Quantum electrodynamics near a photonic bandgap

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1 Single photon bound state calculation

Here we show the derivation of the eigenenergy of the single photon bound state within the band gap. The Hamiltonian of our system is

\[ H = \sum_k \hbar \omega_k a_k^+ a_k + \hbar \frac{\omega_q}{2} \sigma^z + \hbar \sum_k g_k (a_k^+ \sigma^- + a_k \sigma^+) \]

The number of excitations \( \hat{N} = (\sigma_z + 1)/2 + \int_{BZ} d\mathbf{k} a_k^+ a_k \) is a conserved quantity in our model. So in the single-excitation manifold, the eigenstate is in the form of \( |\phi_b\rangle = \cos \theta |0\rangle |e\rangle + \sin \theta \int_{BZ} d\mathbf{k} c_k a_k^+ |0\rangle |g\rangle \) and the eigenstate equation is \( H |\phi_b\rangle = \hbar \omega_b |\phi_b\rangle \). This yields

\[ \hbar (\omega_q - \omega_b) = \pi g^2 \alpha \sqrt{\hbar (\omega_0 - \omega_b)} \] \hspace{1cm} (2)
\[ \tan^2(\theta) = \frac{\omega_q - \omega_b}{2(\omega_0 - \omega_b)} \] \hspace{1cm} (3)
\[ c_k = \frac{g_k}{\tan \theta (\omega_q - \omega_b)} \] \hspace{1cm} (4)

To get an analytical result, we further make two assumptions: the coupling is independant of wavevector \( g_k \approx g \) and the dispersion is quadratic \( \hbar \omega_k = \hbar \omega_0 + \alpha (k - k_0)^2 \). Then extending the integral limits to infinity and performing the integrals yield the following results:

\[ \hbar (\omega_q - \omega_b) = \frac{\pi g^2}{\alpha \sqrt{\hbar (\omega_0 - \omega_b)}} \] \hspace{1cm} (5)
\[ \tan^2(\theta) = \frac{\omega_q - \omega_b}{2(\omega_0 - \omega_b)} \] \hspace{1cm} (6)

Thus, the photonic part of the wavefunction \( |\phi_b\rangle \) is \( \int_{BZ} d\mathbf{k} \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{\tan \theta (\omega_q - \omega_b)} a_k^+ |0\rangle |g\rangle \). By performing a fourier transform \( a_k \rightarrow a_x \) and approximating the Bloch wavefunction \( \psi_k(x) e^{ikx} \) with \( \psi_{k0}(x)e^{ikx} \), we get the photonic part
of the wavefunction is in the following form:

\[
\int dx e^{-x/\lambda} a_+^\dagger |0\rangle |g\rangle
\]

(7)

where \( \lambda \) is the penetration depth defined as \( \lambda = \sqrt{\alpha / \hbar (\omega_0 - \omega_p)} \). The means that photonic part of this polariton state is exponentially localized around the qubit, hence this is often called single photon bound state.

2 Band structure and transfer matrix technique

We first analyze the mode structure (Bloch wavefunction) of an infinite microwave photonic crystal (PhC). It can be obtained by solving the following wave equations for the periodic structure. This calculation leads to the choice of the qubit’s position, the middle of the unit cell, for maximal coupling with the second band.

\[
\frac{d}{dx} V(x,t) = -i(x) \frac{d}{dt} I(x,t)
\]

(8)

\[
\frac{d}{dx} I(x,t) = -c(x) \frac{d}{dt} V(x,t)
\]

Here \( i(x), c(x) \) are the inductance and capacitance per unit length, leading to the following wave equation

\[
\frac{\partial}{\partial x} \left[ \frac{v_p}{Z_c(x)} \frac{\partial V(x,t)}{\partial x} \right] = \frac{1}{v_p Z_c(x)} \frac{\partial^2}{\partial t^2} V(x,t)
\]

(9)

Here \( v_p = \frac{1}{\sqrt{\mu_0}} \) is the phase velocity and \( Z_c(x) = \sqrt{\frac{\mu_0}{\varepsilon_0}} \) is the characteristic impedance. \( Z_c(x) \) is periodically modulated by changing the center pin and gap widths of the coplanar waveguide. This 1D wave equation can be solved using standard Fourier transform technique assuming \( V_k(x) = \sum_n C_n(k) e^{2\pi i n x / d + ikx} \) and \( 1/Z_c(x) = \sum_m \eta_m e^{2\pi i m x / d} \). Then the algebraic equation can be solved numerically. The results are shown in Fig. 1.

To simulate the transmission of our device with a finite number of periods, the transfer matrix (also called ABCD matrix technique) can be employed. The ABCD matrix of a section of coplanar waveguide with characteristic impedance \( Z \) can be written as

\[
M_Z = \begin{bmatrix}
\cos(\omega t/v_p) & jZ\sin(\omega t/v_p) \\
jsin(\omega t/v_p)/Z & \cos(\omega t/v_p)
\end{bmatrix}
\]

(10)

Then the ABCD matrix for one unit cell is \( M_{unit} = M_Z M_{ph} \).

The ABCD matrix for an atom in the single photon regime[1] is given by:

\[
M_a = \begin{bmatrix}
1 & 0 \\
-j2(\gamma/\omega_0)Z_0 & 1
\end{bmatrix}
\]

(11)

Here \( \gamma(\omega_0) \) is the decay constant in a normal waveguide with characteristic impedance \( Z_0 \). This constant is set by the coupling strength between the qubit and the waveguide. To maximize this coupling, one capacitor island of the transmon qubit is fabricated very close (2\( \mu \)m) to the center pin of the waveguide. In the simulation shown in Fig. 2, we have assumed that \( \gamma(\omega_0) \) is constant for all \( \omega_0 \).

The ABCD matrix for the whole device can then be written as \( M = (M_{unit})^N \times M_a \times (M_{unit})^N \) and the transmission coefficient can then derived. The explicit expression is too cumbersome to be presented here, so instead we give the numerical results.

3 Nonlinear response and comments on multiphoton bound states

Neither of the previous theoretical approaches can be easily generalized to the nonlinear regime. A few very recent theoretical studies have used variational ansatz and numerical methods to prove the existence of multi-photon bound states[7, 8]. We did not observe a direct signature of these multiphoton bound states in...
Instead we give the numerical results. The transmission coefficient can then be derived. The explicit expression is too cumbersome to be presented here, so we refer to the simulation shown in Fig. 2. We have assumed that the states are exponentially localized around the qubit, hence this is often called single-photon bound states. To maximize this coupling, one capacitive coupling strength between the qubit and the waveguide is modulated by changing the center pin and gap widths of the coplanar waveguide. This 1D wave equation can be written as:

\[ \text{vp} \left( Z_c / \omega^{\ell} \right) \partial_x I + Z_c \left( \partial_x V - \omega^{\ell} / \text{vp} \right) = \sum \text{Ma} \quad (9) \]

This gives qualitative agreement. But we only use the Hamiltonian approach to fit the experimental data. (c) S21 at \( \Omega / 2 \pi = 5 \text{GHz} \).

Figure S1: Band structure of the bare photonic crystal. (a) Dispersion of the PhC. (b) Measured (at 10mK) and simulated (with ABCD matrix technique) transmission amplitude in the log scale. The small discrepancy comes from fabrication imperfections, additional loss and slight impedance mismatch in the whole measurement chain. Note there are no pronounced resonances in the second band. Mode structure (Bloch wavefunction) of the first (c) and second band (d). The most strongly-coupled modes, which lie near the band-gap, have wavevector \( k = \pi / d \). In the middle of the unit cell, clearly the mode in the first band reaches minimum while the mode in the second band reaches maximum.

Figure S2: ABCD matrix simulation. (a) Measured low-power transmission versus flux bias in log scale. (b) Simulated transmission with ABCD matrix technique in log scale. Here we have assumed \( \gamma / 2 \pi = 0.5 \text{GHz} \). This calculation gives qualitative agreement. But we only use the Hamiltonian approach to fit the experimental data. (c) S21 at \( \omega / 2 \pi = 8.5 \text{GHz} \).
our experiments. As we increase input power, the bound state assisted transmission coefficient decreases accompanying with supersplitting. The supersplitting doublet appears due to saturation of the two-level system and does not correspond to multiphoton transitions. We think that the absence of multiphoton resonances can be attributed to insufficiently strong coupling and relatively large bandwidth of the single photon bound state. The Mollow triplet structure and Autler-Townes splitting clearly shows the quantum nature of this state within the band-gap. Incorporation of low noise amplifiers in the future may reveal multiphoton effects in correlation measurements.

4 Multilevel analysis of dressed-state transitions

The Hamiltonian of the qubit subject to coherent drive has the following form,

\[ H = \sum_{n=0,1,...} [(\omega_n - n\omega_d) |n\rangle \langle n| + \frac{\Omega_n}{2} (|n\rangle \langle n+1| + h.c.)] \] (12)

The above Hamiltonian is written in the frame of the drive and multiple excited states are taken into account. Where \( \Omega_n = \sqrt{n}E \) is the effective Rabi rate for the \( n^{th} \) transition and Fermi’s golden rule dictates that \( \sqrt{n} \) is proportional to the transition matrix of transmon qubit. Note that the energy levels here have taken into account the effect of the photonic crystal, so \( \omega_{d1} \) is really just the bound state frequency \( \omega_d \). The other transition frequencies \( \omega_{d2}, \omega_{d3} \) are found empirically in the experiments, rather than using the transmon anharmonicity \( E_c \). Hence \( \Omega_n = \sqrt{n} + 1 \Omega_0 \). We note that the full quantum analysis has to use input-output theory and consider the coherent coupling between the qubit and photonic crystal modes. However, if the qubit is deep within the gap, the effect of the photonic modes can be described perturbatively with the decay rate \( \gamma \). Diagonizing the matrix involving a few energy levels yields the complete dressed states. We consider two experimentally relevant cases where \( \omega_d = \omega_0 - \omega_n \) and \( \omega_d = \omega_2 - \omega_1 \). These dressed states are fitted to the experimental data. The only fitting parameter is \( \Omega_0 \). The dressed state transition shown in Figure 3 in the main text thus correspond to \( |a\rangle \leftrightarrow |b\rangle \) for \( \omega_d = \omega_{d1} \), and for \( \omega_d = \omega_{d2} \).

5 Effective master equation in photonic crystal

To understand resonance fluorescence in the band-gap medium, we first start from the complete Hamiltonian including both the coherently-driven qubit and the modes of the photonic crystal.

\[ H = \frac{\Delta_d}{2} \sigma_z + \frac{\Omega_0}{2} (\sigma^+ + \sigma^-) + \sum_k \Delta_k a_k^{\dagger} a_k + \sum_k g_k (a_k^{\dagger} \sigma^- + a_k \sigma^+) \] (13)

Where \( \Delta_d = \omega_n - \omega_d, \Delta_k = \omega_k - \omega_d \). We first go to the dressed state of the qubit, defining \( |\tilde{0}\rangle = \cos(\theta) |0\rangle - \sin(\theta) |1\rangle, |\tilde{1}\rangle = \sin(\theta) |0\rangle + \cos(\theta) |1\rangle \), where \( \cos^2(\theta) = \frac{1}{2} + \frac{\Delta_0}{2 \sqrt{\Delta_d^2 + \Delta_k^2}} \).

\[ H = \frac{\Omega}{2} \tilde{\sigma}_z + \sum_k \Delta_k a_k^{\dagger} a_k + \sum_k g_k (\cos^2(\theta) a_k^{\dagger} \tilde{\sigma}^- - \sin^2(\theta) a_k^{\dagger} \tilde{\sigma}^+ + \sin(\theta) \cos(\theta) a_k^{\dagger} \tilde{\sigma}) \] (14)

The Rabi rate is given by \( \Omega = \sqrt{\Omega_0^2 + \Delta_k^2} \). We work in the rotating frame, applying a unitary transformation \( U = \exp[i(\Omega \tilde{\sigma}_z/2 + i \sum_k (\Delta_k a_k^{\dagger} a_k))] \):

\[ H(t) = \sum_k g_k (\cos^2(\theta) a_k^{\dagger} \tilde{\sigma}^- e^{i(\Delta_d - \Omega)t} - \sin^2(\theta) a_k^{\dagger} \tilde{\sigma}^+ e^{i(\Delta_d + \Omega)t} + \sin(\theta) \cos(\theta) e^{i\Delta_d t} a_k^{\dagger} \tilde{\sigma}) \] (15)

From the above Hamiltonian, we can follow the standard procedure involving Born-Markov approximation and rotating wave approximation, deriving the reduced master equation for the qubit. But before we do that, let us analyze it to get some physical intuition. If we assume that the upper sideband is close to the band edge \( \omega_0 \approx \omega_d + \Omega \), then the effective interaction strength will be \( g_k \cos^2(\theta) \), and the coupling of the sideband...
will be effectively smaller than the direct coupling between the qubit and the photonic modes. The reduced density matrix of the qubit is governed by the following equation,

$$\frac{d\rho}{dt} = -\int_0^\tau d\tau T_{R}(H(t), [H(\tau), \rho(\tau) \otimes \rho_R(\tau)])$$  \hspace{1cm} (16)

We assume $\rho(\tau) \to \rho(t)$ and $\rho_R(\tau) \to \rho_R(0)$ (Born-Markov approximation), then we can get

$$2\frac{d\rho}{dt} = \gamma_0 \sin^2(\theta) \cos^2(\theta) (\sigma^z \rho \sigma^z - \sigma^- \sigma^+ \rho) + \gamma_- \sin^4(\theta) (\sigma^+ \rho \sigma^- - \sigma^- \sigma^+ \rho)$$

$$+ \gamma_+ \cos^4(\theta) (\sigma^- \rho \sigma^+ - \sigma^+ \sigma^- \rho) + h.c.$$  \hspace{1cm} (17)

Where $\gamma_0 = 2\pi \sum_k g_k^2 \delta(\omega_k - \omega_L)$, $\gamma_- = 2\pi \sum_k g_k^2 \delta(\omega_k - \omega_L + \Omega)$ and $\gamma_+ = 2\pi \sum_k g_k^2 \delta(\omega_k - \omega_L - \Omega)$. It is easy then to get the steady state of the master equation and get

$$\langle \tilde{1} | \rho | \tilde{1} \rangle = \frac{\gamma_- \sin^4(\theta)}{\gamma_- \sin^4(\theta) + \gamma_+ \cos^4(\theta)}$$  \hspace{1cm} (18)

$$\langle \tilde{0} | \rho | \tilde{0} \rangle = \frac{\gamma_+ \cos^4(\theta)}{\gamma_- \sin^4(\theta) + \gamma_+ \cos^4(\theta)}$$  \hspace{1cm} (19)

If the dephasing is also included, then the above equations shall be modified to be

$$\langle \tilde{1} | \rho | \tilde{1} \rangle = \frac{\gamma_- \sin^4(\theta) + \gamma_p \sin^2(2\theta)}{\gamma_- \sin^4(\theta) + \gamma_+ \cos^4(\theta) + 2\gamma_p \sin^2(2\theta)}$$  \hspace{1cm} (20)

$$\langle \tilde{0} | \rho | \tilde{0} \rangle = \frac{\gamma_+ \cos^4(\theta) + \gamma_p \sin^2(2\theta)}{\gamma_- \sin^4(\theta) + \gamma_+ \cos^4(\theta) + 2\gamma_p \sin^2(2\theta)}$$  \hspace{1cm} (21)

In the case of resonant driving $\theta = \pi/4$, the target dressed state is simply $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. The results can be generalized to many atoms[6].

## 6 Analysis of reservoir engineering

Since we could not directly perform qubit state tomography, we employ two methods to simulate the state purity $\rho_{-\gamma}$ in the reservoir engineering scheme, relying on two different sets of experimental data. Both results are presented in the main text and provide consistent estimates of state fidelity.

The first approach (named A in the main text) takes advantage of the linewidth data to estimate $\gamma_+$. It is apparent that near the band edge, the linewidth within the band reaches a maximum due to strong coupling to the electric field as shown in Fig. 1(d) and high density of states DOS $\sim \frac{1}{\sqrt{\omega - \omega_0}}$. In the perturbative regime, the lifetime of the qubit in the gap can be several orders of magnitude smaller than that in the band. In the strong coupling regime (which is our case here), the difference is smaller due to the formation of the leaky photon bound state. To account for this effect, we added an additional phenomenological dissipation $\gamma_0/2\pi = 25$MHz observed in our experiment to the perturbative formula $\frac{2\pi \Re[Y(\omega)]}{C_\Sigma}$ [4], where $Y(\omega)$ is the input admittance from the port of the qubit and $C_\Sigma$ is the total capacitance of the qubit. The final simulated linewidth (Fig. S3) agrees with the experimental data well both in the gap and in the band. In essense, $\gamma(\omega)$ in the gap is still an order of magnitude smaller than $\gamma(\omega)$ in the band. We will use the simulated linewidth to represent $\gamma(\omega)$. The previous section shows that the formula $\rho_{-\gamma} = 1 - \frac{1}{\gamma_+ \gamma_-}$ gives the dressed state purity in the ideal two-level system. In the presence of higher transmon level, leakage to the other dressed state will decrease the purity of the target state. Nevertheless, all the other dressed state transitions fall within the band gap. This means that their effects will be at most of the order of $\tilde{\gamma}/\gamma_+$, where $\tilde{\gamma} \approx \gamma_-$ is the decay rate in the gap. Based on this understanding, we approximate the state purity as

$$\rho_{-\gamma} \approx 1 - \frac{\gamma_- + \tilde{\gamma}}{\gamma_+} \approx 1 - 2\gamma_-/\gamma_+$$  \hspace{1cm} (22)
Figure S3: Linewidths of the bound state and the qubit transmission dip. The errorbar represents the standard deviation of the Lorenzian fit. This perturbative calculation can be seen as the first order approximation to the real linewidth quantities in the strong coupling regime. The dressed state cooling is most effective in the shaded regions where $\gamma_+$ is an order of magnitude larger than $\gamma_-$. 

Figure S4: Further analysis of the pump-probe data. (a) The resonance linewidth of the upper sideband. The errorbar represents the standard deviation of the Lorenzian fit. (b) The attenuation of the probe signal. The data shows that these two quantities are approximately inversely proportional to each other, which agrees with the theoretical model discussed in this section.
In the reservoir engineering experiment, the upper (lower) sideband is from 7.72GHz (7.16GHz) to 8GHz (6.86GHz) as shown in shaded regions in Fig. 3. The maximum $\gamma_+/2\pi$ is approximately 250MHz and the corresponding $\gamma_-/2\pi$ is about 25MHz. The above equation yields maximum $\rho_- \approx 80\%$.

The second approach (named B in the main text) uses the pump-probe data of the upper sideband in the photonic band to infer $\rho_-$. In Fig. 4, we have extracted the sideband linewidth and amplitude by fitting the dip to a Lorenzian. We first note that they are inversely proportional to each other. For instance, near the band edge $\sim 7.75\text{GHz}$, $\gamma$ reaches a maximum and the transmission amplitude reaches minimum. This actually means that the dressed state cooling is most effective here. In fact, Eq. (4) in the main text directly relates transmission amplitude to the dressed state inversion [5]. The exact expression for $\eta$ depends on specific dressed states and local decay rates. In the strong driving limit $\Omega_p \gg \gamma$ we regard it as a constant for simplicity. Ignoring other dressed states and using the sum rule $\rho_++\rho_- = 1$, we get

$$\rho_- = \frac{1}{2}(1 + \frac{1 - t_q}{\eta}) \geq 1 - t_q/2 \quad (23)$$

The above inequality means that we can use the transmission attenuation in Fig. 4(b) to get a lower bound of $\rho_-\), within the above assumptions. This method yields maximum $\rho_- \approx 86\%$. We quote the maximum fidelity (83%) in the main text as the average of these two methods.

Finally, we remark that pure dephasing in superconducting qubits can be greatly minimized and only relaxation has to be taken into account. Additionally, the $\gamma_+ / \gamma_-$ ratio could easily be made orders of magnitude larger by changing the coupling strength $g_k$ and the number of unit cells in the photonic crystal. In the future, it is very promising that complex many-body states can be prepared with high fidelity.

References


