Inter-qubit interaction mediated by collective modes in a linear array of three-dimensional cavities

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Abstract
A design of LEGO-like construction set that allows assembling of different linear arrays of three-dimensional (3D) cavities and qubits for circuit quantum electrodynamics experiments has been developed. A study of electromagnetic properties of qubit-3D cavity arrays has been done by using high frequency structure simulator (HFSS). A technique for estimation of inter-qubit coupling strength between qubits embedded in different cavities of cavity array, which combines Hamiltonian description of the system with simple HFSS simulations, has been proposed. A good agreement between inter-qubit coupling strengths, which were obtained by using this technique and directly from simulation, demonstrates the suitability of the method for more complex qubit–cavity arrays where usage of finite-element electromagnetic simulators is limited.

1. Introduction

Circuit quantum electrodynamics (cQED) studies light–matter interaction between an artificial atom (qubit) and a coplanar or three-dimensional (3D) waveguide cavity. Nowadays, cQED is widely used in quantum computation [1–8] and quantum simulation [9, 10] where qubit and cavity serve as building blocks for creating complex qubit–cavity arrays. In most of these arrays, preference has been given to on-chip coplanar cavities that facilitate scalability of the sample. However, coplanar cavities have low mode volume and surrounded by different sources of energy dissipation due to the wiring, substrate, radiation etc. In addition, a dense location of elements on a chip leads to appearance of unwanted crosstalk [6]. All these factors hinder measurement and affect qubit performance. A good alternative to coplanar cavity is 3D cavity, which has much higher mode volume and makes the qubit better isolated from the environment. As a result, qubits in 3D cavity demonstrate a significant improvement in lifetimes [11, 12]. In view of this, investigation of qubit-3D cavity arrays is of high scientific relevance.

One of the challenges in qubit-3D cavity arrays is to provide a good coupling between qubits embedded in different cavities of array. Ideally, many properties of the qubit–cavity arrays, including inter-qubit coupling, could be predicted even before sample fabrication by using finite-element electromagnetic simulator such as high frequency structure simulator (HFSS) [13] and black box quantization technique (BBQ) [14–16]. Although this method proposes a very accurate calculation of the energy spectrum of a system, it requires a finite-element simulation of the entire structure for extracting an impedance of the linear part of the circuit. However, with an increase of complexity of simulated model (e.g. introducing additional cavities and qubits into array), the HFSS simulation becomes more time- and resource-consuming. This disadvantage can lead to the limits where HFSS simulation could be applied, forcing us to search a new solution of the problem.

In the past, several methods for control of inter-qubit coupling were proposed theoretically [17–30] and realized experimentally [31–35]. Some of them require only rf pulses [17–20] to control an inter-qubit coupling strength while others, besides dc or rf pulses, require an additional circuit element such as inductance [21, 22], Josephson junction (JJ) [23–25, 31, 32], another qubit [26, 27, 33], qutrit [28] or cavity bus [29, 30, 34, 35]. The later mediates a coupling between distant qubits via exchange of a virtual
For qubits located in different cavities of qubit-3D cavity array, this is the dominant mechanism of the inter-qubit coupling. At the same time, when two or more identical cavities are coupled, their individual resonant frequencies are transforming in to the collective oscillations of the coupled system, which are called normal modes. In cavity array that consists of \( N \) identical cavities, there would be \( N \) normal modes in the vicinity of corresponding resonant frequency of the single cavity. Thus, for qubits located in different cavities of qubit–cavity array, inter-qubit coupling could be mediated by those normal modes. Inter-qubit coupling mediated by normal modes of 3 coupled coplanar resonators was studied in [36] where Hamiltonian describing the system was proposed. According to it, inter-qubit coupling depends on coupling strength between qubits and cavities to which they are directly coupled, detuning between qubits and cavity mode that mediates the coupling and on inter-cavity coupling strength. It turns out that these parameters could be found from a series of HFSS simulations involving simple models, which consist of one or two cavities and only one qubit (if necessary). Knowing these parameters, we can diagonalize Hamiltonian and estimate inter-qubit coupling strength. In this case, we avoid simulation of the entire qubit-3D cavity array, significantly simplifying calculation of the energy spectrum of the system.

In this paper, we have developed qubit-3D cavity arrays for realizing cQED experiments and studied their electromagnetic characteristics by using HFSS. Based on Hamiltonian proposed in [36] and simulated data, inter-qubit coupling for qubits located in different cavities of 3 coupled 3D cavities was found. These values were compared with inter-qubit coupling, which was obtained directly from HFSS simulations of the qubit-3D cavity array. A good agreement between both results demonstrates a perspective to use this approach for estimation of the inter-qubit coupling in more complex qubit–cavity arrays where usage of finite-element electromagnetic simulators is limited.

2. Methods

Figures 1(a) and (b) show a possible assembly of linear 3D cavity array for cQED experiments. The structure consists of five coupled cavities (cavity 1–5) and five chips with qubits (Q1–Q5) inside of each cavity of the array. The base element of the assembly is metallic plate with a square pit. The cavities are formed by stacking the plates one by one. The inner plates of the array have a hole (coupler), which provides coupling with a neighboring cavity. Each terminated plate of the array has two holes where SMA ports (port 1–4) for generation and readout microwave signals could be installed. The structure allows an easy way to assemble many different combinations of linear qubit–cavity arrays, like in a LEGO construction set. This feature is very useful for quantum simulations of one-dimensional lattices [10] where adding or subtracting elements in the chain could be done without affecting properties of the rest of the structure.

Electromagnetic properties of qubit-3D cavity arrays were studied by using HFSS software. For this purpose, different 3D models of either single cavity or cavity arrays were built. In all models, cavities have the shape of a cuboid with width and length of 35 mm \( \times \) 35 mm. These dimensions were chosen in order to obtain resonant frequency of transverse electric fundamental mode for individual cavity (TE101) equal to 6...
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Figure 2. (a) S41-parameters for 2- (bottom), 3- (middle) and 5-cavity arrays (top) with h1 cavity height. For clarity, middle and top S41-parameters are shifted by 50 dB and 140 dB upwards, respectively. (b) Dependence of inter-cavity coupling strength γ on coupler diameter d for h1 (solid circles) and h2 (open circles) cavity heights in 2-cavity array. Solid and dashed lines are fitting functions of γ(d) = αd^4 with α = 11.7 kHz mm^-4 and α = 6.6 kHz mm^-4 for h1 and h2, respectively.

GHz. Cavity arrays with cuboid height either h1 = 1.5 mm or h2 = 3 mm were studied. The cavity array with h1 was used only for obtaining data presented in figure 2. For all other cases, cavities with h2 were simulated. Small cuboid heights were chosen in order not to take much space when plates are stacking up and high enough for installation of a real substrate into the cavity. The thickness of the inner wall between adjacent cavities was equal either to 1.5 mm or 2 mm for h1 or h2 cavity heights, respectively. The diameter of the holes for measurement ports was equal to 2.9 mm and their center-to-center distance was equal to 24 mm. Space inside the structure was assigned as a vacuum while all the walls were assigned as a perfect conductor. The holes on the surface of terminated cavities were assigned as wave ports according to notations in figures 1(a) and (b). The appropriate coupler hole diameter (d) and position were subjects of study and they were chosen depending on simulation. The coupler position is described by (x, y) coordinates in the units of (mm, mm) according to the coordinate system in figure 1(b), i.e. (0, 0) coordinates correspond to the position of the coupler at the cavity center. The coordinates were changed only in the first quadrant of the cavity array due to the symmetry of the structure.

In order to simulate qubit behavior, a 3D model, which is shown in figures 1(c) and (d), was placed inside the cavity. The structure was built by using patch objects and consists of two paddles of dipole antenna, which are well seen in figure 1(c). The pads dimensions are typical for transmon qubit [37] in 3D cavity experiments [11]. The shunt capacitance between antenna pads can be also used for realizing flux qubits with low decoherence [38]. For obtaining impedance (admittance) data of simulated system, a square patch at the antenna feeding point was assigned as a lumped port (LP). A linear part of JJ was simulated by assigning a square patch, connected in parallel to the antenna feeding point, as a parallel LC circuit (LC). LP and LC were connected by two parallel patches. Isometric view of the feeding point of the dipole antenna is depicted in figure 1(d). The JJ capacitance cJ was constant and equal to 10 fF. This value corresponds to the total capacitance of two parallel JJs that form qubit’s SQUID loop with cJ = 5 fF for each junction, which is typical value for the 3D transmon [14]. The qubit resonant frequency was changed by sweeping LC inductance L. All patches, except LC and those connecting it with antenna feeding point, were located on the surface of a substrate with dimensions of 3.5 mm × 7 mm × 0.65 mm. The material of all qubit patches was assigned as a perfect conductor while material of the substrate as a sapphire. If the number of qubits was less than the number of cavities in array, blank substrates without qubit were installed into the rest of the cavities.

3. Inter-cavity coupling

For providing a good coupling between cavities, cavity arrays with different diameters and positions of the coupler were simulated. Figure 2(a) shows S41-parameters data that were obtained from driven modal simulation of 2-, 3- and 5-cavity arrays with h1 cavity height, without qubit and substrate inside. The diameter of the coupler for all arrays was d = 6 mm with (0, 0) coordinates. As is seen, S41-parameters have 2, 3 and 5 resonant peaks for 2-, 3- and 5-cavity arrays, respectively. These peaks correspond to normal mode resonances of cavity array and their frequencies are denoted as ω_Nk, where N is the number of cavities in array and k = 1, . . . , N is the mode index.

In order to study inter-cavity coupling strength, both eigenmode and driven modal simulations of 2- and 3-cavity arrays were done, from which corresponding normal mode frequencies ω21, ω22, ω31, ω32 and
\(\omega_{33}\) were found. A linear array of \(N\) coupled cavities can be described by the many-particle Hamiltonian:

\[
H_N = \sum_{j=1}^{N} \omega_j a_j^\dagger a_j + \sum_{j=1}^{N-1} \gamma_{j+1} \left( a_{j+1}^\dagger a_j + a_j a_{j+1}^\dagger \right),
\]

(1)

in which \(\omega_j\) is the intrinsic cavity frequency of cavity \(j\), and \(\gamma_{j+1}\) are the inter coupling strength between cavity \(j\) and \(j+1\). \(a_j\) and \(a_j^\dagger\) are the annihilation and creation operators of the photons in cavity \(j\). Because the model is non-interacting, the energies of the many-particle system can be simply determined by the spectrum of a 1-particle system. For \(N = 2\) as an example, the 1-particle quantum states are \(|n_1, n_2\rangle = |1, 0\rangle\) and \(|0, 1\rangle\), in which \(n_j\) is the photon number in cavity \(j\). Thus, for \(N = 2\) we can describe the system by the 2 \(\times\) 2 matrix:

\[
H_2 = \begin{pmatrix} \omega_1 & \gamma \\ \gamma & \omega_2 \end{pmatrix} \rightarrow \nu_k = \omega_{2k} \nu_k,
\]

(2)

in which \(\omega_{2k} = \omega_{21,22}\) are eigenmode frequencies of 2-cavity array associated to mode \(\nu_k\). From the spatial symmetry, we can assume that \(\omega_1 = \omega_2 = \omega\). Taking this into account, we can find intrinsic cavity frequency \(\omega\) and inter-cavity coupling strength \(\gamma\) as:

\[
\omega = \omega_{21} + \gamma = \omega_{22} - \gamma, \quad \gamma = (\omega_{22} - \omega_{21})/2.
\]

(3)

For 3-cavity array (\(N = 3\)), the 1-particle quantum states are \(|n_1, n_2, n_3\rangle = |1, 0, 0\rangle, |0, 1, 0\rangle\) and \(|0, 0, 1\rangle\) and the system can be described by the 3 \(\times\) 3 matrix:

\[
H_3 = \begin{pmatrix} \omega_1 & \gamma_{12} & 0 \\ \gamma_{12} & \omega_{2} & \gamma_{23} \\ 0 & \gamma_{23} & \omega_3 \end{pmatrix} \rightarrow \nu_k = \omega_{3k} \nu_k,
\]

(4)

in which \(\omega_{3k} = \omega_{31,32,33}\) are eigenmode frequencies of 3-cavity array associated to mode \(\nu_k\). Although all cavities in 3-cavity array have the same dimensions and should have identical intrinsic frequencies, the presence of the coupler changes the situation. Terminated cavities in a linear array with number of cavities \(N \geq 3\) have only one coupler while others cavities in array have two couplers. Also, in our design each terminated cavity has two holes for input/output microwave ports (see figures 1(a) and (b)), which we use for driven modal simulations. Hence, the intrinsic frequencies of the terminated cavities in the 3-cavity array \(\omega_1\) and \(\omega_3\) should be equal and different from that of the middle cavity \(\omega_2\). Therefore, in equation (4), we assume that \(\omega_1 = \omega_3\) and \(\gamma_{12} = \gamma_{23} = \gamma\). In this case, eigenmode frequencies could be expressed by using following formulas:

\[
\omega_{31} = \frac{1}{2} (\omega_1 + \omega_2 - \sqrt{(\omega_1 - \omega_2)^2 + 8\gamma^2}), \quad \omega_{32} = \omega_1, \quad \omega_{33} = \frac{1}{2} (\omega_1 + \omega_2 + \sqrt{(\omega_1 - \omega_2)^2 + 8\gamma^2}).
\]

(5)

The system of equation (5) has only two unknowns (\(\omega_2\) and \(\gamma\)), which can be easily determined.

In the beginning, dependence of inter-cavity coupling strength \(\gamma\) on diameter of the coupler \(d\) was studied in 2-cavity array. The cavities were empty and the coupler was located at the center of the structure ((0, 0) coordinates). The results of the \(\gamma\) calculation by using eigenmode simulation data and equation (3) for different coupler diameters \(d\) are shown in figure 2(b) as solid and open circles for \(h1\) and \(h2\), respectively. The error bars demonstrate maximum difference between eigenmode and driven modal simulations. As one can see in figure 2(b), \(\gamma\) has a power-law dependence on coupler diameter \(d\) and can be approximated by function \(\gamma(d) = \alpha d^\alpha\) with \(\alpha = 11.7\) kHz mm\(^{-4}\) (solid line) and \(\alpha = 6.6\) kHz mm\(^{-4}\) (dashed line) for \(h1\) and \(h2\), respectively.

The next step was to determine the position of the coupler where maximum inter-cavity coupling can be achieved. For this purpose, eigenmode simulations of 2- and 3-cavity arrays with fixed coupler diameter \(d = 6\) mm and different coupler positions were done. The coordinates of the coupler were changed only in the first quadrant of the cavity arrays due to symmetry of the structures. Inter-cavity coupling strengths were calculated by using results of simulations and equations (3) and (5). Figures 3(a) and (b) show dependences of inter-cavity coupling strength \(\gamma\) on coupler position in 2- and 3-cavity arrays. For both cases maximum values of \(\gamma\) can be achieved when the coupler is located either at the cavity center ((0, 0) coordinates) or close to the cavity walls ((0, 14) and (14, 0) coordinates). The dependence of the difference between intrinsic frequencies \(\omega_2 - \omega_1\) on coupler coordinates in 3-cavity array is shown in figure 3(c). It is seen that when the coupler is at the center of the cavity, \(\omega_2 > \omega_1\), whereas \(\omega_2 < \omega_1\) when the coupler is at the edge.
4. Electrical field distribution in the cavity array

For getting higher inter-cavity and correspondingly inter-qubit coupling, it is more logical to locate the coupler and qubit at the cavity center (0, 0), where usually TE101 mode of the single rectangular cavity has the maximum of electrical field (E-field). However, in this case the coupler hole destroys uniformity of E-field in the cavity center that might affect qubit-normal mode coupling. Therefore, the better choice would be to locate the coupler either at (0, 14) or (14, 0) coordinates while substrate with the qubit at the cavity center.

To study E-field, eigenmode simulations of 3-cavity array with coupler coordinates (0, 14) were done. Since the vector of E-field predominantly propagates along the cavity array structure, scalar values of only this component were retrieved and only from the centroid of the cavity cuboids where JJ of the qubit would be located. In HFSS, eigenmode E-field is always normalized to 1 V m\(^{-1}\), for which a stored energy \(W = 4 \times 10^{-18}\) J in the single cavity was found by using built-in calculator. For cQED experiments, the practical E-field should be rescaled to the single photon level by using the scaling law \(E \propto \sqrt{W}\). The single photon energy for TE101 cavity resonant frequency \((\omega/2\pi = 6\) GHz\) is \(W_{\text{ph}} = \hbar \omega = 4 \times 10^{-24}\) J, giving the single photon electric field in the order of \(10^{-3}\) V m\(^{-1}\). A bar chart with rescaled E-field for 3 normal modes in the cavities of 3-cavity array is presented in figure 4. Arrows over the bars demonstrate relative directions of the vector of E-field in each cavity of the array for corresponding mode.

It is seen from the bar chart that E-fields for each mode in the cavity 1 and 3 are almost identical, demonstrating a reflection symmetry of the structure. At the same time, E-field in the cavity 2 for mode 2 (\(\omega_{32}\)) is almost completely suppressed. The reason of such behavior is vectors of E-field in the cavity 1 and 3, which are approximately equal and directed in counter-phase towards each other, suppressing any excitations in the cavity 2, similar to the eigenmodes in coupled pendulums. Suppression of E-field inside different cavities of cavity array can be also found in arrays with number of cavities \(N > 3\). Thus, \(\omega_{32}\) mode cannot excite the transitions of the qubit located in the cavity 2, in other words, the qubit is darkened in respect to this mode. The evidence of the dark state appearance was observed during simulation of qubit in 3-cavity array (see section 6 and appendix B). However, the thorough investigation of the dark state was out of the scope of this paper.

5. Qubit–cavity coupling

In order to find qubit–cavity coupling strength \(g\), driven modal simulation of the single qubit in the single cavity was done. A qubit–cavity coupling strength can be easy determined from an avoided crossing of qubit and cavity resonances. In turn, the resonances of the system can be found from the zeros of imaginary part of admittance \(\text{Im} \ Y\) at the lumped port LP of the qubit. Figure 5(a) shows the imaginary part of admittance \(\text{Im} \ Y\) as a function of frequency at the lumped port LP of the qubit for \(L_J = 8\) nH. Zeros of \(\text{Im} \ Y\) correspond to resonant frequencies of either qubit or cavity and shown as red and blue open circles, respectively. An avoided crossing of qubit and cavity resonances was obtained by sweeping inductance \(L_J\) of LC circuit and extracting zeros of \(\text{Im} \ Y\), which are shown as blue and red dots in figure 5(b).

The qubit–cavity system could be described by the simple Jaynes–Cummings model [39]:

\[
H_{\text{ef}} = \omega a^\dagger a + \frac{\Delta}{2} \sigma_z + g (a^\dagger \sigma_- + a \sigma_+). \tag{6}
\]

Figure 3. Dependence of inter-cavity coupling strength \(\gamma\) on coupler coordinates \((x, y)\) in 2-cavity array (a) and in 3-cavity array (b). (c) The dependence of the difference between intrinsic frequencies \(\omega_2 - \omega_1\) on coupler coordinates \((x, y)\) in 3-cavity array. Each disc shows coupler position while its color shows corresponding value of the \(\gamma\) (a, b) or \(\omega_2 - \omega_1\) (c) according to the color scale bar. For both arrays, coupler diameter was \(d = 6\) mm and its position was changed only in the first quadrant of cavity array due to the symmetry of the structures.
Figure 4. Single photon E-field for 3 normal modes in the cavities of 3-cavity array with coupler coordinates (0, 14). E-field values were taken at the centroid of the cavity cuboids. The data represent only component of E-field which is propagating along the array (the main contributor to the total E-field). Arrows over the bars demonstrate relative directions of the vector of E-field.

Figure 5. (a) Dependence of imaginary part of admittance Im $Y$ on frequency at the lumped port LP of the qubit, which is located in the single cavity, for $L_J = 8 \text{nH}$. Zeros of Im $Y$ correspond to the cavity (blue open circle) and qubit (red open circle) resonances. (b) An avoided crossing of qubit and cavity resonances, which were obtained from Im $Y$ data by sweeping $L_J$. Zeros of Im $Y$ are shown as dots while data fitting with equation (7) as lines.

By using the similar approximation that was done in section 3, we can write the effective Hamiltonian with quantum states $|1; -\rangle$ and $|0; +\rangle$:

$$H_{qr} = \begin{pmatrix} \omega & g \\ g & q \end{pmatrix},$$

where $q$ is qubit frequency. Since the qubit is simulated by the LC patch, $q$ can be approximated by the standard formula for LC circuit resonance:

$$q = \frac{1}{2\pi \sqrt{c_{\Sigma} L_j}},$$

where $c_{\Sigma}$ is the total capacitance of the qubit–cavity system.

For $L_j = 8 \text{nH}$, qubit and cavity resonances are far detuned and have a small impact on each other. In this case, we can apply equation (8) for finding $c_{\Sigma}$. Thus, for $L_j = 8 \text{nH}$, qubit frequency $q = 6.368 \text{GHz}$, giving $c_{\Sigma} = 78 \text{fF}$. Knowing $c_{\Sigma}$, we can estimate charging energy as $E_C = e^2/(2c_{\Sigma}) = 0.248 \text{GHz}$. Josephson energy can be found as $E_J(\phi) = (\phi_0^2/2L_j \cos \phi)/L_j$, where $\phi$ is the phase difference across the junction, $\phi_0 = \hbar/(2e)$ is the reduced flux quantum. Since in our case $q \gg E_C$, and hence $E_J/E_C \gg 1$, the phase differences would be negligible and $\cos \phi \sim 1$. Therefore, $E_J$ can be approximated as $\phi_0^2/L_j = 20.433 \text{GHz}$. These values are similar to those of transmon qubit.

The eigenvalues of equation (7), where $g$ was a fitting parameter, are depicted as lines in figure 5(b). From the data fitting, the value of the qubit–cavity coupling strength $g = 110 \text{MHz}$. We should notice that an alternative method, which does not require any fitting parameters and based on HFSS data and BBQ model, gives the same value of $g$. More details about this method can be found in appendix A.
It was found that for such a simple model as the single cavity in the single qubit, it is easy to obtain a good convergence in simulations. Therefore, the same results can be obtained if instead of zeros of Im $Y$, we use poles of imaginary part of impedance Im $Z$. The comparison of Im $Y$ and Im $Z$ data is presented in appendix C.

6. Inter-qubit coupling in the qubit-3D cavity array

In order to study inter-qubit coupling in qubit-3D cavity array we have considered an array of 3 coupled 3D cavities with two qubits (Q1 and Q2) that were placed inside different cavities of the array. Without loss of generality, we investigated two configurations: nearest-neighbor (NN) and next-nearest-neighbor (NNN). In both configurations, Q1 was in cavity 1 while Q2 was either in cavity 2 for the NN or in cavity 3 for the NNN configurations.

Quantum electrodynamics in a linear array of $N$ coupled cavities could be described by using following Hamiltonian:

$$H = \sum_{j=1}^{N} \omega_j a_j^\dagger a_j + \sum_{j=1}^{N-1} \gamma_{jj+1} \left( a_{j+1}^\dagger a_j + a_j a_{j+1} \right) + \sum_{j=1}^{N} \frac{q_j}{2} \sigma_z + \sum_{j=1}^{N} g_j \left( a_j^\dagger \sigma_x^+ + a_j \sigma_x^- \right),$$  \hspace{1cm} (9)

in which the first two terms describe the photon energies, the third term describes qubit energies and the last term describes the qubit-photon interactions. $q_j$ and $g_j$ are respectively the qubit frequency and qubit–cavity coupling strength for the qubit placed in cavity $j$. $\sigma_x^+$ and $\sigma_x^-$ are the Pauli matrices. By noting qubit states as $Q = -$ and $Q = +$ for the ground and excited states, respectively, we can consider the 5 quantum states and truncate the others in the Fock space for NN and NNN configurations: $\{\{a\}; \{Q\} = |1, 0, 0; -,-\rangle, |0, 1, 0; -,-\rangle, |0, 0, 1; -,-\rangle, |0, 0, 0; +,-\rangle \text{ and } |0, 0, 0; --+,\}$.

With the 5 states, two $5 \times 5$ Hamiltonian matrices $H_{\text{NN}}$ and $H_{\text{NNN}}$ for NN and NNN configurations, respectively, were built:

$$H_{\text{NN}} = \begin{pmatrix}
\omega_1 & \gamma_{12} & 0 & g_1 & 0 \\
\gamma_{12} & \omega_2 & \gamma_{23} & 0 & g_2 \\
0 & \gamma_{23} & \omega_3 & 0 & 0 \\
g_1 & 0 & 0 & q_1 & 0 \\
g_2 & 0 & 0 & q_2 & 0
\end{pmatrix},$$  \hspace{1cm} (10)

$$H_{\text{NNN}} = \begin{pmatrix}
\omega_1 & \gamma_{12} & 0 & g_1 & 0 \\
\gamma_{12} & \omega_2 & \gamma_{23} & 0 & 0 \\
0 & \gamma_{23} & \omega_3 & 0 & g_2 \\
g_1 & 0 & 0 & q_1 & 0 \\
g_2 & 0 & 0 & q_2 & 0
\end{pmatrix},$$  \hspace{1cm} (11)

Here $\omega_j$ is intrinsic frequency of cavity $j$, $q_1(q_2)$ is resonant frequency of Q1(Q2), $\gamma$ is the inter-cavity and $g_1(q_2)$ is Q1(Q2)-cavity coupling strengths.

Based on geometric features of our structure, the following assumptions can be made: (1) $\gamma_{12} = \gamma_{23} = \gamma$ due to the identity of the coupler between cavities, (2) $g_1 = g_2 = g$ due to the identity of Q1 and Q2. (3) In order to simplify our model we can ignore an impact of the coupler and assume $\omega_1 = \omega_2 = \omega_3 = \omega$.

In this case, all unknown parameters in equations (10) and (11) can be obtained from a series of simple HFSS simulations. Thus, single cavity mode $\omega = 5.642$ GHz was determined from $S_{11}$-parameter data in driven modal simulation of the single cavity. For this simulation, the substrate with qubit antenna and LP but without LC patch, was placed into the cavity. The reason for including the substrate and antenna in the simulation is that they greatly change the dielectric constant, reducing eigenmode frequency from 6.052 GHz to 5.642 GHz. For the same reason, for finding inter-cavity coupling strength $\gamma$, substrates with qubit antennas were placed in both cavities of the 2-cavity array and driven modal simulations were done. The coupler diameter in the array was $d = 8$ mm with (0, 13) coordinates. The inter-cavity coupling strength $\gamma = 20.5$ MHz was obtained from $S_{11}$-parameter data and equation (3). The qubit–cavity coupling strength $g = 110$ MHz was determined in previous section 5 while qubit resonant frequencies $q_1(q_2)$ can be found by using equation (8) with $\omega_C = 78$ FE.

After finding all the unknown parameters, equations (10) and (11) were diagonalized. Eigenvalues were calculated by sweeping $q_1$ for different fixed detunings $\Delta = q_1 - \omega$ of $q_1$ from the single cavity mode $\omega$.

Inter-qubit coupling strengths $J_{12}$ were determined as the half of the minimum distance between $q_1$ and $q_2$ modes, which occurs at $q_2 \sim q_1$. The dependences of $J_{12}$ on detuning $\Delta$ are shown in figure 6(a) as blue and red lines for the NN and NNN configurations, respectively.
Figure 6. (a) Dependences of the inter-qubit coupling strength $J_{12}$ on detuning $\Delta = \omega_1 - \omega$. Results obtained from the model Hamiltonian equations (10) and (11) are shown as blue and red lines for the NN and NNN configurations, respectively. Results obtained directly from HFSS simulations are shown as blue and red circles for the NN and NNN configurations, respectively. (b) Distribution of energy spectrum obtained directly from HFSS simulations of the entire qubit–cavity array for the NN configuration. The data were extracted from Im $Z$ at the LP of Q1 by sweeping inductance $L_{J2}$ of Q2. (c) Magnified region of avoided crossing between $q_1$ and $q_2$, which is shown in (b).

The validity and prediction power of the model Hamiltonian was verified directly from HFSS driven modal simulations of 3-cavity array with two identical qubits (Q1 and Q2) in the same NN and NNN configurations. The coupler diameter was $d = 8$ mm with (0, 13) coordinates. The inter-qubit couplings obtained directly from HFSS simulations of the entire qubit–cavity array are regarded as the benchmark for the model Hamiltonian. In this simulations, for different detunings $\Delta$ of Q1, the frequency $\omega_2$ of Q2 was swept in the vicinity of $\omega_1$ and modes of the cavity array. Unfortunately, achieving a good convergence even for such not very complex models requires long computation times, which we tried to avoid by reducing our demands to the convergence. Therefore, $J_{12}$ data in our simulation was possible to extract not for every $\Delta$ and only from Im $Z$. Poles of Im $Z$ were extracted at the LP of Q1. Figure 6(b) shows energy spectrum for the NN configuration, which was obtained from Im $Z$ data by sweeping inductance $L_{J2}$ of Q2 at $L_{J1} = 10.5$ nH. The absence of few points for $\omega_{32}$ in figure 6(b) is related to the dark state of Q2 at this mode (see section 4 and appendix B). As is seen, $q_1$ and $q_2$ frequencies have an avoided crossing, magnified region of which is depicted in figure 6(c). Inter-qubit coupling strength $J_{12}$ was estimated as the half of the minimum frequency difference between $q_1$ and $q_2$ data points.

The dependences of $J_{12}$ on $\Delta$ obtained directly from HFSS simulations of the entire qubit–cavity array are shown in figure 6(a) as blue and red circles for the NN and NNN configurations, respectively. As it well seen, only few data points and only for positive detuning were extracted for NNN configuration that hindering comparison between two techniques in this configuration. At the same time, figure 6(a) shows that for the NN configuration, a zero detuning ($\Delta = 0$) symmetry of the $J_{12}$ data for the simulation and model Hamiltonian is shifted. The cause of the shift are different total capacitances $c_S$ for two approaches. For the Hamiltonian diagonalization, we used $c_S$ of the single cavity and single qubit system while for the simulation, $c_S$ in the 3-cavity array and 2 qubits system is different. This difference leads to the different calculated and simulated $q_1$ frequencies for the same $L_{J1}$, giving different detunings $\Delta$. Despite this fact, the $J_{12}$ values from the model and simulation for the NN configuration demonstrate a good agreement. For the NN configuration, the maximum values of the inter-qubit coupling strength are $J_{12} = 10.2$ MHz and $J_{12} = 9$ MHz for the model and simulation, respectively. As one can see, the difference between two methods is around 10%. When $\Delta \gg g, \gamma$, analytical results for NN and NNN configurations are respectively $J_{12} = 2g^2\gamma/\Delta^2$ and $J_{12} = 2g^2\gamma^2/\Delta^3$, so the inter-qubit coupling strength for NN configuration is generally bigger than for NNN.
7. Conclusions

We have presented the practical design of linear array of three-dimensional (3D) cavities for experiments in circuit quantum electrodynamics. In order to obtain an efficient inter-cavity, qubit–cavity and inter-qubit coupling, geometry of the structure was optimized by using high frequency structure simulator (HFSS). A method based on Hamiltonian description of the qubit-3D cavity array system for prediction of inter-qubit interaction mediated by normal modes of 3D cavity array was proposed. Unknown parameters in the model Hamiltonian could be found from a series of simple HFSS simulations. The validity of the method was confirmed from direct observation of inter-qubit coupling in simulations, which demonstrate a good agreement. The results obtained allow us to propose this technique for determination of inter-qubit coupling in more complex qubit–cavity systems where finite-element electromagnetic simulators require huge computational resources.

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Appendix A. Calculation of qubit–cavity coupling strength by using BBQ model

BBQ provides an alternative approach for calculation of qubit–cavity coupling strength \( g \), which is based on HFSS simulation data [14]. The only information needed is the dependence of admittance \( \text{Im} Y \) on frequency at LP for the case when qubit is positively far detuned from the cavity resonance. According to the BBQ model, self-Kerr susceptibility \( \chi_p \) of qubit or cavity mode is:

\[
\chi_p = -\frac{L_p e^2}{2J_p c_p},
\]

where \( L_p \) and \( c_p \) are respectively inductance and capacitance of qubit or cavity mode \( \omega_p \). \( L_p \) and \( c_p \) could be found from the following relations:

\[
L_p = \frac{1}{\omega_p^2 c_p},
\]

\[
c_p = \frac{1}{2} \text{Im} \frac{dY(\omega_p)}{d\omega_p}.
\]

Using simulated data of \( \text{Im} Y \) for \( L_1 = 8 \text{ nH} \) (see main text), self-Kerr susceptibilities \( \chi_q = -227 \text{ MHz} \) and \( \chi_r = -0.134 \text{ MHz} \) for the qubit and cavity mode, respectively, could be estimated. Cross-Kerr susceptibility, which is \( \chi_{qr} = -2\sqrt{\chi_q \chi_r} \) is related to the qubit–cavity coupling strength \( g \) as [40]:

\[
\chi_{qr} = -\frac{E_c \frac{G^2}{\Delta_{qr}}}{\Delta_{qr}},
\]

where \( \Delta_{qr} \) is detuning between qubit and cavity mode. Taking into account that for \( L_1 = 8 \text{ nH} \), \( \Delta_{qr} = 739 \text{ MHz} \), we get \( g = 110 \text{ MHz} \), which is the same as those obtained from the data fitting in the main text.

Appendix B. Dark state

The absence of E-field in the cavity 2 for the 2nd normal mode \( \omega_{32} \) in 3-cavity array (see figure 4 in the main text) must lead to the absence of the coupling between qubit located in cavity 2 and \( \omega_{32} \) mode. This effect could be easily revealed by applying the driven modal simulations to 3-cavity array with the qubit located in the cavity 2. The coupler diameter was \( d = 8 \text{ mm} \) with \((0, 13) \) coordinates. Figure B1(a) shows dependence of imaginary part of admittance \( \text{Im} Y \) on frequency at the lumped port LP of the qubit for \( L_1 = 9 \text{ nH} \), with zeros depicted as open circles. Zero associated with the qubit mode is located at 5.93 GHz while two zeros related to two normal modes (\( \omega_{31} \) and \( \omega_{33} \)) are observed at 5.528 GHz and 5.617 GHz. Zeros of \( \text{Im} Y \) for different values of qubit inductance \( L_1 \) present an avoided crossing, which is shown in figure B1(b). The absence of the qubit coupling with \( \omega_{32} \) mode almost in the whole range of qubit
Figure B1. (a) Dependence of imaginary part of admittance $\text{Im } Y$ on frequency at the lumped port LP of the qubit located in cavity 2 of 3-cavity array for $L_J = 9 \text{ nH}$. (b) Avoided crossings of qubit frequency and 2 normal modes ($\omega_{31}$ and $\omega_{32}$) of 3-cavity array. (c) Dependence of imaginary part of admittance $\text{Im } Y$ on frequency at the lumped port LP of the qubit, located in cavity 1 of 3-cavity array for $L_J = 9 \text{ nH}$. (d) Avoided crossings of qubit frequency and 3 normal modes ($\omega_{31}$, $\omega_{32}$ and $\omega_{33}$) of 3-cavity array.

Figure C1. Dependence of imaginary part of admittance $\text{Im } Y$ (blue line and left $y$-axis) and impedance $\text{Im } Z$ (red line and right $y$-axis) on frequency at the lumped port LP of the qubit, which is located in the single cavity, for $L_J = 8 \text{ nH}$. Zero of $\text{Im } Y$ and pole of $\text{Im } Z$, both indicating the cavity resonance, is depicted as a black open circle.

frequencies was observed. For comparison, in figures B1(c) and (d), simulation data for the qubit located in the cavity 1 present 3 zeros, which are related to 3 normal modes ($\omega_{31}$, $\omega_{32}$ and $\omega_{33}$) as well as zero related to the qubit mode.

Appendix C. Comparison of $\text{Im } Y$ and $\text{Im } Z$ data

In most of our simulations, imaginary part of admittance $\text{Im } Y$ and impedance $\text{Im } Z$ data demonstrate a good convergence and interchangeability. For example, figure C1 shows dependence of $\text{Im } Y$ and $\text{Im } Z$ on frequency at the lumped port LP of the qubit for $L_J = 8 \text{ nH}$. The simulation was performed for the the same model, results of which are depicted in figure 5. As one can see, zero of $\text{Im } Y$ and pole of $\text{Im } Z$, which indicate the cavity resonance (black open circle in figure C1), almost coincide. The difference between $\text{Im } Y$
and Im Z data for the qubit and cavity resonances was less than 1 MHz, which is a typical step for frequency sweep in our simulations.

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