Hamiltonian for coupled flux qubits

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An effective Hamiltonian is derived for two coupled three-Josephson-junction (3JJ) qubits. This is not quite trivial, for the customary "free" 3JJ Hamiltonian is written in the limit of zero inductance L. Neglecting the self-flux is already dubious for one qubit when it comes to readout, and becomes untenable when discussing inductive coupling. First, inductance effects are analyzed for a single qubit. For small L, the self-flux is a "fast variable," which can be eliminated adiabatically. However, the commonly used junction phases are *not* appropriate "slow variables," and instead one introduces degrees of freedom that are decoupled from the loop current to leading order. In the quantum case, the zero-point fluctuations (LC oscillations) in the loop current diverge as $L\to 0$. While their effect thus formally dominates over the classical self-flux, it merely renormalizes the Josephson couplings of the effective (two-phase) theory. In the coupled case, the strong zero-point fluctuations render the full (six-phase) wave function significantly entangled in leading order. However, in going to the four-phase theory, this uncontrollable entanglement is integrated out completely, leaving a computationally usable mutual-inductance term of the expected form as the effective interaction.

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I. INTRODUCTION

A commonly considered flux qubit consists of a superconducting loop with three Josephson junctions—a 3JJ qubit.[1] One readily writes down its Hamiltonian,[2]

$$H=\sum_{i=1}^{3}\left[\frac{Q_i^2}{2C_i}-E_i\cos\phi_i\right]+\frac{(\phi_1+\phi_2+\phi_3-\phi_x)^2}{8e^2L}, \quad (1.1)$$

in units with $\hbar=1$, and with the external flux bias Φ_x given in phase units,

$$\phi_x=2e\Phi_x. \quad (1.2)$$

As long as one neglects gate capacitors, etc., the C_i are simply the junction capacitances: for finite inductance L, the redistribution of charges following a tunneling event, often accounted for by an effective capacitance matrix, is not instantaneous (i.e., all three junction charges and phases are independent dynamical variables).[3]

The essence of the 3JJ design is to introduce bistability without relying on magnetic energy so that the superconducting quantum interference device (SQUID) loop can be kept small. For $L\to 0$, the last term in Eq. (1.1) implements the constraint $\phi_3=\phi_x-\phi_1-\phi_2$. This leads to an effective two-phase theory,

$$H_{3JJ}=\tfrac{1}{2}\vec{Q}^{\mathrm{T}}\mathsf{C}^{-1}\vec{Q}-E_1\cos\phi_1-E_2\cos\phi_2 - E_3\cos(\phi_x-\phi_1-\phi_2), \quad (1.3)$$

$$\mathsf{C}=\begin{pmatrix}C_1+C_3 & C_3\\ C_3 & C_2+C_3\end{pmatrix}, \quad (1.4)$$

with $\vec{Q}=(Q_1,Q_2)^{\mathrm{T}}$ [cf. Eq. (4) in Ref. 1, bearing in mind that ϕ_1 and ϕ_2 have the opposite relative sign there].

When scaling to circuits with more than one qubit, the question arises how to generalize the effective Hamiltonian (1.3). Unfortunately, repeating the above reduction merely yields uncoupled 3JJ Hamiltonians. Clearly, by neglecting self-inductances entirely one has missed the effect of mutual inductance (which can never be larger), responsible for qubit-qubit interaction and ultimately entanglement. This can be turned into an advantage: most of the analysis can be done by studying *one* qubit to higher order in L than usual, after which two qubits require only a straightforward generalization.

This is taken up in Sec. II on the level of classical Kirchhoff (circuit) equations. Section III is devoted to the quantum case. Rather than merely confirming the classical result or resolving operator-ordering ambiguities, one finds an additional physical effect: zero-point fluctuations in the loop current wash out (renormalize) the effective Josephson couplings. The results are verified numerically and critically compared to a previous attempt.[4] Section IV contains the generalization to two qubits; it is seen that the four-phase wave function is entangled only in considerably higher order in the inductance than the six-phase one. This integrating out of uncontrollable entanglement may indicate that the effective theory is not merely computationally convenient, but also physically appropriate. Some concluding remarks are made in Sec. V.

For small L, self-fluxes vanish but persistent currents remain finite, so that the latter are often more convenient. When studying dynamics, etc., one needs the current *operator* (as opposed to, say, the ground-state expectation[5]), which is not readily available in the growing literature on the 3JJ qubit. Preliminary to the L expansion proper, it will now be derived quantum-mechanically in both the three- and two-phase theories, which has some independent interest. In fact, one merely needs to add the capacitive and Josephson contributions. In the three-phase theory, one has[6]

$$I_i=-I_{ci}\sin\phi_i-\dot{Q}_i, \quad (1.5)$$

with $I_{ci}\equiv 2eE_i$ and

$$Q_i = \frac{2e}{\mathrm{i}}\frac{\partial}{\partial \phi_i}. \tag{1.6}$$

Then, from Eq. (1.1),

$$\dot{Q}_i = [H, \mathrm{i}Q_i] = \frac{\phi_\mathrm{x} - \sum_j \phi_j}{2eL} - I_{ci}\sin\phi_i \quad \Rightarrow \tag{1.7}$$

$$I_i = \frac{\sum_j \phi_j - \phi_\mathrm{x}}{2eL}. \tag{1.8}$$

That is, $I_i = I$ independent of i as expected; contrast, e.g., arbitrarily picking the Josephson current through one of the junctions.

For $L \to 0$, Eq. (1.8) tends to $\frac{0}{0}$ and a separate derivation from Eq. (1.3) is needed. In this case, however, the canonical variable Q_1 is not simply the charge on capacitor 1 (indeed, two Q's have to account for three C's); to find the latter, we set $\mathsf{C}^{-1} = \left(\begin{smallmatrix} p & r \\ r & q \end{smallmatrix}\right)$ and evaluate

$$\dot{\phi}_1 = \mathrm{i}\left[\tfrac{1}{2}pQ_1^2 + rQ_1Q_2, \phi_1\right] = 2e(pQ_1 + rQ_2). \tag{1.9}$$

Hence,

$$\begin{aligned} I_1^{(0)} &= -\frac{C_1}{2e}\ddot{\phi}_1 - I_{c1}\sin\phi_1 \\ &= (C_1 p - 1)I_{c1}\sin\phi_1 + C_1 r I_{c2}\sin\phi_2 \\ &\quad - C_1(p+r)I_{c3}\sin(\phi_\mathrm{x} - \phi_1 - \phi_2) \\ &= -C\left[\frac{I_{c1}}{C_1}\sin\phi_1 + \frac{I_{c2}}{C_2}\sin\phi_2 + \frac{I_{c3}}{C_3}\sin(\phi_\mathrm{x} - \phi_1 - \phi_2)\right], \end{aligned} \tag{1.10}$$

an appealing and manifestly symmetric form $I_1^{(0)} = I^{(0)}$, involving the loop's series capacitance $C^{-1} = C_1^{-1} + C_2^{-1} + C_3^{-1}$. Interestingly, the junction area κ_i cancels from Eq. (1.10): if, as is often assumed, $I_{ci} \propto C_i \propto \kappa_i$ (with material-dependent constants of proportionality), then the three sines have equal prefactors.

II. CLASSICAL ANALYSIS

The Hamilton equations

$$\dot{\phi}_i = 2e\frac{\partial H}{\partial Q_i}, \quad \dot{Q}_i = -2e\frac{\partial H}{\partial \phi_i} \tag{2.1}$$

yield the classical dynamics of the system (1.1).[7] The last term in H represents a steep and narrow well, so one expects

$$\phi \equiv \phi_1 + \phi_2 + \phi_3 - \phi_\mathrm{x} \tag{2.2}$$

to be small and rapidly oscillating, while the other variables can have excursions of order one but move comparatively slowly—ideal for adiabatic elimination of ϕ. However, from Eq. (2.1) one finds, e.g., $C_1\ddot{\phi}_1 = -\phi/L - 2eI_{c1}\sin\phi_1$, so that determination of the ϕ_1 dynamics to $\mathcal{O}(L)$ apparently involves the ϕ dynamics to $\mathcal{O}(L^2)$, rendering the L expansion quite tedious.

To see what went wrong, consider the rough analogy of a two-dimensional electron gas, where excursions away from the x-y plane carry a large penalty in energy. It is intuitively clear that the fast oscillations in the corresponding potential well occur predominantly in the z direction, orthogonal to the easy plane. While the latter plane is uniquely defined by the potential, in our case "orthogonal" involves the anisotropic capacitance matrix as well (which thus can be said to induce a metric). It is not difficult to scale the phases such that the charging term is $\propto \vec{Q}^\mathrm{T}\vec{Q}$ (in terms of a *three*-vector $\vec{Q}$; in the quantum case, this yields a charging term $\propto -\nabla^2$), upon which the proper coordinates are found by rotation. However, full orthonormalization turns out to be overkill, and the resulting tedious formulas are hard to interpret; crucial is only that the slow coordinates χ, θ are constant along the fast *direction* $(\phi_1, \phi_2, \phi_3) = (C_1^{-1}, C_2^{-1}, C_3^{-1})$. This is readily achieved; the easiest seems[8]

$$\begin{pmatrix} \chi \\ \theta \\ \phi + \phi_\mathrm{x} \end{pmatrix} = \begin{pmatrix} 1 & 0 & -C_3/C_1 \\ 0 & 1 & -C_3/C_2 \\ 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} \quad \Rightarrow \tag{2.3}$$

$$\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{pmatrix} = C\begin{pmatrix} C_2^{-1} + C_3^{-1} & -C_1^{-1} & C_1^{-1} \\ -C_2^{-1} & C_1^{-1} + C_3^{-1} & C_2^{-1} \\ -C_3^{-1} & -C_3^{-1} & C_3^{-1} \end{pmatrix}\begin{pmatrix} \chi \\ \theta \\ \phi + \phi_\mathrm{x} \end{pmatrix}. \tag{2.4}$$

The Kirchhoff equations become

$$\frac{C_1\ddot{\chi}}{2e} = I_{c3}\sin\phi_3 - I_{c1}\sin\phi_1, \tag{2.5}$$

$$\frac{C_2\ddot{\theta}}{2e} = I_{c3}\sin\phi_3 - I_{c2}\sin\phi_2, \tag{2.6}$$

$$\frac{1}{2e}\left(\ddot{\phi} + \frac{\phi}{LC}\right) = -\frac{I_{c1}}{C_1}\sin\phi_1 - \frac{I_{c2}}{C_2}\sin\phi_2 - \frac{I_{c3}}{C_3}\sin\phi_3, \tag{2.7}$$

where the ϕ_i's on the right-hand side are simply shorthand for the linear combinations in Eq. (2.4). Indeed, the terms $\sim L^{-1}$ have canceled in Eqs. (2.5) and (2.6). For an interpretation, note that $\ddot{\chi} \propto C_1\dot{Q}_1 - C_3\dot{Q}_3$ describes the charging of the *island* between junctions 1 and 3; unlike the charging of, e.g., *capacitor* 1, $\ddot{\chi}$ thus has no net direct contribution from the loop current, and is affected by it only indirectly [in $\mathcal{O}(L)$] through the flux-quantization condition.

In these variables, the L expansion to the required order is almost trivial. In $\mathcal{O}(L^0)$, one simply sets $\phi = 0$ in Eqs. (2.5) and (2.6), which is readily verified to yield dynamics equivalent to Eq. (1.3). In $\mathcal{O}(L)$, ϕ can be neglected on the right-hand side of Eq. (2.7) because it does not occur with a large coefficient. The leading adiabatic solution is then

$$\phi = 2eLI^{(0)}(\chi, \theta), \tag{2.8}$$

or explicitly $I^{(0)}(\chi, \theta, \phi = 0)$ in Eq. (1.10). Subsequently, Eq. (2.8) can be substituted into the right-hand sides of

Eqs. (2.5) and (2.6), yielding a self-contained dynamical system with two degrees of freedom.

In preparation for the quantum analysis, it is instructive to also consider a canonical formulation. The Lagrangian reads

$$\mathcal{L}(\chi,\theta,\phi)=\sum_{i=1}^{3}\frac{C_i\dot{\phi}_i^2}{8e^2}-V \tag{2.9}$$

$$=\frac{C}{8e^2}\left[\left(\frac{C_1}{C_2}+\frac{C_1}{C_3}\right)\dot{\chi}^2-2\dot{\chi}\dot{\theta}+\left(\frac{C_2}{C_1}+\frac{C_2}{C_3}\right)\dot{\theta}^2+\dot{\phi}^2\right]-V, \tag{2.10}$$

in which one is to substitute Eq. (2.8) for ϕ. The transformation (2.3) has achieved that Eq. (2.10) does not contain $\dot{\chi}\dot{\phi}$ or $\dot{\theta}\dot{\phi}$. Such terms, which *do* occur in $\mathcal{L}(\phi_1,\phi_2,\phi)$, would in $\mathcal{O}(L)$ result in an extremely unpleasant phase-dependent capacitance matrix in the effective Lagrangian (or Hamiltonian). However, in Eq. (2.10) with Eq. (2.8), $\dot{\phi}^2(\chi,\theta)$ is $\mathcal{O}(L^2)$, hence, negligible for the (χ,θ) dynamics. The effective Hamiltonian follows from $Q_\chi=2e\partial\mathcal{L}/\partial\dot{\chi}$, etc., as

$$H(\chi,\theta;Q_\chi,Q_\theta)\equiv\frac{Q_\chi\dot{\chi}+Q_\theta\dot{\theta}}{2e}-\mathcal{L} \tag{2.11}$$

$$=\frac{1}{2}\left[\frac{1}{C_1}\left(1+\frac{C_3}{C_1}\right)Q_\chi^2+\frac{2C_3}{C_1C_2}Q_\chi Q_\theta+\frac{1}{C_2}\left(1+\frac{C_3}{C_2}\right)Q_\theta^2\right]+V. \tag{2.12}$$

The potential V merits closer inspection: to $\mathcal{O}(L)$,

$$V(\chi,\theta)=U_J(\chi,\theta,\phi=0)+\left.\frac{\partial U_J}{\partial\phi}\right|_{\phi=0}\phi(\chi,\theta)+\frac{\phi^2(\chi,\theta)}{8e^2L}. \tag{2.13}$$

Using Eq. (2.4) to perform the differentiation in the second term explicitly *at constant* χ,θ, one finds $\partial_\phi U_J|_0=-I^{(0)}(\chi,\theta)/2e$.[9] Substituting Eq. (2.8) for $\phi(\chi,\theta)$, this means that this term inverts the sign of the third term,[10] yielding

$$H(\chi,\theta;Q_\chi,Q_\theta)=H_0-\frac{L}{2}I^{(0)}(\chi,\theta)^2, \tag{2.14}$$

$$\begin{aligned}H_0=&\frac{1}{2}\left[\frac{1}{C_1}\left(1+\frac{C_3}{C_1}\right)Q_\chi^2+\frac{2C_3}{C_1C_2}Q_\chi Q_\theta+\frac{1}{C_2}\left(1+\frac{C_3}{C_2}\right)Q_\theta^2\right]\\&-E_1\cos\left[C\left\{\left(\frac{1}{C_2}+\frac{1}{C_3}\right)\chi-\frac{\theta}{C_1}+\frac{\phi_x}{C_1}\right\}\right]\\&-E_2\cos\left[C\left\{-\frac{\chi}{C_2}+\left(\frac{1}{C_1}+\frac{1}{C_3}\right)\theta+\frac{\phi_x}{C_2}\right\}\right]\\&-E_3\cos\left[\frac{C}{C_3}\{\phi_x-\chi-\theta\}\right].\end{aligned} \tag{2.15}$$

Here, H_0 plays the role of H_{3JJ} in (χ,θ) coordinates. The combination of "Josephson" and "inductive" corrections in Eq. (2.14) would *not* have occurred in, say, (ϕ_1,ϕ_2,ϕ), where, thus, an awkward potential term would have compensated an awkward charging term [cf. below Eq. (2.10)]. The sign-flipping of the magnetic term has also been observed around Eq. (2) in Ref. 11, though not in terms of the detailed current operator $I^{(0)}$ in Eq. (1.10). Thus, the semiclassical analysis in Ref. 10 seems a valid approximation for stationary currents in the low-lying qubit states.

Because H is invariant, one can here and in the following increase the similarity to the conventional treatment by introducing $\underline{\phi}_1=C\{(C_2^{-1}+C_3^{-1})\chi-\theta/C_1+\phi_x/C_1\}$ and $\underline{\phi}_2=C\{-\chi/C_2+(C_1^{-1}+C_3^{-1})\theta+\phi_x/C_2\}$, so that formally $H_0(\underline{\vec{\phi}})=H_{3JJ}(\vec{\phi})$. Since comparison to Eqs. (2.4) and (2.8) shows that $\underline{\phi}_{1,2}$ do not coincide with the junction phases to $\mathcal{O}(L)$, this formulation is not very useful in derivations. However, in terms of $\underline{\vec{\phi}}$, the double periodicity of V and any additional symmetries are expressed conveniently, which may be effective numerically [cf. below Eq. (3.28)]. Figure 1 shows both the zeroth-order potential V_0 and the corrected V of Eq. (2.13), for standard parameters $E_1=E_2$, $C_1=C_2$, and $\alpha\equiv E_3/E_1=C_3/C_1=0.8$. In this case $V_0(\underline{\phi}_1,\underline{\phi}_2)=V_0(\underline{\phi}_2,\underline{\phi}_1)$, which is preserved in V. Since we have chosen a degenerate bias $\phi_x=\pi$, one also has $V_{(0)}(\underline{\phi}_1,\underline{\phi}_2)=V_{(0)}(-\underline{\phi}_1,-\underline{\phi}_2)$. The small self-flux has a clear physical effect: $(I^{(0)})^2=\nabla_{\underline{\vec{\phi}}}(I^{(0)})^2=0$ for $\underline{\vec{\phi}}^{\mathrm{T}}\in\{(0,0),(0,\pi),(\pi,0)\}$ by symmetry, so both the location and the height of all saddle points are unchanged.[12] Since clearly $-\frac{1}{2}L(I^{(0)})^2<0$ in the wells, both the "easy" (intra-) and "hard" (intercell) barriers are increased, and this term's suppression of the tunneling amplitude may not always be negligible. Finally, the lines $\underline{\phi}_1+\underline{\phi}_2=\pi \pmod{2\pi}$, which are *straight* equipotentials[13] through the intercell saddle points of V_0, cease to play this role in V.

III. QUANTUM ANALYSIS

A. Expansion of the Schrödinger equation

In quantum mechanics, one can advantageously use the same variables (2.3), avoiding $\partial_\chi\partial_\phi$ and $\partial_\theta\partial_\phi$ in Eq. (3.2) below. The large inductive term in Eq. (1.1) for H now causes the system to remain in its ground state with respect to ϕ. To leading order this is a harmonic-oscillator ground state $\psi\sim e^{-\lambda\phi^2}$, and one readily finds

$$\lambda=\frac{1}{8e^2}\sqrt{\frac{C}{L}}. \tag{3.1}$$

This unfortunately means that formally $\phi\sim L^{1/4}$ $(\partial_\phi\sim L^{-1/4})$ and strikingly $I\sim L^{-3/4}$. Hence, the expansion to $\mathcal{O}(L)$ will turn out to be sixth order while it was first order in Sec. II, and keeping the calculation organized is essential. Since it suffices to study the time-independent problem, the expansion will be analogous to, e.g., fast-variable elimination in (Fokker-Planck) diffusion operators.[14]

Using Eqs. (1.6) and (2.3) in Eq. (1.1), in the eigenvalue equation $(H-\mathcal{E})\psi=0$ we expand

$$H=-\frac{2e^2}{C}\partial_\phi^2+\frac{\phi^2}{8e^2L}+H_0+H_1\phi+H_2\phi^2+\cdots, \tag{3.2}$$

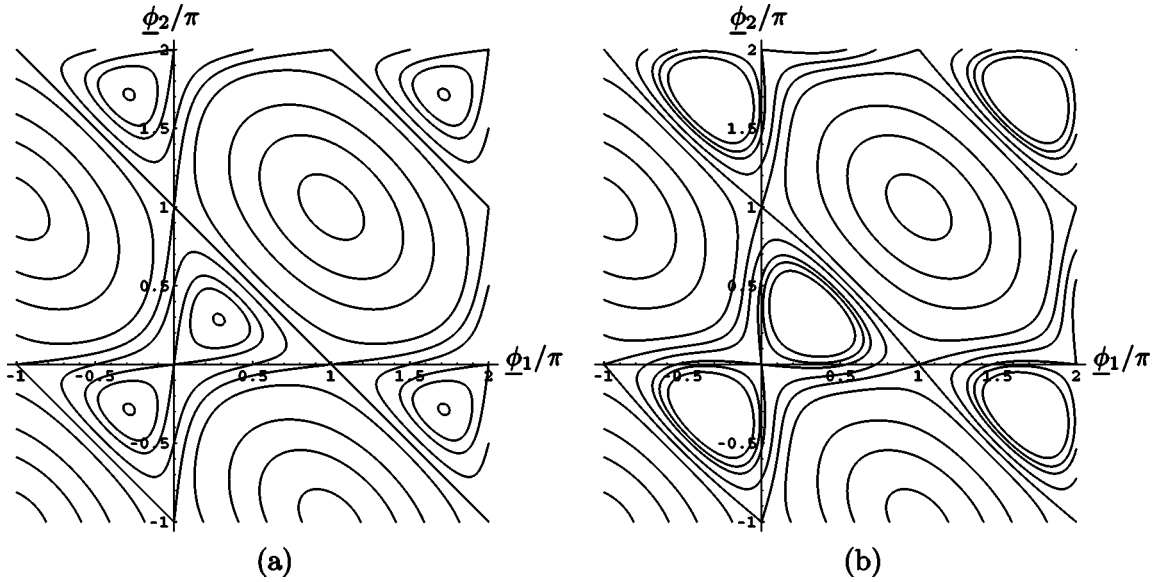

FIG. 1. The zeroth-order potential V_0 (a) and the first-order potential V (b), for $\alpha=0.8$ and $\phi_x=\pi$. In (b), we also use $e^2LE_1=0.3$. The contours correspond to $V_{(0)}/E_1=-1.42$, -1.3, $-1.2(=\alpha-2)$, -1, $-0.8(=-\alpha)$, -0.5, 0.5, 1.5, and 2.5, the latter encircling the maximum at $\underline{\phi}_1=\underline{\phi}_2=\pi$. The wells $V_0(\pm\underline{\phi}^*,\pm\underline{\phi}^*)/E_1=-\alpha-1/2\alpha=-1.425$ at $\underline{\phi}^*=\arccos(1/2\alpha)\approx 0.8957$ are shifted to $V(\pm\underline{\xi}^*,\pm\underline{\xi}^*)/E_1\approx -1.7983$ at $\underline{\xi}^*\approx 0.9602$. While the shifts in well location thus are appreciable, just evaluating the persistent current in the unshifted ones, i.e., $V(\pm\underline{\phi}^*,\pm\underline{\phi}^*)/E_1=-\alpha-1/2\alpha-e^2LE_1(2-1/2\alpha^2)\approx -1.7906$, gives a good estimate of the well depth.

$$\mathcal{E}=\mathcal{E}_{\rm zp}+\mathcal{E}_0+\mathcal{E}_1+\cdots, \tag{3.3}$$

$$\psi=\psi_0+\psi_2+\cdots, \tag{3.4}$$

with the zero-point energy $\mathcal{E}_{\rm zp}\sim L^{-1/2}$ and H_0 as in Eq. (2.15), with $\mathcal{E}_i$, $\psi_i\sim L^{i/4}$, and where we have been able to omit an $L^{-1/4}$ ($L^{1/4}$) term in $\mathcal{E}$ (ψ) from the outset because H does not have an $L^{-1/4}$ term. One has $H_n=(1/n!)\partial_\phi^n|_0 U_{\rm J}$ for $n\geqslant 1$, and because the calculation below Eq. (2.13) is just as valid in quantum as in classical mechanics, $H_1=-I^{(0)}(\chi,\theta)/2e$.

In $\mathcal{O}(L^{-1/2})$, one has

$$\left[-\frac{2e^2}{C}\partial_\phi^2+\frac{\phi^2}{8e^2L}-\mathcal{E}_{\rm zp}\right]\psi_0=0 \quad\Rightarrow \tag{3.5}$$

$$\psi_0(\chi,\theta,\phi)=\psi_0'(\chi,\theta)\mathrm{e}^{-\lambda\phi^2},\quad \mathcal{E}_{\rm zp}=\frac{1}{2\sqrt{LC}}, \tag{3.6}$$

the obvious answer for zero-point fluctuations of the loop current.

One can use Eq. (3.6) to factorize the operator in brackets in Eq. (3.5). In $\mathcal{O}(L^0)$, this leads to

$$-\frac{2e^2}{C}\mathrm{e}^{\lambda\phi^2}\partial_\phi[\mathrm{e}^{-2\lambda\phi^2}\partial_\phi(\mathrm{e}^{\lambda\phi^2}\psi_2)]+(H_0-\mathcal{E}_0)\psi_0'\mathrm{e}^{-\lambda\phi^2}, \tag{3.7}$$

where one can commute $\mathrm{e}^{-\lambda\phi^2}$ through $H_0-\mathcal{E}_0$. Operating with $\int \mathrm{d}\phi\,\mathrm{e}^{-\lambda\phi^2}$, the first term vanishes, so that one obtains the *solvability condition*

$$(H_0-\mathcal{E}_0)\psi_0'=0, \tag{3.8}$$

equivalent to the standard 3JJ theory (1.3). Substitution back into Eq. (3.7) renders the latter identical to the leading order, so that

$$\psi_2(\chi,\theta,\phi)=\psi_2'(\chi,\theta)\mathrm{e}^{-\lambda\phi^2}. \tag{3.9}$$

Proceeding to $\mathcal{O}(L^{1/4})$, one has

$$-\frac{2e^2}{C}\mathrm{e}^{\lambda\phi^2}\partial_\phi[\mathrm{e}^{-2\lambda\phi^2}\partial_\phi(\mathrm{e}^{\lambda\phi^2}\psi_3)]+\left(-\frac{I^{(0)}}{2e}\phi-\mathcal{E}_1\right)\psi_0'\mathrm{e}^{-\lambda\phi^2}=0, \tag{3.10}$$

for a solvability condition

$$\mathcal{E}_1=0 \tag{3.11}$$

because the term $\propto I^{(0)}\phi$ cancels by parity. This term does, however, contribute to ψ_3 itself,[15]

$$\psi_3(\chi,\theta,\phi)=\left[\frac{CI^{(0)}\psi_0'}{16e^3\lambda}\phi+\psi_3'(\chi,\theta)\right]\mathrm{e}^{-\lambda\phi^2}, \tag{3.12}$$

where the first term in square brackets is readily verified to shift the center of the Gaussian in Eq. (3.6) to[16] $\langle\phi\rangle_{\chi,\theta}$ in accordance with Eq. (2.8).

In $\mathcal{O}(L^{1/2})$, one obtains the first nontrivial solvability condition,[17]

$$(H_0-\mathcal{E}_0)\psi_2'+\left(\frac{H_2}{4\lambda}-\mathcal{E}_2\right)\psi_0'=0, \tag{3.13}$$

where the prefactor is obtained as $\int \mathrm{d}\phi\,\phi^2\mathrm{e}^{-2\lambda\phi^2}=(4\lambda)^{-1}\int \mathrm{d}\phi\,\mathrm{e}^{-2\lambda\phi^2}$. While we are only expanding the linear Schrödinger equation, it apparently "knows" that the proper

statistical weight is $|\psi_0|^2$ not ψ_0. The correction to ψ follows as

$$\psi_4(\chi,\theta,\phi)=\left[-\frac{CH_2\psi_0'}{16e^2\lambda}\phi^2+\psi_4'(\chi,\theta)\right]e^{-\lambda\phi^2}. \quad (3.14)$$

In $\mathcal{O}(L^{3/4})$, the solvability condition reads

$$(H_0-\mathcal{E}_0)\psi_3'-\mathcal{E}_3\psi_0'=0, \quad (3.15)$$

apparently posing the obstacle that both ψ_3' and $\mathcal{E}_3$ are unknown in this order. However, one can operate with $\int d\chi\, d\theta\, (\psi_0')^*$ and use Eq. (3.8), yielding

$$\mathcal{E}_3=0 \quad (3.16)$$

and $\psi_3'\propto\psi_0'$, so that

$$\psi_3'=0 \quad (3.17)$$

is a convenient choice of normalization. Determination of ψ_5 presents no problems, but is not required.

Finally, one arrives at $\mathcal{O}(L)$, finding a solvability condition

$$(H_0-\mathcal{E}_0)\psi_4'-e^2L(H_0-\mathcal{E}_0)H_2\psi_0'-\frac{L}{2}(I^{(0)})^2\psi_0'+\left(\frac{H_2}{4\lambda}-\mathcal{E}_2\right)\psi_2'+\left(\frac{12e^4L}{C}H_4-\mathcal{E}_4\right)\psi_0'=0. \quad (3.18)$$

What remains is to interpret this in terms of an effective two-phase Schrödinger equation.

B. Effective theory

While odd powers in $L^{1/4}$ were important in the above, most clearly through $I^{(0)}$ in Eq. (3.12) implementing the quantum counterpart of Eq. (2.8), they cancel in final results, such as Eqs. (3.11) and (3.16), by ϕ parity. What emerges is a two-phase theory involving an expansion in terms of $\sqrt{L}$ in which the zero-point motion (3.5) is absent, the leading order being simply

$$(\tilde{H}_0-\tilde{\mathcal{E}}_0)\tilde{\psi}_0=0, \quad (3.19)$$

$$\tilde{H}_0=H_0,\quad \tilde{\mathcal{E}}_0=\mathcal{E}_0,\quad \tilde{\psi}_0=\psi_0'. \quad (3.20)$$

Subsequently, Eq. (3.13) is recognized as the first-order part of

$$[\tilde{H}_0+\tilde{H}_1+\cdots-(\tilde{\mathcal{E}}_0+\tilde{\mathcal{E}}_1+\cdots)](\tilde{\psi}_0+\tilde{\psi}_1+\cdots)=0, \quad (3.21)$$

if one sets

$$\tilde{H}_1=\frac{H_2}{4\lambda},\quad \tilde{\mathcal{E}}_1=\mathcal{E}_2,\quad \tilde{\psi}_1=\psi_2'. \quad (3.22)$$

For the next and final relevant order, care is needed in identifying the effective wave function. Since probability should be conserved, $\tilde{\psi}$ must obey $|\tilde{\psi}(\chi,\theta)|^2=\int d\phi\,|\psi(\chi,\theta,\phi)|^2$, in which ψ_3 cancels to $\mathcal{O}(L)$ by Eqs. (3.12) and (3.17). Combining Eqs. (3.4), (3.6), (3.9), and (3.14), one has

$$|\psi_0'|^2+2\,\mathrm{Re}[(\psi_0')^*\psi_2']+|\psi_2'|^2+2\,\mathrm{Re}[(\psi_0')^*\psi_4']-2e^2LH_2|\psi_0'|^2+\mathcal{O}(L^{3/2})=|\tilde{\psi}_0+\tilde{\psi}_1+\tilde{\psi}_2+\cdots|^2, \quad (3.23)$$

which is satisfied by

$$\tilde{\psi}_2=\psi_4'-e^2LH_2\psi_0'. \quad (3.24)$$

Substituting this into Eq. (3.18), the latter is identified as the second order[18] of Eq. (3.21), with[19]

$$\tilde{\mathcal{E}}_2=\mathcal{E}_4,\quad \tilde{H}_2=\frac{12e^4L}{C}H_4-\frac{L}{2}(I^{(0)})^2. \quad (3.25)$$

Combining the above, one sees that the effective quantum Hamiltonian $\tilde{H}$ again has the form (2.14), but with renormalized Josephson couplings

$$E_i\mapsto E_i'=E_i\left(1-\frac{e^2\sqrt{LC^3}}{C_i^2}+\frac{e^4LC^3}{2C_i^4}\right). \quad (3.26)$$

To this order, the latter is exactly what one would expect from a Gaussian averaging $\tilde{U}_J(\chi,\theta)=\int d\phi\, e^{-2\lambda\phi^2}U_J(\chi,\theta,\phi)/\int d\phi\, e^{-2\lambda\phi^2}$: the zero-point fluctuations in ϕ behave as uncertainty in ϕ_x in Eq. (2.15), which washes out the Josephson potential. The systematic expansion is not prejudiced about "Josephson" versus "inductive" contributions to the energy, and instead directly provides a term $-\frac{1}{2}L(I^{(0)})^2$ to $\tilde{H}$ with the correct sign.

C. Numerics

To test the above analysis numerically, introduce the dimensionless inductance $\beta=2\pi LI_c/\Phi_0=4e^2LE_1$ (Φ_0 is the flux quantum) and $g=E_1/E_C$ (with the charging energy $E_C=e^2/2C_1$), and measure all energies in units E_1. Evaluation of the L-expansion is only meaningful for $\beta<1$, and β should be varied by at least an order of magnitude. These imply that for some of our parameter values, the energy levels of the full and effective theories will be very close. Hence, we focus on the simplest junction systems (to which the above for the 3JJ qubit is readily adapted), stressing accuracy rather than generality.

First, consider the rf-SQUID, $H=-(4/g)\partial_\phi^2-\cos(\phi+\phi_x)+\phi^2/2\beta$, for which the effective $\tilde{H}=\sqrt{2/\beta g}-(1-\sqrt{\beta/2g}+\beta/4g)\cos\phi_x-\frac{1}{2}\beta\sin^2\phi_x$ is zero-dimensional, i.e., a closed expression.[20] To evaluate H, we use that ϕ has an effective range $\sim\lambda^{-1/2}$ [cf. Eq. (3.1)], by truncating the potential with hard walls at $\phi=\pm m\sqrt[4]{\beta/g}$. Discretizing the resulting Dirichlet boundary value problem, the ground-state energy $\mathcal{E}$ is found by direct diagonalization, checking for convergence both with respect to the grid spacing Δ and $m=6,7,8,\ldots$.[21] Using the known error $\sim\Delta^2$ of lowest-order discretization of ∂_ϕ^2, one can perform a (highly effective) Richardson extrapolation $\mathcal{E}(\Delta\downarrow 0)\approx[4\mathcal{E}(\Delta)-\mathcal{E}(2\Delta)]/3$. The resulting data (not shown) confirm that the effective theory has an error $\mathcal{O}(\beta^{3/2})$.

TABLE I. The ground-state energy $\mathcal{E}$ of a symmetric dc-SQUID, compared to the standard estimate $\mathcal{E}_0$, which ignores inductance effects entirely, and to the prediction of the effective theory $\tilde{\mathcal{E}}$, accounting for renormalization of the Josephson coupling and for self-flux. Special attention has been paid at $g=40$, $\phi_x=\pi/4$, and $\beta=0.02$ to obtain the very small $\tilde{\mathcal{E}}-\mathcal{E}$ reliably. For $\phi_x=\pi$, the zeroth-order problem reduces to a free rotor, hence $\mathcal{E}_0=2/\sqrt{\beta g}$.

g	ϕ_x	β	$\mathcal{E}$	$\mathcal{E}_0$	$\tilde{\mathcal{E}}$
40	π	0.32	0.471441	0.559017	0.463997
40	π	0.08	1.097919	1.118034	1.097038
40	π	0.02	2.231116	2.236068	2.231006
40	$\pi/4$	0.32	−1.057313	−1.076987	−1.059445
40	$\pi/4$	0.08	−0.503724	−0.517970	−0.503857
40	$\pi/4$	0.02	0.608463	0.600064	0.608456
1	$\pi/4$	0.32	2.998577	2.870307	2.996471
1	$\pi/4$	0.08	6.476253	6.405841	6.476015
1	$\pi/4$	0.02	13.513825	13.476908	13.513799

For a system with a non-trivial effective theory, consider the symmetric dc-SQUID, $H=-(4/g)(\partial_{\phi_1}^2+\partial_{\phi_2}^2)-\cos\phi_1-\cos\phi_2+(\phi_1+\phi_2-\phi_x)^2/2\beta$. With fast and slow variables $\phi\equiv\phi_1+\phi_2-\phi_x$, $\chi\equiv\frac{1}{2}(\phi_1-\phi_2)$ respectively, this becomes

$$H=-\frac{8}{g}\partial_\phi^2-\frac{2}{g}\partial_\chi^2-2\cos\left(\frac{\phi+\phi_x}{2}\right)\cos\chi+\frac{\phi^2}{2\beta}, \qquad (3.27)$$

$$\tilde{H}=\frac{2}{\sqrt{\beta g}}-\frac{2}{g}\partial_\chi^2-2\left(1-\frac{1}{4}\sqrt{\frac{\beta}{g}}+\frac{\beta}{32g}\right)\cos\left(\frac{\phi_x}{2}\right)\cos\chi-\frac{\beta}{2}\sin^2\left(\frac{\phi_x}{2}\right)\cos^2\chi. \qquad (3.28)$$

In both Eqs. (3.27) and (3.28), 2π-periodic boundary conditions are imposed on χ. This is not the only possible choice, and corresponds to a zero offset charge in the two arms of the SQUID; for large g, the effect of this boundary condition will be small. Observing that both H and $\tilde{H}$ are even in χ, the even sector (containing the ground state[22]) can be treated as a Neumann boundary value problem on $0\leqslant\chi\leqslant\pi$. Further details areas for the rf-SQUID.[23]

Some results are shown in Table I, together with the standard zeroth-order prediction $\mathcal{E}_0$, which results by dropping all correction terms in Eq. (3.28). In all cases, reducing β by a factor of 4 reduces the error $\tilde{\mathcal{E}}-\mathcal{E}$ by at least a factor of ~ 8, as predicted. We note without explanation that for $g=40$, $\phi_x=\pi/4$, this factor seems to be rather ~ 16, as if the next $\mathcal{O}(\beta^{3/2})$ correction were very small numerically or canceled altogether. In contrast, $\mathcal{E}_0-\mathcal{E}$ only goes down by a factor of ~ 2, except for $\phi_x=\pi$, in which case the effective theory has a zero Josephson coupling so that its $\mathcal{O}(\sqrt{\beta})$ renormalization does not matter. Still, even in the latter case the self-flux term is nontrivial, so that an $\mathcal{O}(\beta)$ error renders $\mathcal{E}_0$ less accurate than $\tilde{\mathcal{E}}$. The last three rows emphasize that, in spite of this paper's title, our L expansion is not at all limited to the "flux-qubit" regime $g\gg 1$. This is useful, since small-L, small-C dc-SQUIDs are commonly used as tunable compound junctions, and 3JJ qubits in an intermediate-g regime have also been considered recently.[24]

In summary, the transparent effective Hamiltonian $\tilde{H}$ can be used with excellent accuracy also in many cases where the zeroth-order H_0 would be unsatisfactory. In the actual computations, the advantages in speed and storage requirements are evident; these will persist even when more sophisticated algorithms are employed in the study of more complex devices. In particular, let us reemphasize that, while the magnetic effects look small in the example of Table I, these effects constitute 100% of the interaction energy for two inductively coupled SQUID-type loops.

D. Comparison

Inductance effects in flux qubits have previously been studied in Ref. 4,[25] with the examples of loops containing one through three junctions. For one junction, the rf-SQUID, the two treatments are still largely equivalent and agree on the $\mathcal{O}(\sqrt{L})$ contribution to the energy [due to the second term in Eq. (3.26)]; this presumably is the main reason for the improved agreement with numerics in their Fig. 1(b). In $\mathcal{O}(L)$, the last term in Eq. (5) gives the self-flux contribution $-\frac{1}{2}L(I^{(0)})^2$; however, in the same order the renormalization effect [third term in Eq. (3.26)] is missing, because in the transition from Eq. (3) to Eq. (4), the Josephson potential was expanded to second instead of to the required fourth order in I.

For loops with multiple junctions, several problems arise in the treatment of Ref. 4. First, the physical role of the loop's series capacitance is not identified,[26] as is most clearly seen in the third term of Eq. (9), written in terms of the parallel capacitance $2C$ (the appropriate effective mass for the Θ coordinate) while this term can be naturally expressed as $\frac{1}{2}(C/2)L^2\dot{I}^2$ [cf. Eq. (3.27)]. Observing that the series capacitance of the 3JJ qubit is $[\alpha/(1+2\alpha)]C$ would have uncovered the missing factor $\frac{1}{2}$ in the third term of Eq. (14), which presently carries through to underestimating ω_0 below

Eq. (16) by a factor $\sqrt{2}$—which is not detected in their Fig. 3(b) because the latter does not feature three-phase numerics.

Second, the renormalization effect is not estimated correctly. The last term of Eq. (10) is neglected because it involves L^2, which is small, without checking whether $\tilde{I}^2$ could possibly be large. In fact, this term's counterpart in Eq. (4) yields the dominant correction in Eq. (5). For three junctions, the corresponding term is simply omitted from Eq. (15). Note that their Fig. 2(b) is given on such a scale, and for such extremely small β, that the apparent agreement with numerics only verifies the zeroth-order result, which never was in doubt.

Third and most serious, the analysis is conceptually incorrect in averaging the dynamics of the fast variable over the dynamics of the slow ones [first below Eq. (9)] instead of the other way round. In the final results (11) and (16), this leads (in our notation) to a perturbative energy correction $-\frac{1}{2}L\langle I^{(0)}\rangle^2$ instead of the proper $-\frac{1}{2}L\langle (I^{(0)})^2\rangle$ (cf. Ref. 19). This is inconsistent with the classical limit of Sec. II and underestimates the magnitude of the self-flux effect—most dramatically for the two lowest eigenstates of the degenerately biased 3JJ qubit (cf. our Fig. 1), where it would incorrectly predict this effect to vanish entirely. See also the remark on the coupled case in Sec. V.

IV. TWO COUPLED QUBITS

Consider two SQUIDs a and b side by side. The directions of the fluxes have to be chosen consistently in each loop with respect to the external field, and their magnitude is given as

$$\mathbf{\Phi} - \mathbf{\Phi}_{\mathrm{x}} = \mathbb{L}\boldsymbol{I}, \tag{4.1}$$

where $\mathbf{\Phi}=(\Phi_a,\Phi_b)^{\mathrm{T}}$, etc., and where

$$\mathbb{L} = \begin{pmatrix} L_a & -M \\ -M & L_b \end{pmatrix} \tag{4.2}$$

so that the antiferromagnetic coupling is characterized by a positive M. We can assume a homogeneous external field, so that the applied fluxes $\mathbf{\Phi}_{\mathrm{x}}=(A_a,A_b)^{\mathrm{T}}B_{\mathrm{x}}$ are proportional to the loop areas $A_{a,b}$. The magnetic energy can now be written as[27]

$$\begin{aligned} H_{\mathrm{M}} &= \frac{1}{2}\boldsymbol{I}^{\mathrm{T}}\mathbb{L}\boldsymbol{I} \qquad (4.3)\\ &= \frac{1}{2}(\mathbf{\Phi}-\mathbf{\Phi}_{\mathrm{x}})^{\mathrm{T}}\mathbb{L}^{-1}(\mathbf{\Phi}-\mathbf{\Phi}_{\mathrm{x}})\\ &= \frac{(\Phi_a - A_aB_{\mathrm{x}})^2}{2L_a(1-k^2)} + \frac{(\Phi_b - A_bB_{\mathrm{x}})^2}{2L_b(1-k^2)}\\ &\quad + \frac{M(\Phi_a - A_aB_{\mathrm{x}})(\Phi_b - A_bB_{\mathrm{x}})}{L_aL_b(1-k^2)}, \qquad (4.4) \end{aligned}$$

where $k^2 \equiv M^2/L_aL_b \ll 1$ will never (need to) be assumed. The factors[28] $(1-k^2)^{-1}$ are often ignored, but should not be surprising given the nontrivial effective capacitances one is used to seeing in charge-qubit Hamiltonians. Physically, they arise since, e.g., $\Phi_a - A_aB_{\mathrm{x}}$ is not simply the self-flux of loop a, but includes a mutual contribution.[29]

Two coupled 3JJ qubits can now be described by[30]

$$H = \sum_{c=a,b}\sum_{i=1}^{3}\left[\frac{Q_{ic}^2}{2C_{ic}} - E_{ic}\cos\phi_{ic}\right] + H_{\mathrm{M}}, \tag{4.5}$$

with $\Phi_c=\Sigma_{i=1}^{3}\phi_{ic}/2e$ in Eq. (4.4). This description is valid for arbitrary inductances; the price to pay is that Eq. (4.5) involves 6 DOF. Let us turn to the quantum expansion right away, limiting ourselves to outlining the proper generalization of Sec. III.

In $\mathcal{O}(L^{-1/2})$, the anisotropic oscillator problem is solved by

$$\psi_0 = \psi_0'(\chi_a,\theta_a;\chi_b,\theta_b)\mathrm{e}^{-\boldsymbol{\phi}^{\mathrm{T}}\Lambda\boldsymbol{\phi}}; \tag{4.6}$$

the inverse covariance matrix Λ is found from $\Lambda\mathbb{C}^{-1}\Lambda = \mathbb{L}^{-1}/64e^4$, with $\mathbb{C}\equiv\mathrm{diag}(C_a,C_b)$ diagonal since the coupling between the qubits is purely inductive. One obtains

$$\Lambda = \frac{1}{8e^2}\sqrt{\mathbb{C}}[\sqrt{\mathbb{C}}\mathbb{L}\sqrt{\mathbb{C}}]^{-1/2}\sqrt{\mathbb{C}}, \quad \mathcal{E}_{\mathrm{zp}} = 4e^2\left(\frac{\Lambda_{aa}}{C_a} + \frac{\Lambda_{bb}}{C_b}\right). \tag{4.7}$$

Since even 2×2 matrix square roots are slightly tedious, we leave Λ unevaluated in most formulas [cf. Eq. (5.1)]. The correlation (entanglement) expressed by the Gaussian in Eq. (4.6) seems physically reasonable: for, e.g., again two small loops on top of each other, deviations of $\Phi_{a,b}$ from each other should be even more strongly suppressed than deviations from Φ_{x}.

In $\mathcal{O}(L^0)$, one has

$$-2e^2\mathrm{e}^{\boldsymbol{\phi}^{\mathrm{T}}\Lambda\boldsymbol{\phi}}\nabla_{\boldsymbol{\phi}}^{\mathrm{T}}\mathrm{e}^{-2\boldsymbol{\phi}^{\mathrm{T}}\Lambda\boldsymbol{\phi}}\mathbb{C}^{-1}\nabla_{\boldsymbol{\phi}}\mathrm{e}^{\boldsymbol{\phi}^{\mathrm{T}}\Lambda\boldsymbol{\phi}}\psi_2 + \mathrm{e}^{-\boldsymbol{\phi}^{\mathrm{T}}\Lambda\boldsymbol{\phi}}(H_0-\mathcal{E}_0)\psi_0' = 0. \tag{4.8}$$

Since $\nabla_{\boldsymbol{\phi}}^{\mathrm{T}}$ has two components, one needs a double integral $\int \mathrm{d}\phi_a\,\mathrm{d}\phi_b\,\mathrm{e}^{-\boldsymbol{\phi}^{\mathrm{T}}\Lambda\boldsymbol{\phi}}$ to cancel it, yielding a single solvability condition formally equal to Eq. (3.8). However, in the present case we additionally observe the decoupling

$$H_0 = H_{0a} + H_{0b} \quad \Rightarrow$$

$$\mathcal{E}_0 = \mathcal{E}_{0a} + \mathcal{E}_{0b}, \quad \psi_0' = \psi_{0a}'(\chi_a,\theta_a)\psi_{0b}'(\chi_b,\theta_b). \tag{4.9}$$

Thus, the leading six-phase wave function ψ_0 can be strongly entangled, while the leading four-phase one ψ_0' factorizes. Subsequently, ψ_2 is obtained analogously to Eq. (4.6).

In $\mathcal{O}(L^{1/4})$, one again finds $\mathcal{E}_1=0$, while

$$\psi_3 = \left[\boldsymbol{\phi}^{\mathrm{T}}\frac{\mathbb{C}\Lambda^{-1}\boldsymbol{I}^{(0)}}{16e^3}\psi_{0a}'\psi_{0b}' + \psi_3'(\chi_a,\theta_a;\chi_b,\theta_b)\right]\mathrm{e}^{-\boldsymbol{\phi}^{\mathrm{T}}\Lambda\boldsymbol{\phi}}. \tag{4.10}$$

A Gaussian vector integral, followed by use of Eq. (4.7), confirms the expected $\langle\boldsymbol{\phi}\rangle = 2e\mathbb{L}\boldsymbol{I}^{(0)}$.

In $\mathcal{O}(L^{1/2})$, the correction to H takes the form $H_{2a}\phi_a^2 + H_{2b}\phi_b^2$ since Eq. (4.5) has no Josephson interaction [cf. the remark below Eq. (4.6)]. This does *not* generate any interac-

tion when $\boldsymbol{\phi}$ is integrated out with the entangled weight $e^{-2\boldsymbol{\phi}^T\Lambda\boldsymbol{\phi}}$, so that

$$\psi_2' = \psi_{2a}'(\chi_a,\theta_a)\psi_{2b}'(\chi_b,\theta_b), \quad \mathcal{E}_2 = \mathcal{E}_{2a} + \mathcal{E}_{2b}, \quad (4.11)$$

$$(H_{0a} - \mathcal{E}_{0a})\psi_{2a}' + \left[\tfrac{1}{4}(\Lambda^{-1})_{aa}H_{2a} - \mathcal{E}_{2a}\right]\psi_{0a}' = 0 \quad (4.12)$$

and similarly for $a \leftrightarrow b$. One could proceed to solve for ψ_4 but this will be omitted, since all that really matters is its relation to the effective wave function $\tilde{\psi}_2 = \int d\phi_a\, d\phi_b\, \psi_4 e^{-\boldsymbol{\phi}^T\Lambda\boldsymbol{\phi}} / \int d\phi_a\, d\phi_b\, e^{-2\boldsymbol{\phi}^T\Lambda\boldsymbol{\phi}}$.

The next order $\mathcal{O}(L^{3/4})$ again is comparatively uninteresting, as it mainly justifies taking $\mathcal{E}_3 = \psi_3' = 0$.

Finally, in $\mathcal{O}(L)$, everything can be combined, and the effective Hamiltonian can be read off. Doing so leads to the central result of this paper,

$$\tilde{H} = H_{0a}' + H_{0b}' - \tfrac{1}{2}(\boldsymbol{I}^{(0)})^T\mathbb{L}\boldsymbol{I}^{(0)}, \quad (4.13)$$

where H_{0a}', H_{0b}' are as in Eq. (2.15) (with $\phi_{xc} = 2eA_cB_x$), except for the renormalizations

$$E_{ic} \mapsto E_{ic}' = E_{ic}\left[1 - \left(\frac{C_c}{C_{ic}}\right)^2\frac{(\Lambda^{-1})_{cc}}{8} + \left(\frac{C_c}{C_{ic}}\right)^4\frac{(\Lambda^{-1})_{cc}^2}{128}\right]$$

$$(c = a,b). \quad (4.14)$$

V. DISCUSSION

Let us first of all return to this paper's motivation. In a classical potential, such as in Fig. 1, inductance effects are typically on the order of a few percent. However, this is compared to the Josephson coupling, i.e., to a typical tunneling *barrier*. For two coupled 3JJ qubits, the magnetic interaction energy may well be comparable to the tunnel *splitting*, so nontrivial interplay[31] between the two is expected, prompting the present systematic derivation.

One can view Eq. (4.13) in at least two ways. Experimentally, the bare couplings E_{ic} will usually be unknown and the diagonal contributions from the last term may be comparatively small. In that case, most interesting will be the interaction $MI_a^{(0)}(\chi_a,\theta_a)I_b^{(0)}(\chi_b,\theta_b)$, derived with the antiferromagnetic sign without any remaining ambiguity. Also, this interaction is given in terms of explicitly known current operators so that, in, e.g., the two-level (qubit) approximation, one has $H_{\text{int}} = M|I_a||I_b|\sigma_a^z\sigma_b^z$ in the flux basis without additional handwaving. Contrast Ref. 4, where improper averaging of the $I^{(0)}$'s would have led to $\langle H\rangle = \cdots + M\langle I_a^{(0)}\rangle\langle I_b^{(0)}\rangle$, which for instance vanishes for all four two-qubit Bell states.

On the other hand, for detailed numerical comparison between the four- and six-phase theories, every last bit of parameter dependence needs to be made explicit. Therefore, we take the square root in Eq. (4.7) in the eigenbasis, yielding

$$(\Lambda^{-1})_{aa} = \frac{2\sqrt{2}e^2}{C_a}\left[\left(1 + \frac{L_aC_a - L_bC_b}{\Omega}\right)\sqrt{L_aC_a + L_bC_b + \Omega} + \left(1 + \frac{L_bC_b - L_aC_a}{\Omega}\right)\sqrt{L_aC_a + L_bC_b - \Omega}\right], \quad (5.1)$$

$$\Omega = \sqrt{(L_aC_a - L_bC_b)^2 + 4M^2C_aC_b}, \quad (5.2)$$

$$\det\Lambda = \frac{1}{64e^4}\sqrt{\frac{C_aC_b}{L_aL_b(1-k^2)}}, \quad (5.3)$$

while $(\Lambda^{-1})_{bb}$ follows by $a \leftrightarrow b$. The second square root in Eq. (5.1) has a positive argument because $k^2 < 1$ (positive-definiteness of $\mathbb{L}$). Note that Eq. (5.1) reduces to λ_a^{-1} as in Eq. (3.1) for $\Omega \to \pm(L_aC_a - L_bC_b)$ (i.e., regardless of which of the uncoupled qubits has the larger LC).

As already seen in Sec. III C, the L expansion involves two different dimensionless parameters—as expected in a system with Coulomb, Josephson, and magnetic energies. "Classical" self-flux effects go as $LI^2/E_1 \sim \beta$. On the other hand, from Eq. (3.26) one reads off that the "quantum" zero-point effects go as $e^2\sqrt{L/C} \sim \lambda^{-1} \sim E_C/\omega_{LC}$. Thus, the former (latter) parameter does not contain the charging (Josephson) energy, which is also the reason why, to the given order, their contributions are separated in the final results. In particular, for comparatively large junctions and not too small area, the $\mathcal{O}(L)$ self-flux effect could dominate over the $\mathcal{O}(\sqrt{L})$ renormalization within the domain of validity of our expansion—as was implicitly used in Fig. 1. However, in the experiments for which all parameters are available, one has[32] $(LI_c/\Phi_0, e^2\sqrt{L/C}) = (0.003, 0.015)$ and[33,34] (0.007, 0.02) respectively, so that, if anything, the renormalization effect dominates.

Extension to >2 qubits, using the same vector notation, is immediate. It is hoped that the methods presented will have additional use in other devices with near-constrained variables.

Note added in proof. Let us finally raise a question slightly beyond this paper's scope, about the proper form of the two-level approximation for multi-flux-qubit systems. The conventional approach is to determine a two-level single-qubit Hamiltonian involving both bias and tunneling terms, and subsequently add interactions involving products of Pauli matrices. However, the free and coupled systems are simply different, and therefore tunneling amplitudes should properly be evaluated using the interacting multi-qubit potential. The simplest case consists of two inductively coupled rf-SQUIDs, having a two-dimensional potential landscape. For the qubit approximation to this system, one should calculate the four lowest states in this potential. The resulting effective Hamiltonian may well contain, e.g., a direct $|\uparrow\uparrow\rangle \leftrightarrow |\downarrow\downarrow\rangle$ tunneling amplitude—a transition which is second-order in the conventional approach. To study this question for 3JJ qubits, it is vital to have a well-defined interaction *operator*, as derived in this paper.

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[1] T. P. Orlando, J. E. Mooij, L. Tian, C. H. van der Wal, L. Levitov, S. Lloyd, and J. J. Mazo, Phys. Rev. B **60**, 15 398 (1999).

[2] As always, ϕ_i in Eq. (1.1) are properly gauge-invariant "phases," defined as line integrals along the SQUID loop. Thus, there is no reason for H to be 2π-periodic even though the Josephson term is, and, indeed, ϕ_i's differing by multiples of 2π correspond to physically distinguishable magnetic field configurations.

[3] A nontrivial capacitance matrix will be essential in Eq. (1.3). Note also that, for this pure series circuit, H does not depend on how the inductance is distributed along the loop.

[4] D. S. Crankshaw and T. P. Orlando, IEEE Trans. Appl. Supercond. **11**, 1006 (2001).

[5] E.g., Ya. S. Greenberg, A. Izmalkov, M. Grajcar, E. Il'ichev, W. Krech, H.-G. Meyer, M. H. S. Amin, and A. Maassen van den Brink, Phys. Rev. B **66**, 214525 (2002), Eq. (13).

[6] When choosing conventions, one needs a minus sign somewhere for the final Eq. (1.8) with Eq. (1.2) to come out as $\Phi - \Phi_x = LI$.

[7] Since superconductivity is not a "classical" phenomenon, the term is a bit tenuous. Indeed, if H is written in terms of phases (fluxes), the inductive (Josephson) terms would involve $\hbar$ in SI units. Of course, the dynamics (2.1) do emerge from the full quantum theory in the limit of large capacitances (cf. Sec. V).

[8] The coordinates Θ_1, Θ_2 (plus $I_m \propto \phi$) in Eq. (13) of Ref. 4 satisfy the same criterion. They correspond to choosing two zero entries in Eq. (2.4) rather than Eq. (2.3), and are physically equivalent to χ, θ.

[9] By the same token, one has $I^{(0)} = -2e\partial H_0/\partial\phi_x|_{\chi,\theta}$ for H_0 as in Eq. (2.15). This seemingly obvious relation is simply not true for $\partial H_{3JJ}/\partial\phi_x|_{\phi_1,\phi_2}$ in Eq. (1.3), even though $I = -2e\partial H/\partial\phi_x|_{\vec{\phi}}$ does hold between Eqs. (1.1) and (1.8) in the three-phase theory. For coupled qubits, one likewise has $\partial H/\partial B_x = -A_a I_a - A_b I_b$ in Eqs. (4.4) and (4.5).

[10] The negative sign of the second term in (2.13) is most readily understood for degenerate bias, where any self-flux will effectively reduce the maximum flux frustration imposed externally.

[11] J. Q. You, J. S. Tsai, and F. Nori, Phys. Rev. Lett. **89**, 197902 (2002); J. Q. You, Y. Nakamura, and F. Nori, cond-mat/0309491 and references therein (unpublished).

[12] The same holds for the maximum $V_{(0)}(\pi,\pi)/E_1 = 2+\alpha$, but this should have few physical consequences.

[13] This may be a new observation and holds for general ϕ_x even though the saddle-points themselves will move along this line.

[14] N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).

[15] Only solutions bounded in ϕ are acceptable.

[16] Properly, $\langle\phi\rangle_{\chi_0,\theta_0} = \langle\phi\delta(\chi-\chi_0)\delta(\theta-\theta_0)\rangle/\langle\delta(\chi-\chi_0)\delta(\theta-\theta_0)\rangle$ is a conditional quantum-mechanical expectation. The vector version below Eq. (4.10) is analogous.

[17] Of course, one can operate on Eq. (3.13) with $\int d\chi\, d\theta\, (\psi_0')^*$, yielding $\mathcal{E}_2 = \langle\psi_0'|(H_2/4\lambda)|\psi_0'\rangle/\langle\psi_0'|\psi_0'\rangle$, upon which ψ_2' is determined up to a multiple of ψ_0' (a trivial change in normalization). However, our focus is on deriving the effective theory, not solving it.

[18] The occurrence of $\tilde{H}_1\tilde{\psi}_1$ in this order represents the effect of $\tilde{H}_1$ in second-order perturbation theory, not a new term in $\tilde{H}$.

[19] Again, one can solve $\tilde{\mathcal{E}}_2 = [\langle\tilde{\psi}_0|\tilde{H}_2|\tilde{\psi}_0\rangle + \langle\tilde{\psi}_1|\tilde{\mathcal{E}}_0 - \tilde{H}_0|\tilde{\psi}_1\rangle]/\langle\tilde{\psi}_0|\tilde{\psi}_0\rangle$, cf. Ref. 17. However, in practice direct numerical solution of $\tilde{H}$—though no more accurate—seems preferable over a perturbative approach.

[20] For convenient comparison, $\mathcal{E}_{zp}$ (usually an irrelevant constant) is included in $\tilde{H}$.

[21] Increasing m too fast, e.g., successive doubling, wastes grid points on the wave function's large-$|\phi|$ tail.

[22] The ground state tends to be found with the highest accuracy for a given Δ, but other states are readily found and compared as well.

[23] The used matrix representation [W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C*, 2nd Edition (Cambridge University Press, Cambridge, England, 1992)] makes it convenient to allocate only half of a symmetric matrix in a way that is transparent to the rest of the program, as long as the latter never accesses matrix elements above the main diagonal.

[24] M. H. S. Amin, Phys. Rev. B **71**, 024504 (2005).

[25] In that paper's opening paragraph, $2\pi I_c/\Phi_0$ defines L_J^{-1} not L_J. The order estimates below Eq. (1) give the number of grid points, while the "computational time" grows faster. Equation (3) and the one right above have a sign problem when compared to Eq. (2) and Fig. 1(a). A constant $2E_J$ is lost between Eqs. (6) and (7) on the one hand and Eq. (9) on the other. In the definition of $\tilde{\Theta}_m$ below Eq. (14), the factor 2 in the second term is spurious. In the expression for $\hbar\omega_0$ below Eq. (16), E_c/E_J should read $E_c E_J$. The figures are irreproducible since E_J/E_c is not given.

[26] In general, not taking independent capacitances and Josephson couplings makes it more difficult to conceptually separate the effects of the two.

[27] Expanding the bilinear form in Eq. (4.3), the *anti*ferromagnetic interaction is seen to involve a term $-MI_aI_b$, in contrast to the positive last term in Eq. (4.4). This is counterintuitive, but a simple consequence of 2×2 matrix inversion. It may be clarifying to compare (anti)ferromagnetic configurations *at constant absolute fluxes in the loops*. Due to the mutual inductance, antiparallel fluxes can be generated with smaller $|I|$'s, reducing thevalue of $\frac{1}{2}L_aI_a^2$, etc., which one would naively discard as a small part of the "free" Hamiltonian. That is, while total energy is conserved, the designation of an "interaction" part can be somewhat arbitrary, so it is best to be as consistent as possible and retain all terms in Eq. (4.3). The electrostatic counterpart may be more familiar in the field [cf. the remark below Eq. (4.4)].

[28] E.g., J. F. Ralph, T. D. Clark, M. J. Everitt, and P. Stiffell, Phys. Rev. B **64**, 180504(R) (2001).

[29] For $k \uparrow 1$, Eq. (4.4) seems to diverge. However, physically this limit can only be achieved with two loops right on top of each other. The resulting *ferro*magnetic interaction is described by $M<0$ in Eq. (4.2), so that the last term in Eq. (4.4) tends to cancel the other two. Indeed, we have merely rewritten the finite Eq. (4.3).

[30] Not all of our assumptions (cf. Ref. 3) may hold in a figure-8 geometry [J. B. Majer, F. G. Paauw, A. C. J. ter Haar, C. J. P. M. Harmans, and J. E. Mooij, cond-mat/0308192 (unpublished)] if part of the inductance is distributed along the shared leg. Therefore, this case deserves special attention. Furthermore, incorporating a (large) Josephson junction into a shared leg is known to cause an antiferromagnetic coupling in close analogy to the inductive one discussed here. See L. S. Levitov, T. P. Orlando, J. B. Majer, and J. E. Mooij, cond-mat/0108266; J. R. Butcher,

graduation thesis, Delft University of Technology, Delft, 2002; M. Grajcar, A. Izmalkov, S. H. W. van der Ploeg, S. Linzen, E. Il'ichev, Th. Wagner, U. Hübner, H.-G. Meyer, A. Maassen van den Brink, S. Uchaikin, and A. M. Zagoskin, cond-mat/0501085 (unpublished).

[31] A. Izmalkov, M. Grajcar, E. Il'ichev, Th. Wagner, H.-G. Meyer, A. Yu. Smirnov, M. H. S. Amin, A. Maassen van den Brink, and A. M. Zagoskin, Phys. Rev. Lett. **93**, 037003 (2004).

[32] C. H. van der Wal, A. C. J. ter Haar, F. K. Wilhelm, R. N. Schouten, C. J. P. M. Harmans, T. P. Orlando, S. Lloyd, and J. E. Mooij, Science **290**, 773 (2000).

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[34] M. Grajcar, A. Izmalkov, E. Il'ichev, Th. Wagner, N. Oukhanski, U. Hübner, T. May, I. Zhilyaev, H. E. Hoenig, Ya. S. Greenberg, V. I. Shnyrkov, D. Born, W. Krech, H.-G. Meyer, A. Maassen van den Brink, and M. H. S. Amin, Phys. Rev. B **69**, 060501(R) (2004).