Two-polariton bound states in the Jaynes-Cummings-Hubbard Model

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We examine the eigenstates of the one-dimensional Jaynes-Cummings-Hubbard (JCH) model in the two-excitation subspace. We discover that two-excitation bound states emerge when the ratio of vacuum Rabi frequency to the tunneling rate between cavities exceeds a critical value. We determine the critical ratio as a function of the quasi-momentum quantum number, and indicate that the bound states carry a strong correlation in which the two polaritons appear to be spatially confined together.

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The investigation of quantum electrodynamics in coupled-cavity systems provides insight about the behavior of strongly interacting photons and atoms via a variety of interaction schemes [1]. With the capability of tunable coupling and measurement of individual cavity fields, Coupled-cavity QED could serve as a useful tool to address the control of quantum many-body phenomena [2, 3]. The Jaynes-Cummings-Hubbard (JCH) model corresponds to a fundamental configuration exhibiting the quantum phase transition of light [4–11]. In this paper we will focus on states \( \{|\psi\rangle\} \) with two excitations only, i.e., \( \langle \hat{N}_A + \hat{N}_c \rangle = 0 \) in this paper we will focus on states \( \{|\psi\rangle\} \) with two excitations only, i.e., \( \langle \hat{N}_A + \hat{N}_c \rangle = 0 \).

Defining the atomic and photonic excitation number operators as \( \hat{N}_A = \sum_{n=1}^{N} \sigma_n^+ \sigma_n^- \) and \( \hat{N}_c = \sum_{n=1}^{N} \hat{a}_n^+ \hat{a}_n \), it is easy to check that the excitation number (or the polariton number) is a conserved quantity, i.e., \( [H, \hat{N}_A + \hat{N}_c] = 0 \). In this paper we will focus on states \( \{|\psi\rangle\} \) with two excitations only, i.e., \( \langle \hat{N}_A + \hat{N}_c \rangle = 2 \). In order to exploit the translational invariance, we define the following operators via discrete Fourier transform:

\[
\begin{align*}
b_k &= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-\frac{2\pi ikn}{N}} a_n \\
s_k &= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-\frac{2\pi ikn}{N}} \sigma_n^-
\end{align*}
\]

where \( k = 0, 1, 2, \ldots, N - 1 \) is related to the (discrete) quasi-momentum of the excitation. The commutation relations for the operators are given by:

\[
\begin{align*}
[b_k, b_j^+] &= \delta_{kj} \\
[s_k, s_j^+] &= -\frac{1}{N} \sum_{n=1}^{N} e^{\frac{2\pi i n(j-k)}{N}} \sigma_n^+
\end{align*}
\]

where \( \sigma_n^+ \) is the Pauli-Z matrix for the \( n \)-th atom. The Hamiltonian in term of operators defined in [2] and [3] is partially diagonalized:

\[
H = \sum_{k=0}^{N-1} \Omega_k b_k^+ b_k + g \sum_{k=0}^{N-1} (b_k s_k^+ + b_k^+ s_k)
\]

where \( \Omega_k = \Delta + 2J \cos \frac{2\pi k}{N} \) are normal mode frequencies (shifted by \( \omega_a \)) of the field in the coupled-cavity system.
in the absence of atoms. For later purpose, the ground state of the system is denoted by $|\Phi_0\rangle$ which is the state with vacuum cavity fields and all atoms being in their ground levels.

The two-polariton subspace can be spanned by the kets: $|k,j\rangle_F = b_k^{|j\rangle|\Phi_0\rangle}$, $|k,j\rangle_A = s_k^{|j\rangle|\Phi_0\rangle}$, and $|k\rangle_F|j\rangle_A = b_k^{|j\rangle|\Phi_0\rangle}$ with $k$ and $j$ ranging from 0 to $N-1$. The subscripts $F$ and $A$ are used to denote the field and atomic excitations respectively. For convenience, $|k,j\rangle_F$ and $|k,j\rangle_A$ are not normalized. Note that $|k,j\rangle_A$ are generally not orthogonal to each other because

$$
\langle kj|kj\rangle_A = \delta_{kk}\delta_{jj}-\frac{2}{N}\delta_{k+j,k'+j'}.
$$

Furthermore, it can be shown that

$$
\begin{align}
(b_k^{|j\rangle|F\rangle}_k + s_k^{|j\rangle|A\rangle})|k,j\rangle_F = b_k^{|j\rangle|F\rangle}_k + s_k^{|j\rangle|A\rangle}\rangle_A \quad \text{(7)}
\end{align}
$$

$$
\begin{align}
\delta_{kk}^{|j\rangle|F\rangle}_k + \delta_{jj}^{|j\rangle|A\rangle} = -\frac{2}{N}\delta_{k+j,k'+j'} \quad \text{(8)}
\end{align}
$$

$$
\begin{align}
\frac{2}{N}|l\rangle |F\rangle |[k+j-l]\rangle_A
\end{align}
$$

with $|x\rangle \equiv (x \mod N)$. Eqs. (7-9) imply that when $H$ operates on $|k,j\rangle_F$, $|k,j\rangle_A$ or $|k\rangle_F$, the quantum number $P \equiv k+j \mod N$ remains unchanged. We may call this as a conservation of quasi-momentum which is the key to construct eigenvectors.

A general two-polariton eigenvector with a given quasi-momentum quantum number $P$ is given by:

$$
|\Psi_P\rangle = \sum_{(k,j)\in S_P} (\alpha_{kj}|k,j\rangle_F + \beta_{kj}|k,j\rangle_A + \gamma_{kj}|kj\rangle_A)
$$

where $S_P$ denotes the set of $(k,j)$ satisfying $k+j \equiv P \mod N$ and $j \geq k$. To avoid double counting, we set $\beta_{kk}' = 0$. Next by the Schrödinger equation, assuming $\lambda$ is the eigenvalue, $H|\Psi_P\rangle = \lambda|\Psi_P\rangle$, we have, for $j > k$,

$$
\begin{align}
\lambda\alpha_{kj} &= (\Omega_k + \Omega_j)\alpha_{kj} + g(\beta_{kj} + \beta_{kj}') \quad \text{(11)}
\end{align}
$$

$$
\begin{align}
\lambda\beta_{kj} &= g\alpha_{kj} + \Omega_k\beta_{kj} + g\gamma_{kj} - \frac{2g}{N}\sum_{S_P} \gamma_{kj'} \quad \text{(12)}
\end{align}
$$

$$
\begin{align}
\lambda\beta_{kj}' &= g\alpha_{kj} + \Omega_j\beta_{kj} + g\gamma_{kj} - \frac{2g}{N}\sum_{S_P} \gamma_{kj'} \quad \text{(13)}
\end{align}
$$

$$
\begin{align}
\lambda\gamma_{kj} &= g(\beta_{kj} + \beta_{kj}') \quad \text{(14)}
\end{align}
$$

and for $j = k$,

$$
\begin{align}
\lambda\alpha_{kk} &= 2\Omega_k\alpha_{kk} + g\beta_{kk} \quad \text{(15)}
\end{align}
$$

$$
\begin{align}
\lambda\beta_{kk} &= 2g\alpha_{kk} + \Omega_k\beta_{kk} + 2g\gamma_{kk} - \frac{2g}{N}\sum_{S_P} \gamma_{kj'} \quad \text{(16)}
\end{align}
$$

$$
\begin{align}
\lambda\gamma_{kk} &= g\beta_{kk}. \quad \text{(17)}
\end{align}
$$

It is worth noting that the case of even $N$ and odd $P$ is simpler because this excludes the possibility $k = j$.

We may cast Eqs. (11-17) in the matrix form and solve the eigensystem directly by standard numerical packages. Since we are interested in systems with a large $N \gg 1$, the corresponding eigenvectors are expected to be insensitive to parity of $N$ and $P$ and this has been verified in our numerical calculations. To facilitate our discussions, we shall focus on the case of even $N$ and odd $P$ so that Eq. (15-17) are not needed, and Eqs. (11-14) become:

$$
H_P|\Psi_P\rangle = \lambda|\Psi_P\rangle
$$

where $H_P$ is a $2N \times 2N$ matrix:

$$
H_P = \begin{pmatrix}
\hbar_{k_1,j_1} & w_0 & \cdots & w_0 \\
w_0 & \hbar_{k_2,j_2} & w_0 & \cdots \\
w_0 & \cdots & \hbar_{k_{N/2},j_{N/2}} \\
\end{pmatrix}
$$

where $(k_1,j_1) \in S_P$, and $\hbar_{k_{\ell},j_{\ell}}$ and $w_0$ are $4 \times 4$ submatrices:

$$
\begin{pmatrix}
\Omega_k + \Omega_j & g & g & 0 \\
g & \Omega_k & 0 & g - \frac{2g}{N} \\
g & 0 & \Omega_j & g - \frac{2g}{N} \\
0 & g & g & 0 \\
\end{pmatrix}
$$

$$
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & -\frac{2g}{N} & 0 \\
0 & 0 & 0 & -\frac{2g}{N} \\
0 & 0 & 0 & 0 \\
\end{pmatrix}
$$

In this way the eigenvector $V$ takes the form:

$$
V = (v_{k_1,j_1}, v_{k_2,j_2}, \cdots, v_{k_{N/2},j_{N/2}})^T
$$

with $v_{k,j} = (\alpha_{kj}, \beta_{kj}, \beta_{kj}', \gamma_{kj})^T$. We remark that $H_P$ is not symmetric and this is due to the fact that non-orthogonal atomic basis vectors $|kj\rangle_A$ have been used to express the eigenvectors.

In Fig. 1, we illustrate the eigenvalues of $H$ as a function of $P$ at resonance ($\Delta = 0$) for various photon-atom interaction strengths. We find that if $g/J$ is sufficiently large (Fig. 1c and 1d), then there exist two branches of discrete eigenvalues (marked in red). The discrete eigenvalues correspond to bound states in the large $N$ limit and they are isolated from the quasi-continuous bands of eigenvalues. By lowering the photon-atom interaction (Fig. 1b), the bands and the discrete eigenvalues become closer, and eventually the discrete eigenvalues disappear in the bands if $g$ is too small (Fig. 1a). We will estimate the critical value of $g$ for the occurrence of bound states near the end of this paper.

Let $|\lambda_0\rangle$ be the normalized eigenvector with the discrete eigenvalue $\lambda_0$. Although the notion bound states is for infinite $N$ systems, the confined nature of $|\lambda_0\rangle$ starts to emerge in real space at finite large $N$. This is illustrated in Fig. 2 in which the probability distribution of excitations in real space are plotted. Specifically, we
calculate the joint probabilities defined by,

\[ p^{FF}_{nm} = | \langle \lambda_b \Phi_0 | a_n^\dagger a_m^\dagger | \rangle|^2 \]  \hfill (23)

\[ p^{AA}_{nm} = | \langle \lambda_b \sigma_n^+ \sigma_m^+ | \rangle|^2 \]  \hfill (24)

\[ p^{FA}_{nm} = | \langle \lambda_b | a_n^\dagger \sigma_m^+ | \rangle|^2 \]  \hfill (25)

Here \( m \) and \( n \) are indices for the cavity positions, and hence \( p^{FF}_{nm} (p^{AA}_{nm}) \) is the joint probability of having photonic (atomic) excitations in the \( n \)-th and \( m \)-th cavity. Similarly, \( p^{FA}_{nm} \) is the joint probability of a single photon in \( n \)-th cavity and an excited atom in the \( m \)-th cavity. For a given value of \( P \), all the three joint probabilities depend on \( n - m \) only.

In Fig. 2(a-c), we see that the joint probabilities are strongly localized around \( m = n \) when the interaction strength \( g \) is sufficiently away from the critical value \( (g_c \approx \sqrt{3}J) \). Note that \( p^{AA}_{nm} \) vanishes at \( n = m \) because \( \sigma_n^+ \sigma_m^+ = 0 \), but \( p^{AA}_{nm} \) peaks at \( n = m \pm 1 \). The localized feature means that the two polaritons are spatially confined together and behave like a composite object. As the photon-atom interaction \( g \) decreases, the binding becomes weaker. This is shown in the wider distributions in Fig. 2(d-e) in which \( g/J \) is slightly above the critical ratio. We remark that although Fig. 2 is plotted with \( P = 1 \) as an illustration, our numerical results indicate that the localized feature of bound states appear for the whole range of \( P \). For example, in the case \( N = 50 \) and \( g/J = 5 \), by adding up the same site probabilities and the nearest neighbor probabilities, the sum is over 98.5\% for \( 0 \leq P \leq N - 1 \).

In the strong coupling limit with \( g \gg J \), we find that the eigenvalues \( \lambda_b \) for bound states are approximately given by,

\[ \lambda_b \approx \pm \sqrt{2} \left[ g - \frac{J^2}{2g} \left( 4 + 5 \cos \frac{2\pi P}{N} \right) \right]. \]  \hfill (29)

This is obtained by noting that at \( J = 0 \) (i.e., when the cavities are decoupled), the \( \pm \sqrt{2}g \) are dressed energies known in the resonance Jaynes-Cummings model. Treating this as a zeroth order approximation, we can make a Taylor expansion of Eq. (26) in a power series \( J/g \). Eq. (29) is then obtained as an approximation solution of \( \lambda_b \) up to the first order in \( J/g \).

In the \( N \gg 1 \) limit, Eq. (26) can also be used to estimate the critical value of \( g \) below which bound states cease to exist. This is done by observing that the function
Therefore $g_c$ can be estimated by determining when the band edges overlap. In the $N \gg 1$ limit, the bands are filled up by those $\lambda$’s that give zero denominators in (26) [i.e., $G(\lambda) \rightarrow \pm \infty$] as shown in Fig. 3, and hence the band edges can be estimated. Base on this estimation scheme, the critical value $g_c$ in the $N \rightarrow \infty$ limit is plotted as a function of $P$ (Fig. 4). Note that $g_c$ is a maximum at $P = 0$ and $P = N - 1$ and it equals $\sqrt{3}J$.

To conclude, we have addressed the spectrum as well as the conditions for the existence of two-polariton bound states of the JCH model. These bound states are composite objects characterized by the quasi-momentum quantum number $P$ and they process a strong spatial correlation. In view of the previously studied bound atom pairs in Bose-Hubbard model [16–18], our work is a generalization to bound polariton pairs in a coupled cavity QED system. Although our analysis have been confined to the zero detuning case, bound states are also found for detuned systems according to our numerical solutions of Eq. (18). The effect of detuning would control the nature of polaritons such that the two excitations can be mainly photonic (atomic) at positive (negative) large $\Delta$. We also remark that the dynamics of a single polariton in the JCH model has been discussed recently [19], and we expect the two-polariton problem may have richer dynamical features because bound states would enable interesting correlated two-polariton transport. We hope to address this issue in the future.

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