Importance of counter-rotating coupling in the superfluid-to-Mott-insulator quantum phase transition of light in the Jaynes-Cummings lattice

Hang Zheng\(^{1}\) and Yasutami Takada\(^{2}\)

\(^{1}\)Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), Department of Physics, Shanghai Jiao Tong University, China
\(^{2}\)Institute for Solid State Physics, The University of Tokyo, Kashiwa, Chiba 277-8581, Japan

(Received 23 May 2011; published 11 October 2011)

The quantum phase transition between Mott insulator and superfluid is studied in the two-dimensional Jaynes-Cummings lattice. The counter-rotating coupling (CRC) is included. Both the ground state and the spectra of low-lying excitations are obtained with use of a sophisticated unitary transformation. This CRC is shown not only to induce a long-range interaction between cavities, favoring the long-range superfluid order, but also to break the conservation of local polariton number at each site, leading to the absence of the Mott lobes in the phase diagram, in sharp contrast with the case without the CRC as well as that of the Bose-Hubbard model.

The quantum phase transition between Mott insulator and superfluid is studied in the two-dimensional Jaynes-Cummings lattice (JCL) as

\[ H = \sum_l \left( H_l^{\text{RWA}} + H_l^{\text{CRC}} - \mu N_l^0 \right) - J \sum_l \sigma^+_l \sigma^-_l, \]

with \( b^+_l \) (\( b_l \)) the creation (annihilation) operator of cavity mode at site \( l \) with frequency \( \omega \), \( J \) the hopping strength between nearest-neighbor cavities \( l \) and \( \Gamma \), and \( \mu \) the chemical potential associated with \( N_l^0 \) (\( = \sigma^+_l \sigma^-_l + b^+_l b_l \)), the polariton number operator at site \( l \). The term \( H_l^{\text{RWA}} \) describes the JC model in the RWA as

\[ H_l^{\text{RWA}} = \epsilon \sigma^+_l \sigma^-_l + \omega b^+_l b_l + g (b_l^+ \sigma^-_l - \sigma^+_l b_l^+), \]

with \( \sigma^\pm \) the Pauli matrices representing the two-level-atom system characterized by the level difference \( \epsilon \) and \( g \) the atom-photon coupling.

The counter-rotating coupling (CRC) term \( H_l^{\text{CRC}} \) is obtained as

\[ H_l^{\text{CRC}} = g (b_l^+ \sigma^+_l - \sigma^-_l b_l). \]

II. UNITARY TRANSFORMATION

In the single-site JC problem, the ground state can be found rather trivially in the RWA, but it is not the case if the CRC is included. In order to overcome this difficulty, we perform a series of unitary transformations on \( H \) under the same guiding principles as described in Ref. [12] to obtain \( H' = e^{\delta_k} e^{\delta_l} H e^{-\delta_k} e^{-\delta_l} = H_0' + H'_1 + H'_2 \), where \( S_1 \) is a displacement transformation

\[ S_1 = \frac{1}{\sqrt{N}} \sum_k g \sum_l \frac{1}{\omega_l} \delta_l \sigma^+_l (b^+_l - b_l) e^{-\delta_{l-k}}, \]

and \( S_2 \) is a squeezing transformation [13]

\[ S_2 = \frac{1}{2} \sum_k \ln(\tau_k) (b_k b^+_k - b^+_k b_k). \]
where $b_k$ is the Fourier transform of $b$, $N$ is the total number of cavities, $\omega_k = \omega - \mu - z J \gamma(k)$ ($z$ the coordinate number), and $\gamma(k) = [\cos(k_x) + \cos(k_y)]/2$ for a two-dimensional square lattice. The actual functional forms for the displacement $\xi_k$ and the squeezing $r_k$ will be given later.

The calculation along these transformations can be done straightforwardly to the end and the result is

$$H'_0 = \frac{N}{2} \Delta - NV_0 + \frac{1}{4} \sum_k \omega_k \left( \tau_k^2(b_{-k}^d + b_{-k})^2 + \tau_k^{-2}(b_{-k} + b_{-k})^2 - 2 \right)
+ \frac{1}{2} \sum_k \eta \Delta \sigma_k^z \left( \frac{g^2 \xi_k}{\omega_k} - \frac{\xi_k}{\omega_k} \right)
+ \frac{1}{2} \sum_k \eta \Delta \sigma_k^z \left( \frac{g^2 \xi_k}{\omega_k} - \frac{\xi_k}{\omega_k} \right)
\times \left( b_{-k}^d b_{-k} + b_{-k} b_{-k} - 2b_{-k}^2 \right)
- \frac{1}{N} \sum_k \sigma_k^z \sigma_k^z \left( \frac{g^2 \xi_k(2 - \xi_k)}{\omega_k} - V_0 \right) e^{i k \cdot (r - r')}, \quad (6)$$

$$H'_1 = \frac{1}{\sqrt{N}} \sum_k \sum_l g \tau_k (1 - \xi_k) \sigma_k^z (b_{-k} + b_{-k}) e^{-i k l} - \frac{1}{\sqrt{N}} \sum_k \sum_l \frac{g \eta \Delta}{\omega_k \tau_k} \xi_k \sigma_k^z (b_{-k} + b_{-k}) e^{-i k l} - \frac{1}{2} \sum_k \sigma_k^z \left( \cosh(X_1) - \eta - \frac{N}{\Delta} \right)
\times \sum_k \frac{2g^2 \xi_k^2}{\omega_k^2 \tau_k} (b_{-k}^d b_{-k} + b_{-k} b_{-k} - 2b_{-k}^2 \right)
- \frac{1}{2} \sum_k i \sigma_k^z \sinh(X_1) - \eta X_1, \quad (7)$$

$$H'_2 = \frac{\Delta}{2} \sum_k \sigma_k^z \left( \cosh(X_1) - \eta - \frac{1}{N} \right)
\times \sum_k \frac{2g^2 \xi_k^2}{\omega_k^2 \tau_k} (b_{-k}^d b_{-k} + b_{-k} b_{-k} - 2b_{-k}^2 \right)
- \frac{1}{2} \sum_k i \sigma_k^z \sinh(X_1) - \eta X_1, \quad (8)$$

where the parameters $\Delta$ and $\eta$ are defined as

$$\Delta = \epsilon - \mu \quad \text{and} \quad \eta = \exp \left( - \frac{2}{N} \sum_k \frac{g^2 \xi_k^2}{\omega_k^2 \tau_k} \right). \quad (9)$$

respectively, and the operator $X_1$ is introduced as

$$X_1 = \frac{2}{\sqrt{N}} \sum_k \frac{g \xi_k}{\omega_k \tau_k} e^{-i k l} (b_{-k}^d - b_{-k}). \quad (10)$$

The last term in $H'_0$ is an induced long-range Ising-type interaction between atoms in different cavities, in which $V_0$, defined as

$$V_0 = \frac{1}{N} \sum_k \frac{g^2 \xi_k^2}{\omega_k^2} (2 - \xi_k). \quad (11)$$

is subtracted so as to eliminate a constant self-interaction at the same site.

The terms in proportion to $\eta$ in $H'_0$ and $H'_1$ are exactly canceled by the corresponding ones in $H'_2$, but it is very important to define $H'_2$ in the present form of Eq. (8), as we shall explain in the following: Basically, the “photon-dressing” parameter $\eta$ arises from the rearrangement of the operator $\exp(X_1)$ into the form of normal ordering with respect to the photon operators:

$$\exp(X_1) = \eta \exp \left( - \frac{2}{N} \sum_k \lambda_k e^{-i k l} b_{-k} \right)
\times \exp \left( - \frac{2}{N} \sum_k \lambda_k e^{-i k l} b_{-k} \right), \quad (12)$$

where $\lambda_k = g^2 \xi_k^2/\omega_k \tau_k$. Then, it is easy to see that $\sinh(X_1) - \eta X_1$ in the second term in $H'_2$ consists of the products of at least three photon operators in normal ordering. ( Needless to say, this photon operator is not a bare one, but an effective one renormalized by the unitary transformations.) On the other hand, the dominant contribution to the first term in $H'_2$ is proportional to the operator

$$\sum_k \left\{ \cosh(X_1) - \eta - \frac{2\eta}{N} \right\}
\times \left[ \frac{2g^2 \xi_k^2}{\omega_k^2 \tau_k} (b_{-k}^d b_{-k} + b_{-k} b_{-k} - 2b_{-k}^2 \right)$$

because $\sigma_k^z$ is well approximated to be $-1$, a constant independent of site index $k$, as we shall see in the linearized spin-wave approximation. Then, the predominant contribution originates from the products of at least four photon operators in normal ordering.

As a result, one can see that the dominant parts of $H'_1$ in the form of Eq. (8) are composed of terms of three, or a higher number of, photon operators, which enables us to drop $H'_2$ hereafter. Note, however, that this neglect of $H'_2$ does not mean that our calculation is valid only up to second order in $g$; it is a well-known fact in the physics of polarons and bipolarons that the strong-coupling effects on the ground and low-lying excited states can be included to a satisfactory degree up to infinite order of $g$ in terms of the photon-dressing parameter $\eta$. Therefore, as long as we employ $H'_0$ and $H'_1$ in the forms of Eqs. (6) and (7), respectively, with using $\eta$ in Eq. (9), we believe that our calculation scheme of neglecting $H'_2$ will work very well even for the strong-coupling region of $g$.

For the substantiation of our belief, we have assessed the accuracy of our scheme by checking the single- and double-site JC model. (Details are given in Appendices A and B.) In Fig. 1, we have favorably compared our results for the ground-state energy $E_0$ of the single-site JC model [Eq. (A6)] with the exact ones obtained numerically by exact diagonalization of $H$ in Eq. (1) for the single-site case. We have also obtained satisfactory agreement between our results for $n$ as the ground-state-average polariton number per site [Eq. (A10)] with those in the exact calculation. In addition to such numerical calculations, we have also calculated the perturbation contribution of $H'_2$ to the ground-state properties for the single-site JC model in Appendix A and have found that it is less than $2\%$, even for the resonant and moderately strong coupling case of $\epsilon = \mu = g$.

Similar comparison is made in Fig. 2 for the double-site JC model to confirm enough accuracy of our calculation scheme in the weak-hopping region. It must be noted here that the level crossover, which is predicted to occur in the RWA and constitutes an important ingredient for the emergence of the Mott lobes, is eliminated by the CRC. Concomitantly, the
ground-state polariton number changes continuously in both the exact and our approximate results, in sharp contrast with the jump in the excitation number found in the RWA.

In order to estimate the degradation of our approximation scheme with the increase of $J$, the hopping parameter between two cavities, we plot the results of both $E_g$ and $n$ as a function of $J/g$ for the double-site JC model at $\epsilon = g = \omega$. One can see that, although the RWA always gives poor results, our approach provides satisfactory results for $E_g$ and reasonably good estimates for $n$, even if $J$ is increased by an order of magnitude from the case in Fig. 2. Thus, we are confident of the accuracy of our scheme.

**III. INSULATING PHASE**

The Pauli matrices in $H' \approx H'_0 + H'_c$, $\sigma^z, \sigma^x, \sigma^y$ may be treated by the linearized spin-wave approximation [14] as

$$\sigma^z = 2\sigma^0_1 \sigma^0_1 - 1, \sigma^x = \sigma^0_1, \text{ and } \sigma^y = \sigma^0_1$$

with $\sigma^0_1$ bosonic operators. Then, $H'$ is approximated as

$$H' \approx H'_0 = \frac{1 - \eta}{2} \Delta N - NV_0 + \frac{1}{4} \sum_k \omega_k (\tilde{\tau}_k^+ + \tilde{\tau}_k^- - 2) + \sum_k \omega_k \tilde{\tau}_k^- b_k^+ b_k + \sum_k \eta \Delta \tilde{\delta}_k a_k^+ a_k$$

$$- \sum_k \left( \begin{array}{c} \eta \Delta \tilde{\delta}_k \tilde{\tau}_k b_k^+ - V_0 \end{array} \right) (\tilde{a}_k^+ - a_k)(\tilde{a}_k^+ + a_k - \tilde{a}_k)$$

$$+ \sum_k g \tilde{\tau}_k (1 - \tilde{\xi}_k)(b_k^+ + b_k)(\tilde{a}_k^+ - a_k)$$

$$- \sum_k \eta \Delta \tilde{\delta}_k \tilde{\tau}_k b_k^+ b_k(\tilde{a}_k^+ - \tilde{a}_k),$$

where $\tilde{\tau}_k$ is the running-wave operator of $\sigma^0_1$ and $\tilde{\tau}_k$ is the squeezing function, given by

$$\tilde{\tau}_k^2 = \sqrt{1 + 4 \eta \Delta g^2 \tilde{\delta}_k^2 / \tilde{\xi}_k^2 \omega_k^3}.$$  

In Eq. (13), we have kept only the quadratic operator terms, neglecting all cubic and quartic terms so as to focus on the ground and low-lying excited states.

We further apply a Bogoliubov transformation to $H'$ as

$$e^{S_1} H' e^{-S_1} = E_g + \sum_k \omega_k \tilde{\tau}_k^+ b_k^+ b_k + \sum_k \eta \Delta \tilde{\delta}_k^2 a_k^+ a_k$$

$$+ \sum_k \tilde{g}_k (b_k a_k - \tilde{a}_k b_k),$$

with

$$S_1 = \frac{1}{2} \sum_k \ln(\rho_k)(\tilde{a}_k^+ a_k^+ - a_k^+ a_k).$$

where $\tilde{g}_k = 2g \tilde{\tau}_k (1 - \tilde{\xi}_k) / \rho_k$, with $\rho_k$ and $\tilde{\xi}_k$ given by

$$\rho_k^2 = \sqrt{1 - 4 \eta \Delta g^2 \tilde{\delta}_k^2 / \tilde{\xi}_k^2 \omega_k^3},$$

$$\tilde{\xi}_k = \omega_k \tilde{\tau}_k^+ (\omega_k \tilde{\tau}_k - \eta \Delta \tilde{\delta}_k).$$
The ground-state energy of the insulating phase is obtained as

\[ E_g^I = \frac{1}{2} N (1 - 2\eta) \Delta - N V_0 + \frac{1}{2} \sum \omega_k (r_k^2 + t_k^2 - 2) + \frac{1}{2} \eta \Delta \sum \rho_k^2. \]  

(19)

Note that, because of the choice of \( \xi_k \) and \( t_k^2 \), \( e^{S_I} H^I e^{-S_I} \) is of the form of rotating-wave coupling between \( a_k \) and \( b_k \), allowing us to write the ground state of the form of \( |G_I\rangle = |(a_k^0 b_k^0 = 0)\rangle |(b_k^0 b_k^0 = 0)\rangle \).

Diagonalization of \( H^I \) determines the excitation energies of two branches \( E^I_+(k) \) in the insulating phase as

\[ E^I_+(k) = \frac{1}{2} (\eta \Delta \rho_k^2 + \omega_k \tau_k^2) \pm \frac{1}{2} \sqrt{(\eta \Delta \rho_k^2 - \omega_k \tau_k^2)^2 + 4 \xi_k^2}. \]  

(20)

In Fig. 4, the lower branch \( E^I_-(k) \) is plotted for the resonant case of \( \omega = \epsilon \) and \( \Delta/g = 1.1 \). In the weak-hopping situation, there exists a gap at \( k = 0 \) in the excitation spectrum, as can be seen at \( zJ/g = 0.08 \), but the gap disappears at \( zJ/g = 0.08876 \), and for \( zJ/g > 0.08876 \), \( E^I_-(0) \) becomes negative, indicating that the insulating phase is no longer stable for this situation, suggesting that the superfluid phase should occur instead. Thus, the condition for the presence of the stable insulating phase may be written as

\[ \eta \Delta \rho_0^2 \omega_0 \tau_0^2 \geq \frac{\xi_0^2}{\rho_0^2} \Rightarrow 2G_0 \leq \eta \Delta, \]  

(21)

where \( G_0 = 2(\xi_0^2 + \omega_0 - V_0) \).

This condition can be used to determine the phase boundary between the insulating and the superfluid phases, and the result is shown in Fig. 5. For comparison, the Mott lobes predicted in the RWA are also plotted to show that we have obtained a totally different phase boundary.

FIG. 4. (Color online) Dispersion relation of the lower-branch excitation for the two-dimensional JC square lattice at \( \omega = \epsilon \) and \( \Delta/g = 1.1 \). Energies are in units of \( \omega \). The excitation energies are gapped in both insulating (\( zJ/g = 0.08 \)) and superfluid (\( zJ/g = 0.092 \)) phases except for the case of \( zJ/g = 0.08876 \), at which the phase transition occurs.

FIG. 5. (Color online) Phase diagram in \((zJ/g, (\mu - \omega)/g)\) space for the two-dimensional JC square lattice at the resonant condition \( \omega = \epsilon \).

IV. SUPERFLUID PHASE

In the superfluid phase with \( 2G_0 > \eta \Delta \), we introduce a static displacement of the \( k = 0 \) photon mode to transform \( H_0' \) and \( H_I' \) as

\[ e^{R} H_0' e^{-R} = \frac{N \Delta}{2} - N V_0 + \frac{N G_0 \sigma_0^2}{2} + \frac{1}{4} \sum \omega_k \left( \tau_k^2 (a_k^0 a_k^0 + b_k^0 b_k^0)^2 - \tau_k^2 (b_k^0 b_k^0 - b_k^0 b_k^0)^2 - 2 \right) + \frac{1}{N} \sum g^2 \xi_k^2 (b_k^0 b_k^0 + b_k^0 b_k^0 - b_k^0 b_k^0 - b_k^0 b_k^0) \times \sum \eta \Delta \sigma_i^2 \left( e^{2i \xi_k} + \frac{1}{2} \sum \eta \Delta \sigma_i^2 - \sum G_0 \sigma_0 \sigma_i^2 \right) - \frac{1}{N} \sum \left( \frac{g^2 \xi_k}{\omega_k} - V_0 \right) \times \sum e^{i(k_{ij} - \xi_k) (\sigma_i^0 - \sigma_0) (\sigma_j^0 - \sigma_0)}, \]  

(22)

\[ e^{R} H_I' e^{-R} = \frac{1}{\sqrt{N}} \sum \omega_k \left( \xi_k (1 - \xi_k) (b_k^0 + b_k^0) \right) \times \sum e^{-i k_{ij} (\sigma_i^0 - \sigma_0)} - \frac{1}{\sqrt{N}} \sum \frac{g \eta \Delta}{\omega_k^2} \times \xi_k (b_k^0 - b_k^0) \sum \xi_k (\sigma_i^0 - \sigma_0)^2 e^{-i k_{ij}}, \]  

(23)

with the operator \( R \) defined by

\[ R = \sqrt{N} g \sigma_0 (1 - \xi_k) (b_k^0 + b_k^0)/\omega_0 \tau_0. \]  

(24)

The subscript \( 0 \) in Eq. (24) refers to the case of \( k = 0 \). Then, after a rotation of the Pauli matrices at every site \( l \) as

\[ H'' = U^\dagger e^{R} (H_0'' + H_I'') e^{-R} U = H_0'' + H_I'', \]  

(25)

with a unitary matrix \( U \) given by

\[ U = \prod_l (\sigma_i^0 - u \sigma_i^0). \]  

(26)
where the squeezing function \( \xi \) is not the same as the one in the insulating case [Eq. (14)], but is given by
\[
\xi = \sqrt{1 + 4\eta^2\Delta^2 g^2\xi_k^2 / W\omega_k^2}.
\] (30)

After a Bogoliubov transformation with use of the generator \( S_4 \), defined by
\[
S_4 = \frac{1}{2} \sum_k \text{ln}(\theta_k)(a_k^+ a_{-k}^+ - a_k a_{-k}),
\] (31)

we finally obtain the expression for the Hamiltonian as
\[
e^{S_4} H^S e^{-S_4} = E^S + \sum_k \omega_k \xi_k^2 b_k^+ b_k + \sum_k W\theta_k^2 a_k a_k^+
- \sum_k \xi_k \xi_k^+ b_k^+ a_k + \xi_k^+ b_k a_k^+.
\] (32)

where \( \xi_k = 2g\eta\Delta k/(1 - \xi_k) / W\theta_k \) with \( \theta_k \) and \( \xi_k \) given by
\[
\theta^2(k) = \sqrt{1 - 4\eta^2\Delta^2 [g^2\xi_k^2(2 - \xi_k)/\omega_k - V_0]/W^2},
\] (33)

\[
\xi_k = \omega_k \xi_k^2 / (\omega_k^2 + W^2)
\] (34)

Note that the displacement function \( \xi_k \) in Eq. (34) is different from the one in the insulating case [Eq. (18)].

By referring to the fact that the structure of the coupling between \( \alpha_k^+ b_k \) in \( e^{S_4} H^S e^{-S_4} \) is the same as that in the rotating-wave coupling, we can immediately write the ground state of \( e^{S_4} H^S e^{-S_4} \) in the form of \( |G_S \rangle = |(a_k^+ a_k = 0)\rangle |(b_k^+ b_k = 0)\rangle \) with the corresponding ground-state energy of the superfluid phase as
\[
E^S_S = \frac{1}{2} N(\Delta - 2W - 2V_0 + G_0\sigma_0^2)
+ \frac{1}{4} \sum_k \omega_k (\tau_k^2 + \tau_k^{-2} - 2) + \frac{1}{2} \sum_k W\theta_k^2.
\] (35)

Two branches of excitations in the superfluid phase \( E^S_\pm(k) \) are obtained by diagonalization of \( e^{S_4} H^S e^{-S_4} \) as
\[
E^S_\pm(k) = \frac{1}{2} (W\theta_k^2 + \omega_k \xi_k^2) \pm \frac{1}{2} [W\theta_k^2 - \omega_k \xi_k^2]^2 + 4g^2\xi_k^2.
\] (36)

Obviously, the following condition must be satisfied for \( E^S_\pm(k) \) to be a stable excitation mode:
\[
W\theta_0^2 \omega_0^2 \xi_0^2 \geq 3g^2 \Rightarrow 2G_0 \geq \eta\Delta.
\] (37)

This condition is exactly the complementation of the condition (21). At the transition point, \( E^S_\pm(k) \) is the same as \( E^S_\pm(k) \) (see Fig. 4). But, for \( zJ/g = 0.092 (0.38876) \), \( E^S_\pm(k) \) has a positive gap as shown in Fig. 4.

The gap in the lower-branch excitation spectrum and the order parameter estimated by \( \langle G^H | b_k | G^H \rangle \) are shown in Fig. 6 as a function of the hopping parameter \( zJ/g \), where \( |G^H \rangle \) denotes the ground state of the original Hamiltonian \( H \). This
The hopping for the two-dimensional JC square lattice at \( \omega = \epsilon \) and \( \Delta / g = 1.1 \), leading to a totally different phase diagram from that in the JC lattice. The coupling breaks the local conservation of the polariton between cavities, which favors the long-range superfluid order-

The counter-rotating coupling induces a long-range interaction long-range superfluid may occur at some critical parameters.

The squared order parameter\(^{38}\)
\[
\langle G^H | b_G | G^H \rangle = \langle G_S | e^{S_1 \hat{e}^R e^{S_1} b_G e^{-S_1} e^{-R} U e^{-S_1}} | G_S \rangle
\]
\[
= \frac{g \sigma_0}{\omega_0} (A3)
\]
is calculated as the ground-state average of the photonic annihilation operator, and the result is given as \( g \sigma_0 / \omega_0 \). One can see that the gap vanishes at the transition point, and the order parameter grows up from zero for \( z J / g \geq 0.08876 \), indicating a second-order phase transition.

Finally, we add a comment on the gapped excitations from the viewpoint of the Goldstone theorem: For the JC lattice in the RWA, the polariton number \( \sum_{l} (\sigma_l^+ \sigma_l^- + b_l^+ b_l) \) is conserved, which is similar to the conservation of the total boson number in the Bose-Hubbard model. In the superfluid phase, the emergence of the order parameter \( \langle G^H | b_G | G^H \rangle \neq 0 \) breaks the number conservation in both models, leading to the Goldstone theorem according to which the gapless bosons should appear to restore the symmetry. When the RSC is included in the JC lattice as in the present case, however, the number conservation is broken from the outset; in this case, we have only the parity conservation with parity operator defined by \( \exp[i \pi \sum_l (\sigma_l^+ \sigma_l^- + b_l^+ b_l)] \), which is a discrete symmetry. Thus, the Goldstone theorem does not apply to our case.

V. CONCLUSION

In summary, we have studied the ground state and the spectra of low-lying excitations of a two-dimensional JC square lattice in both the insulating and the superfluid phases and have shown that, as a result of the competition between the intrasite JC coupling and the intersite photon hopping, a quantum phase transition between the Mott insulator and the long-range superfluid may occur at some critical parameters. The counter-rotating coupling induces a long-range interaction between cavities, which favors the long-range superfluid ordering. The coupling breaks the local conservation of the polariton number, leading to a totally different phase diagram from that in the Bose-Hubbard model. More specifically, the Mott lobes, which are a conspicuous feature in the phase diagram in the Bose-Hubbard model, are totally absent in the JCL.

ACKNOWLEDGMENTS

This work was supported by the National Basic Research Program of China (Grant No. 2011CB922202) and the National Natural Science Foundation of China (Grant No. 10734020). This work was also supported by a Grant-in-Aid for Scientific Research (C) (Grant No. 21540353) as well as Innovative Area “Materials Design through Computics: Complex Correlation and Non-Equilibrium Dynamics” (Grant No. 22104011) from MEXT, Japan.

APPENDIX A: SINGLE-SITE JC MODEL

After the first two unitary transformations with the use of \( S_1 \) and \( S_2 \), the transformed Hamiltonian \( H' \) for the single-site JC model may be written as the sum of three terms \( H'_0, H'_1, \) and \( H'_2 \), each of which is given as follows:

\[
H'_0 = \frac{1}{2} \epsilon + \frac{1}{2} \frac{g \eta \epsilon}{\omega_0} - \frac{g^2 \lambda^2}{\omega_0} \xi (2 - \xi)
\]
\[
+ \frac{1}{4} \frac{g \eta ^2}{\omega_0} \tau^2 (b_1^+ b_1 - \tau^{-2} b_1^+ b_1 - 2)
\]
\[
- \frac{1}{4} \frac{g \eta \lambda^2}{\omega_0} b_1^+ b_1 - b_1 b_1 - \frac{1}{2} \frac{g \eta \epsilon}{\omega_0} (\sigma^z + 1) \lambda^2 b_1^+ b_1,
\]
\[
(H'_1 = g \tau (1 - \xi) \sigma^x (b_1^+ b_1 - b_1^+ b_1 - b_1 b_1 - b_1^+ b_1)
\]
\[
- \frac{g \eta}{\omega_0 \tau} \eta \lambda \xi \sigma^x (b_1^+ b_1 - b_1^+ b_1 - b_1 b_1 - b_1^+ b_1),
\]
\[
+ \frac{g \eta}{\omega_0 \tau} \eta \lambda \xi \sigma^x (b_1^+ b_1 - b_1^+ b_1 - b_1 b_1 - b_1^+ b_1),
\]
\[
+ \frac{g \eta}{\omega_0 \tau} \eta \lambda \xi \sigma^x (b_1^+ b_1 - b_1^+ b_1 - b_1 b_1 - b_1^+ b_1),
\]
where \( \lambda = 2 g \xi / \omega_0 \) and \( \eta \) is the photon dressing of the level difference, given by \( \epsilon \eta = \exp(-\lambda^2 / 2) \). At this point, no approximation is made and all terms in \( H' \) are retained, although some rearrangements among them are made.

By choosing the squeezing parameter \( \tau \) as
\[
\tau^2 = \sqrt{1 + 4 \eta \epsilon g^2 \xi^2 / \omega_0^3},
\]
we may diagonalize \( H'_0 \) into the following form:

\[
H'_0 = E_g + \frac{g \eta}{\omega_0} (1 + \sigma^z) + \frac{1}{4} \omega (1 - \sigma^z) \tau^{-2} b_1^+ b_1
\]
\[
+ \frac{1}{2} \omega (1 + \sigma^z) \tau^{-2} b_1^+ b_1,
\]
where the constant energy \( E_g \) is defined as
\[
E_g = \frac{1}{2} \epsilon (1 - \xi) - \frac{g^2}{\omega_0} \xi (2 - \xi) + \frac{1}{4} \omega (\tau^2 + \tau^{-2} - 2).
\]
Similarly, by choosing the displacement parameter \( \xi \) as
\[
\xi = \frac{\omega \tau^2}{\omega \tau^2 + \eta \epsilon},
\]
we may eliminate the CR terms in \( H'_1 \), leading to the expression for \( H'_1 \) as
\[
H'_1 = \eta \epsilon \lambda (b_1^+ \sigma^- + \sigma^+ b_1),
\]
in which only the RW terms are present.
An eigenstate of $H'_2$ in Eq. (A5) is described in a form of the direct product $|\pm i\rangle$, where $|\pm i\rangle$ is the eigenstate of $\sigma_z$: $|+\rangle = (1/\sqrt{2})$ or $|-\rangle = (1/\sqrt{2})$, and $|i\rangle$ is the phononic number state with $i$ phonons. Then, it is easy to check that the ground state of $H'_0 + H'_1$ is described by $|G_1\rangle = |-\rangle|0\rangle$ with the ground-state energy $E_g$ in Eq. (A6), namely,

$$ (H'_0 + H'_1)|G_1\rangle = E_g|G_1\rangle. \quad (A9) $$

With this state $|G_1\rangle$, the ground-state-average polariton number $n$ is given by

$$ n = \langle G_1| e^{S_z} e^{S_i}(\sigma^+ \sigma^- + b^\dagger b) e^{-S_z} e^{-S_i}|G_1\rangle = 1 + n + \frac{1}{4}(\tau^2 + \tau^{-2} - 2) + \frac{g^2}{\omega^2} \xi^2. \quad (A10) $$

The results in Eqs. (A6) and (A10) are used in plotting Fig. 1. Let us examine the effects of $H'_2$ on this state $|G_1\rangle$. The photon operators in $H'_2$ may be expanded as

$$ \cosh(\lambda(b^\dagger - b)) - \eta - \frac{\lambda^2}{2}(b^\dagger b^\dagger + bb - 2b^\dagger b) = \frac{1}{2}\eta[\exp(\lambda b^\dagger) - \exp(-\lambda b) - \lambda b^\dagger - \exp(-\lambda b^\dagger) + \exp(\lambda b^\dagger) + \exp(-\lambda b^\dagger) - \lambda b^\dagger - \exp(-\lambda b^\dagger)] = O(\lambda^4), \quad (A11) $$

$$ \sinh(\lambda(b^\dagger - b)) - \eta\lambda(b^\dagger - b) = \frac{1}{2}\eta[\exp(\lambda b^\dagger + \exp(-\lambda b^\dagger) + \exp(\lambda b^\dagger - \exp(-\lambda b^\dagger) + \exp(\lambda b^\dagger) - \lambda b^\dagger - \exp(-\lambda b^\dagger)] = O(\lambda^3). \quad (A12) $$

Here, all photon operators are arranged in normal ordering and the renormalization factor $\eta$ arises from the relation $\exp(\lambda(b^\dagger - b)) = \eta \exp(\lambda b^\dagger) \exp(-\lambda b)$. The results in Eqs. (A11) and (A12) indicate that all zeroth-, first-, and second-order terms of $\lambda$ are removed from $H'_0$ and, instead, they are put into $H'_0$ and $H'_1$. Thus, the effects of $H'_2$ on the ground-state energy appear through multiphoton nondiagonal virtual transitions from $|G_1\rangle$.

With this recognition, the correction to $E_g$ due to $H'_2$ may be estimated by perturbation theory with the formula $\Delta E_g = \sum_m |\langle m|H'_2|G_1\rangle|^2/(E_g - E_m)$, where $|m\rangle$ is an excited state of $H'_0$ with energy $E_m$. Concretely, the correction from the first term in $H'_2$ is given by [see Eq. (A11)]

$$ C_1 = -\frac{\eta^2 e^2}{4\omega\tau^2} \sum_{j=0}^{\infty} \frac{(j^2)^{2j}}{2(j+1)!} = -\frac{\eta^2 e^2}{4\omega\tau^2} \left[ \int_0^{\pi} \frac{\cos(x) - 1}{x} dx - \frac{\lambda^4}{4} \right]. \quad (A13) $$

Similarly, the correction from the second term in $H'_2$ is less than the quantity $C_2$, given by [see Eq. (A12)]

$$ C_2 = -\frac{\eta^2 e^2}{4\omega\tau^2} \sum_{j=1}^{\infty} \frac{(\lambda^2)^{2j+1}}{(2j+1)(2j+1)!} = -\frac{\eta^2 e^2}{4\omega\tau^2} \left[ \int_0^{\pi} \frac{\sin(x) \sin(x)}{x} dx - \lambda^4 \right]. \quad (A14) $$

We have estimated the values of $C_1$ and $C_2$ for the resonant case with moderately strong coupling ($\omega = g = 1$) to find that $E_g$(exact) = -1.1479 (numerical exact diagonalization), $E_g$(our scheme) = -1.1330 [Eq. (A6)], $C_1 = -0.0027$, and $C_2 = -0.0183$, implying that the perturbation correction from $H'_2$ is less than 2%. Thus, we believe that for calculating the ground-state properties, the contribution from $H'_2$ may be safely dropped.

**APPENDIX B: DOUBLE-SITE JC MODEL**

Calculations for the double-site JC model can be done by extending those for the single-site JC model. A complication arises from the existence of two kinds of photons: in-phase photon with $k = 0, \omega_0 = \omega = J$ and antiphase photon with $k = \pi, \omega_\pi = \omega = J$. After the first two transformations with the use of $S_1$ and $S_2$, the transformed Hamiltonian $H'$ containing all terms may be written as the sum of three terms $H'_0$, $H'_1$, and $H'_2$, each of which is given as follows:

$$ H'_0 = -\frac{g^2}{\omega_0} \xi_0(2 - \xi_0) - \frac{g^2}{\omega_\pi} \xi_\pi(2 - \xi_\pi) + \frac{1}{2}\eta\epsilon(\sigma^+_1 + \sigma^-_1) - V\sigma^+_1 \sigma^-_1 + \frac{\alpha_0}{4} \left[ \tau_0^2(\hat{b}_0^\dagger \hat{b}_0 + \hat{b}_0^\dagger \hat{b}_0) - 2\tau_0^2(\hat{b}_0^\dagger \hat{b}_0 - \hat{b}_0^\dagger \hat{b}_0) \right] $$

$$ + \frac{\alpha_\pi}{4} \left[ \tau_\pi^2(\hat{b}_\pi^\dagger \hat{b}_\pi + \hat{b}_\pi^\dagger \hat{b}_\pi) - 2\tau_\pi^2(\hat{b}_\pi^\dagger \hat{b}_\pi - \hat{b}_\pi^\dagger \hat{b}_\pi) \right] + \frac{i\eta\epsilon}{\sqrt{2}} \lambda_0(\hat{b}_0^\dagger - \hat{b}_0)(i\sigma^+_1 + i\sigma^-_1) $$

$$ + \frac{i\eta\epsilon}{\sqrt{2}} \lambda_\pi(\hat{b}_\pi^\dagger - \hat{b}_\pi)(i\sigma^+_\pi + i\sigma^-_\pi), \quad (B1) $$

$$ H'_1 = \frac{g}{\sqrt{2}} \tau_0(1 - \xi_0)(\hat{b}_0^\dagger + \hat{b}_0)(\sigma^+_1 + \sigma^-_1) - \frac{\eta\epsilon}{\sqrt{2}} \lambda_0(\hat{b}_0^\dagger + \hat{b}_0)(i\sigma^+_1 + i\sigma^-_1) $$

$$ + \frac{g}{\sqrt{2}} \tau_\pi(1 - \xi_\pi)(\hat{b}_\pi^\dagger + \hat{b}_\pi)(\sigma^+_\pi + \sigma^-_\pi) - \frac{\eta\epsilon}{\sqrt{2}} \lambda_\pi(\hat{b}_\pi^\dagger + \hat{b}_\pi)(i\sigma^+_\pi + i\sigma^-_\pi), \quad (B2) $$

$$ H'_2 = -\frac{\xi}{2} \sum_{l=1}^{2} i\sigma^+_l [\sinh(X_l) - \eta X_l] $$

$$ + \frac{\xi}{2} \sum_{l=1}^{2} \sigma^-_l \left[ \cosh(X_l) - \eta - \frac{\lambda^2_0(\hat{b}_0^\dagger \hat{b}_0 + \hat{b}_0^\dagger \hat{b}_0) - \lambda^2_\pi(\hat{b}_\pi^\dagger \hat{b}_\pi + \hat{b}_\pi^\dagger \hat{b}_\pi) - 2\eta^2 \hat{b}_0^\dagger \hat{b}_0 - 2\hat{b}_\pi^\dagger \hat{b}_\pi] \right], \quad (B3) $$

$$ + \frac{\xi}{2} \sum_{l=1}^{2} \sigma^-_l \left[ \cosh(X_l) - \eta - \frac{\lambda^2_0(\hat{b}_0^\dagger \hat{b}_0 + \hat{b}_0^\dagger \hat{b}_0) - \lambda^2_\pi(\hat{b}_\pi^\dagger \hat{b}_\pi + \hat{b}_\pi^\dagger \hat{b}_\pi) - 2\eta^2 \hat{b}_0^\dagger \hat{b}_0 - 2\hat{b}_\pi^\dagger \hat{b}_\pi] \right]. \quad (B4) $$

043819-7
where the operator $X_l$ and the parameter $V$ are, respectively, introduced as
\begin{equation}
X_l = \sqrt{2} \lambda_0 (b_l^\dagger - b_l) - \sqrt{2}(-1)^l \lambda_\pi (b_\pi^\dagger - b_\pi),
\end{equation}
and the squeezing parameters $\lambda_0 = g\xi_0/\omega_0\tau_0$, $\lambda_\pi = g\xi_\pi/\omega_\pi\tau_\pi$, and $\eta = \exp(-\lambda_0^2 - \lambda_\pi^2)$.

The ground state of $H'_0$, $|G_2\rangle$ is represented by the sum of two direct products:
\begin{equation}
|G_2\rangle = (u|−,−⟩ + v|+,+⟩)|0_0,0_\pi\rangle,
\end{equation}
where $|−,−⟩$ is the state for both spins in the “−” state, $|0_0,0_\pi⟩$ is the vacuum state for both in-phase and antiphase photons, the squeezing parameters $\tau_0$ and $\tau_\pi$ are given by
\begin{equation}
\tau_0^2 = \frac{1 + 4\eta^2 \epsilon^2 \sqrt{g^2 \xi_0^2}}{2} \omega_0^2, \quad \tau_\pi^2 = \frac{1 + 4\eta^2 \epsilon^2 \sqrt{g^2 \xi_\pi^2}}{2} \omega_\pi^2,
\end{equation}
and the parameters $u$ and $v$ are given as $u = \sqrt{(1 + \eta \epsilon / Y)/2}$ and $v = \sqrt{(1 - \eta \epsilon / Y)/2}$, respectively, with $Y = \sqrt{\eta^2 \epsilon^2 + V^2}$.

The corresponding ground-state energy $E_g$ is obtained as
\begin{align*}
E_g &= \epsilon - \sqrt{\eta^2 \epsilon^2 + V^2} - \frac{g^2}{\omega_0} \xi_0 (2 - \xi_0) - \frac{g^2}{\omega_\pi} \xi_\pi (2 - \xi_\pi) \\
&\quad + \frac{1}{4} \frac{\omega_0 (\tau_0^2 + \tau_0^{-2} - 2)}{\omega_\pi} (\tau_\pi^2 + \tau_\pi^{-2} - 2).
\end{align*}
By choosing the displacement parameters $\xi_0$ and $\xi_\pi$ as
\begin{equation}
\xi_0 = \frac{\omega_0 \tau_0^2}{\omega_0 \tau_0^2 + Y - V}, \quad \xi_\pi = \frac{\omega_\pi \tau_\pi^2}{\omega_\pi \tau_\pi^2 + Y + V},
\end{equation}
we can eliminate the CR terms in $H'^0$ to give $H'_1|G_2\rangle = 0$.

Finally, the ground-state-average polariton number per site $n$ for the two-site JC model is calculated as
\begin{align*}
2n &= \langle G_2 | e^{S^\dagger} e^{S^\prime} \sum_{k=0,1,2} (\sigma_k^+ \sigma_k^- + b_k^\dagger b_k) e^{-S^\dagger} e^{-S^\prime}| G_2 \rangle \\
&= 1 - \eta^2 \epsilon / Y + \sum_{k=0,\pi} (\tau_k^2 + \tau_k^{-2} - 2)/4 \\
&\quad + \sum_{k=0,\pi} g^2 \xi_k^2 / \omega_k^2 + g^2 V (\xi_0^2 / \omega_0^2 - \xi_\pi^2 / \omega_\pi^2) / Y.
\end{align*}
The results in Eqs. (B9) and (B11) are used in plotting Figs. 2 and 3.