

# Superconducting qubits beyond the dispersive regime

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(Received 8 July 2018; revised manuscript received 11 June 2019; published 17 July 2019)

Superconducting circuits consisting of a few low-anharmonic transmons coupled to readout and bus resonators can perform basic quantum computations. Since the number of qubits in such circuits is limited to not more than a few tens, the qubits can be designed to operate within the dispersive regime where frequency detunings are much stronger than coupling strengths. However, scaling up the number of qubits will bring the circuit out of the regime, and this invalidates current theories. We develop a formalism that allows to consistently diagonalize the superconducting circuit Hamiltonian beyond the dispersive regime. This will allow to study qubit-qubit interaction unperturbatively, therefore, our formalism remains valid and accurate at small or even negligible frequency detuning; thus, our formalism serves as a theoretical ground for designing qubit characteristics for scaling up the number of qubits in superconducting circuits. We study the most important circuits with single- and two-qubit gates, i.e., a single transmon coupled to a resonator and two transmons sharing a bus resonator. Surprisingly, our formalism allows to determine the circuit characteristics, such as dressed frequencies and Kerr couplings, in closed-form formulas that not only reproduce perturbative results, but also extrapolate beyond the dispersive regime and can ultimately reproduce (and even modify) the Jaynes-Cummings results at resonant frequencies.

DOI: [10.1103/PhysRevB.100.024509](https://doi.org/10.1103/PhysRevB.100.024509)

## I. INTRODUCTION

Quantum computation is rapidly progressing toward practical technology [1–4]. So far, quantum bits have been well developed on superconducting circuits [5]. When cooled to millikelvin temperatures, coherent tunneling of the Cooper pairs through the Josephson junction (JJ) exhibits slightly nonlinear harmonic oscillations with addressable energy levels [6]. Such quantum states have long coherent times and can operate on nanosecond scales. Moreover, they are compatible with microwave control technology and can scale up in number. All these features makes superconducting qubits one of the prominent platforms for constructing a multiqubit quantum processor [7,8].

The state-of-the-art superconducting circuits contain a few tens of qubits with an operational gate error rate about 0.1% for single qubit gates [9] and 1% for two-qubit gates [10] below the threshold for error detection in the surface code [11]. Scaling up the qubit number beyond this limit dramatically increases errors, and the key milestone of the next few years is to reduce the errors [12,13]. Achieving this not only requires further enhancements in the circuit quality [14], but also needs progressive advancement in theory [15]. So far, the Jaynes-Cummings model, originally introduced in quantum optics [16], and its generalization have been routinely applied on superconducting circuits. These models have been, so far, well studied for parameters admissible by perturbation theory, namely, within the “dispersive regime” [17,18] as well as special resonant frequency solutions [19,20]. However, scaling up the number of qubits within the narrow domain of parameters will introduce new issues, such as circuit frequency crowding

[21], that must be avoided. Recently, it has been discussed that significant advantages can be made in engineering circuits outside of the dispersive regime [22]. However, those studies have been performed numerically in the absence of established theory.

Motivated by the “black box quantization” method, here, we develop a formalism for evaluating the qubit characteristics in circuits consisting of transmons and resonators at arbitrary frequencies and coupling strengths. Black box quantization has been recently introduced in Ref. [23] for circuits consisting of low anharmonic transmons coupled to resonators. The low anharmonicity allows dividing the circuit Hamiltonian into harmonic and anharmonic sectors. In the absence of anharmonicity, the transmons and the resonators can be treated on equal footing, thus, the Foster decomposition [24] can replace the harmonic circuit with a set of lumped imaginary impedances seen by the anharmonic sector. Identifying the characteristic impedances is of central importance in this method for which Ref. [23] proposes iterative feedback between experiment and theory. This formalism has initiated, so far, several progressive improvements for extracting circuit parameters from electromagnetic simulation [25–27]. In Fig. 1, the harmonic sector is made of  $N$  qubits (in blue boxes) coupled to cavity modes (in the gray area). The curly (red) crosses denote anharmonic sectors.

After introducing a unitary transformation matrix in the space of the total number of qubits and resonators, we find a normal-mode basis for the harmonic sector of a multiqubit circuit. Using the transformation, we determine all dressed frequencies and Kerr nonlinear terms in the leading order of anharmonicity. The simplicity and accuracy of this method

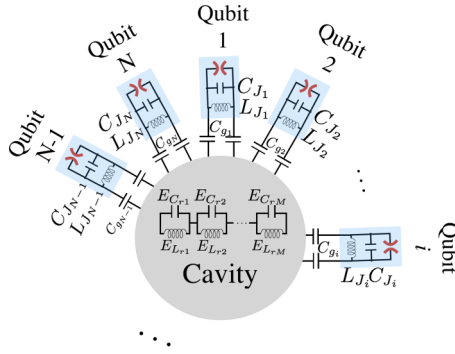


FIG. 1.  $N$  transmons (blue boxes) coupled to a multimode resonator; the curly (red) crosses are the nonlinear JJs that represent the anharmonicity sector, everything else makes the harmonic one.

allow us to present the results of a transmon and two transmons in closed-form formulas. For complex circuits, this method provides insightful Hamiltonian diagonalization inside and outside of the dispersive regime, which will be progressively useful in scaling up the number of qubits. We explain the formalism first in the single transmon, then, we generalize it before we solve another example of two transmons.

## II. SINGLE TRANSMON COUPLED TO A RESONATOR

*A transmon coupled to a resonator.* The canonical variables are charges and phases [28], i.e.,  $(q_i, \phi_i)$  with  $i$  being  $t, r$  for transmon and resonator. The transmon is coupled to the center conductor of the resonator by the capacitance  $C_g$ . The dipole interaction  $H_{\text{int}} = \beta V_r q_t$  couples the transmon charge and the resonator voltage  $V_r = q_r/C_r$  with  $C_{r/t}$  being the resonator/transmon capacitance and  $\beta \equiv C_g/C_t$ . Keeping  $\beta \ll 1$  guarantees the increase in qubit coherence time [29]. The circuit harmonic and anharmonic sectors sum to define the circuit classical Hamiltonian,

$$H = H_{\text{har}} + H_{\text{anhar}}, \quad H_{\text{anhar}} = -\frac{E_C}{3Z_t^2 \hbar^2} \phi_t^4, \quad (1)$$

$$H_{\text{har}} = \sum_{i=r,t} \frac{q_i^2}{2C_i} + \frac{\phi_i^2}{2L_i} + H_{\text{int}},$$

The characteristic impedances and the harmonic frequencies in the circuit are  $Z_i = \sqrt{L_i/C_i}$  and  $\omega_i = 1/\sqrt{L_i C_i}$ , respectively, with  $E_C$  being the total capacitive energy of transmon (including the JJ and shunt capacitances as well as capacitive coupling between transmon and voltage sources), and  $\hbar$  being the reduced Planck constant. We define canonical variables  $(Q_i, X_i) \equiv (q_i/\sqrt{L_i}, \phi_i/\sqrt{L_i})$  such that the harmonic part of Eq. (2) can be transformed to

$$H_{\text{har}} = \frac{1}{2} \mathbf{Q}^T \mathbf{M} \mathbf{Q} + \frac{1}{2} \mathbf{X}^T \mathbf{X}, \quad \mathbf{M} = \begin{bmatrix} \frac{\omega_t^2}{g\sqrt{4\omega_t\omega_r}} & g\sqrt{4\omega_t\omega_r} \\ g\sqrt{4\omega_t\omega_r} & \omega_r^2 \end{bmatrix}, \quad (2)$$

with  $g \equiv \beta\omega_r\sqrt{Z_r/4Z_t}$ ,  $\mathbf{Q} \equiv (Q_t, Q_r)$ , and  $\mathbf{X} \equiv (X_t, X_r)$ .

This Hamiltonian can be diagonalized by unitarily transforming  $\mathbf{Q}$  and  $\mathbf{X}$  into new canonical variables  $\mathcal{Q}$  and  $\mathcal{X}$ , i.e.,  $Q_i = \sum_j S_{ij} Q_j$  and  $X_i = \sum_j T_{ij} X_j$ . Given that the variables in the new and the old frames must satisfy the Poisson

brackets of canonical coordinates, i.e.,  $\{Q_i, X_j\} = \delta_{ij}$ , one can find that  $T_{ij} = S_{ij}$  (see Appendix A). The only term in Eq. (2) that needs diagonalization is  $\mathbf{Q}^T \mathbf{M} \mathbf{Q}$ , which, in the new basis, must look like  $\mathcal{Q}^T \Omega \mathcal{Q}$  with  $\Omega$  being a diagonal matrix  $\Omega_{tt} = \bar{\omega}_t^2$ ,  $\Omega_{rr} = \bar{\omega}_r^2$ , and zero otherwise. The unitary transformation  $\mathbf{S}$  is, therefore, the matrix of columns of normalized eigenvectors of  $\mathbf{M}$ .

In the new basis, the following dressed frequencies can be found in the linear sector:  $\bar{\omega}_t \equiv K_-^2$  and  $\bar{\omega}_r \equiv K_+^2$  with  $K_{\pm} \equiv 2^{-(1/4)}(\omega_t^2 + \omega_r^2 \pm \Delta \Sigma s^{-1})^{1/4}$  and  $s \equiv [1 + 16(g/\Delta)^2 \omega_r \omega_t / \Sigma^2]^{-1/2}$ ,  $\Sigma \equiv \omega_r + \omega_t$ , and  $\Delta \equiv \omega_r - \omega_t$ . The unitary transformation matrix  $\mathbf{S}$  is made of columns of the following normalized eigenvectors  $[\pm\sqrt{(1 \mp s)/2}, \sqrt{(1 \pm s)/2}]^T$  associated with the eigenvalues  $K_{\pm}^2$ . (In Appendix H, similar results have been found using the Bogoliubov transformations [30].) In this basis, the anharmonic term proportional to  $X_t^4$  should be transformed using the phase transformation  $X_t = -\sqrt{(1+s)/2} \mathcal{X}_t + \sqrt{(1-s)/2} \mathcal{X}_r$ , and this can make many types of terms possible, e.g.,  $C_m \mathcal{X}_r^m \mathcal{X}_t^{4-m}$  with coupling strengths  $C_m(s)$  and  $m = 0-4$ . In the original eigenbasis  $|n_j\rangle$  with  $j = t, r$ , the ladder operators  $\hat{a}_j = \sum_{n_j} \sqrt{n_j+1} |n_j+1\rangle \langle n_j+1|$  can help to rewrite the charge operator  $\hat{Q}_j = \sqrt{\hbar/2\omega_j}(\hat{a}_j^\dagger + \hat{a}_j)$  and the phase operator  $\hat{X}_j = i\sqrt{\hbar\omega_j/2}(\hat{a}_j^\dagger - \hat{a}_j)$  [28]. Similarly, in the normal-mode basis, the ladder operators  $\hat{\alpha}_k$  determine the new charge and phase operators:  $\hat{Q}_j$  and  $\hat{X}_j$ . These two bases can be transformed into one another using the following Bogoliubov-Velatin transformation:  $\hat{a}_t^\dagger - \hat{a}_t = U_{tt}(\hat{\alpha}_t^\dagger - \hat{\alpha}_t) + U_{tr}(\hat{\alpha}_r^\dagger - \hat{\alpha}_r)$  with  $U_{tt} = -[(1+s)\bar{\omega}_t/2\omega_t]^{1/2}$  and  $U_{tr} = [(1-s)\bar{\omega}_r/2\omega_t]^{1/2}$ .

The anharmonic quantum Hamiltonian from Eq. (2) can be written as  $H_{\text{anhar}} = -(\delta/12)(\hat{a}_t^\dagger - \hat{a}_t)^4$  with  $\delta \equiv E_C$  being the anharmonicity coefficient. In the new basis, this Hamiltonian is transformed to  $-\frac{\delta}{12}[U_{tt}(\hat{\alpha}_t^\dagger - \hat{\alpha}_t) + U_{tr}(\hat{\alpha}_r^\dagger - \hat{\alpha}_r)]^4$ , defining the self-Kerr coefficient [31] of the transmon  $\chi_t = \delta U_{tt}^4$  and that of the resonator  $\chi_r = \delta U_{tr}^4$ . Note that the anharmonic Hamiltonian is not diagonal in the normal-mode basis, however, we can simplify it by ignoring irrelevant terms to first order and applying a secular approximation. This reformulates the total Hamiltonian to

$$H = \sum_{i=t,r} \bar{\omega}_i \hat{\alpha}_i^\dagger \hat{\alpha}_i - \frac{\chi_i}{2} \left[ (\hat{\alpha}_i^\dagger \hat{\alpha}_i)^2 + \hat{\alpha}_i^\dagger \hat{\alpha}_i + \frac{1}{2} \right] - 2\chi_{rt} \left( \hat{\alpha}_t^\dagger \hat{\alpha}_t + \frac{1}{2} \right) \left( \hat{\alpha}_r^\dagger \hat{\alpha}_r + \frac{1}{2} \right), \quad (3)$$

The transmon state in the normal-mode basis makes a shift proportional to  $\chi_{rt}$ , namely, the cross-Kerr coefficient in the resonator frequency. It is simple to show that  $\chi_{rt} = \sqrt{\chi_r \chi_t}$  and, therefore, it linearly scales with the anharmonicity  $\delta$ . Defining “dressed frequency”  $\tilde{\omega}_i$  to be the coefficient of  $\hat{\alpha}_i^\dagger \hat{\alpha}_i$  after summing over all relevant terms, we find the following closed-form formula for the dressed frequencies:

$$\tilde{\omega}_t = K_-^2 - \frac{\chi_t}{2} - \chi_{rt}, \quad \tilde{\omega}_r = K_+^2 - \frac{\chi_r}{2} - \chi_{rt}, \quad (4)$$

$$\chi_t = \delta(1+s)^2 K_-^4/4\omega_t^2, \quad \chi_r = \delta(1-s)^2 K_+^4/4\omega_r^2, \quad (5)$$

which indicate  $E_{n_t n_r} = \sum_i \tilde{\omega}_i n_i - \chi_t^2 n_t^2/2 - 2\chi_{rt} n_t n_r$ . The validity of these formulas are much wider than the dispersive

regime, in fact, they are valid for *arbitrary* coupling strength and frequency detuning.

Let us compare our results with other models. In general, two sets of analytical results are known for the circuit: (i) within the dispersive regime, which defines the validity of perturbation theory, or (ii) at resonant frequencies in the Jaynes-Cummings model. In the dispersive regime, the detuning frequency is much stronger than the coupling strength, i.e.,  $g/\Delta \ll 1$ , and, within this regime, Eqs. (4) and (5) are expanded in polynomials of  $g/\Delta$ . This will result in the following dressed frequencies:  $\tilde{\omega}_t \approx \omega_t - 2\omega_r g/\Delta \Sigma$ ,  $\tilde{\omega}_r \approx \omega_r + 2g^2\omega_t/\Delta \Sigma$ , and the self-Kerr nonlinearities  $\chi_t = \delta[1 - 4g^2\omega_r(\omega_r^2 + \omega_t^2)/\omega_t \Sigma^2 \Delta^2]$  and  $\chi_r = 16\delta(g/\Delta)^4 \omega_r^4/\Sigma^4$ . These expressions are in agreement with the non-rotating-wave approximation (non-RWA) results recently reported in Ref. [32] using perturbation theory. In the RWA regime  $g \ll \Delta \ll \Sigma$ , therefore, we can simplify these expressions by using Ref. [32]:  $\omega_r/\Sigma \approx \omega_t/\Sigma \approx 1/2$ . The RWA dressed frequencies are  $\tilde{\omega}_t^{\text{RWA}} \approx \omega_t - \delta/2 - g^2/\Delta - \delta g^2/\Delta^2$ ,  $\tilde{\omega}_r^{\text{RWA}} \approx \omega_r + g^2/\Delta - \delta g^2/\Delta^2$ ,  $\chi_t^{\text{RWA}} \approx \delta[1 - 2(g/\Delta)^2]$ ,  $\chi_r^{\text{RWA}} \approx \delta(g/\Delta)^4$ . These results are in agreement with the original perturbative Lamb and ac Stark shifts reported by Koch *et al.* in Ref. [33] and experimentally observed [34].

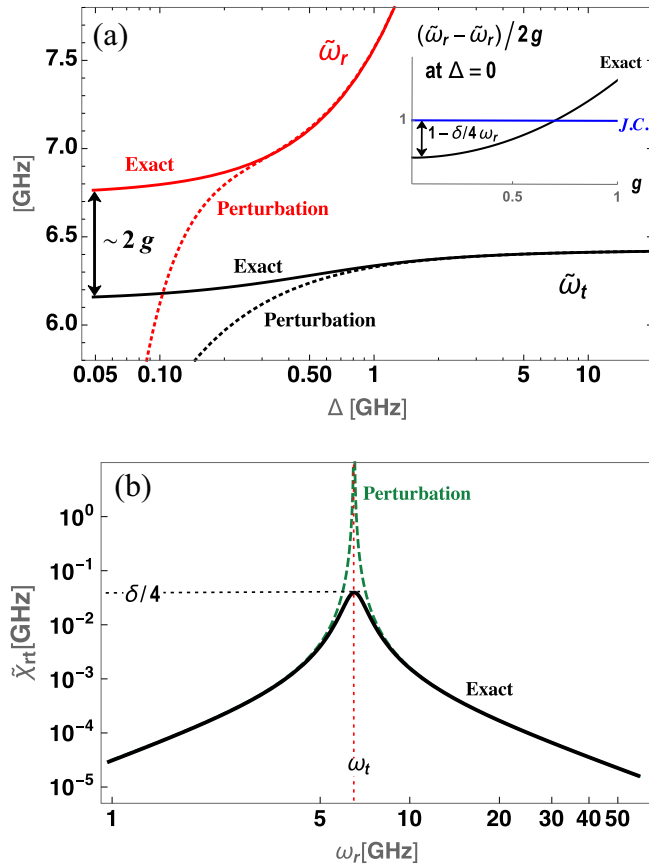


FIG. 2. Exact (solid) and perturbative (dashed) results for (a) dressed frequencies (b) cross Kerr in the circuit with  $\omega_t = 6.5$  GHz,  $\omega_r = \Delta + \omega_t$ ,  $g = 0.3$  GHz, and  $\delta = 0.15$  GHz. (Inset) Rescaled dressed frequency detuning at resonant bare frequency in the Jaynes-Cummings and the exact models.

Figure 2(a) shows the transmon and the resonator dressed frequencies at different detuning frequencies  $\Delta$  and a fixed coupling strength  $g$ . For the choice of circuit parameters, there is a negligible mismatch between RWA and non-RWA perturbative results, therefore, on the logarithmic scales, the lines labeled by perturbation can be plotted using both formulations. In large detuning  $\Delta$ , the exact dressed frequencies of Eq. (4), on the solid lines, are in good agreement with the perturbative (dotted) results. However, as  $g/\Delta$  increases almost above  $\sim 1/3$ , the difference between exact and perturbative results starts to appear. Another regime of interest is the special solution of the resonant point where bare frequency of the transmon and the resonator are the same. Perturbation theory at this point diverges, however, the Jaynes-Cummings model predicts that due to atom-photon coupling, a  $2g$  frequency gap between the two dressed frequencies is produced [19,20]. Our exact formalism in Eq. (4) not only confirms this result, but also provides a modification in it due to the presence of finite anharmonicity in transmons, which makes the dressed frequency detuning  $2g(1 - \delta/4\omega_r)$ . Figure 2(b) inset shows this gap rescaled by  $2g$  at different coupling strengths  $g$ , which is unity for infinite anharmonicity (labeled J.C.); and is nonlinear for finite anharmonicity. Figure 2(b) shows cross-Kerr coefficient—defined below Eq. (3)—in the solid line and compares it with the perturbative results in the dashed lines. At the resonant point as expected, the perturbation theory diverges, however, in contrast, the exact solution reveals the finite value of  $\delta/4 + o(g^2)$  for any choice of bare frequencies.

### III. GENERAL METHOD: $N$ ATOMS COUPLED TO A RESONATOR

*$N$  transmons coupled to a  $M$  resonator.* The black box quantization in the original form has been proposed as an experimental method to get theoretical feedback on fitting parameters. Here, we study a purely theoretical approach to generalize it to  $N$  modes and  $M$  transmons. This will help not only to scale up quantum circuits, but also to study nonperturbative solutions.

Scaling up entanglement is one of the purely quantum phenomena that is most crucial for quantum computing. Such phenomena can take place in large-scale quantum circuits with  $N$  transmons interacting with  $M$  resonators. A total of  $N + M$  pairs of canonical variables can be defined: the charge vector  $\mathbf{Q} = (Q_1, \dots, Q_{N+M})^T$  and the phase vector  $\mathbf{X} = (X_1, \dots, X_{N+M})^T$ . The circuit Hamiltonian can be divided into a harmonic sector and a weakly anharmonic sector. The harmonic Hamiltonian is  $H_{\text{har.}} = \frac{1}{2} \sum_{i=1}^{N+M} \omega_i^2 Q_i^2 + \frac{1}{2} X_i^2 + \sum_{i=1}^N \sum_{j=N+1}^{N+M} g_{ij} \sqrt{4\omega_i \omega_j} Q_i Q_j$ . Using a generalization of the  $\mathbf{M}$  matrix in Eq. (2), this Hamiltonian is simplified to  $H_{\text{har.}} = \frac{1}{2} \mathbf{Q}^T \mathbf{M} \mathbf{Q} + \frac{1}{2} \mathbf{X}^T \mathbf{X}$  with the matrix  $\mathbf{M}$  being nonzero only at  $M_{RR} = \omega_r^2$ ,  $M_{TT} = \omega_a^2$ ,  $M_{TR} = M_{RT} = g_r \sqrt{4\omega_t \omega_r}$ ; subindices  $T$  labels transmons  $\{1, 2, \dots, N\}$  and  $R$  labels the resonators  $\{N+1, \dots, M\}$ . Consider that the following unitary transformations charge  $Q_i = \sum_j S_{ij} Q_j$  and phases  $X_i = \sum_j T_{ij} X_j$  take them to a normal-mode basis. As discussed in Appendix A, these unitary transformations are identical, i.e.,  $T_{ij} = S_{ij}$ . They transform the harmonic Hamiltonian to  $\frac{1}{2} \sum_i \tilde{\omega}_i Q_i^2 + \chi_i^2$ . Detailed analysis show that  $S$  is

the matrix of normalized eigenvectors of the  $\mathbf{M}$  matrix. This evaluates dressed frequencies in the absence of anharmonicity, which, in this paper, we determine them exactly in a closed-form formula for circuits with one and two transmons and one resonator, however, for larger circuits the  $\mathbf{M}$  matrix can be evaluated numerically, and this determines all exact dressed frequencies.

Once  $S$  is found, charges and phases can be promoted to operators and rewritten in terms of ladder operator  $\hat{a}$  in the original basis and  $\hat{\alpha}$  in the new basis. They transform to one another as follows:

$$\hat{a}_i^\dagger - \hat{\alpha}_i = \sum_{j=1}^{N+M} U_{ij}(\hat{\alpha}_j^\dagger - \hat{\alpha}_j), \quad U_{ij} \equiv \sqrt{\frac{\bar{\omega}_j}{\omega_i}} S_{ij}. \quad (6)$$

The anharmonic Hamiltonian  $\sum_{i=1}^N (\delta_i/12)(\hat{a}_i - \hat{\alpha}_i^\dagger)^4$  can be similarly taken to the normal-mode basis—see Appendix H for details. The smallness of anharmonicity in transmons allows the nonlinear physical parameters to be evaluated in leading order.

#### IV. TWO TRANSMONS COUPLED TO A RESONATOR

*Two transmons sharing a bus resonator.* This is an important circuit for two-qubit gate calibration [35,36]. Let us denote  $\omega_i$  with  $i = 1-3$  for the two transmons and the resonator, respectively—alternatively, we sometimes use  $r$  (instead of 3) to emphasize the resonator. The coupling strengths between the transmons and the resonator are  $g_1, g_2$ . The  $\mathbf{M}$  matrix is

$$\mathbf{M} = \begin{bmatrix} \omega_1^2 & 0 & g_1\sqrt{4\omega_1\omega_3} \\ 0 & \omega_2^2 & g_2\sqrt{4\omega_2\omega_3} \\ g_1\sqrt{4\omega_1\omega_3} & g_2\sqrt{4\omega_2\omega_3} & \omega_3^2 \end{bmatrix}. \quad (7)$$

The  $\mathbf{M}$ -matrix can be taken to a normal-mode basis within a wide domain of parameters. The cubic equation  $\lambda^3 + b\lambda^2 + c\lambda + d = 0$  determines the eigenvalues  $\lambda$  of Eq. (7) with  $b \equiv -\sum_{i=1-3} \omega_i^2$ ,  $c \equiv \omega_1^2\omega_2^2 + \omega_1^2\omega_3^2 + \omega_2^2\omega_3^2 - \sum_{i=1,2} 4g_i^2\omega_i\omega_3$ , and  $d \equiv 4g_2^2\omega_1^2\omega_2\omega_3 + 4g_1^2\omega_1\omega_2^2\omega_3 - \omega_1^2\omega_2^2\omega_3^2$ . Note that the eigenvalues  $\lambda_k$  determine the circuit dressed frequencies, i.e.,  $\bar{\omega}_k \equiv \sqrt{\lambda_k}$  with  $k = 1-3$ . By defining  $\theta \equiv \lambda + b/3$ , the quadratic term is eliminated, i.e.,  $\theta^3 - f\theta + h = 0$ ,  $f \equiv b^2/3 - c$ , and  $h \equiv (2b^3 - 9bc + 27d)/27$ . We solve this equation using trigonometric trials functions and find

$$\bar{\omega}_k^2 = 2\sqrt{\frac{f}{3}} \cos \frac{\cos^{-1}\left[-\frac{h}{2}\left(\frac{3}{f}\right)^{3/2}\right] - 2\pi(k-1)}{3} - \frac{b}{3}. \quad (8)$$

A relabeling of indices might be needed to identify corresponding frequencies. Should the inverse cosine be always between  $-1$  and  $1$ ,  $h^2/4 - f^3/27 < 0$  must be satisfied for real-valued solutions. In circuits suitable for quantum computation, however, since coupling strengths are much smaller than individual frequencies, this condition is trivially satisfied, see Appendix B.

The anharmonic Hamiltonian transformed into the normal-mode basis in the leading order can be written as

$$\begin{aligned} H = & \sum_{i=1-3} \bar{\omega}_i \hat{\alpha}_i^\dagger \hat{\alpha}_i - \sum_{i=1-3} \left\{ \frac{\chi_i}{2} (\hat{\alpha}_i^\dagger \hat{\alpha}_i)^2 + 2 \sum_{k>i} \chi_{ik} (\hat{\alpha}_i^\dagger \hat{\alpha}_i) (\hat{\alpha}_k^\dagger \hat{\alpha}_k) \right. \\ & + \sum_{k>i} \left( \mathcal{J}_{ik} + \sum_{l \neq i,k} \mathcal{L}_{ikl} \hat{\alpha}_l^\dagger \hat{\alpha}_l \right) (\hat{\alpha}_i^\dagger \hat{\alpha}_k^\dagger + \hat{\alpha}_i^\dagger \hat{\alpha}_k) \\ & \left. + \sum_{k \neq i} \mathcal{K}_{ik} [(\hat{\alpha}_i^\dagger \hat{\alpha}_i) \hat{\alpha}_i^\dagger \hat{\alpha}_k^\dagger + \hat{\alpha}_i^\dagger \hat{\alpha}_k (\hat{\alpha}_i^\dagger \hat{\alpha}_i)] \right\}, \end{aligned} \quad (9)$$

with self-Kerr  $\chi_i = \sum_{j=1,2} \delta_j U_{ji}^4$ , cross-Kerr  $\chi_{ik} = \sum_{j=1,2} \delta_j U_{ji}^2 U_{jk}^2$ , and  $U_{ij}$  being defined in Eq. (6)—see Appendix C for details. One can evaluate the Kerr cofactors and see that, in general, there is no simple relation between cross-Kerr and self-Kerr coefficients.

In Eq. (9), the  $\mathcal{J}$  coupling indicates a direct interaction between two oscillators. The  $\mathcal{K}$  and  $\mathcal{L}$  terms are multiplied by  $\hat{\alpha}_i^\dagger \hat{\alpha}_i$ , therefore, they are effectively  $n_l \mathcal{L}_{ikl}$  and  $n_i \mathcal{K}_{ik}$  with  $n$  being integer quantum numbers. These couplings linearly depend on anharmonicity  $\delta$  and are stronger in higher excited states. Detailed analysis—see Appendices D and E—shows that after block diagonalization these three interactions appear in the effective Hamiltonian of the two-qubit circuit only in the higher-order  $\delta^2$ , thus, they are negligible in the leading order.

The dressed frequency of the transmons and resonator is

$$\bar{\omega}_i = \bar{\omega}_i - \frac{\chi_i}{2} - \sum_{j(\neq i)} \chi_{ij}, \quad (10)$$

and the energy levels are  $E_{n_1-n_3} = \sum_{i=1}^3 n_i \bar{\omega}_i - \chi_i n_i^2/2 - 2 \sum_{k>i} \chi_{ik} n_i n_k$ . Figure 3(a) shows all dressed frequencies given the bare values  $\omega_1 = 3$  GHz,  $\omega_2 = \alpha\omega_1$ , and  $\omega_r = \omega_1 + \Delta_{r1}$ . We obtain perturbative results (dotted) using the formalism explained in Refs. [37,38]—more explicitly Eqs. (4.3)–(4.5) of the first reference. For the fixed coupling strength  $g$  and large  $\Delta_{r1} \gg g$ , the results of perturbation theory and Eq. (10) are in good agreement. Far from the dispersive regime, however, the two become much deviated. For example, in a circuit with the frequency of transmon 1 and a resonator in resonance, perturbation theory diverges, however, Eq. (10) predicts a finite dressed frequency gap as shown in Fig. 3(a). In the case of  $\alpha < 1$  and  $g/\omega_1 < (1 - \alpha^2)/3\sqrt{6}$ , a series expansion of Eq. (10) in terms of  $g$  shows that in the absence of anharmonicity  $\tilde{\Delta}_{r1} \approx 2g$  and  $\tilde{\Delta}_{12} \approx \Delta_{12} - g + [(1 + \alpha)^{-1} + (1 + \alpha)/2]g^2/\Delta_{12} + o(g^3)$ . Figure 3(b) shows the special case of resonant transmons with  $\omega_1 = \omega_2 \equiv \omega$ . Our exact evaluation indicates that all dressed frequencies become off-resonant at the values of  $\omega$ ,  $\sqrt{(\omega^2 + \omega_r^2 \pm \Delta \Sigma r^{-1})/2}$  with  $r^{-2} \equiv 1 + 32g^2\omega\omega_r/\Delta_{r1}^2 \Sigma_{r1}^2$ . The special case of maximal resonance, i.e.,  $\omega_r = \omega$ , the dressed frequencies will be found to be  $\tilde{\Delta}_{r1} \approx \tilde{\Delta}_{12} \approx \sqrt{2}g$  in the absence of anharmonicity, see Appendix F for details. These are all previously unknown results that can be used, for instance, to identify bad samples in circuit fabrications.



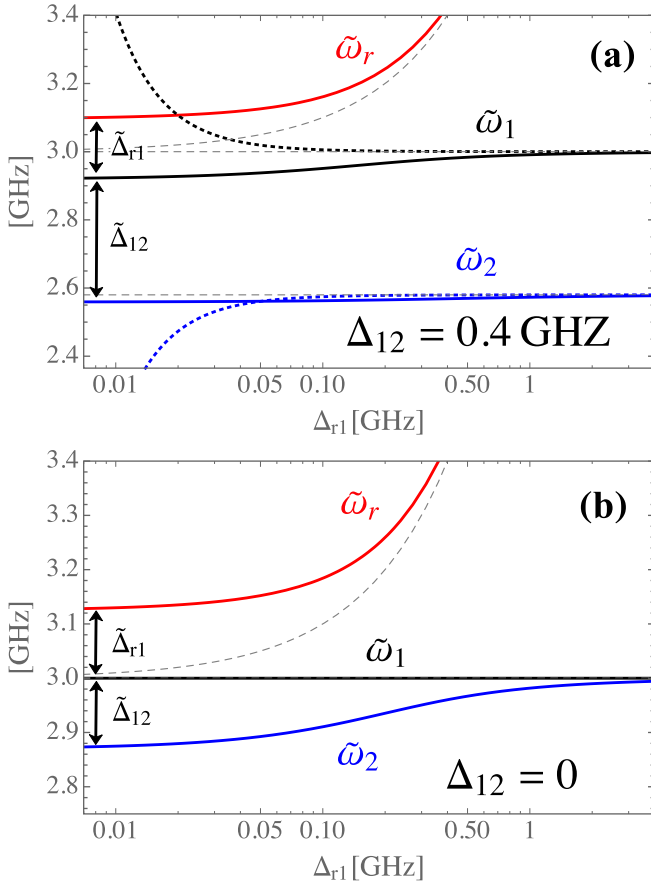


FIG. 3. Perturbative (dotted) and exact (solid) dressed frequencies in the circuit with bare frequencies (dashed) of transmons  $\omega_1 = 3$  GHz,  $\omega_2 = \alpha\omega_1$ , and the resonator  $\omega_r = \omega_1 + \Delta_{r1}$ , couplings  $g \equiv g_{1,2} (=0.1$  GHz) and  $\delta \equiv \delta_{1,2} (=0.1$  GHz). (a)  $\alpha = 0.86$ , and (b) three-body resonance  $\alpha = 1$ .

Before the Discussion, let us comment on evaluating the effective impedances introduced by the black box quantization [23]. They are assumed to be unknown parameters and can be evaluated in iterative feedback between theory and experiment. Our formalism, however, reveals a number of constraints that link between the effective impedances that make the simpler be theoretically estimated. For the simple example of a transmon coupled to a resonator, the effective impedances can be found analytically:  $Z_t^{\text{eff}} = \tilde{\omega}_t(1+s)Z_t/2\omega_t$  and  $Z_r^{\text{eff}} = \tilde{\omega}_r(1-s)Z_t/2\omega_r$ . Their ratio in the dispersive regime is  $Z_r^{\text{eff}}/Z_t^{\text{eff}} \sim (g/\Delta)^2$ , which indicates the characteristic impedance associated with the transmon exceeds that of the resonator.

## V. DISCUSSION

We presented a rigorous method to exactly obtain effective qubit parameters from the Hamiltonian of superconducting circuits consisting of resonators and JJs at arbitrary coupling strengths and frequency detunings. Using this formalism, we exhibited a single transmon and two transmons outside of the dispersive regime in closed-form formulas. For complicated circuits, finding analytical expressions may not be easy, however, our formalism can determine qubit parameters

numerically much easier and more accurately compared to perturbation theory in the charge basis because the  $\mathbf{M}$  matrix (defined in the text) linearly scales with the number of qubits and resonators and all we need is to find its eigenvectors. This simplicity and accuracy will play an essential role for scaling up superconducting circuits as it allows to explore the possibilities of new domains of parameters for elevated fidelities.

## ACKNOWLEDGMENTS

We thank D. DiVincenzo for many useful discussions. Support from Intelligence Advanced Research Projects Activity (IARPA) under Contract No. W911NF-16-0114 is gratefully acknowledged.

## APPENDIX A: UNITARY TRANSFORMATION OF CANONICAL VARIABLES

Consider two  $N$ -dimensional vectors of canonical variables  $\mathbf{q} = (q_1, q_2, \dots, q_N)$  and  $\mathbf{p} = (p_1, p_2, \dots, p_N)$ . These variables satisfy the Poisson bracket relation  $\{q_i, p_j\} = \delta_{ij}$  with  $i, j = 1, 2, \dots, N$  and the definition of  $\{f, g\} = \sum_{i=1}^N (\partial f / \partial q_i)(\partial g / \partial p_i) - (\partial f / \partial p_i)(\partial g / \partial q_i)$ .

Let us consider the following unitary transformations take place on these variables:  $Q_i = \sum_{j=1}^N S_{ij}q_j$  and  $P_i = \sum_{j=1}^N T_{ij}p_j$ . In order to have the two new variables  $\mathbf{Q}$  and  $\mathbf{P}$  be canonical variables, they must satisfy a similar Poisson bracket relation as those of old variables:  $\{Q_i, P_j\} = \delta_{ij}$ . This indicates that  $\{Q_i, P_j\} = \sum_{k=1}^N (\partial Q_i / \partial q_k)(\partial P_j / \partial p_k) - (\partial Q_i / \partial p_k)(\partial P_j / \partial q_k)$ . One can easily simplify these relations into  $\sum_{k=1}^N S_{ik}T_{jk} = \delta_{ij}$ . Because of the unitarity of the transformation matrices  $S$  and  $T$ , one can see that  $\sum_{k=1}^N S_{ik}S_{kj}^\dagger = \delta_{ij}$ . For real matrices, we have  $S_{kj}^\dagger = S_{jk}$ , thus,  $\mathbf{T} = \mathbf{S}$ .

## APPENDIX B: CONSTRAINTS WITHIN THE EXACT FORMULA FOR A TWO-TRANSMON CIRCUIT

Another condition that can be concluded from Eq. (8) of the main article is the following:

$$2\sqrt{\frac{f}{3}} \cos \frac{\cos^{-1}(-\frac{b}{2}(\frac{3}{f})^{3/2}) - 2\pi(k-1)}{3} - \frac{b}{3} \geq 0. \quad (\text{B1})$$

By definition, we have always  $b \leq 0$ , therefore, the condition can be checked in the cases where the cos function is negative, therefore, we need to check the following condition:  $-2\sqrt{f/3} + |b|/3 \geq 0$ , which can be further simplified to  $b^2/3 > c$ . Substituting the definitions will introduce the following condition to hold:

$$\omega_1^4 + \omega_2^4 + \omega_3^4 \geq \omega_1^2\omega_2^2 + \omega_1^2\omega_3^2 + \omega_2^2\omega_3^2 - 4g_1^2\omega_1\omega_2 - 4g_2^2\omega_2\omega_3.$$

We take the first three terms from the right side to the left, then simplify the left side to arrive at the following condition:

$$(\omega_1^2 - \omega_2^2)^2 + (\omega_2^2 - \omega_3^2)^2 + (\omega_3^2 - \omega_1^2)^2 \geq -4g_1^2\omega_1\omega_2 - 4g_2^2\omega_2\omega_3,$$

which trivially holds valid without imposing any limitations on parameters.

### APPENDIX C: UNITARY TRANSFORMATION FOR TWO TRANSMONS COUPLED TO A RESONATOR

The unitary transformation to the diagonal basis in the harmonic sector is carried out by the matrix of normalized eigenstates with columns being eigenvectors, which is

$$S = \begin{bmatrix} \frac{V_1 \gamma_{12}}{N_1} & \frac{V_1 \gamma_{22}}{N_2} & \frac{V_1 \gamma_{32}}{N_3} \\ \frac{V_2 \gamma_{11}}{N_1} & \frac{V_2 \gamma_{21}}{N_2} & \frac{V_2 \gamma_{31}}{N_3} \\ \frac{\gamma_{11} \gamma_{12}}{N_1} & \frac{\gamma_{21} \gamma_{22}}{N_2} & \frac{\gamma_{31} \gamma_{32}}{N_3} \end{bmatrix}, \quad (C1)$$

with  $V_i \equiv g_i \sqrt{4\omega_r \omega_i}$ ,  $\gamma_{ij} = \bar{\omega}_i^2 - \omega_j^2$ , and  $N_i = \sqrt{V_2^2 \gamma_{i1}^2 + V_1^2 \gamma_{i2}^2 + \gamma_{i1}^2 \gamma_{i2}^2}$ .

### APPENDIX D: ADDITIONAL INTERACTION TERMS

In the circuit made of two transmons coupled to a shared resonator, the anharmonic part of the Hamiltonian can be simplified to Eq. (9) in the main article. Below are detailed interaction couplings in terms of bare parameters,

$$\begin{aligned} \mathcal{J}_{ik} &= \sum_{j=1,2} \delta_j \left[ \frac{1}{3} U_{ji}^3 U_{jk} + U_{jk}^3 U_{ji} + \frac{2}{3} \frac{(U_{ji} U_{jk} U_{j3})^2}{U_{j1} U_{j2}} \right], \\ \mathcal{K}_{ik} &= \sum_{j=1,2} \delta_j U_{ji}^3 U_{jk}, \quad \mathcal{S}_{ikl} = \frac{4}{3} \sum_{j=1,2} \delta_j \frac{(U_{ji} U_{jk} U_{j3})^2}{U_{ji} U_{jk}}. \end{aligned} \quad (D1)$$

### APPENDIX E: BLOCK DIAGONALIZATION

Let us consider the Hamiltonians of two harmonic oscillators (labeled 1 and 2) coupled to a resonator (labeled 3),

$$\begin{aligned} H &= H_0 + \epsilon H_{\text{int}}, \quad H_0 \equiv \sum_{i=1-3} \omega_i \hat{\alpha}_i^\dagger \hat{\alpha}_i, \\ H_{\text{int}} &\equiv \sum_{k=1,2} g_k (\hat{\alpha}_3 \hat{\alpha}_k^\dagger + \hat{\alpha}_3^\dagger \hat{\alpha}_k). \end{aligned}$$

The unperturbed part  $H_0$  in the eigenbasis of itself is diagonal, however,  $H_{\text{int}}$  is not. In general, we may not be able to find a transformation to a fully diagonal matrix, but instead, we can separate out a subset of states from the rest of the states. The Schrieffer-Wolff transformation is one way to block diagonalize the interacting Hamiltonian into low-energy and high-energy sectors (see Ref. [39]). This usually takes place by transforming the Hamiltonian by the anti-Hermitian operator  $\exp S$  in the following way:  $H_{BD} = \exp(-S) H \exp S$ , which can be expanded into  $H_{BD} = \sum_{n=0} [H, S]_n / n!$  with  $[H, S]_{n+1} = [[H, S]_n, S]$  and  $[H, S]_0 = H$ . One can, in principle, assume a geometric series expansion of the transformation matrix:  $S = \sum_{i=0} (\epsilon)^i S_i$ ; however, given that the zeroth order or order of  $H_{BD}$  is  $H_{BD_0} = [H_0, S_0] = H_0$ , therefore,  $S_0$  must be diagonal too, which is, in fact, inconsistent with the definition of  $S$  to be anti-Hermitian and block off diagonal (bod), therefore, always  $S_0 = 0$ . In the first order, the Hamiltonian is already given by  $H_{\text{int}}$  which can be made of block-diagonal (bd) and bod matrices  $H_{\text{int}} = H_{\text{int}}^{\text{bd}} + H_{\text{int}}^{\text{bod}}$ .

Therefore,  $H_{BD_1} = [H_0, S_1] = -H_{\text{int}}^{\text{bod}}$ . In the second order,  $H_{BD_2} = [H_0, S_2] + [H_{\text{int}}, S_1] + (1/2)[[H_0, S_1], S_1]$ , and so on. Putting all together, one can find the effective Hamiltonian up to the second-order  $H_{BD} = H_0 + H_{\text{int}}^{\text{bd}} + (1/2)[H_{\text{int}}^{\text{bod}}, S_1]$ .

Using the relations above for the Hamiltonian of Eq. (E1) in which the interaction is block off diagonal, one can use the following ansatz:

$$S_1 = - \sum_{k=1,2} g_k (\hat{\alpha}_3 \hat{\alpha}'_k^\dagger - \hat{\alpha}_3^\dagger \hat{\alpha}'_k), \quad (E1)$$

with  $\hat{\alpha}'_k \equiv \sum_{n=0}^{\infty} \sqrt{n+1} (\omega_3 - \omega_k)^{-1} |n\rangle \langle n+1|$  being the modified ladder operator for the  $k$ th transmon, given that the normal ladder operator for the same transmon is  $\hat{\alpha}_k \equiv \sum_{n=0}^{\infty} \sqrt{n+1} |n\rangle \langle n+1|$ .

One can explicitly determine the effective Hamiltonian up to the second order of perturbation theory becoming

$$H_{BD} = H_0 - \sum_{i,j=1,2; (i \neq j)} \frac{g_i g_j}{2} (\hat{\alpha}_i \hat{\alpha}'_j^\dagger + \hat{\alpha}_i^\dagger \hat{\alpha}'_j). \quad (E2)$$

### APPENDIX F: RESONANT TRANSMONS

In a circuit with two transmons in resonance  $\omega_1 = \omega_2 \equiv \omega$  and homogeneous coupling and anharmonicity  $g_1 = g_2 \equiv g$  and  $\delta_1 = \delta_2 \equiv \delta$ , the harmonic Hamiltonian is  $H_{\text{har.}} = \frac{1}{2} \omega^2 (Q_1^2 + Q_2^2) + \frac{1}{2} \omega_r^2 Q_r^2 + \frac{1}{2} (X_1^2 + X_2^2 + X_r^2) + g \sqrt{4\omega\omega_r} (Q_1 + Q_2) Q_3$ . Defining the vectors  $\mathbf{Q} = (Q_1, Q_2, Q_r)^T$  and  $\mathbf{P} = (P_1, P_2, P_r)^T$ , this Hamiltonian can be rewritten as  $H_{\text{har.}} = \frac{1}{2} \mathbf{Q}^T \mathbf{M} \mathbf{Q} + \frac{1}{2} \mathbf{X}^T \mathbf{X}$  with matrix  $\mathbf{M}$  being

$$\mathbf{M} = \begin{bmatrix} \omega^2 & 0 & V \\ 0 & \omega^2 & V \\ V & V & \omega_r^2 \end{bmatrix}, \quad (F1)$$

with  $V \equiv g \sqrt{4\omega\omega_r}$ . Because the off-diagonal elements are identical, it is easy to find the eigenvalues, which are

$$\omega, \quad \sqrt{\frac{\omega^2 + \omega_r^2 \pm \sqrt{(\omega^2 - \omega_r^2)^2 + 8V^2}}{2}}.$$

At the extreme resonance with  $\omega_r = \omega$ , the eigenenergies will become

$$\omega, \quad \omega \sqrt{1 \pm \frac{2\sqrt{2}g}{\omega}}.$$

In the limit of small coupling  $g \ll \omega$ , this can be simplified to

$$\omega, \quad \omega \pm \sqrt{2}g.$$

### APPENDIX G: ANHARMONICITY

Consider the following Bogoliubov transformations for the transmon ladder operator:

$$\hat{a}_n = \sum_m A_{nm} \hat{\alpha}_m + B_{nm} \hat{\alpha}_m^\dagger, \quad (G1)$$

and using the relation between transmon charge number and phase and the ladder operator  $\hat{a}_n = \sqrt{\frac{\omega_n}{2}} \hat{q}_n + i \sqrt{\frac{1}{2\omega_n}} \hat{p}_n$  and its

conjugate as well as similarly in the transformed basis  $\hat{\alpha}_n = \sqrt{\frac{\omega_n}{2}} \hat{Q}_n + i\sqrt{\frac{1}{2\omega_n}} \hat{P}_n$ , one can find

$$A_{nm} = \left( \sqrt{\frac{\omega_n}{8\tilde{\omega}_m}} + \sqrt{\frac{\tilde{\omega}_m}{8\omega_n}} \right) S_{nm},$$

$$B_{nm} = \left( \sqrt{\frac{\omega_n}{8\tilde{\omega}_m}} - \sqrt{\frac{\tilde{\omega}_m}{8\omega_n}} \right) S_{nm},$$

in which  $\tilde{\omega}$  is the frequency in the transformed basis.

The anharmonicity in the Hamiltonian will be  $-\frac{\delta_i}{12}(a_i - a_i^\dagger)^4$ . The operator part can be Bogoliubov transformed to the new basis, keeping terms with as many creations as annihilations, ignoring frequencies,

$$\begin{aligned} (a_n - a_n^\dagger)^4 = & 6 \sum_{m=1}^3 (A_{nm} - B_{nm})^4 [(\hat{\alpha}_m^\dagger \hat{\alpha}_m)^2 + \hat{\alpha}_m^\dagger \hat{\alpha}_m] \\ & + 6 \sum_{m < k} (A_{nm} - B_{nm})^2 (A_{nk} - B_{nk})^2 [\hat{\alpha}_m^2 \hat{\alpha}_k^{\dagger 2} \\ & + \hat{\alpha}_m^{\dagger 2} \hat{\alpha}_k^2 + 4\hat{\alpha}_m^\dagger \hat{\alpha}_m \hat{\alpha}_k^\dagger \hat{\alpha}_k + 2\hat{\alpha}_m^\dagger \hat{\alpha}_m + 2\hat{\alpha}_k^\dagger \hat{\alpha}_k] \\ & + 4 \sum_{m \neq k} (A_{nm} - B_{nm})^3 (A_{nk} - B_{nk}) (\hat{\alpha}_m^2 \hat{\alpha}_m^\dagger \hat{\alpha}_k^\dagger \\ & + \hat{\alpha}_m^{\dagger 2} \hat{\alpha}_m \hat{\alpha}_k + 2\hat{\alpha}_m^\dagger \hat{\alpha}_m \hat{\alpha}_m \hat{\alpha}_k^\dagger \\ & + 2\hat{\alpha}_m^\dagger \hat{\alpha}_m \hat{\alpha}_m^\dagger \hat{\alpha}_k + \hat{\alpha}_m^\dagger \hat{\alpha}_k^\dagger + \hat{\alpha}_m^\dagger \hat{\alpha}_k) \\ & + 8 \sum_{m \neq k \neq l} (A_{nm} - B_{nm})^2 (A_{nk} - B_{nk}) (A_{nl} - B_{nl}) \\ & \times (\hat{\alpha}_m^2 \hat{\alpha}_l^\dagger \hat{\alpha}_k^\dagger + \hat{\alpha}_m^{\dagger 2} \hat{\alpha}_l \hat{\alpha}_k + 2\hat{\alpha}_m^\dagger \hat{\alpha}_m \hat{\alpha}_l \hat{\alpha}_k^\dagger \\ & + 2\hat{\alpha}_m^\dagger \hat{\alpha}_m \hat{\alpha}_l^\dagger \hat{\alpha}_k + \hat{\alpha}_l \hat{\alpha}_k^\dagger + \hat{\alpha}_l^\dagger \hat{\alpha}_k). \end{aligned}$$

## APPENDIX H: BOGOLIUBOV TRANSFORMATION FOR HAMILTONIAN DIAGONALIZATION

In this Appendix, we use the quantum Hamiltonian of a transmon coupled to a resonator  $H = 4E_C n - E_J \cos \phi + H_{\text{res}}$ . Separating the harmonic sector and the anharmonic sector and using Bogoliubov transformation, we diagonalize the interacting harmonic sector into a diagonal quantum harmonic Hamiltonian. We find all Bogoliubov transformation coefficients, which turns out to be similar to the results we took from semiclassical analysis.

Given that the charge number operator is proportional to ladder operators  $n \sim 2^{-(1/4)}(a + a^\dagger)$ , the phase is the conjugate variable  $\phi \sim 2^{1/4}(a - a^\dagger)$ , and the resonator Hamiltonian is  $H_{\text{res}} = \omega_r b^\dagger b$ ; the circuit Hamiltonian can be written as

$H = \omega_q a^\dagger a - \frac{\delta}{12}(a - a^\dagger)^4 + \omega_r b^\dagger b + g(a + a^\dagger)(b + b^\dagger)$  with harmonic part being  $H_{\text{har}} = \omega_q a^\dagger a + \omega_r b^\dagger b + g(a + a^\dagger)(b + b^\dagger)$ .

We would like to Bogoliubov transform the Hamiltonian into a diagonal Hamiltonian  $\mathcal{H}$ ,

$$\mathcal{H} = \tilde{\omega}_q \alpha^\dagger \alpha + \tilde{\omega}_r \beta^\dagger \beta - \frac{1}{12}[\chi_q^{1/4}(\alpha - \alpha^\dagger) + \chi_r^{1/4}(\beta - \beta^\dagger)]^4.$$

We use a technique widely used in second quantized quantum field theory, which is to Bogoliubov transform creation and annihilation operators,

$$\hat{a} = A\hat{\alpha} + B\hat{\beta} + C\alpha^\dagger + D\beta^\dagger,$$

$$\hat{b} = E\hat{\alpha} + F\hat{\beta} + G\alpha^\dagger + H\beta^\dagger.$$

Eight equations are needed to determine coefficients; four by enforcing that the transformed Hamiltonian preserves eigenvalues, which is equivalent to equating  $H_{ho}$  and  $\mathcal{H}_{ho}$  and setting coefficients of  $\hat{\alpha}\hat{\alpha}$ ,  $\hat{\beta}\hat{\beta}$ ,  $\hat{\alpha}\hat{\beta}$ , and  $\hat{\alpha}\hat{\beta}^\dagger$  to zero, respectively,

$$\omega_q AC^* + \omega_r EG^* + g(A + C^*)(E + G^*) = 0, \quad (\text{H1})$$

$$\omega_q BD^* + \omega_r FH^* + g(B + D^*)(F + H^*) = 0, \quad (\text{H2})$$

$$\omega_q (BC^* + AD^*) + \omega_r (FG^* + EH^*) + g[(A + C^*) \times (F + H^*) + (B + D^*)(E + G^*)] = 0, \quad (\text{H3})$$

$$\omega_q (DC^* + AB^*) + \omega_r (HG^* + EF^*) + g[(A + C^*) \times (F + H^*) + (B + D^*)(E + G^*)] = 0. \quad (\text{H4})$$

The other four are determined by enforcing commutation relations, i.e.,  $[a, a^\dagger] = [b, b^\dagger] = 1$  and  $[a, b] = [a, b^\dagger] = 0$ , respectively, given that  $[\alpha, \alpha^\dagger] = [\beta, \beta^\dagger] = 1$  and zero otherwise,

$$|A|^2 + |B|^2 - |C|^2 - |D|^2 = 1, \quad (\text{H5})$$

$$|E|^2 + |F|^2 - |G|^2 - |H|^2 = 1, \quad (\text{H6})$$

$$AG + BH - CE - DF = 0, \quad (\text{H7})$$

$$AE^* + BF^* - CG^* - DH^* = 0. \quad (\text{H8})$$

For simplicity, we assume coefficients are real valued, but the equations are difficult to be analytically solved. A practical simplification can be achieved by defining new variables,

$$A_\pm \equiv A \pm C, \quad B_\pm \equiv B \pm D,$$

$$E_\pm \equiv E \pm G, \quad F_\pm \equiv F \pm H,$$

which reformulates the equations given above to the following:

$$\begin{aligned} \omega_q(A_+^2 - A_-^2) + \omega_r(E_+^2 - E_-^2) + 4gE_+A_+ &= 0, \\ \omega_q(B_+^2 - B_-^2) + \omega_r(F_+^2 - F_-^2) + 4gF_+B_+ &= 0, \\ \omega_q(A_+B_+ - A_-B_-) + \omega_r(E_+F_+ - E_-F_-) + 2g(A_+F_+ + B_+E_+) &= 0, \\ \omega_qA_-B_- + \omega_rE_-F_- = 0, \quad A_-A_+ + B_+B_- = 1, \quad E_-E_+ + F_+F_- = 1, \\ A_-E_+ + B_-F_+ = 0, \quad A_+E_- + B_+F_- = 0. \end{aligned}$$

Given that one may solve the Bogoliubov coefficient equations, we can determine new frequencies in  $\mathcal{H}$ ,

$$\begin{aligned}\bar{\omega}_r &= \frac{\omega_q}{2}(B_+^2 + B_-^2) + \frac{\omega_r}{2}(F_+^2 + F_-^2) + 2gB_+F_+, \\ \bar{\omega}_q &= \frac{\omega_q}{2}(A_+^2 + A_-^2) + \frac{\omega_r}{2}(E_+^2 + E_-^2) + 2gA_+E_+.\end{aligned}$$

One can easily prove that  $F_+F_- = A_+A_-$ , which simplifies equations and helps to find the following two important equalities:

$$E_+^2 = \frac{\omega_r A_+(1 - A_-A_+)}{\omega_q A_-}, \quad E_-^2 = \frac{\omega_q A_-(1 - A_-A_+)}{\omega_r A_+}. \quad (\text{H9})$$

Substituting them in Eq. (H10), we find one equation between  $A_\pm$ ,

$$\begin{aligned}& [\omega_q^2 A_-(A_+^3 - A_-) + \omega_r^2 A_+^2(1 - A_+A_-)]^2 \\ & - 16\omega_r\omega_q g^2 A_+^5 A_-(1 - A_-A_+) = 0.\end{aligned} \quad (\text{H10})$$

This is one of the main equations we need to solve. Another one can be determined taking some nontrivial steps listed below: We use Eq. (H10), substitute  $B_\pm$  from the unnumbered equation in the sentence beginning with ‘‘Given that one...’’, multiply two sides in  $E_+F_-^2F_+$ , and simplify it, and magically the final equation is again a second equation that relation  $A_\pm$ ,

$$(1 - A_-A_+)A_+A_- \left( \frac{\omega_r^2}{2\omega_q} - \frac{\omega_q}{2} \right)^2 - (2A_-A_+ - 1)^2 = 0. \quad (\text{H11})$$

Now, we solve these two equations together. To do so, we first define  $x = A_+A_-$  and substitute in Eq. (H11)  $a(1-x)x - (2x-1)^2 = 0$  with  $a \equiv \frac{\Delta^2 \Sigma^2}{4g^2 \omega_r \omega_q}$ ,  $\Sigma = \omega_r + \omega_q$ , and  $\Delta = \omega_r - \omega_q$ . The exact real-valued solution is

$$A_-A_+ = \frac{1}{2} + \frac{1}{2}s, \quad s^{-1} \equiv \sqrt{1 + \frac{16g^2 \omega_r \omega_q}{\Delta^2 \Sigma^2}},$$

and substituting in Eq. (H10) determines exact real-valued  $A_\pm$ ,

$$\begin{aligned}A_- &= 2^{-(3/4)} \omega_q^{-(1/2)} \sqrt{1+s} (\omega_q^2 + \omega_r^2 - \Delta \Sigma s^{-1})^{1/4}, \\ A_+ &= 2^{-(1/4)} \omega_q^{1/2} \sqrt{1+s} (\omega_q^2 + \omega_r^2 - \Delta \Sigma s^{-1})^{-(1/4)}, \\ E_- &= -2^{-(3/4)} \omega_r^{-(1/2)} \sqrt{1-s} (\omega_q^2 + \omega_r^2 - \Delta \Sigma s^{-1})^{1/4}, \\ E_+ &= -2^{-(1/4)} \omega_r^{1/2} \sqrt{1-s} (\omega_q^2 + \omega_r^2 - \Delta \Sigma s^{-1})^{-(1/4)}, \\ F_- &= 2^{-(3/4)} \omega_r^{-(1/2)} \sqrt{1+s} (\omega_q^2 + \omega_r^2 + \Delta \Sigma s^{-1})^{1/4}, \\ F_+ &= 2^{-(1/4)} \omega_r^{1/2} \sqrt{1+s} (\omega_q^2 + \omega_r^2 + \Delta \Sigma s^{-1})^{-(1/4)}, \\ B_- &= 2^{-(3/4)} \omega_q^{-(1/2)} \sqrt{1-s} (\omega_q^2 + \omega_r^2 + \Delta \Sigma s^{-1})^{1/4}, \\ B_+ &= 2^{-(1/4)} \omega_q^{1/2} \sqrt{1-s} (\omega_q^2 + \omega_r^2 + \Delta \Sigma s^{-1})^{-(1/4)}.\end{aligned}$$

In order to find  $F_\pm$ , yet we need to simplify Eq. (H10) by multiplying on both sides of  $F_-F_+$  and rewriting  $B_\pm$  in terms

of  $A_\pm$ ,  $E_\pm$ , and  $F_\pm$  as Eq. (H9)

$$\left( \frac{F_-}{F_+} \right)^2 = \frac{1}{2} \frac{\omega_q^2 + \omega_r^2 + \Delta \Sigma s^{-1}}{\omega_r^2}.$$

Defining

$$K_\pm \equiv 2^{-(1/4)} (\omega_q^2 + \omega_r^2 \pm \Delta \Sigma s^{-1})^{1/4},$$

then,

$$\begin{aligned}A &= \frac{\sqrt{1+s}}{2^{3/2}} \left( \frac{\sqrt{\omega_q}}{K_-} + \frac{K_-}{\sqrt{\omega_q}} \right), \\ B &= \frac{\sqrt{1-s}}{2^{3/2}} \left( \frac{\sqrt{\omega_q}}{K_+} + \frac{K_+}{\sqrt{\omega_q}} \right), \\ C &= \frac{\sqrt{1+s}}{2^{3/2}} \left( \frac{\sqrt{\omega_q}}{K_-} - \frac{K_-}{\sqrt{\omega_q}} \right), \\ D &= \frac{\sqrt{1-s}}{2^{3/2}} \left( \frac{\sqrt{\omega_q}}{K_+} - \frac{K_+}{\sqrt{\omega_q}} \right), \\ E &= \frac{-\sqrt{1-s}}{2^{3/2}} \left( \frac{\sqrt{\omega_r}}{K_-} + \frac{K_-}{\sqrt{\omega_r}} \right), \\ F &= \frac{\sqrt{1+s}}{2^{3/2}} \left( \frac{\sqrt{\omega_r}}{K_+} + \frac{K_+}{\sqrt{\omega_r}} \right), \\ G &= \frac{-\sqrt{1-s}}{2^{3/2}} \left( \frac{\sqrt{\omega_r}}{K_-} - \frac{K_-}{\sqrt{\omega_r}} \right), \\ H &= \frac{\sqrt{1+s}}{2^{3/2}} \left( \frac{\sqrt{\omega_r}}{K_+} - \frac{K_+}{\sqrt{\omega_r}} \right).\end{aligned}$$

We can expand the functions in terms of small coupling  $g$  to any order. Below are results up to the fourth order:

Substituting in the definition of new frequencies, one finds

$$\begin{aligned}\bar{\omega}_r &= (2s)^{-(1/2)} \sqrt{(\omega_q^2 + \omega_r^2)s + \Delta \Sigma}, \\ \bar{\omega}_q &= (2s)^{-(1/2)} \sqrt{(\omega_q^2 + \omega_r^2)s - \Delta \Sigma}.\end{aligned}$$

In the weak interaction limit, these frequencies turn into Lamb and Stark shifts. Below we evaluate them up to fourth order,

$$\begin{aligned}\bar{\omega}_r &= \omega_r + \frac{2\omega_q g^2}{\Delta \Sigma} - \frac{2g^4 \omega_q^2 (5\omega_r^2 - \omega_q^2)}{\omega_r \Delta^3 \Sigma^3} + O(g^5), \\ \bar{\omega}_q &= \omega_q - \frac{2g^2 \omega_r}{\Delta \Sigma} - \frac{2g^4 \omega_r^2 (\omega_r^2 - 5\omega_q^2)}{\omega_q \Delta^3 \Sigma^3} + O(g^5).\end{aligned}$$

Anharmonicity can be easily derived using the following relation:

$$\begin{aligned}(a - a^\dagger)^4 &= 6(A - C)^4 [(\alpha^\dagger \alpha)^2 + \alpha^\dagger \alpha], \\ &+ 6(B - D)^4 [(\beta^\dagger \beta)^2 + \beta^\dagger \beta] \\ &+ 12(A - C)^2 (B - D)^2 (2\alpha^\dagger \alpha \beta^\dagger \beta + \alpha^\dagger \alpha + \beta^\dagger \beta).\end{aligned}$$



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