Universal Formalism for Superconducting Quantum Circuits

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Currently the number of various qubit designs is vastly growing: from early-generation phase and charge qubits to modern transmons and fluxonia and their more complex modifications. Moreover, more complicated qubits with better predicted qualities are now being designed and tested. All these qubit designs require simple and efficient modeling that allows to predict various qubit properties and compare them with experiments.

Here we propose a simple formalism that allows to naturally write a Hamiltonian of any superconducting circuit consisting capacitors, inductors and Josephson junctions. The formalism allows to "untangle" the phase coordinates of different nodes of the circuit and write the Hamiltonian as a set of maximally independent variables. It automatically separates generalized coordinates into two distinct categories based on whether or not they obey charge quantization condition. Eventually the formalism allows to reduce Hamiltonian of any circuit to the one consisting of (1) set of independent harmonic oscillators, (2) set of superconducting islands with quantized charges and (3) set of Josephson junctions that facilitate interaction between elements (1) and (2). This allows to formally isolate inductors from the rest of the superconducting circuit and treat cooper pairs and photons stored in harmonic oscillators separately.

Typically superconducting circuits are treated using formalism described in[2]. This formalism, allows to write a Hamiltonian for a complicated superconducting circuit, but in order to numerically find eigenstates and eigenenergies of such Hamiltonian one needs to choose a set of orthogonal basis states in which the Hamiltonian needs to be represented. Formalism [2] provides a large degree of freedom in both: choice of the generalized circuit coordinates and in the choice of their quantization. However, for purposes of analysis and numerical modeling some choices for of generalized coordinates can be better, more natural, then others. This requires further analysis to figure out which degrees of freedom are more critical to the functioning of the circuit and require more detailed approach. Formalism proposed here provides no freedom in choosing the generalized coordinates, but in turn suggests basis wavefunctions that are natural for each coordinate: charge eigenstates for coordinates that obey charge quantization and harmonic oscillator eigenstates for coordinates that are associated with inductors and hence violate charge quantization. This makes analysis of any circuit formalizable and easily automatizable.

Moreover, in many cases it is important to model charge and flux offset fields that vary with time. While formalism [2] assumes static fields and localization of offset fluxes depends on the choice of generalized coordinates, our approach

allows to place and distribute flux offsets anywhere in the circuit. It becomes critical when modeling circuits with time-dependent fields. For example, in the closed loop of a superconducting circuit, a static flux can be modeled by adding a flux offset to a phase drop only on one of the elements (inductors or Josephson junctions), but a phase drops due to a dynamic flux must be distributed between the elements according to their capacitances[3]. Our formalism allows to easily implement that.

Overview. Typically superconducting circuits (e.g. random circuit in Figure 1) and qubits can be represented as a set of inductors, capacitors and Josephson junctions. The latter ones give qubits and other superconducting devices their useful non-trivial properties. In absence of the Josephson junctions the circuit is simply a set of interacting harmonic oscillator modes. Without Josephson junctions the simplest way to treat a problem is to perform a coordinate transformation that transforms the circuit Hamiltonian into a set of independent harmonic oscillators (call it **transformation I**). Then, Josephson junctions are introduced in the picture as an interaction Hamiltonian that describes tunneling of Cooper pairs between different parts of the circuit. However, as will be shown later, such straightforward approach has a critical flaw. Many circuits, such as transmon-based ones contain so-called "clusters" – segments of the circuit that are not connected to the ground via inductors or wires (Fig.1). Obviously the net charge on such cluster has to be quantized in multiples of $2e$. Unfortunately coordinate transformation that untangles harmonic oscillators also partially violates this charge quantization: it requires non-integer quantization of charge states, which manifests itself in the fact that in the new coordinates Josephson junction potential no longer has a 2π periodicity in phase. To correct this issue we suggest a second coordinate transformation (**transformation II**) that restores the integer charge quantization. After these two transformations the Hamiltonian is split into two parts: Hamiltonian of a set of independent harmonic oscillators and an interaction term represented by the energies of the Josephson junctions. For example, the formalism effectively transforms circuit in Fig.1 that has a complex graph topology into a simply structured circuit displayed in Figure 2 preserving number of charge clusters and closed loops.

After this the Hamiltonian can be easily quantized by describing each degree of freedom either in terms of harmonic oscillator eigenstates or in terms of charge eigenstates. This choice of basis automatically diagonalizes most part of the Hamiltonian and the problem can be then solved numerically with minimal computational expenses. In other words, the proposed formalism allows to distinguish generalized coordinates of a circuit that behave like coordinates of an oscillator from "cyclic coordinates" – coordinates that are cyclic in phase and hence correspond to quantized charge. This, in turn, ultimately allows to to find the basis vector set that naturally describes the two types of coordinates. Then the Hamiltonian can be written in a matrix form without a need for excessively large and computationally expensive dimensionality: the proposed formalism allows to reasonably predict the number of eigenstates sufficient for description of each coordinate.

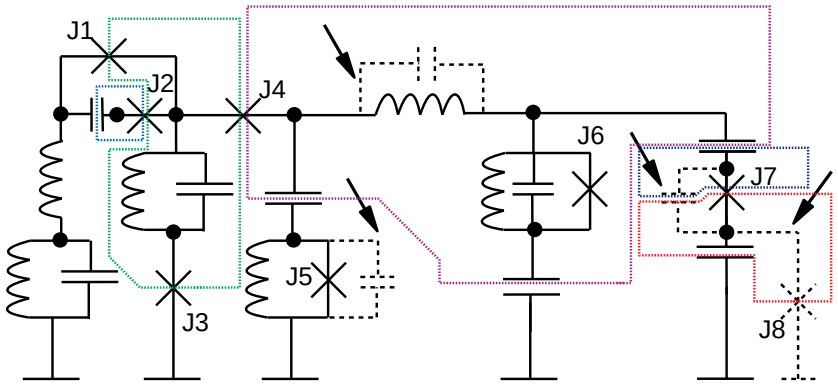

Figure 1. Example of a complex superconducting circuit. Thick black dots represent nodes with total node number $N^{\rm tot}$ (not counting ground being node 0). The dashed colored contours indicate the the clusters not connected to ground through inductors. Dashed capacitors marked with arrows exemplify parasitic capacitances. Josephson junctions are named as J1, J2,...J8. Dashed Josephson junction J8 marked with an arrow represent ad-hoc zero Josephson junction whose only function is to enforce charge quantization on the cluster.

Setting up the Hamiltonian. The general idea is (e.g. G-mon, X-mon,...) to write the Hamiltonian as a sum of energies contained in capacitances and inductances ($\mathcal{H}_{LC}$) and in Josephson junctions ($\mathcal{H}_{\rm jos}$):

$$\mathcal{H} = \mathcal{H}_{LC} + \mathcal{H}_{\rm jos}. \tag{1}$$

Here

$$\mathcal{H}_{LC}\left(\vec{\phi},\vec{n}\right) = \frac{1}{2}C^{-1}_{jk}n_j n_k + \frac{1}{2}\phi_k G^T_{k\widetilde{K}} L^{-1}_{\widetilde{K}\widetilde{M}} G_{\widetilde{M}m}\phi_m; \tag{2}$$

$$\mathcal{H}_{\rm jos}\left(\vec{\phi}\right) = -\sum_{\widehat{J}} E_{\widehat{J}}\cos(H_{\widehat{J}j}\phi_j) \tag{3}$$

with L^{-1} and C^{-1} being inductance and Maxwell capacitance matrices respectively; G and H being inductance and Josephson connectivity matrices respectively that will be discussed below; ϕ_j being phase on the j-th node and $n_j = -i\partial/\partial\phi_j$ – charge on the j-th node. One of the nodes (zeroth node) is assumed to be a ground one and hence is not counted by index j. Note that summation over repeating indexes is implied unless explicitly noted otherwise. Lower-case Latin indexes $(j,k,...)$ shall count nodes and upper case-indexes with either tildes or hats ($\widetilde{J},\widetilde{K},\widetilde{M}...$ or $\widehat{J},\widehat{K}...$) count inductors and Josephson junctions respectively. Later we will also use bold lower-case indexes $(\mathbf{p},\mathbf{r},\mathbf{s},...)$ to count quantum states. This will help us keep track of multiple index types. We use units of $\hbar = 2e = \Phi_0/2\pi = 1$.

We assume that any two nodes are connected with at least small parasitic capacitance (Fig. 1) rendering C^{-1}-matrix invertible and positively-defined[1]. Matrix $G_{\widetilde{K}k}$ is called an "inductance connectivity matrix" – generally a rectangular matrix that converts phases on the nodes (counted by index k) into phase drop across the $\widetilde{K}$-th inductance. Thus, number of rows in $G_{\widetilde{K}k}$ corresponds to the number of inductors in the circuit and number of columns – to the number of nodes. If $\widetilde{K}$-th inductor connects nodes k and l, then the $\widetilde{K}$-th row of G contains $+1$ in the k-th column, -1 – in the l-th column and zeros everywhere else. If, however, the inductor connects k-th node to the ground then only the k-th column of the corresponding row needs to be filled with 1, keeping other columns filled with zeros. Thus, matrix G acting on a vector of node phases $\vec{\phi}$ renders a vector of phase drops across the inductances $G\vec{\phi}$. In the same way $H_{\widehat{J}j}$ is a "Josephson connectivity matrix" that transforms phases on different nodes into phase drops across Josephson junctions. Having N_{jos} Josephson junctions in the circuit, H has N_{JOS} rows. External flux and charge offsets ($\Phi_{\widetilde{K}}$ and Q_j respectively) can be included later by substitutions $G_{\widetilde{K}k}\phi_k \to G_{\widetilde{K}k}\phi_k - \Phi_{\widetilde{K}}$ and $n_j \to n_j - Q_j$. Thus we assume that external phase is gained inside inductors.

Now, after defining the main notations we start performing coordinate transformations untangling the circuit elements.

Coordinate transformation I: untangling oscillators. The first step to simplification is standard: we want to "untangle" interacting harmonic oscillators in $\mathcal{H}_{LC}$ and formally get a set of independent harmonic oscillators. The Hamiltonian $\mathcal{H}_{LC}$ can be easily diagonalized using coordinate transformation

$$\phi_j = C_{jk}^{-1/2} U_{k(e.g. G-mon, X-mon, \ldots)l} z_l. \tag{4}$$

Here U is a unitary matrix that diagonalizes the matrix $C^{-1/2}G^T L^{-1} G C^{-1/2}$ in the following way:

$$U\omega^2 U^T = C^{-1/2}G^T L^{-1} G C^{-1/2} \tag{5}$$

with $\omega = \text{diag}\{\omega_j\}$ being the diagonal matrix containing mode frequencies ω_j of $\mathcal{H}_{LC}$ from lowest (left-top corner) to highest (right-bottom) values. Note that while phases on nodes are denoted by Greek letter "ϕ", after coordinate transformation they are denoted using lower-case Latin letters "z". In these coordinates

$$\mathcal{H}_{LC}\left(\vec{z}, \vec{k}\right) = \sum_j \left\{ \frac{1}{2} k_j^2 + \frac{1}{2} \omega_j^2 z_j^2 \right\}. \tag{6}$$

Here z_j are new phase coordinates and $k_j = -i\partial/\partial z_j$ are canonically conjugated charges. Thus, the network of interlinked harmonic oscillators splits into a set of independent harmonic oscillators with mode frequencies ω_j and zero-point amplitudes of $\omega_j^{-1/2}$. Formally the total number of oscillators is equal to the number of nodes. However, some of the nodes can be combined into a "cluster" – set of nodes that may be connected to each other via inductors but

are not connected to the ground or to other clusters or nodes via inductors. Total charge of such "cluster" is therefore quantized. Examples of clusters are shown with dashed contours in Figure 1. It is important to note that the number of zeros among $\{\omega_j\}$ is equal to the number of clusters in the circuit. This happens because the cluster's net charge k_{cluster} quantization requires periodicity of the Hamiltonian in the corresponding phase variable z_{cluster} and hence zero coefficient in front of the corresponding quadratic phase term $0 \times z^2_{\text{cluster}}$ in $\mathcal{H}_{LC}$. Quadratic terms would only be caused by presence of an inductor (or continuous chain of inductors) that allows charges to freely leave the cluster and go into the ground. However, by our definition of the cluster, such inductors cannot be present. It is then important to distinguish two types of coordinates: cyclic coordinates z_j^{cyc} for which no terms quadratic in z_j exist in $\mathcal{H}_{LC}\left(\vec{z},\vec{k}\right)$ and oscillatory z_j^{osc} coordinates for which finite quadratic z_j^2 terms do exist in $\mathcal{H}_{LC}\left(\vec{z},\vec{k}\right)$. When counting coordinates z_j we put cyclic coordinates first (smaller js) and oscillatory – last (larger js).

Coordinate transformation II: proper charge quantization. While diagonalization procedure described above "untangles" harmonic oscillators, it creates another issue. The problem is that the Josephson Hamiltonian $\mathcal{H}_{\text{jos}}$ written in terms of z_j,

$$\mathcal{H}_{\text{jos}} = -\sum_{\hat{\jmath}} E_{\hat{\jmath}} \cos(H_{\hat{\jmath}m} C^{-1/2}_{mk} U_{kj} z_j) \tag{7}$$

will now contain terms like $\cos(\{\text{prefactor}\} \times z_j)$ with a non-integer prefactor. That is not a problem for oscillatory coordinates because no periodicity in z_j^{osc} is expected anyway. However, cyclic coordinates are expected to show integer charge quantization. Hence, it is desirable to perform another coordinate transformation that would yield integer prefactors inside $\cos(\{\text{prefactor}\} \times z_j^{\text{cyc}})$ for cyclic coordinates and thus restoring integer charge quantization. Note that transformation II will yield oscillatory coordinates intact.

This transformation can be performed in the following way. Assume we have N^{tot} nodes and N^{cyc} clusters leading to $N^{\text{osc}} = N^{\text{tot}} - N^{\text{cyc}}$ oscillatory coordinates. Consider a matrix $M = HC^{-1/2}U$ from (7) that now determines prefactors in front of z_js inside cosines in $\mathcal{H}_{\text{jos}}$. This matrix has N_{jos} (number of Josephson junctions in the circuit) rows and N^{tot} columns. We can now split this matrix into a cyclic part and an oscillatory part

$$M = \left[\mathrm{M}^{\text{cyc}} \middle| \mathrm{M}^{\text{osc}}\right] \tag{8}$$

by allocating first N^{cyc} columns of M to create M^{cyc} and the rest – for M^{osc} (remember that we enumerated transformed coordinates z so that cyclic coordinates go first). Through multiple numerical experimentations with various M^{cyc} we found out that it has a following curious property. If we create a matrix m^{cyc} that consists only of linearly-independent rows of M^{cyc}, then division of one matrix by another $\mathrm{M}^{\text{cyc}}/\mathrm{m}^{\text{cyc}} = \mathrm{Z}^{\text{cyc}}$ results into a matrix Z^{cyc} that consists only of integers. Thus, M^{cyc} can be always written in the form

$$\mathrm{M}^{\mathrm{cyc}} = \mathrm{Z}^{\mathrm{cyc}}\mathrm{m}^{\mathrm{cyc}}. \tag{9}$$

We thereby split $\mathrm{M}^{\mathrm{cyc}}$ into a desired integer-valued part $\mathrm{Z}^{\mathrm{cyc}}$ with dimensions $N_{\mathrm{jos}} \times N^{\mathrm{cyc}}$ and square invertible matrix $\mathrm{m}^{\mathrm{cyc}}$. In short, $\mathrm{m}^{\mathrm{cyc}}$ is the largest invertible submatrix of $\mathrm{M}^{\mathrm{cyc}}$. Matrix $\mathrm{m}^{\mathrm{cyc}}$ acts on cyclic coordinates $\vec{z}^{\mathrm{cyc}}$ and hence is required to have dimensions of $N^{\mathrm{cyc}} \times N^{\mathrm{cyc}}$. It is critical to note that in order to be able to extract $\mathrm{m}^{\mathrm{cyc}}$ from $\mathrm{M}^{\mathrm{cyc}}$, the number of Josephson junctions N_{jos} (i.e. number of rows in $\mathrm{M}^{\mathrm{cyc}}$) should not be less than the number of clusters N_{cyc} (i.e. number of columns in $\mathrm{M}^{\mathrm{cyc}}$). This can be guaranteed by connecting all clusters with the ground via Josephson junctions even if Josephson energies of those junctions are zero. Physical significance of these ad-hoc junctions is that they provide the measure for the unit of charge $2e = 1$ and thereby enforce integer charge quantization on clusters (Fig. 1). Otherwise, the proper charge unit in this formalism will not be properly defined.

Finally, we perform the desired transformation only on cyclic coordinates, leaving oscillatory coordinates intact:

$$\vec{v}^{\mathrm{cyc}} = \mathrm{m}^{\mathrm{cyc}}\vec{z}^{\mathrm{cyc}}. \tag{10}$$

Thus, inside the cosines of $\mathcal{H}_J$ we obtain values

$$\left[\left[\mathrm{M}^{\mathrm{cyc}}\middle|\,\mathrm{M}^{\mathrm{osc}}\right]\begin{pmatrix}\vec{z}^{\mathrm{cyc}}\\ \vec{z}^{\mathrm{osc}}\end{pmatrix}\right]_{\widehat{J}} = \left[\left[\mathrm{Z}^{\mathrm{cyc}}\middle|\,\mathrm{M}^{\mathrm{osc}}\right]\begin{pmatrix}\vec{v}^{\mathrm{cyc}}\\ \vec{z}^{\mathrm{osc}}\end{pmatrix}\right]_{\widehat{J}} = \mathrm{Z}^{\mathrm{cyc}}_{\widehat{J}_j} v_j^{\mathrm{cyc}} + \mathrm{M}^{\mathrm{osc}}_{\widehat{J}_j} z_j^{\mathrm{osc}} \tag{11}$$

yielding only integer prefactors in front of our new cyclic coordinates v_j^{cyc}. Thus, our final set of coordinates is

$$\begin{pmatrix}\vec{v}^{\mathrm{cyc}}\\ \vec{z}^{\mathrm{osc}}\end{pmatrix} = \begin{pmatrix}\mathrm{m}^{\mathrm{cyc}} & 0\\ 0 & 1\end{pmatrix}\vec{z} = \begin{pmatrix}\mathrm{m}^{\mathrm{cyc}} & 0\\ 0 & 1\end{pmatrix} U^T C^{1/2}\vec{\phi} \tag{12}$$

In this case the LC part of the Hamiltonian reads:

$$\mathcal{H}_{LC} = \sum_{j,k=1}^{N^{\mathrm{cyc}}} \frac{1}{2}\left(\mathrm{c}^{\mathrm{cyc}}\right)^{-1}_{jk} q_j^{\mathrm{cyc}} q_k^{\mathrm{cyc}} + \frac{1}{2}\sum_{j=N^{\mathrm{tot}}-N^{\mathrm{osc}}}^{N^{\mathrm{tot}}} \left\{\left(k_j^{\mathrm{osc}}\right)^2 + \left(\omega_j z_j^{\mathrm{osc}}\right)^2\right\}. \tag{13}$$

Here $\vec{q}^{\mathrm{cyc}} = -i\partial/\partial\vec{v}^{\mathrm{cyc}}$ and $(\mathrm{c}^{\mathrm{cyc}})^{-1} = \mathrm{m}^{\mathrm{cyc}}(\mathrm{m}^{\mathrm{cyc}})^T$. The Josephson part of the Hamiltonian yields:

$$\mathcal{H}_{\mathrm{jos}} = -\mathrm{Re}\sum_{\widehat{J}=1}^{N_{\mathrm{jos}}} E_{\widehat{J}} \exp\left\{i\mathrm{Z}^{\mathrm{cyc}}_{\widehat{J}_j} v_j^{\mathrm{cyc}}\right\} \exp\left\{i\mathrm{M}^{\mathrm{osc}}_{\widehat{J}_j} z_j^{\mathrm{osc}}\right\}. \tag{14}$$

Inclusion of flux and charge offsets. In order to include flux and charge offsets Φ_K and Q_j we substitute $G_{\widetilde{K}k}\phi_k \to G_{\widetilde{K}k}\phi_k - \Phi_{\widetilde{K}}$ and $n_j \to n_j - Q_j$.

After corresponding coordinate transformations the Josephson Hamiltonian (14) needs to be modified via substitutions

$$E_{\hat{\jmath}} \to E_{\hat{\jmath}} \exp\left(iF_{\hat{\jmath}}\right); \tag{15}$$

and LC Hamiltonian (13) – via substitution

$$\begin{pmatrix} \vec{q}^{\,\mathrm{cyc}} \\ \vec{k}^{\,\mathrm{osc}} \end{pmatrix} \to \begin{pmatrix} \vec{q}^{\,\mathrm{cyc}} \\ \vec{k}^{\,\mathrm{osc}} \end{pmatrix} - \begin{pmatrix} (\mathrm{m}^{\mathrm{cyc}})^{-T} & 0 \\ 0 & 1 \end{pmatrix} U^T C^{-1/2} \vec{Q}. \tag{16}$$

Here $\vec{F} = H(G\backslash\vec{\Phi})$ with "\" denoting left division of matrices. We denote the second term in (16) as $\vec{K} = \mathrm{diag}\left\{(\mathrm{m}^{\mathrm{cyc}})^T, 1\right\} U^T C^{-1/2}\vec{Q}$. To sum up, the final Hamiltonian after all transformations reads:

$$\begin{aligned} \mathcal{H} = \;& \tfrac{1}{2}\left[(\mathrm{m}^{\mathrm{cyc}})^T\left(\vec{q}^{\,\mathrm{cyc}} - \vec{K}^{\mathrm{cyc}}\right)\right]^2 + \tfrac{1}{2}\left[\left(\vec{k}^{\,\mathrm{osc}} - \vec{K}^{\mathrm{osc}}\right)^2 + (\omega^{\mathrm{osc}}\vec{z}^{\,\mathrm{osc}})^2\right] - \\ & -\mathrm{Re}\sum\nolimits_{\hat{\jmath}=1}^{N_{\mathrm{JOS}}} E_{\hat{\jmath}} e^{iF_{\hat{\jmath}}} \exp\left\{iZ^{\mathrm{cyc}}_{\hat{\jmath}_j} v_j^{\mathrm{cyc}} + i\mathrm{M}^{\mathrm{osc}}_{\hat{\jmath}_j} z_j^{\mathrm{osc}}\right\} \end{aligned} \tag{17}$$

Quantizing the Hamiltonian. This Hamiltonian can now be easily quantized by substituting generalized coordinate variables with finite matrices. After that the eigenvelues and eigenvectors of the Hamiltonian can be found numerically. It is convenient to use the following basis: we calculate matrix elements of the oscillatory part of the Hamiltonian using harmonic oscillator eigenvectors and matrix elements of the cyclic part of the Hamiltonian – using charge state eigenvectors, i.e. plane waves in the phase space:

$$\left|\mathbf{p}_1^{\mathrm{cyc}} \cdots \mathbf{p}_{N^{\mathrm{cyc}}}^{\mathrm{cyc}} \mathbf{p}_{N^{\mathrm{cyc}}+1}^{\mathrm{osc}} \cdots \mathbf{p}_{N^{\mathrm{tot}}}^{\mathrm{osc}}\right\rangle = \bigotimes_{j=1}^{N^{\mathrm{cyc}}} |\mathbf{p}_j; \mathrm{cyc}\rangle \bigotimes_{j=N^{\mathrm{cyc}}+1}^{N^{\mathrm{tot}}} |\mathbf{p}_j; \mathrm{osc}\rangle\,. \tag{18}$$

Here the eigenvectors in the phase representation are as follows:

$$\langle v_j\,|\mathbf{p}_j; \mathrm{cyc}\,\rangle = (2\pi)^{-1/2}\exp\left(i\mathbf{p}_j v_j\right); \tag{19}$$

natural for charge-quantized clusters and

$$\langle z_j\,|\mathbf{p}_j; \mathrm{osc}\,\rangle = i^{\mathbf{p}_j} e^{-iK_j\phi_j}\omega_j^{1/4}\Psi_{\mathbf{p}_j}\left(\sqrt{\omega_j}z_j\right). \tag{20}$$

natural for oscillatory coordinates (no summation over repeating js).

Bold indexes $\mathbf{n}_j$ count quantum states corresponding to the j-th generalized coordinate and $\Psi_{\mathbf{p}}$ is the harmonic oscillator eigenfunction $\Psi_{\mathbf{p}}(x) = \pi^{-1/4}(2^m\mathbf{p}!)^{-1/2}\exp(-x^2/2)\mathrm{H}_{\mathbf{p}}(x)$. Note that (20) prescribes specific width for each oscillator eigenfunction according to the oscillator mode impedance.

After choosing a finite number $\mathbf{p}_j^{\max}$ of eigenfunctions for each j-th coordinate the LC Hamiltonian $\mathcal{H}_{LC}$ is diagonalized automatically. Cyclic charge operator q_j is substituted with

$$\hat{q}_j^{\rm cyc} \approx 1_1 \otimes 1_2 \otimes ... \otimes 1_{j-1} \otimes \hat{\boldsymbol{N}}_j^{\rm cyc} \otimes 1_{j+1} \otimes ... \otimes 1_{N^{\rm tot}}. \qquad (21)$$

Here 1_k is a $\mathbf{p}_j^{\max} \times \mathbf{p}_j^{\max}$ identity matrix and $\hat{\boldsymbol{N}}_j^{\rm cyc}$ is a charge number operator $\hat{\boldsymbol{N}}_j^{\rm cyc} = {\rm diag}\{-\mathbf{p}_j^{\max}, -\mathbf{p}_j^{\max}+1, .., -1, 0, 1, ...\mathbf{p}_j^{\max}\}$. Matrices approximating quantum operators shall be written as capital bold letters with a 'hat' $(\hat{\boldsymbol{N}}, \hat{\boldsymbol{V}}, ...)$. Oscillatory modes are substituted as

$$\frac{1}{2}\left(\hat{k}_j^{\rm osc} - K_j^{\rm osc}\right)^2 + \frac{1}{2}\omega_j^2 \left(\hat{z}_j^{\rm osc}\right)^2 \approx \omega_j 1_1 \otimes ... \otimes \hat{\boldsymbol{N}}_j^{\rm osc} \otimes ... \otimes 1_{N^{\rm tot}}. \qquad (22)$$

No summation implied here. The offset $K_j^{\rm osc}$ is included in the definition of eigenfunction (20) and $\hat{\boldsymbol{N}}_j^{\rm osc}$ is an oscillator number operator $\hat{\boldsymbol{N}}_j^{\rm osc} = {\rm diag}\left\{0, 1, ..., \mathbf{p}_j^{\max}\right\}$. While charge number operators $\hat{\boldsymbol{N}}^{\rm cyc}$ count cooper pairs, oscillator number operators $\hat{\boldsymbol{N}}^{\rm osc}$ count photons of oscillator modes.

Thus, we have decoupled charge and oscillator number operators and $\mathcal{H}_{\rm jos}$ acts as an interaction Hamiltonian. In order to evaluate $\mathcal{H}_{\rm jos}$ of (14,17) one needs to calculate matrix elements of exponential operators $\exp\{i{\rm Z}^{\rm cyc}_{\widehat{J}_j} v_j^{\rm cyc}\}$ and $\exp\{i{\rm M}^{\rm osc}_{\widehat{J}_j} v_j^{\rm osc}\}$ (no summation implied). For the cyclic coordinates the matrix elements are:

$$\hat{\boldsymbol{V}}_{\mathbf{pr}}^{(\widehat{J},j)} = \left\langle \mathbf{p}_j; {\rm cyc} \left| \exp\left\{ i{\rm Z}^{\rm cyc}_{\widehat{J}_j} v_j^{\rm cyc} \right\} \right| \mathbf{r}_j; {\rm cyc} \right\rangle = \left\{ \begin{array}{ll} 1 & , \mathbf{p}-\mathbf{r} = Z^{\rm cyc}_{\widehat{J}_j} \\ 0 & , {\rm otherwise} \end{array} \right. . \qquad (23)$$

Again, no summation over j is implied here. The matrix elements $\hat{\boldsymbol{V}}_{\mathbf{pr}}^{(\widehat{J},j)} = \langle \mathbf{p}_j; {\rm osc}| \exp\{i{\rm M}^{\rm osc}_{\widehat{J}_j} z_j^{\rm osc}\} |\mathbf{r}_j; {\rm osc}\rangle$ for oscillatory eigenfunctions $|\mathbf{p}; {\rm osc}\rangle$ cannot be simplified in the same way and have to be obtained numerically. However, a slightly simpler expression is possible for $\hat{\boldsymbol{V}}$-matrices in oscillatory coordinates:

$$\hat{\boldsymbol{V}}_{\mathbf{pr}}^{(\widehat{J},j)} = (-1)^{\mathbf{r}} \sum_{\mathbf{s}=0}^{\min(\mathbf{p},\mathbf{r})} (-1)^{\mathbf{s}} \frac{\sqrt{\mathbf{p}!\mathbf{r}!}}{\mathbf{s}!(\mathbf{p}-\mathbf{s})!(\mathbf{r}-\mathbf{s})!} \left(\frac{Q}{\sqrt{2}}\right)^{\mathbf{p}+\mathbf{r}-2\mathbf{s}} e^{-Q^2/4} \qquad (24)$$

with $Q = {\rm M}^{\rm osc}_{\widehat{J}_j} \omega_j^{-1/2}$ (no summation implied). Note that i^m-prefactor for the harmonic oscillator eigencfunctions in (20) was intentionally introduced to keep corresponding $\hat{V}$-matrices non-hermitian but real-valued. Without $i^{\mathbf{p}}$-prefactor for oscillator eigenfunctions, prefactor in (24) would be $i^{\mathbf{p}+\mathbf{r}}$ instead of $(-1)^{\mathbf{r}}$. Expression (24) is obtained by re-writing matrix element in the charge basis (which results in an expression for convolution of two harmonic oscillator functions) and then using property ${\rm H}_{\mathbf{p}}(x+y) = \sum_{\mathbf{s}=0}^{\mathbf{p}} C_{\mathbf{p}}^{\mathbf{s}} {\rm H}_{\mathbf{s}}(x)(2y)^{\mathbf{p}-\mathbf{s}}$ of Hermite polynomials (here $C_{\mathbf{p}}^{\mathbf{s}}$ are binomial coefficients $\mathbf{p}$ choose $\mathbf{s}$).

The Josephson Hamiltonian then becomes:

$$\mathcal{H}_{\text{jos}} \approx -\frac{1}{2}\sum_{\hat{\jmath}} e^{iF_{\hat{\jmath}}} E_{\hat{\jmath}} \bigotimes_{j=1}^{N^{\text{tot}}} \hat{\boldsymbol{V}}^{(\hat{J},j)} + (h.c.). \tag{25}$$

The total Hamiltonian is then

$$\mathcal{H} \approx \sum_{j,k=1}^{N^{\text{cyc}}} \frac{1}{2} \left(\mathrm{c}^{\text{cyc}}\right)^{-1}_{jk} \left(\hat{\boldsymbol{N}}_j^{\text{cyc}} - K_j\right)\left(\hat{\boldsymbol{N}}_k^{\text{cyc}} - K_k\right) +$$

$$+ \sum_{j=N^{\text{tot}}-N^{\text{osc}}}^{N^{\text{tot}}} \omega_j \left(\hat{\boldsymbol{N}}_j^{\text{cyc}} + \frac{1}{2}\right) + \mathcal{H}_{\text{jos}}. \tag{26}$$

Choosing number of eigenstates. Since the cost of numerical calculations grows exponentially with the number of nodes it is critical to have a minimal but sufficient number of eigenstates to represent each coordinate. In order to do that, for oscillatory coordinates, we want to make sure that there are enough eigenfunctions to adequately model the cosine ripples superimposed onto the harmonic oscillator potential because of the Josephson Hamiltonian. Thus, for j-th coordinate the quasiperiod of the highest $\mathbf{p}_j^{\max}$-th oscillatory eigenfunction has to be mush shorter than $1/\max(\mathrm{M}^{\text{osc}}_{\hat{J}_j})$ – the period of the "quickest" cosine containing z_j^{osc} in the Josephson Hamiltonian. Number of cyclic eigenfunctions needs to be large enough to approximate Mathieu functions with characteristic widths of $\sim \min\{\mathrm{c}_{jk}\}/\max\{E_{\hat{\jmath}}\}$.

Additionally, often we want to model devices that include dc-SQUIDs. In our approach fluxes can only be inserted into inductances. Thus to describe a flux-tunable dc-SQUID it is insufficient to have two Josephson junctions in parallel – an infinitesmall inductance has to be inserted in the loop. Introduction of such inductance will create an additional node and additional high frequency mode $\omega_j^{\text{high-freq.}}$. However since the first excited state of a corresponding oscillator mode will be high, it is sufficient to take only one lowest eigenfunction for such coordinate. Thus, introduction of infinitesmall inductances in the circuit comes at no computational cost. Note that it is important to match small inductance and parasitic capacitance of this ad-hoc inductor so that $L^{\text{small}}/C^{\text{parasit}} \to 0$ to avoid quantum phase fluctuations across the inductor. Such additional coordinates shall be called "classical".

Addendum: Transformation III. Although transformations above are sufficient for numerical modeling or analytical treatment of superconducting circuits, they contain an unpleasant unit mismatch between unitless transformed cyclic coordinates $\{v_j^{\text{cyc}}\}$ and oscillatory coordinates $\{z_j^{\text{osc}}\}$ that have dimensions of $[\omega_j^{-1/2}]$. It is easy to get rid of this mismatch by switching oscillatory coordinates to

$$v_j^{\text{osc}} = \omega_j^{1/2} z_j^{\text{osc}} \tag{27}$$

(no summation). In vector form that reads: $\vec{v}^{\rm osc} = \omega^{\rm osc}\vec{z}^{\rm osc}$. In this case the Hamiltonian (without flux or charge biases) reads:

$$\mathcal{H} = \sum_{j,k=1}^{N^{\rm cyc}} \frac{1}{2}\left(\mathrm{c}^{\rm cyc}\right)^{-1}_{jk} q_j^{\rm cyc} q_k^{\rm cyc} + \sum_{j=N^{\rm tot}-N^{\rm osc}}^{N^{\rm tot}} \frac{\omega_j}{2}\left\{\left(q_j^{\rm osc}\right)^2 + \left(v_j^{\rm osc}\right)^2\right\} -$$

$$-{\rm Re}\sum_{\widehat{\jmath}=1}^{N_{\rm jos}} E_{\widehat{\jmath}} \exp\left\{ i \sum_j M^{\rm (III)}_{\widehat{\jmath}j} v_j \right\}. \tag{28}$$

Here $q_j^{\rm osc} = -i\partial/\partial v_j^{\rm osc}$ and

$$M^{\rm (III)}_{\widehat{\jmath}j} = \left[\mathrm{Z}^{\rm cyc} \middle| \mathrm{M}^{\rm osc} (\omega^{\rm osc})^{-1/2} \right]. \tag{29}$$

The final coordinate transformation reads:

$$\vec{v} = \begin{pmatrix} \mathrm{m}^{\rm cyc} & 0 \\ 0 & \sqrt{\omega^{\rm osc}} \end{pmatrix} U^T C^{1/2} \vec{\phi}. \tag{30}$$

This transformation can also be used to introduce external flux and charge biases.

Momentum transformation reads:

$$\vec{q} = \begin{pmatrix} (\mathrm{m}^{\rm cyc})^{-T} & 0 \\ 0 & (\omega^{\rm osc})^{-1/2} \end{pmatrix} U^T C^{-1/2} \vec{n}. \tag{31}$$

These transformations render final coordinates $\vec{v}$ unitless.

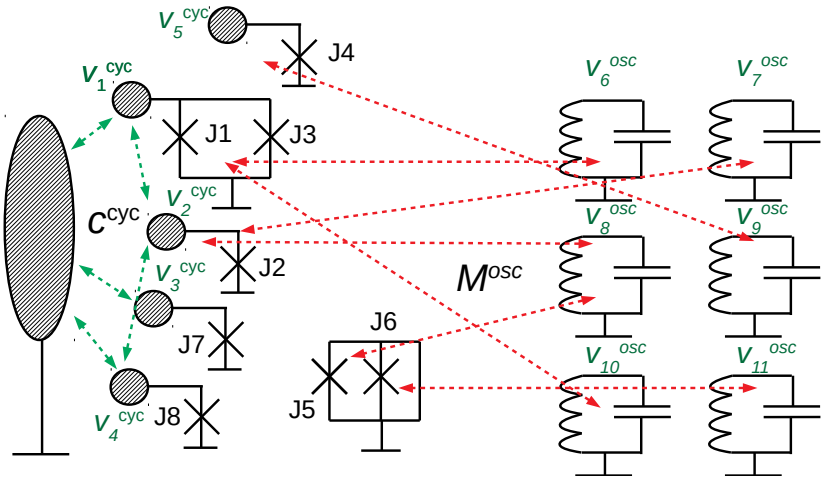

Figure 2. Circuit described in Figure 1 re-drawn. Shaded circles/ovals represent capacitor pads that couple to the ground (big oval pad on the left) and to each other creating capacitance matrix $\mathrm{c}^{\mathrm{cyc}}$ for cyclic coordinates. Green double-sided arrows represent capacitive coupling between the pads. Left part of the circuit represents Josephson junction part of the Hamiltonian along with capacitive interaction between cyclic degrees of freedom. Right part of the figure represents Hamiltonian of the harmonic oscillators that are inductively coupled to the Josephson junctions (red arrows). Particularly, Josephson junctions J1,2,3,4,7,8 along with capacitor pads form the cyclic part of the Hamiltonian. Number of capacitor pads corresponds to the number of charge clusters in the original circuit. In order to figure out which Josephson junctions correspond to which pad, one needs to look at non-zero elements of matrix $\mathrm{Z}^{\mathrm{cyc}}_{\hat{J}_j}$: Josephson junctions $\hat{J}_1$ and $\hat{J}_3$ should be connected to the same pad (i.e. cyclic coordinate) j iff $\hat{J}_1$'th and $\hat{J}_3$'th rows of $\mathrm{Z}^{\mathrm{cyc}}_{\hat{J}_j}$ contain non-zero value in the j'th position. Josephson junctions J5,6 form a closed flux-sensitive loops where these junctions are shorted to the ground and their energy is only defined by magnetic fields due to other coordinates. Cyclic and oscillatory coordinates are denoted as v_j^{cyc} and v_j^{osc}.

Conclusions. We demonstrated a rigid formalism that allows to write a Hamiltonian of any superconducting circuit in terms of two types of variables: cyclic variables that obey charge quantization and are associated with superconducting charge islands and oscillatory variables that are associated with inductors in the circuit and behave lake (an)harmonic oscillators. In essence using this formalism we effectively "pull" the inductors out of the circuit. For example, applying our formalism to the circuit described in Fig. 1, The Hamiltonian is split into a cyclic part consisting of Josephson junctions interacting through a cyclic capacitance matrix $\mathrm{c}^{\mathrm{cyc}}$ and oscillatory part consisting of harmonic oscillator which interact with Josephson junctions via mutual inductances $\mathrm{M}^{\mathrm{osc}}$. This allows to redraw the circuit in the form as shown in Figure 2. This equivalent circuit has same number of nodes and loops as the original circuit. In fact, any circuit can be reduced to such universal form. Any circuit can be represented as consisting of three types of elements: (i) cascades of Josephson junctions capacitively coupled with the ground and between each other, (ii)

cascade of Josephson junctions shorted to the ground forming a flux-sensitive loop and (iii) Harmonic oscillators that are inductively coupled to the Josephson junctions. This allows for automatic optimization of numeric modeling of the circuit and for more abstract view of that circuit.

Contributions. Andrey R. Klots developed the formalism and implemented it as a SuperQuant python package. Lev B. Ioffe supervised the project.

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