Theory of spectrum in qubit-Oscillator systems in the ultrastrong coupling regime

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Recent measurement on an LC resonator magnetically coupled to a superconducting flux qubit[arXiv:1005.1559] shows that the system operates in the ultra-strong coupling regime and crosses the limit of validity for the rotating-wave approximation of the Jaynes-Cummings model. By using extended bosonic coherent states, we solve the Jaynes-Cummings model exactly without the rotating-wave approximation. Our numerically exact results for the spectrum of the flux qubit coupled to the LC resonator are fully consistent with the experimental observations. The smallest Bloch-Siegert shift obtained is consistent with that observed in this experiment. In addition, the Bloch-Siegert shifts in arbitrary level transitions and for arbitrary coupling constants are predicted.

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I. INTRODUCTION

The Jaynes-Cummings (JC) model[1] describes the interaction of a two-level atom with a single bosonic mode, which is fundamental model in quantum optics. Recently, the JC model is also closely related to condensed matter physics. It can be realized in some solid-state systems, such as one Josephson charge qubit coupling to an electromagnetic resonator, the superconducting quantum interference device coupled with a nanomechanical resonator, and the LC resonator magnetically coupled to a superconducting qubit. In conventional quantum optics, the coupling between the "natural" two-level atom and the single bosonic mode is quite weak, the rotating-wave approximation (RWA) has been usually employed. With the advent of circuit quantum electro-dynamics (QED), on-chip superconducting qubits (the "artificial " two-level atoms) could be engineered to interact very strongly with oscillators (cavities). RWA can not describe well the strong coupling regime, so the studies to the JC model without RWA is highly called for.

However, it is more difficult to solve the JC model without RWA than with RWA. In the absence of RWA, due to the presence of the counter-rotating terms, the photonic number is not conserved, so the photonic Fock space has infinite dimensions. The standard diagonalization procedure (see, for example, Ref. [5]) is the first candidate, which is to apply a truncation procedure considering only a truncated number of photons. Typically, the convergence is assumed to be achieved if the numerical results are determined within very small relative errors. Within this method, one has to diagonalize very large, sparse Hamiltonian in strong coupling regime. Furthermore, the calculation might become prohibitive for higher excited states where more photons should be involved.

Fortunately, several non-RWA approaches[10,11] has been recently proposed in a few contexts. Especially, by using extended bosonic coherent states, three of the present authors and a collaborator have solved the Dicke model without RWA exactly in the numerical sense[11]. The JC model is just special Dicke model with only one two-level atom.

Recently, the spectrum for an LC resonator magnetically coupled to a superconducting qubit was measured experimentally. A 50 MHz Bloch-Siegert shift when the qubit is in its symmetry point was observed, which clearly shows that the system enter the ultra-strong coupling regime. Therefore JC model with RWA is invalid to describe this strong coupling system. In this paper, we numerically solve JC model without RWA exactly. Based on the some key data drew from the spectrum, we obtain a fit of the experimental parameters. All spectrum line can then be calculated. The Bloch-Siegert shifts in arbitrary level transitions and in a wide range of the coupling parameters can also be estimated.

The paper is organized as follows. In Sec.II, the numerically exact solution to the JC model is proposed in detail. The numerical results and discussions are given in Sec.III. The brief summary is presented finally in the last section.

II. MODEL

The interaction between the flux qubit and the LC resonator in the experiment[5] is described by

\[ H_{\text{int}} = h g (a^\dagger a) \sigma_z \]  (1)

where \(a^\dagger, a\) are the photon creation and annihilation operators in the basis of Fock states of the LC resonator, \(g\) is the flux qubit-cavity coupling constant. The RWA has not been employed here. The effective Hamiltonian for the flux qubit can be written as the standard one for a two-level system

\[ H = - (\epsilon \sigma_z + \Delta \sigma_x) / 2 \]  (2)
where $\Delta$ and $\epsilon$ are the tunneling coupling between the two persistent current states and the transition frequency of the flux qubit. $\epsilon = I_p(\Phi - \Phi_0/2)$ with $I_p$ the persistent current in the qubit loop, $\Phi$ an externally applied magnetic flux, and $\Phi_0$ the flux quantum. In the above two equations, the Pauli matrix notations $\sigma_k(k = x, y, z)$ are used in the basis of the two persistent current states. Then the Hamiltonian for the whole system reads

$$H = -(\epsilon \sigma_z + \Delta \sigma_z)/2 + \hbar \omega_r \left( a^\dagger a + \frac{1}{2} \right) + \hbar g (a^\dagger + a) \sigma_z$$

(3)

where $\omega_r$ is the cavity frequency. For convenience, we denote

$$\hbar \omega_q = \sqrt{\epsilon^2 + \Delta^2}, \tan \theta = \Delta/\epsilon$$

Then the final Hamiltonian is ($\hbar$ is set to unity)

$$H = -\frac{\omega_q}{2} [\cos(\theta) \sigma_z + \sin(\theta) \sigma_x] + \omega_r \left( a^\dagger a + \frac{1}{2} \right)$$

$$+ g (a^\dagger + a) \sigma_z$$

(4)

By introducing the new operators

$$A = a + \alpha, B = a - \alpha, \alpha = g/\omega_r$$

we have

$$H = \left( \omega_r (A^\dagger A - \alpha^2) + \epsilon_- - \omega_q \sin(\theta)/2 \right)$$

$$- \omega_q \sin(\theta)/2 \omega_r \left( B^\dagger B - \alpha^2 \right) + \epsilon_+$$

(6)

where $\epsilon_{\pm} = (\omega_r \pm \omega_q \cos \theta)/2$. Note that the linear term for the original bosonic operator $a^\dagger(a)$ is removed, and only the number operators $A^\dagger A$ and $B^\dagger B$ are left. Therefore the wavefunction can be expanded in terms of these new operators as

$$|\psi\rangle = \left( \sum_{n=0}^{\infty} c_m |n\rangle \right)_A \left( \sum_{n=0}^{\infty} d_n |n\rangle \right)_B$$

(7)

For $A$ operator, we have

$$|n\rangle_A = \frac{A^n}{\sqrt{n!}} |0\rangle_A = \frac{(a + \alpha)^n}{\sqrt{n!}} |0\rangle_A$$

(8)

$$|0\rangle_A = e^{-\alpha^2 + \alpha a^\dagger} |0\rangle_a$$

(9)

$B$ operator has the same properties. Inserting Eqs. (6) and (7) into the Schrödinger equation, we have

$$[\epsilon_+ + \omega_r (m - \alpha^2)] c_m$$

$$- \frac{\omega_q}{2} \sin(\theta) \sum_n D_{mn} d_n = Ec_m$$

(10)

$$[\epsilon_- + \omega_r (m - \alpha^2)] d_m$$

$$- \frac{\omega_q}{2} \sin(\theta) \sum_n D_{mn} c_n = Ed_m$$

(11)

where

$$D_{mn} = \exp(-2\alpha^2) \sum_{k=0}^{\min[m,n]} (-1)^k \sqrt{m!n!(m+n-k)!} k!$$

In principle, all eigenvalues and eigenfunctions can be obtained in Eqs. (10) and (11). As before, to obtain the true exact results, the truncated number $N_m$ should be taken to infinity. Fortunately, it is not necessary. It is found that finite terms in state (7) are sufficient to give very accurate results with a relative errors less than $10^{-5}$ in the whole parameter space. We believe that we have exactly solved the JC model numerically. The numerical results are given in the next section.

**Solutions in the symmetry point.** The spectrum in the symmetry point ($\epsilon = 0$) is particularly interesting in experiments. In this case, Eq. (3) becomes

$$H_0 = -\frac{\Delta}{2} \sigma_x + \hbar \omega_r \left( a^\dagger a + \frac{1}{2} \right) + g (a^\dagger + a) \sigma_z$$

(12)

Associated with this Hamiltonian is a conserved parity $\Pi$, such that $[H_0, \Pi] = 0$, which is given by

$$\Pi = e^{i\pi \sigma_x/4} e^{i\pi N/4} e^{-i\pi \sigma_y/4}, N = a^\dagger a + \sigma_z/2 + 1/2, \quad (13)$$

where $\tilde{N}$ is the excitation number operator. $\Pi$ has two eigenvalues $\pm 1$, depending on whether the excitation number is even or odd. So the system has the corresponding even or odd parity. It is easily proven that the wavefunction (6) with even and odd parity is of the form

$$|\Psi_\pm\rangle = \left( \sum_{n=0}^{N_f} f_n |n\rangle \right)_A \left( \sum_{n=0}^{N_f} f_n |n\rangle \right)_B$$

(14)

where $\Psi_+$ ($\Psi_-$) is corresponding to wavefunction with even(odd) parity. Inserting Eq. (13) into Eq. (3) gives

$$\left[ \omega_r + \omega_r (m - \alpha^2) \right] f_m + \frac{\Delta}{2} \sum D_{mn} f_n = E f_m$$

(15)

The level transition is only allowed between the even and odd parity, i.e. $E_i^{(\pm)} \Leftrightarrow E_j^{(\mp)}$. The transition between the levels with the same parity is forbidden, $E_i^{(\pm)} \not\Leftrightarrow E_j^{(\pm)}$. The optical selection rules related to the parity have been discussed in the microwave-assisted transitions of superconducting quantum circuits [2, 16].

**III. RESULTS AND DISCUSSIONS**

Diaz et al diagonalize a restricted Hilbert space to a certain number of photon states (in the Fock basis) and obtained fitted parameters [5, 17]. The optimum fit of the experimental results within the present theoretical scheme gives $I_p = 515nA, g/2\pi = 0.82GHz, \omega_r/2\pi = 8.13GHz, \Delta/h = 4.25GHz$, very close to their values.
The calculations in this paper are based on these parameters, unless specified.

We plot the numerical results for the spectrum for $E_n \rightarrow E_0$ (n = 1, 2, and 3) in Fig. 1. The experimental three spectral lines are just corresponding to the transitions between a few low energy levels, such as $E_3 \rightarrow E_0$ (upper), $E_2 \rightarrow E_0$ (middle), and $E_1 \rightarrow E_0$ (down). It is very interesting that our theoretical results for the spectrum are in excellent agreement with the experimental ones in Fig. 3 of Ref. [5]. Using these fitted parameters, the energy splitting on resonance ($E_2 - E_3$)/$h$ obtained within the present approach is around 0.957 GHz, just in the scope of the experimental observation.

In Fig. 3 of Ref. [3], a weakly visible spectrum line just below the middle spectrum line was attributed to the thermally excited qubit. We calculate the spectrum line for the transition $E_3 \rightarrow E_1$, as also list in Fig. 1 with a yellow line. Interestingly, it is just in the location observed experimentally shown in their Fig. 3. We believe that the state with $E_1$ is just corresponding to the qubit excited thermally mentioned in Ref. [3].

We would like to mention here that the experimentally observed spectrum lines have been explicitly related to the specified energy level transitions in the JC model without RWA. Then the comparison are easily performed.

Next, we specially consider the case in the symmetry point. Fig. 2(a) presents the energy levels from the numerically exact calculations. It was suggested in Ref. [3] that in the blue sideband spectral line the minimum vanishes since the qubit is in the symmetry point where it produces no net flux and the transition is forbidden. In the symmetry point, the transition from $E_1^{(+)} \rightarrow E_0^{(+)}$ is forbidden due to the same parity, as shown in Fig. 2

This is the reason that the upper spectrum line around the symmetry point of Fig. 3 in Ref. [3] is almost invisible. It is perhaps just the optical selection rules related to the parity makes the qubit to produce no net flux.

As also indicated in Fig. 2 the other two transitions between levels with the different parity are allowed, so the intensities in the middle and down spectrum lines in the symmetry point are nearly the same as in the whole spectrum line.

Fig. 2(b) shows the first 10 spectrums $E_n^{(-)} \rightarrow E_0^{(+)}$ theoretically. In the experimental accessible detection, one can check the existence of these spectrums.

We then turn to the Bloch-Siegert shift, which is just energy shift of the level transition with the consideration of the counter-rotating terms in the ultrastrong coupling regime. The Bloch-Siegert shift of the level transitions $E_i \rightarrow E_0$ in the symmetry point are exhibited in Fig. 8. The smallest Bloch-Siegert shift is around 50 MHz, nearly the same as that measured in the experiment [3]. Note that some level transitions $E_i \rightarrow E_0$ are forbidden in the symmetry point due to the same parity, which are also presented here only for the estimation of the magnitude of the Bloch-Siegert shift in the corresponding spectrum. For the main spectrum $E_i \rightarrow E_0$, the Bloch-Siegert shift becomes larger as $i$ increases, and its sign changes alternatively with either $i$, as shown in Fig. 3(b).

To show the effect of the qubit-cavity coupling strength on the Bloch-Siegert shift, we fix all parameters fitted from experiments except the coupling parameter $g$. The Bloch-Siegert shift of the level transitions $E_1 \rightarrow E_0$ in the symmetry point as a function of the effecting coupling constant $\alpha = g/\omega_r$ defined in Eq. (5) are plotted in Fig. 4. In the weak coupling regime, say $\alpha \leq 0.01$, the Bloch-Siegert shift is so small (less than 1 MHz) that it could not be distinguished from the spectrum line. When $\alpha \geq 0.1$, the Bloch-Siegert shift increases considerably with the coupling constant, and can reach the regime of GHz. This observation is also of practical interest. Recently, the coupling could easily be further enhanced in the circuit QED [18, 20] where $g$ is comparable with $\omega_r$, i.e. $\alpha$ is in the order of magnitude of
observed to exceed 80 MHz, the qubit line width at the symmetry point around 4 GHz, it is predicted that the Bloch-Siegert shift could be clearly resolved experimentally in this strong-coupling regime, like the Lamb shift \[21\].

IV. CONCLUSIONS

In summary, by using extended bosonic coherent states, we solve the Jaynes-Cummings model without RWA exactly in the numerical sense. Within this technique, we can reproduce excellently the spectrum measured in a recent experiments on an LC resonator magnetically coupled to a superconducting qubit [2], which was demonstrated in the ultra-strong coupling regime. The Bloch-Siegert shift \( E_1 \rightarrow E_0 \) in the symmetry point is estimated to be 50 MHz, very close to the experimental value. For the transition between the higher excited state \( i > 1 \) and the ground-state, the magnitude of the Bloch-Siegert shift monotonously increases, but the sign changes as \((-1)^{i+1}\). The considerable Bloch-Siegert shift in turn demonstrate that the counter-rotating terms should be considered. The effect of the qubit-cavity coupling strength on the Bloch-Siegert shift is also investigated. It is predicted that the Bloch-Siegert shift can be distinguished experimentally for \( \alpha > 0.15 \). The present technique are more suited for the stronger coupling regime, which experimental realizations may appear in the near future [18–20].

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