of answering the questions of main interest to us, it suffices to focus on the case where the external bias parameters are set to fixed values. We therefore treat a time-independent Hamiltonian. Since we are assuming that we can speak of three distinct quantum objects, we must be able to write down a Hamiltonian that reflects this clear separation of the different objects in the system. We therefore express the Hamiltonian as

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_C + \hat{H}_{12} + \hat{H}_{1C} + \hat{H}_{2C}, \tag{1}$$

where the first three terms are the Hamiltonians of the separate objects in the system, and the last three terms describe coupling between those objects. As a realistic, representative case, we take the different terms in the Hamiltonian to have the forms

$$\hat{H}_1 = \frac{\Delta_1}{2}\hat{\sigma}_z^{(1)} + \frac{\epsilon_1}{2}\hat{\sigma}_x^{(1)}, \tag{2}$$

$$\hat{H}_2 = \frac{\Delta_2}{2}\hat{\sigma}_z^{(2)} + \frac{\epsilon_2}{2}\hat{\sigma}_x^{(2)}, \tag{3}$$

$$\hat{H}_C = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & \eta_1 & 0 & \\ 0 & 0 & \eta_2 & \\ \vdots & & & \ddots \end{pmatrix}, \tag{4}$$

$$\hat{H}_{12} = J_0\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)} = \begin{pmatrix} 0 & 0 & 0 & J_0 \\ 0 & 0 & J_0 & 0 \\ 0 & J_0 & 0 & 0 \\ J_0 & 0 & 0 & 0 \end{pmatrix}, \tag{5}$$

$$\hat{H}_{1C} = \hat{\sigma}_x^{(1)} \otimes \hat{A}, \tag{6}$$

$$\hat{H}_{2C} = \hat{\sigma}_x^{(2)} \otimes \hat{B}, \tag{7}$$

with the coupler energies $0, \eta_1, \eta_2, \ldots$. arranged in increasing order,

$$\hat{A} = \begin{pmatrix} A_{00} & A_{01} & A_{02} & \cdots \\ A_{10} & A_{11} & A_{12} & \\ A_{20} & A_{21} & A_{22} & \\ \vdots & & & \ddots \end{pmatrix}, \tag{8}$$

and similarly for $\hat{B}$. For the case of superconducting flux qubits, Δ_j is the minimum gap of qubit j, ϵ_j represents the deviation from the degeneracy point of half-integer flux quantum threading the qubit loop [i.e., $\epsilon_j = I_{p,j}(\Phi_{\mathrm{ext},j} - \Phi_0/2)$, where $I_{p,j}$ is the persistent current of qubit j, $\Phi_{\mathrm{ext},j}$ is the externally applied flux in the loop of qubit j, and Φ_0 is the flux quantum], J_0 is the direct qubit-qubit coupling strength, and $\hat{\sigma}_\alpha^{(j)}$ are the usual Pauli matrices of qubit j. Note that the minimum gap Δ_j is the coefficient of $\hat{\sigma}_z^{(j)}$ above, in contrast with some alternative conventions used in the literature where Δ_j is the coefficient of $\hat{\sigma}_x^{(j)}$. Note also that the operators $\hat{A}$ and $\hat{B}$ must satisfy the relations $A_{ij} = A_{ji}^*$ and $B_{ij} = B_{ji}^*$. The coupler's Hamiltonian $\hat{H}_C$ is written in its own eigenbasis (thus, it is diagonal), and its ground-state energy has been set to zero. We shall express Hamiltonians and energies in frequency units throughout this paper.

We now make the assumption that the largest energy scale in the problem is the excitation energy of the coupler. In other words, η_1 is larger than any relevant energy scale in the Hamiltonian excluding $\hat{H}_C$. We shall not make any assumption regarding the relation between the qubit energy scale $\sqrt{\Delta_j^2 + \epsilon_j^2}$ and the qubit-coupler coupling energy scale (i.e., the scale of the matrix elements in $\hat{A}$ and $\hat{B}$). Although it is not crucial for most of our analysis below, we shall generally take the direct coupling energy scale J_0 to be smaller than the qubit energy scale.

III. SEMICLASSICAL TREATMENT

Before embarking on the semiclassical description of our system, it is instructive to recall the problem of calculating interatomic forces within the hydrogen molecule.[35] One starts by assuming that the nuclei have fixed locations in space, leaving the degrees of freedom associated with electron motion as the only variables in the problem. The ground state of the electronic degrees of freedom is calculated and expressed as a function of the distance between the nuclei. At this point, the total energy (direct Coulomb energy of the nuclei plus electronic ground-state energy) is expressed as a function of the relative position operator between the nuclei, and the nuclear motion is treated quantum mechanically. One can now obtain information related to atomic motion or molecular states without having to worry about electronic motion. The first step in the calculation ensures that the effects of the electrons' adiabatic adjustment to nuclear motion are properly taken into account. The reason why the electronic degrees of freedom can adjust adiabatically to nuclear mo-

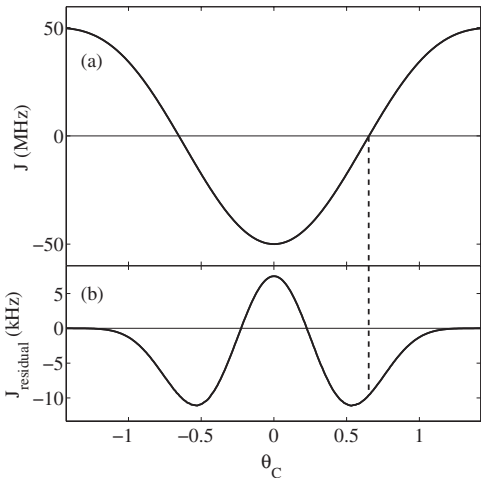

FIG. 1. Coefficients of the (a) main and (b) residual coupling terms (i.e., J and J_{residual}) as functions of the coupler's bias point θ_C. In generating this figure, we took $\Delta_1=4$ GHz, $\Delta_2=5$ GHz, $\Delta_C=30$ GHz, $J_0=50$ MHz, and $J_{1C}=J_{2C}=\sqrt{J_0\Delta_C}$. It should be noted, however, that the results are only weakly dependent on the exact choice of parameters.

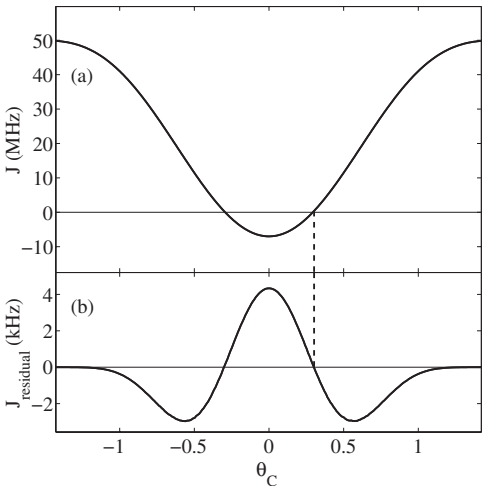

FIG. 2. Same as in Fig. 1, except that $J_{1C}=J_{2C}=0.75\sqrt{J_0\Delta_C}$. As opposed to Fig. 1, J and J_{residual} now vanish at the same bias point.

tion is that they are associated with a much higher energy scale and thus changes that result from nuclear motion are felt by the electrons as very slow variations.

A similar procedure can be applied when dealing with interqubit couplers. Since the qubit-coupler interactions contain the operators $\hat{\sigma}_x^{(j)}$, one first assumes that the qubits are in eigenstates of $\hat{\sigma}_x^{(j)}$. One therefore needs to calculate the ground-state energy of the Hamiltonian (or, more precisely, the four Hamiltonians),

$$\hat{H}_{C,\text{eff}} \equiv \hat{H}_C + \hat{H}_{1C} + \hat{H}_{2C} \overset{\sigma_x^{(j)}=\pm 1}{\rightarrow} \hat{H}_C \pm \hat{A} \pm \hat{B}. \tag{9}$$

The ground-state energy [i.e., the four values obtained from Eq. (9)] can then be expressed in the form[36]

$$E_0\{\hat{H}_{C,\text{eff}}\} = c_1 + c_2\sigma_x^{(1)} + c_3\sigma_x^{(2)} + c_4\sigma_x^{(1)} \otimes \sigma_x^{(2)}. \tag{10}$$

Note that we have started with the assumption that the qubits have well-defined values of $\sigma_x^{(j)}$. One could therefore say that the above expression is not a quantum operator. However, it is straightforward to follow the adiabaticity argument: the coupler will, to a very good approximation, always be in the ground state that corresponds to the instantaneous values of $\sigma_x^{(j)}$ (including the possibility of quantum superpositions). One can therefore turn back to the qubits and analyze their dynamics using the effective Hamiltonian,

$$\hat{H}_{q,\text{eff}} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{12} + \hat{H}_{\text{mediated}}, \tag{11}$$

where

$$\hat{H}_{\text{mediated}} = c_1 + c_2\hat{\sigma}_x^{(1)} + c_3\hat{\sigma}_x^{(2)} + c_4\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)}. \tag{12}$$

The above derivation shows that the response of the coupler to external perturbations (induced by the qubits and represented by the terms $\pm\hat{A}$ and $\pm\hat{B}$) translates into a renormalization of the qubit bias points [second and third terms in Eq. (12)] and an additional coupling term between the qubits [last term in Eq. (12)].

It is interesting to note here that in the semiclassical treatment above, the effect of the coupler on the qubits is completely described by the Hamiltonian $\hat{H}_{\text{mediated}}$. Therefore, if the bias point is chosen such that the coefficient c_4 in Eq. (12) cancels the direct coupling strength J_0, there would be no residual coupling between the qubits. The off state would therefore correspond to complete decoupling between the qubits. In contrast, we shall show below that the fully quantum treatment predicts the presence of finite residual coupling effects.

IV. QUANTUM TREATMENT

We now take the Hamiltonian of Sec. II [Eq. (1)] and treat it quantum mechanically. In particular, we would like to analyze the properties of the eigenvalues and eigenstates of the total Hamiltonian. For the purposes of the calculations in this section, we divide the Hamiltonian into two parts as follows:

$$\hat{H} = \hat{H}_0 + \hat{V}, \tag{13}$$

where

$$\hat{H}_0 = \frac{\Delta_1}{2}\hat{\sigma}_z^{(1)} + \frac{\Delta_2}{2}\hat{\sigma}_z^{(2)} + \hat{H}_C, \tag{14}$$

$$\hat{V} = \frac{\epsilon_1}{2}\hat{\sigma}_x^{(1)} + \frac{\epsilon_2}{2}\hat{\sigma}_x^{(2)} + \hat{H}_{12} + \hat{H}_{1C} + \hat{H}_{2C}. \tag{15}$$

We use the basis $\{|00\underline{0}\rangle, |01\underline{0}\rangle, |10\underline{0}\rangle, |11\underline{0}\rangle, |00\underline{1}\rangle, |01\underline{1}\rangle, |10\underline{1}\rangle, |11\underline{1}\rangle, |00\underline{2}\rangle, \ldots\}$, where the first, second, and third quantum numbers describe, respectively, the state of the first qubit, second qubit, and coupler (the state of the coupler will be distinguished from those of the qubits using an underline throughout this paper); note that we allow the coupler to have more than two levels, and we shall assume an infinite number of levels in the expressions below. We can now express $\hat{H}_0$ as

$$\hat{H}_0 = \begin{pmatrix} \frac{-\Delta_1-\Delta_2}{2} & 0 & 0 & 0 & & & & & \cdots \\ 0 & \frac{-\Delta_1+\Delta_2}{2} & 0 & 0 & & & 0 & & \\ 0 & 0 & \frac{\Delta_1-\Delta_2}{2} & 0 & & & & & \\ 0 & 0 & 0 & \frac{\Delta_1+\Delta_2}{2} & & & & & \\ & & & & \eta_1+\frac{-\Delta_1-\Delta_2}{2} & 0 & 0 & 0 & \\ & 0 & & & 0 & \eta_1+\frac{-\Delta_1+\Delta_2}{2} & 0 & 0 & \\ & & & & 0 & 0 & \eta_1+\frac{\Delta_1-\Delta_2}{2} & 0 & \\ & & & & 0 & 0 & 0 & \eta_1+\frac{\Delta_1+\Delta_2}{2} & \\ \vdots & & & & & & & & \ddots \end{pmatrix}. \tag{16}$$

A. Coupling strength: Leading term

In order to calculate the effective coupling strength, we now calculate the energies of the lowest four energy levels. We therefore want to construct a 4×4 effective-Hamiltonian matrix describing the lowest energy levels while taking into account the effects of the higher levels.

We now follow a standard calculation[37] (see Appendix) that gives

$$\hat{H}_{\text{eff}} \approx \hat{H}_{\text{eff}}^{(0)} + \hat{H}_{\text{eff}}^{(1)} + \hat{H}_{\text{eff}}^{(2)}, \tag{17}$$

where

$$\hat{H}_{\text{eff}}^{(0)} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{12} = \frac{1}{2}\begin{pmatrix} -\Delta_1-\Delta_2 & \epsilon_2 & \epsilon_1 & 2J_0 \\ \epsilon_2 & -\Delta_1+\Delta_2 & 2J_0 & \epsilon_1 \\ \epsilon_1 & 2J_0 & \Delta_1-\Delta_2 & \epsilon_2 \\ 2J_0 & \epsilon_1 & \epsilon_2 & \Delta_1+\Delta_2 \end{pmatrix}, \tag{18}$$

$$\hat{H}_{\text{eff}}^{(1)} = A_{00}\sigma_x^{(1)} + B_{00}\sigma_x^{(2)} = \begin{pmatrix} 0 & B_{00} & A_{00} & 0 \\ B_{00} & 0 & 0 & A_{00} \\ A_{00} & 0 & 0 & B_{00} \\ 0 & A_{00} & B_{00} & 0 \end{pmatrix}, \tag{19}$$

$$\hat{H}_{\text{eff}}^{(2)} = \sum_{l=1}^{\infty} \sum_{k=00,01,10,11} \hat{P}\frac{\hat{V}|k,l\rangle\langle k,l|\hat{V}}{\hat{H}_{\text{eff}} - E_{k,l}}\hat{P}, \tag{20}$$

where the operator $\hat{P}$ projects the state onto the space of the lowest four eigenstates of H_0 ($|00\underline{0}\rangle, |01\underline{0}\rangle, |10\underline{0}\rangle$, and $|11\underline{0}\rangle$); alternatively, one could say that the operator $\hat{P}$ removes the size mismatch between the four-dimensional Hilbert space of interest and the infinite-dimensional operator $\hat{V}$. The sum over l in Eq. (20) runs over states where the coupler is in one of its excited states. The energies $E_{k,l}$ are the eigenvalues of $\hat{H}_0$ with the qubits in state k and the coupler in state l. In order to find the lowest-order expression for the mediated coupling term, we make the approximation $\hat{H}_{\text{eff}} - E_{k,l} \approx -\eta_l$ in Eq. (20). Thus, we obtain the expression

$$\hat{H}_{\text{eff}}^{(2)} = \hat{H}_{\text{coupling}}^{(2)} + \hat{H}_{\text{shift}}^{(2)},$$

$$\hat{H}_{\text{coupling}}^{(2)} \approx \begin{pmatrix} 0 & 0 & 0 & -J_1 \\ 0 & 0 & -J_1 & 0 \\ 0 & -J_1 & 0 & 0 \\ -J_1 & 0 & 0 & 0 \end{pmatrix} = -J_1\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)},$$

$$\hat{H}_{\text{shift}}^{(2)} \approx -\Delta_{\text{shift}}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{21}$$

where

$$J_1 = \sum_{l=1}^{\infty} \frac{A_{0l}B_{l0} + B_{0l}A_{l0}}{\eta_l},$$

$$\Delta_{\text{shift}} = \sum_{l=1}^{\infty} \frac{|A_{0l}|^2 + |B_{0l}|^2}{\eta_l}. \tag{22}$$

The overall shift $\hat{H}^{(2)}_{\text{shift}}$ does not have any physical consequences to this order of the calculation and can be neglected.

The effective Hamiltonian can now be expressed as

$$\hat{H}_{\text{eff}} = \tilde{H}_0 + \tilde{H}_{\text{coupling}}, \tag{23}$$

where

$$\tilde{H}_0 = \frac{\Delta_1}{2}\hat{\sigma}_z^{(1)} + \frac{\tilde{\epsilon}_1}{2}\hat{\sigma}_x^{(1)} + \frac{\Delta_2}{2}\hat{\sigma}_z^{(2)} + \frac{\tilde{\epsilon}_2}{2}\hat{\sigma}_x^{(2)},$$

$$\tilde{H}_{\text{coupling}} = J\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)},$$

with the parameters

$$\tilde{\epsilon}_1 = \epsilon_1 + 2A_{00},$$

$$\tilde{\epsilon}_2 = \epsilon_2 + 2B_{00},$$

$$J = J_0 - J_1. \tag{24}$$

The above results agree with those of Ref. 29 when the parameters of our model are taken to correspond to those considered in Ref. 29.

First, we mention the physical interpretation of the terms $2A_{00}$ and $2B_{00}$ in the expressions for $\tilde{\epsilon}_j$. Taking the experimentally relevant case of flux qubits as an example, these terms describe the fluxes generated by the coupler (in its ground state) and going through the qubit loops. As a result, if one wishes to bias the qubits at their optimal points, the externally applied fluxes through the qubit loops are not set to $\Phi_0/2$, but they are shifted from that value to compensate for the coupler-induced contributions. This is the physical explanation of the difference between ϵ_j and $\tilde{\epsilon}_j$.[38]

We can now answer the question of how high the coupler's energy splitting can be. We note that the mediated coupling strength J_1 is second order in the scale of $\hat{A}$ and $\hat{B}$, and it is inversely proportional to the scale of η_l. Although this means that we cannot simply take $\eta_1 \to \infty$ keeping the other parameters fixed (otherwise $J_1 \to 0$), it also means that if we increase A_{nm}, B_{nm}, and η_l (keeping the ratio $A_{0l}B_{l0}/\eta_l$ fixed), we can in fact take $\eta_1 \to \infty$ while maintaining the same level of mediated coupling. We shall see below that this situation is desirable for purposes of reducing residual-coupling effects.

We are also in a position to comment on the question of monostability of the coupler (i.e., the idea that a single energy level of the coupler is relevant in the system under consideration). The presence of the matrix elements A_{l0} and B_{l0}, which describe coupling between the coupler's ground and excited states, in the expression for the mediated coupling strength [Eq. (22)] demonstrates that the excited states of the coupler play an important role in the coupling mechanism. The semiclassical treatment relies on the fact that the relevant information contained in these matrix elements is also encoded, and more easily accessible experimentally, in the response of the coupler's ground state to weak perturbations. As a result, knowledge of the matrix elements themselves is not necessary; knowledge of simple response parameters is sufficient in order to calculate the mediated coupling strength.

B. Residual coupling in the off state

In Sec. IV A, we have derived the leading-order terms in the effect of the coupler on the two-qubit system. The results agree with the predictions of the semiclassical treatment (although no explicit expressions were given in Sec. III). Our main motivation for using the fully quantum treatment, however, is that it allows us to go further in the calculation, e.g., evaluating any off-state residual coupling terms in the two-qubit effective Hamiltonian. Such closer examination of the off state will be the subject of this and the following subsection (as well as part of Sec. V).

Since we are interested in an ideal off state with the qubits at their optimal points, we consider the case where $J = \tilde{\epsilon}_1 = \tilde{\epsilon}_2 = 0$ (we shall allow J to take nonzero values in the course of the discussion below). In order to enhance the robustness of the decoupling between the qubits, we take $\Delta_1 \neq \Delta_2$. The effective Hamiltonian [Eq. (23)] is diagonal to lowest order in this case. We can therefore proceed with calculating higher-order corrections using the states $|00\underline{0}\rangle$, $|01\underline{0}\rangle$, $|10\underline{0}\rangle$, and $|11\underline{0}\rangle$.

The calculation of the residual-coupling Hamiltonian is now carried out by calculating the energies of the lowest four levels of the entire system (we shall refer to them as $E_{00\underline{0}}$, $E_{01\underline{0}}$, $E_{10\underline{0}}$, and $E_{11\underline{0}}$). The four values that we obtain for the energies in the four-level spectrum can then be used to extract four quantities: (1) an overall energy that can be neglected, [(2) and (3)] the corrected (i.e., renormalized) values of the qubit splittings Δ_j, and (4) a residual-coupling energy (given by $E_{00\underline{0}} + E_{11\underline{0}} - E_{01\underline{0}} - E_{10\underline{0}}$). It is this last quantity that is of most interest to us here. It characterizes a coupling Hamiltonian of the form

$$\hat{H}_{\text{residual}} = J_{\text{residual}}\hat{\sigma}_z^{(1)} \otimes \hat{\sigma}_z^{(2)}, \tag{25}$$

where

$$J_{\text{residual}} = \frac{E_{00\underline{0}} + E_{11\underline{0}} - E_{01\underline{0}} - E_{10\underline{0}}}{4}. \tag{26}$$

Note that in writing Eq. (25), we have used our assumption that the qubits are biased at their optimal points.

Although one can make analytic progress calculating the energies using the pseudodegenerate perturbation theory approach, reaching the relevant results requires several steps of the iterative procedures explained in the Appendix (the lowest-order corrections to the individual energies do not contribute to the combination $E_{00\underline{0}} + E_{11\underline{0}} - E_{01\underline{0}} - E_{10\underline{0}}$). We therefore only present the results of numerical calculations that find the energy levels of the entire system. It also turns out that proceeding with the rather general model used so far

complicates the extraction of the important results. We therefore have to make some simplifying assumptions. From now on, we focus on a simple case that also happens to be relevant to recent experiments: We take the coupler to be a two-level system, such that

$$\hat{H}_C = \frac{\epsilon_C}{2}\hat{\sigma}_x^{(C)} + \frac{\Delta_C}{2}\hat{\sigma}_z^{(C)} = \frac{\Delta_C}{2}(\tan\theta_C\hat{\sigma}_x^{(C)} + \hat{\sigma}_z^{(C)}),$$

$$\hat{H}_{1C} = J_{1C}\hat{\sigma}_x^{(1)} \otimes \sigma_x^{(C)},$$

$$\hat{H}_{2C} = J_{2C}\hat{\sigma}_x^{(2)} \otimes \sigma_x^{(C)} \tag{27}$$

(note that, unlike the convention used in Sec. II, $\hat{H}_C$ is not diagonal here). We therefore have $\eta_1 = \sqrt{\Delta_C^2 + \epsilon_C^2} = \Delta_C/|\cos\theta_C|$, $A_{00} = -A_{11} = -J_{1C}\sin\theta_C$, $A_{10} = A_{01} = J_{1C}\cos\theta_C$, and similarly for $\hat{B}$. As a result, we find from Eq. (22) that

$$J = J_0 - \frac{2J_{1C}J_{2C}\cos^3\theta_C}{\Delta_C}. \tag{28}$$

.

For clarity and definiteness in the following analysis, we now focus on the parametric-coupling scheme,[28–30] and we start by noting three factors that can contribute to determining the ideal dc bias point (it is worth mentioning at this point that in general it will not be possible, nor necessary, to satisfy all three conditions simultaneously). First, we note from Eq. (28) that the range of values for the effective coupling strength J extends from $J_0 - 2J_{1C}J_{2C}/\Delta_C$ (at $\theta_C = 0$) to J_0 (at $\theta_C = \pi/2$). In order to maximize the effective coupling strength of the parametric-coupling scheme, it would be desirable to set the dc bias point such that $J = J_0 - J_{1C}J_{2C}/\Delta_C$, i.e., halfway between the two extremes. This situation would be obtained by setting $\theta_C \approx 0.65 \approx \pi/5$, irrespective of the specific system parameters. At this bias point, the allowed amplitude of the ac driving signal (i.e., before encountering nonlinearities in J) is maximized [see Fig. 1(a)]. Second, it is desirable to set $J = 0$ at the dc bias point. Third, it is also desirable to set the residual coupling energy $J_{\text{residual}} = 0$.

We now proceed with the numerical calculations as follows: We first fix the parameters Δ_1, Δ_2, Δ_C, and J_0 (e.g., $\Delta_1 = 4$ GHz, $\Delta_2 = 5$ GHz, $\Delta_C = 30$ GHz, and $J_0 = 50$ MHz). The coupling strengths J_{1C} and J_{2C} are then chosen as $J_{1C} = J_{2C}$ and $J_{1C}J_{2C}/\Delta_C = J_0$. This choice ensures that a single dc bias point satisfies at least two of the three desirable conditions mentioned above, i.e., J vanishes while maximizing the achievable effective coupling strength for the parametric-coupling scheme. The coupler's bias point, determined by the angle θ_C, is now treated as the only variable in the problem. For each value of θ_C, we (numerically) bias the qubits at their optimal points (determined by simultaneously minimizing both qubit energy splittings) and calculate the residual coupling energy. The results are shown in Fig. 1. We can clearly see that there is some residual coupling in the off state (i.e., at $\theta_C \approx 0.65$); however, the residual coupling strength in Fig. 1 is very small compared to typical relaxation and dephasing times. After varying all the parameters by at least a factor of 2 in either direction, we can identify that the residual-coupling term is given by

$$J_{\text{residual}} \approx 4\frac{\Delta_1\Delta_2 J_0 J_{1C}J_{2C}}{\Delta_C^4}\cos^6\theta_C - \alpha\frac{\Delta_1\Delta_2 J_{1C}^2 J_{2C}^2}{\Delta_C^5}\cos^5\theta_C\sin^2(2\theta_C), \tag{29}$$

where the coefficient α is approximately 20.

It is encouraging for future experimental efforts that the residual-coupling term obtained above decreases rapidly with increasing coupler gap Δ_C, even if the mediated coupling strength is kept at a fixed level. Furthermore, it is possible to adjust the system parameters such that the conditions of vanishing J and J_{residual} are simultaneously satisfied. An example of this situation is shown in Fig. 2. Note that the achievable effective coupling strength for the parametric-coupling scheme has been reduced from that in Fig. 1 because the dc bias point has now moved away from the desirable point $\theta_C \approx 0.65$ mentioned above.

Another relevant quantity when analyzing the ideality of the off state is how the effective coupling strength changes in response to changes in the coupler's bias point. This quantity can be derived easily from Eq. (28),

$$\frac{dJ}{d\epsilon_C} = \frac{6J_{1C}J_{2C}\cos^4\theta_C\sin\theta_C}{\Delta_C^2}. \tag{30}$$

With proper design parameters, this quantity also decreases rapidly with increasing Δ_C.

C. Entanglement in the energy eigenstates

In addition to the residual-coupling Hamiltonian, another natural question to ask when analyzing the ideality of the off state is how much entanglement there is between the qubits and the coupler, and between the qubits themselves, in the different energy eigenstates. Unlike the residual-coupling Hamiltonian, where we had to resort to numerical calculations, this entanglement can be evaluated using the analytic approach. The analysis of how the energy-eigenstate entanglement manifests itself as errors in a quantum calculation will be postponed until Sec. V.

Here, we are interested in the nearly ideal situation where any residual entanglement is treated as a small error. We therefore take the situation analyzed in the previous subsection ($J = \tilde{\epsilon}_1 = \tilde{\epsilon}_2 = 0$, $\Delta_1 \neq \Delta_2$, and the coupler is a two-level system), and we analyze the degree of entanglement to lowest nonvanishing orders.

As explained earlier in this section, we can start our calculation using the states $|00\underline{0}\rangle$, $|01\underline{0}\rangle$, $|10\underline{0}\rangle$, and $|11\underline{0}\rangle$. For the lowest order of this calculation, we can use the pseudodegenerate perturbation theory calculation explained in the Appendix. We find that

$$|\psi_{00}\rangle \approx |00\underline{0}\rangle - \frac{J_0}{2\eta_1}|11\underline{0}\rangle - \frac{A_{10}}{\eta_1}|10\underline{1}\rangle - \frac{B_{10}}{\eta_1}|01\underline{1}\rangle,$$

$$|\psi_{01}\rangle \approx |01\underline{0}\rangle - \frac{J_0}{2\eta_1}|10\underline{0}\rangle - \frac{A_{10}}{\eta_1}|11\underline{1}\rangle - \frac{B_{10}}{\eta_1}|00\underline{1}\rangle$$

$$|\psi_{10}\rangle \approx |10\underline{0}\rangle - \frac{J_0}{2\eta_1}|01\underline{0}\rangle - \frac{A_{10}}{\eta_1}|00\underline{1}\rangle - \frac{B_{10}}{\eta_1}|11\underline{1}\rangle,$$

$$|\psi_{11}\rangle \approx |11\underline{0}\rangle - \frac{J_0}{2\eta_1}|00\underline{0}\rangle - \frac{A_{10}}{\eta_1}|01\underline{1}\rangle - \frac{B_{10}}{\eta_1}|10\underline{1}\rangle, \quad (31)$$

up to a normalization constant slightly smaller than 1. Note that the above expressions can be collectively summarized as[39]

$$\begin{aligned}|\psi_{nm}\rangle \approx |nm\underline{0}\rangle - \frac{J_0}{2\eta_1}|\bar{n}\bar{m}\underline{0}\rangle - \frac{A_{10}}{\eta_1}|\bar{n}m\underline{1}\rangle - \frac{B_{10}}{\eta_1}|n\bar{m}\underline{1}\rangle = \Bigg(1 \\ - \frac{J_0}{2\eta_1}\hat{\sigma}_x^{(1)}\otimes\hat{\sigma}_x^{(2)} - \frac{A_{10}}{\eta_1}\hat{\sigma}_x^{(1)}\otimes\hat{\sigma}_x^{(C)} - \frac{B_{10}}{\eta_1}\hat{\sigma}_x^{(2)}\otimes\hat{\sigma}_x^{(C)}\Bigg) \\ \times|nm\underline{0}\rangle = \Bigg(1 - \frac{J_0\cos\theta_C}{2\Delta_C}\hat{\sigma}_x^{(1)}\otimes\hat{\sigma}_x^{(2)} \\ - \frac{J_{1C}\cos^2\theta_C}{\Delta_C}\hat{\sigma}_x^{(1)}\otimes\hat{\sigma}_x^{(C)} - \frac{J_{2C}\cos^2\theta_C}{\Delta_C}\hat{\sigma}_x^{(2)}\otimes\hat{\sigma}_x^{(C)}\Bigg) \\ \times|nm\underline{0}\rangle. \quad (32)\end{aligned}$$

Two notes are in order here. (1) The mixing of computational-basis states in the energy eigenstates [Eq. (32)] cannot be identified as arising from a simple residual-coupling Hamiltonian. In other words, one cannot find a two-qubit Hamiltonian that reproduces any of the corrections in Eq. (32). This can be perhaps most clearly seen in the fact that the signs in front of the small terms in Eq. (32) are independent of the state. In contrast, one always expects different states to acquire corrections of different signs when dealing with a direct coupling Hamiltonian. Higher-order effects in this system therefore cannot be completely described by simply using small corrections to the reduced (i.e., 4×4) two-qubit Hamiltonian. (2) The above expressions were obtained assuming only that the coupling strength J vanishes, $\tilde{\epsilon}_1=\tilde{\epsilon}_2=0$, and $\Delta_1\neq\Delta_2$. They are not affected by the value of the residual-coupling Hamiltonian discussed in Sec. IV B. This fact demonstrates that the vanishing of both J and J_{residual} does not imply that the qubits are entirely decoupled. Corrections to the energy eigenstates still have to be considered when calculating possible errors, as will be explained in Sec. V.

As in the case of the residual-coupling Hamiltonian, it is encouraging for scalability considerations that the entanglement in the energy eigenstates decreases and approaches zero with increasing Δ_C, assuming that J_0 and J_1 are kept fixed. One can therefore say that the coupler becomes more and more ideal as Δ_C is increased. It should be noted that the superconducting gap for aluminum is ~50 GHz. It would be interesting to investigate in the future how serious a constraint this number imposes on the maximum allowed value of Δ_C.

D. Harmonic oscillator as a coupler

We can use the results derived above for a two-level coupler to infer the corresponding results for a harmonic-oscillator coupler. We now consider the situation where

$$\hat{H}_C = \omega_C\hat{a}^\dagger\hat{a},$$

$$\hat{H}_{1C} = J_{1C}\hat{\sigma}_x^{(1)}\otimes(\hat{a}+\hat{a}^\dagger),$$

$$\hat{H}_{2C} = J_{2C}\hat{\sigma}_x^{(2)}\otimes(\hat{a}+\hat{a}^\dagger), \quad (33)$$

where $\hat{a}^\dagger$ and $\hat{a}$ are the creation and annihilation operators for the coupler. The above coupling Hamiltonians change the state of the coupler by one excitation. It should therefore be a good approximation to truncate the coupler to its lowest two energy levels. We now find that

$$J = J_0 - \frac{2J_{1C}J_{2C}}{\omega_C} \quad (34)$$

and

$$J_{\text{residual}} \approx 4\frac{\Delta_1\Delta_2 J_0 J_{1C}J_{2C}}{\omega_C^4}. \quad (35)$$

In order to study the tunability of a harmonic-oscillator coupler, we now consider the effect of an applied external field on the mediated coupling, adding the term

$$\hat{H}_{\text{field}} = h(\hat{a}+\hat{a}^\dagger) \quad (36)$$

to the Hamiltonian. By defining $\hat{b}\equiv\hat{a}+2h/\omega_C$, we can see that the new Hamiltonian takes the same form it had in the absence of $\hat{H}_{\text{field}}$, except that $\hat{a}$ and $\hat{a}^\dagger$ are replaced by $\hat{b}$ and $\hat{b}^\dagger$, and the qubit bias parameters ϵ_1 and ϵ_2 are shifted to $\tilde{\epsilon}_1$ and $\tilde{\epsilon}_2$ (just as discussed in the general case above). In particular, the values of J and J_{residual} are not affected by the applied field. The mediated coupling is therefore not tunable, assuming that the coupler's bias point is set by an applied linear field, i.e., a field that affects the coupler according to Eq. (36).

If the frequency of the harmonic oscillator (or alternatively J_{1C} and J_{2C}) were tunable, one would be able to obtain a tunable value of J [see Eq. (34)]. Possible designs for such tunable couplers have been proposed theoretically,[40] but they have not been realized experimentally. Given the advantages they could provide in terms of tunable coupling, it would be highly desirable to fabricate such tunable oscillators in the future.

A related design would be to use a (possibly nontunable) harmonic-oscillator element, which can be made large in size, in the circuit and add a tunable coupler between this oscillator and each qubit around it. With this design, one would gain the advantages of both (1) the large "cavity" being able to function as a data bus connecting a large number of qubits and (2) the coupling being tunable. With this design, one would also be able to use the parametric-coupling scheme to perform entangling operations on any

qubit in the circuit and the cavity relatively easily (using red- or blue-sideband transitions), with the qubits biased at their optimal points.

E. Coupler that is near resonance with the qubits

So far, we have focused on the case where the coupler's excitation energy is the largest energy scale in the problem. For completeness, we consider in this section the case where the coupler's excitation energy is close to those of the two qubits, but with sufficient detuning to avoid exciting the coupler. In other words, we consider a situation similar to the experiment of Ref. 20, but not that of Ref. 19.

The largest energy scale in the problem is now the qubit and coupler energy splittings, which are almost equal. The next largest energy scale is the detuning between the qubits and the coupler (this assumption is made in order to avoid large entanglement between the qubits and the coupler in the energy eigenstates, in which case we would have to deal with real excitations in the coupler). The detuning between the qubits, direct interqubit coupling strength, and qubit-coupler coupling strength can take any values.

Because the qubit energy scale is the largest energy scale in the problem, the mediated-coupling term now describes an excitation transfer between the two qubits. As such, the form of the effective-coupling term will only make sense in connection with the single-qubit Hamiltonians, not the physically defined operators $\hat{\sigma}_x$ and $\hat{\sigma}_z$ as in the case of a high excitation energy coupler. Assuming that the qubits are biased at their optimal points and the coupler is a harmonic oscillator with only one relevant excited state (and using the notation of Sec. IV D), the mediated-coupling term for this excitation-transfer process is well described by the Hamiltonian

$$\hat{H}_{\text{mediated}} = -\frac{J_{1C}J_{2C}}{\omega_C - \bar{\Delta}}(\hat{\sigma}_+^{(1)}\hat{\sigma}_-^{(2)} + \text{H.c.}), \tag{37}$$

where $\bar{\Delta}=(\Delta_1+\Delta_2)/2$ (note that $|\Delta_1-\Delta_2|$ is assumed to be much smaller than $|\omega_C-\bar{\Delta}|$; note also that the qubit splittings Δ_j will be slightly modified because of the interaction with the coupler). Using numerical calculations, we find that the residual-coupling term is given by Eq. (25) with

$$J_{\text{residual}} \approx \frac{J_0 J_{1C} J_{2C}}{(\omega_C - \bar{\Delta})^2}. \tag{38}$$

The fact that the residual-coupling strength scales inversely with the second power of the qubit-coupler detuning as opposed to the fourth power of the coupler's energy splitting indicates that residual coupling can be a more serious issue in this case than in the case of a high excitation energy coupler. It should be noted, however, that in the experiment of Ref. 20, J_0 was essentially zero, in which case residual coupling should be negligible.

V. ESTIMATING ERRORS IN A TYPICAL EXPERIMENT

In this section, we discuss a typical present-day experimental procedure. Using concrete examples, we will be able to discuss rather clearly the possible errors that the residual coupling and energy-eigenstate entanglement might cause.

In most, if not all, present-day experiments, the qubits are controlled using a single microwave line. This situation, however, cannot be maintained for larger multiqubit systems, where the energy levels of the entire system become densely packed. We shall therefore assume that local control lines are used to address the individual qubits.

A. Two-qubit system

The usual theoretical approach to describing a quantum system that is composed of several distinct objects commonly runs along the following line of reasoning. First, we assume that these objects are in a separable initial state, then we controllably evolve the system using the total Hamiltonian, we take the trace over the degrees of freedom of the unused objects (in this case the coupler), and we find the answer to the physical questions of interest. Given the entangled form of the energy eigenstates obtained in Sec. IV, one might expect that this "contamination" of the states will reduce the observed coherence effects. Indeed, following the above-described recipe, one finds such a reduction in observable coherence effects, e.g., reduced gate fidelities. As we now explain, however, this is not the correct description of a typical experiment, and the resulting errors and limitations are also described incorrectly in this way.

First, let us consider the assumption about the initial conditions. In a real two-qubit experiment (assuming essentially zero temperature), the system starts in its ground state $|\psi_{00}\rangle \neq |00\underline{0}\rangle$. When preparing the desired initial state (e.g., a product of two single-qubit states), single-qubit operations are performed using small-amplitude pulses that are resonant with individual qubits. These pulses are typically weak enough that the single-qubit operations are performed over times that are long compared to $1/|\Delta_1-\Delta_2|$ (the energy difference $|\Delta_1-\Delta_2|$ is used here because it is, to a good approximation, the smallest energy difference in the spectrum of the four lowest energy levels). Rather than perform ideal single-qubit operations, such weak pulses drive transitions between the eigenstates of the Hamiltonian of the entire system, regardless of the form of these eigenstates. One could therefore ignore the fact that $|\psi_{nm}\rangle \neq |nm\underline{0}\rangle$ and simply use the eigenstates of the Hamiltonian (i.e., $|\psi_{00}\rangle$, $|\psi_{01}\rangle$, $|\psi_{10}\rangle$ and $|\psi_{11}\rangle$) as the computational basis for performing a quantum algorithm. One can then use weak pulses with properly calibrated frequencies to perform any operation on this effective two-qubit system. Thus, the initial and all subsequent states in the experiment can be very close to the desired form, except that the basis states do not have the simple, separable form [e.g., the state $(|\psi_{00}\rangle+|\psi_{10}\rangle)/\sqrt{2}$ is prepared instead of the state $(|00\underline{0}\rangle+|10\underline{0}\rangle)/\sqrt{2}$].

There are two main possible sources of errors that can affect the above picture. They are both related to the fact that in most quantum algorithms, one needs to perform operations on a certain qubit without knowing the states of the other qubits. The residual-coupling Hamiltonian [Eq. (25)] provides the first source of errors. For example, the resonance frequencies for the transitions $|\psi_{00}\rangle \leftrightarrow |\psi_{10}\rangle$ and

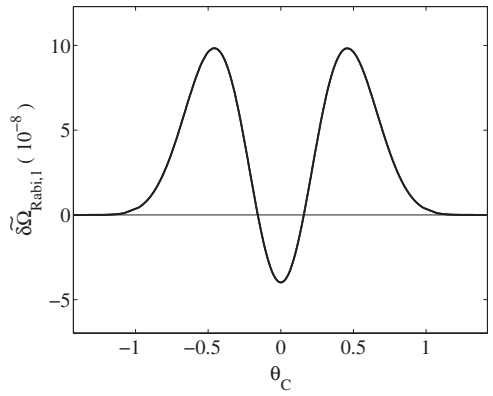

FIG. 3. The error-estimating quantity $\delta\tilde{\Omega}_{\mathrm{Rabi},1} \equiv (\langle\psi_{00}|\hat{\sigma}_x^{(1)}|\psi_{10}\rangle - \langle\psi_{01}|\hat{\sigma}_x^{(1)}|\psi_{11}\rangle)/2$ for the relative spread in the Rabi frequency of qubit 1 as a function of the coupler's bias point θ_C for the same parameters as in Fig. 2. Similar results would be obtained for qubit 2.

$|\psi_{01}\rangle \leftrightarrow |\psi_{11}\rangle$ are shifted from each other by a frequency difference given by $4J_{\mathrm{residual}}$. As a result, the resonance frequency for performing operations on qubit 1 depends on the state of qubit 2, and vice versa. In principle, one could perform a single-qubit gate using two pulses, with each pulse being resonant with one of the transitions. This approach, however, is impractical for many-qubit systems, where resonance lines generally split into an exponentially large number of lines. A more scalable alternative is to perform single-qubit operations using driving amplitudes that are large compared to the spread in the relevant resonance frequencies, such that the pulse can be considered on resonance for all the relevant transitions. However, the residual-coupling Hamiltonian will then cause an undesirable phase accumulation over the course of running the algorithm. Until this residual coupling is suppressed in future experiments (e.g., by increasing Δ_C, as discussed in Sec. IV B), one might need to apply refocussing pulses to reduce its effects. As can be seen from Figs. 1 and 2, pushing J_{residual} to the kilohertz range should be possible using realistic experimental parameters. The other possible source of errors is the fact that the Rabi frequency of qubit 1 oscillations generally depends on the state of qubit 2, and vice versa (this splitting of the Rabi frequencies is a result of the mixing in the energy eigenstates). Such errors can be described by quantities of the form $\delta\tilde{\Omega}_{\mathrm{Rabi},1} \equiv (\langle\psi_{10}|\hat{\sigma}_x^{(1)}|\psi_{00}\rangle - \langle\psi_{11}|\hat{\sigma}_x^{(1)}|\psi_{01}\rangle)/2$. It is straightforward to see that, to the lowest order given in Sec. IV C,

$$\langle\psi_{10}|\hat{\sigma}_x^{(1)}|\psi_{00}\rangle = \langle\psi_{11}|\hat{\sigma}_x^{(1)}|\psi_{01}\rangle. \tag{39}$$

In order to obtain an estimate for $\delta\tilde{\Omega}_{\mathrm{Rabi},1}$, we perform some numerical calculations. We show in Fig. 3 the results for the parameters of Fig. 2. With these parameters we can see that $\delta\tilde{\Omega}_{\mathrm{Rabi},1} \sim 10^{-8}$. This type of errors can therefore be made extremely small using realistic experimental parameters.

A third, but less serious, point of potential concern relates to quantities of the form $\langle\psi_{00}|\hat{\sigma}_x^{(1)}|\psi_{01}\rangle$. This quantity describes, in some sense, how much qubit 2 "feels" a signal applied to qubit 1 (similar to the splitting of Rabi frequencies mentioned above, this type of error is a result of the mixing in the energy eigenstates). Using the parameters of Fig. 2, the error estimator $\langle\psi_{00}|\hat{\sigma}_x^{(1)}|\psi_{01}\rangle$ is of order of 10^{-2} and vanishes close to the point where $J=0$. This type of errors can be suppressed further by using microwave amplitudes such that the small fraction of a signal applied to qubit 1 that is felt by qubit 2 is small enough to be considered far off resonance. Alternatively, one could say that single-qubit operations on qubit 1 must be performed on a time scale that is long compared to $|\langle\psi_{00}|\hat{\sigma}_x^{(1)}|\psi_{01}\rangle|/|\Delta_1 - \Delta_2|$. This is a very mild constraint, even for existing experiments.

Finally, a tricky issue related to the usual theoretical approach mentioned at the beginning of this section is when the coupler degrees of freedom are traced out at the end of the actual quantum calculation. Here again, the measurement process in typical experiments does not follow the simple picture of a sudden, accurate measurement device that probes the basis 0/1. For flux qubits, for example, one typically designs the readout device to simply be a very accurate device for measuring magnetic fields [measuring the flux generated by the qubits and going through the loop of a readout superconducting quantum interference device (SQUID)]. If the qubit-SQUID coupling is weak compared to the qubits' energy scale and it acts for a sufficiently long duration, the readout device will perform the measurement in the basis of the eigenstates of the system Hamiltonian, not the physically defined clockwise and counterclockwise current states. If, in addition, the relevant decoherence rates in the SQUID are small enough, the readout fidelity will not be limited by the exact amount of mixing between the clockwise and counterclockwise current states in the energy eigenstates.[41] Therefore, the readout device can, in principle, give the correct reading (0 or 1) essentially 100% of the time even if the energy eigenstates that are being used in the experiment contain finite amplitudes of the "wrong" state [in particular, here we have in mind the states in Eq. (32)]. We should emphasize here that present-day readout techniques are far from this ideal limit.

B. Multiqubit systems

We now generalize some of the results concerning possible errors in a typical experiment to the case where the system contains more than two qubits. The discussion below also demonstrates an interesting issue related to the significance of setting $J=0$ in the off state (here we have in mind the parametric coupling scheme).

In order to clearly identify whether a given effect is related to mediated coupling or not, we start by considering a multiqubit system with no couplers (the expressions obtained below for the errors also apply if we integrate out the couplers in the circuit and use the effective, i.e., direct plus mediated, coupling strengths between the qubits). We first take the two-qubit Hamiltonian,

$$\hat{H} = \frac{\Delta_1}{2}\hat{\sigma}_z^{(1)} + \frac{\Delta_2}{2}\hat{\sigma}_z^{(2)} + J_{12}\hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)}. \tag{40}$$

The above Hamiltonian has the interesting property that, with the proper assignment of the labels 00, 01, 10, and 11 to

the eigenstates of the Hamiltonian, the relations

$$E_{10} - E_{00} = E_{11} - E_{01},$$

$$E_{01} - E_{00} = E_{11} - E_{10},$$

$$\langle \psi_{10} | \hat{\sigma}_x^{(1)} | \psi_{00} \rangle = \langle \psi_{11} | \hat{\sigma}_x^{(1)} | \psi_{01} \rangle,$$

$$\langle \psi_{01} | \hat{\sigma}_x^{(2)} | \psi_{00} \rangle = \langle \psi_{11} | \hat{\sigma}_x^{(2)} | \psi_{10} \rangle \tag{41}$$

hold regardless of the values of the different parameters in the Hamiltonian. The above relations imply that the first two sources of error discussed in the previous section vanish completely for this system. It is therefore not required to have $J_{12} < |\Delta_1 - \Delta_2|$ in order to perform an almost error-free quantum algorithm in this system.

The question now is whether this situation persists for a system with more than two qubits. We approach this question by performing numerical simulations of a one-dimensional chain of three to ten qubits with the Hamiltonian

$$\hat{H} = \sum_{j=1}^{N} \frac{\Delta_j}{2} \hat{\sigma}_z^{(j)} + \sum_{j=1}^{N-1} J_{j,j+1} \hat{\sigma}_x^{(j)} \otimes \hat{\sigma}_x^{(j+1)}. \tag{42}$$

From the numerical calculations, we find that the generalized version of the relations in Eq. (41) holds only for the two qubits at the ends of the chain. The generalized version of the resonance-frequency relation [i.e., the first two lines in Eq. (41)] continues to hold for all the qubits (i.e., the resonance frequency for flipping qubit j is independent of the states of all the other qubits). The Rabi frequency of qubit j oscillations, however, now generally depends on the states of the other qubits.

In order to get an estimate for the above-mentioned errors, we take the three-qubit case and calculate the standard deviation $\delta\widetilde{\Omega}_{\mathrm{Rabi},2}$ in the quantity $\langle \psi_{n1m} | \hat{\sigma}_x^{(2)} | \psi_{n0m} \rangle$. When the coupling strengths $J_{j,j+1}$ are small compared to the differences between qubit gaps, we find that

$$\widetilde{\delta\Omega}_{\mathrm{Rabi},2} \propto \frac{J_{12}^2 J_{23}^2}{|(\Delta_1 - \Delta_2)(\Delta_2 - \Delta_3)(\Delta_1 - \Delta_3)^2|}, \tag{43}$$

with a prefactor of order one (we also find that this expression remains valid when we add a few more qubits at the ends of the chain). It is for this reason that one would like to set $J=0$ (for all pairs of qubits) in the off state, even though violating this requirement does not necessarily have detrimental effects on a two-qubit experiment.[42] It will also be highly desirable to set the gaps Δ_j to different values, even if they are not nearest neighbors.

We now take a three-qubit chain with couplers, and we perform numerical simulations for several sets of parameters with the leading-order coupling strengths (i.e., the parameters that correspond to J in the two-qubit case) set to zero. We calculate the resonance frequencies for qubit j ($j=1,2,3$) for the four different states of the two other qubits. We find that the resonance-frequency shifts are consistent with the residual coupling strength given in Eq. (29). We therefore expect our results concerning the residual coupling to hold for systems with more than two qubits. We also expect the form of the energy eigenstates to follow the rather straightforward generalization of Eq. (32). If a distant pair of qubits have the same value of Δ_j, the energy scale associated with any possible hybridization of energy levels (e.g., involving states of the form $|0\underline{0}n_2\underline{0}n_3\underline{0}n_4\underline{0}1\underline{0}n_6\cdots\rangle$ and $|1\underline{0}n_2\underline{0}n_3\underline{0}n_4\underline{0}\underline{0}\underline{0}n_6\cdots\rangle$) will be small enough that it can be neglected. Similarly, hybridization between energy levels that require flipping the states of several qubits should be greatly suppressed.

Next, we consider a loop of three or four qubits, i.e., in triangle and square geometries. Denoting the typical scale of the coupling strengths between neighboring qubits by J and the detuning between the qubits by $\Delta\omega$, which is taken to be much smaller than the qubit frequencies, we find that the standard deviation in the resonance frequency $\delta\omega_{\mathrm{resonance}}$ and the standard deviation in the transition matrix element $\delta\widetilde{\Omega}_{\mathrm{Rabi}}$ when attempting to change the state of a given qubit are given by

$$\delta\omega_{\mathrm{resonance}} \sim \frac{J^3}{\Delta\omega^2},$$

$$\widetilde{\delta\Omega}_{\mathrm{Rabi}} \sim \left(\frac{J}{\Delta\omega}\right)^3 \tag{44}$$

in the three qubit case and

$$\delta\omega_{\mathrm{resonance}} \sim \frac{J^4}{\Delta\omega^3},$$

$$\widetilde{\delta\Omega}_{\mathrm{Rabi}} \sim \left(\frac{J}{\Delta\omega}\right)^4 \tag{45}$$

in the four qubit case. The detailed expressions for the above quantities depend rather nontrivially on the values of the different parameters in the problem. Errors stemming from the spreads in resonance and Rabi frequencies therefore depend on the geometry of the multiqubit system, e.g., chain versus closed loop. A two-dimensional lattice would belong to the latter category.

Finally, we consider the geometry where every qubit is coupled to every other qubit, which is relevant to the case of a single coupler mediating coupling between several qubits. We find that the scaling of errors in this case follows the triangle geometry discussed above, with $\Delta\omega$ representing the typical spacing of frequencies in the system. In particular, adding qubits to the system at distant frequencies has little effect on the errors associated with a given qubit.

The main result of this subsection is the fact that certain errors that have not been relevant to past experiments (i.e., two-qubit experiments) will likely arise in future experiments. Although this result might seem somewhat discouraging, it is encouraging that the errors, quantified by the spreads in the resonance and Rabi frequencies, follow scaling laws that make them less serious than one might intuitively expect (e.g., $\delta\widetilde{\Omega}_{\mathrm{Rabi}}$ scales as the third or fourth power of $J/\Delta\omega$, as opposed to being linearly proportional to $J/\Delta\omega$).

VI. CONCLUSION

We have analyzed the problem of a high excitation energy quantum object mediating coupling between two qubits. After reviewing some known results concerning the leading-order term in the mediated coupling, we obtained expressions that describe the residual coupling in the off state and the entanglement in the energy eigenstates of the system. We have argued that our approach analyzing the properties of the eigenvalues and eigenstates of the total Hamiltonian is the appropriate one to describe recent and possibly future experiments. We have also estimated the expected errors originating from the nonideality of the off state in typical experimental situations. Our results should be helpful in designing future circuits that employ the mediated-coupling approach in order to achieve tunable coupling between qubits. In particular, our results suggest that with properly chosen design parameters, the residual coupling in the off state could be greatly reduced in future experiments.

We have focused on the case of a two-qubit system, which is the relevant case for present-day experiments. However, we expect our results for the errors in a two-qubit system to apply to multiqubit systems as well. As we have shown, other sources of error that are absent in a two-qubit system arise for systems with more than two qubits. It would therefore be interesting and important in the future to analyze in more detail the properties of large, many-qubit systems.

Finally, we should mention that although a large part of our analysis was formulated in the language of superconducting systems, our results are quite general and should apply to other systems that employ similar mediated-coupling mechanisms.[43]

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APPENDIX: QUASIDEGENERATE PERTURBATION THEORY

In this appendix, we present a perturbation-theory procedure for the case where the separation between some energy levels is not large compared to the energy scale of the perturbation.[37]

Let us take the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V}, \tag{A1}$$

where we want to treat $\hat{V}$ as a perturbation. We assume, however, that the energy scale of $\hat{V}$ is not necessarily small compared to the energy separations within a subset of n eigenstates of $\hat{H}_0$. The energy scale of $\hat{V}$ is small compared to the energy separation between this subset of levels and all the levels outside it.

We now want to find the approximate energy levels and eigenstates of $\hat{H}$ in the vicinity of these n original energy levels of $\hat{H}_0$. We proceed by assuming that these closely spaced eigenstates can have a large amount of mixing among themselves because of the added perturbation $\hat{V}$, but we assume that mixing with all other states will be small. In other words, we express (any one of) the eigenstates of interest as

$$|\Psi_i\rangle = \sum_{j=1}^{n} f_{ij}|\psi_j\rangle + \sum_{j=n+1}^{\infty} g_{ij}|\psi_j\rangle, \tag{A2}$$

where $|\psi_j\rangle$ are the eigenstates of $\hat{H}_0$ with

$$\hat{H}_0|\psi_j\rangle = \epsilon_j|\psi_j\rangle \tag{A3}$$

the states $|\Psi_i\rangle$ with $j=1,2,\ldots,n$ represent the states of interest, and g_{ij} are understood to be small enough to be treated perturbatively (this is the only reason we express the amplitudes f_{ij} and g_{ij} using two different symbols). We can now express the eigenvalue problem as

$$\sum_{j=1}^{n} f_{ij}\epsilon_j|\psi_j\rangle + \sum_{j=n+1}^{\infty} g_{ij}\epsilon_j|\psi_j\rangle + \sum_{k=1}^{\infty}\left(\sum_{j=1}^{n} f_{ij}V_{kj}|\psi_k\rangle + \sum_{j=n+1}^{\infty} g_{ij}V_{kj}|\psi_k\rangle\right) = E_i\left(\sum_{j=1}^{n} f_{ij}|\psi_j\rangle + \sum_{j=n+1}^{\infty} g_{ij}|\psi_j\rangle\right). \tag{A4}$$

If we multiply the above equation from the left by $\langle\psi_l|$ with $1\le l\le n$, we obtain the equation

$$f_{il}\epsilon_l + \sum_{j=1}^{n} f_{ij}V_{lj} + \sum_{j=n+1}^{\infty} g_{ij}V_{lj} = E_i f_{il}. \tag{A5}$$

If we multiply the equation by $\langle\psi_l|$ with $l>n$, we obtain instead

$$g_{il}\epsilon_l + \sum_{j=1}^{n} f_{ij}V_{lj} + \sum_{j=n+1}^{\infty} g_{ij}V_{lj} = E_i g_{il}, \tag{A6}$$

which can be rewritten as

$$g_{ij} = \frac{\sum_{j=1}^{n} f_{ij}V_{lj} + \sum_{j=n+1}^{\infty} g_{ij}V_{lj}}{E_i - \epsilon_l}. \tag{A7}$$

Equation (A7) is now treated using a perturbative (or rather iterative) approach. If we neglect the sum over the states with $j=n+1,\ldots$, we obtain

$$g_{il} \approx \frac{\sum_{j=1}^{n} f_{ij}V_{lj}}{E_i - \epsilon_l}. \tag{A8}$$

Substituting this expression into Eq. (A5), we obtain (for every l with $1\le l\le n$)

$$\sum_{j=1}^{n}\left(\epsilon_l\delta_{lj}+V_{lj}+\sum_{j'=n+1}^{\infty}\frac{V_{lj'}V_{j'j}}{E_i-\epsilon_{j'}}\right)f_{ij}=E_if_{il}, \tag{A9}$$

where δ_{lj} is the Kronecker delta function.

If we want to obtain more accurate results, we can take Eq. (A8) and substitute it into the right-hand side of Eq. (A7). Expressing g_{ij} in Eq. (A8) as g_{ij}^{prev}, we obtain

$$g_{il}\approx\frac{\sum_{j=1}^{n}f_{ij}V_{lj}}{E_i-\epsilon_l}+\frac{1}{E_i-\epsilon_l}\left(\sum_{j=n+1}^{\infty}g_{ij}^{\text{prev}}V_{lj}\right)=\frac{\sum_{j=1}^{n}f_{ij}V_{lj}}{E_i-\epsilon_l}+\frac{1}{E_i-\epsilon_l}\left(\sum_{j=n+1}^{\infty}\frac{\sum_{j'=1}^{n}f_{ij'}V_{jj'}}{E_i-\epsilon_j}V_{lj}\right). \tag{A10}$$

Using this expression for g_{ij} in Eq. (A5), we find that to the next order,

$$\sum_{j=1}^{n}\left(\epsilon_l\delta_{lj}+V_{lj}+\sum_{j'=n+1}^{\infty}\frac{V_{lj'}V_{j'j}}{E_i-\epsilon_j'}+\sum_{j'=n+1}^{\infty}\sum_{j''=n+1}^{\infty}\frac{V_{lj'}V_{j'j''}V_{j''j}}{(E_i-\epsilon_{j'})(E_i-\epsilon_{j''})}\right)f_{ij}=E_if_{il}. \tag{A11}$$

The generalization to all orders is now obvious, if needed. One must be careful, of course, that the denominators on the left-hand side of Eqs. (A9) and (A11) contain the eigenvalue E_i. The solution is therefore not yet obtained by a straightforward diagonalization of an $n\times n$ matrix. However, it is usually a good first approximation to use some (averaged) value for E_i on the left-hand side of the equation. This value can be taken from the energy levels of the original Hamiltonian $\hat{H}_0$. One can then obtain more accurate results by introducing a second iterative procedure. Every time we obtain an approximate value of the energy E_i, we can substitute it into the left-hand side of Eq. (A9) and (A11) to obtain an even more accurate result. Note that this iterative procedure is independent of the other one introduced above, i.e., the iterative substitution of Eq. (A8) into Eq. (A7). In order to reach a given level of accuracy, both procedures must be performed to the appropriate order.

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