CROSSOVER FROM EXCITONIC TO PHOTONIC CONDENSATION IN MICROCAVITY POLARITON SYSTEMS

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Abstract. We determine the mean-field ground state of a closed microcavity polariton condensation for various experimentally tunable and material-dependent parameters such as excitation density, detuning and ultraviolet cutoff. The condensate changes its character from excitonic to photonic ones as increasing excitations. This change can be a crossover or a first-order transition depending on these parameters.

1. Introduction
Recently, new family of systems undergoing Bose-Einstein condensation (BEC) was found in semiconductor microcavities [1, 2]. What is different from other BEC systems of neutral atoms [3] is that: “polariton” is a Bose particle composed of the light field (photon) and the polarization field (exciton). It is important for applications that the polariton BEC can be realized even at room temperature due to the light mass (typically $10^{-4}$ times the free electron mass) [4]. Another important difference is that the quantum degenerate state is obtained with the pumping laser focused onto the system and hence it is a nonequilibrium stationary state with balanced injection and ejection of energy. Thus, the polariton BEC does possibly have different properties from those of BEC in a thermodynamic equilibrium. Discussions in this context can be found in some papers [5, 6], however, their difference is not yet clearly understood. Finally, polariton BEC is followed by a coherent emission of light. Due to photonic features of polaritons, the BEC can be characterized by the light properties. As seen in experiments [7, 8], the coherent emission shows differences from that of the conventional laser.

The polariton condensation satisfies two conditions: (i) the excitation density is fixed by nonresonant pumping, and (ii) macroscopic occupation of the lowest energy state. Therefore it will be described, to some extent, by the ground state of a closed microcavity polariton system with fixed excitation density. In this paper, we discuss the ground state at zero temperature, as a function of experimentally variable parameters: excitation density, detuning, ultraviolet cutoff determined by the lattice constant. There are mean field theories in which two limits of low excitation-density [9, 10] and high excitation-density [11, 12] are discussed. Apart from them, here we also investigate the intermediate region where the internal structure of polariton wavefunction comes up in our theory. We show the ground state energy and the wavefunctions gradually change from those of excitons to photons as the excitation density increases. It is also
shown that the change can be a crossover or a first-order transition depending on the detuning parameter and the ultraviolet cutoff.

Calculations are done for three-dimensional systems, and we omit the electron spins and the mass difference between electrons and holes \((m_e = m_h = m)\) to simplify discussions. In addition, to get more sophisticated answer, we need to solve the self-consistent loop taking into account Coulomb screenings which we did not. Therefore, conclusions drawn here seem to be correct only qualitatively. Results for two-dimensional systems will be shown elsewhere.

2. Formulation

The polariton system is described as interacting electrons and photons where they are coupling with each other through the electric dipole interaction. We suppose the stationary state under a normalization condition. The polariton system is described as interacting electrons and photons where they are coupling based microcavity, where

\[
E_{\psi} = \sum_{q} \frac{1}{2} V_q (\rho_q \rho_{-q} - N_e - N_h) = \sum_{q} \frac{2 \pi c^2}{\kappa V} q^{-2} : \rho_q \rho_{-q} : ,
\]

\[
H_{el} = \sum_{k} \left( \frac{\hbar^2 k^2}{2 m_e} + \frac{E_g - \mu}{2} \right) a_k^\dagger a_k + \left( \frac{\hbar^2 k^2}{2 m_h} + \frac{E_g - \mu}{2} \right) b_k b_k^\dagger ,
\]

\[
H_{el-el} = \sum_{q} \frac{1}{2} \hbar \omega (\rho_q \rho_{-q} - N_e - N_h) = \sum_{q} \frac{2 \pi c^2}{\kappa V} q^{-2} : \rho_q \rho_{-q} :,
\]

\[
H_{ph} = \sum_{k} \left( \sqrt{\left( c k \right)^2 + \left( \hbar \omega_c \right)^2} - \mu \right) \psi_k^\dagger \psi_k ,
\]

\[
H_{el-ph} = -g \sum_{k,q} (\psi_q a_k^\dagger b_k + \psi_k^\dagger b_q^\dagger a_k) .
\]
There are two advantages in using Eq. (6): (i) it can reduce the infinite numbers of unknown parameters, $u_k$ and $v_k$, to two parameters, $\zeta$ and $\Omega$ only; (ii) it gives correct answer at least in the low and the high density limit when the polariton condensation are exciton-like such as in the case of weak light-matter couplings. It is easily found $\chi_k = 0$ for all $k$ to minimize the electron-hole exchange and dipole coupling energies. Now three parameters $\zeta$, $\Omega$ and $\lambda$ are left to be determined.

### 3. Results

There are two solutions to this variational problem. One approaches smoothly that of exciton BEC [14] in the low-density region where matter-light coupling is weak. For another, photonic fraction of the condensate is nearly 100 percent regardless of the density. Here, we call the former “polariton solution” and the latter “photon solution”. Which solution corresponds to the system ground state is determined by a comparison of the energies.

It is found that polariton solution depends very weakly on $k_c$ as far as $k_c a_0 \gg 1$. The ground state energy par particle $\varepsilon$ is plotted as a function of the excitation density in Fig. 1. In Fig. 1(a), $\varepsilon$ is plotted for several values of the detuning for not too large cutoff ($k_c a_0 = 20$) where the polariton solution is always the ground sate. It approaches the energy of exciton BEC for low density and slightly below the photon energy level ($=d$) for high density. This indicates the polariton BEC becomes excitonic to photonic as the density increases. The photonic character arises above the excitation density where the curves move apart from that of exciton BEC (black thick solid). Depending on the detuning, the condensate wavefunctions can be those of tightly-bound excitons, weakly-bound excitons, or electron-hole plasma (red dashed) before photonic character appears. As seen in Fig. 1(b), energy for the photon solution can be lower than that of polariton solution (thin dotted) for large $k_c a_0$. The system experiences a first-order transition from polariton to photon solutions around $R_s = 1.5$ when $k_c a_0 = 100$, while the photon solution remains the ground state for any value of $R_s$ when cutoff is very large as $k_c a_0 = 200$.

To clarify the difference between the two solutions, we plot in Fig. 2 the wavefunction of polarization $P(r) = (1/V) \sum_k (a_k^\dagger b_k) e^{ikr}$ where $r$ is the relative coordinate between an electron
Figure 2. Plots of polarization field $P(r)$ for (a) $R_s = 2.9$ where the polariton solution is stable and (b) $R_s = 1.1$ where the photon solution is stable. We set $d = 1$, $k_c a_0 = 100$ and $\tilde{g} = 0.1$.

and a hole. As shown in Fig. 2(a), $P(r)$ is very similar to that of 1s exciton for polariton solution in the low-density where the bound electron-hole pair is formed due to the Coulomb attraction. For photon solution in the higher density, the wavefunction is very narrow as shown in Fig. 2(b) since the bound pair is due to the electric dipole interaction. Narrow width of the wavefunction is understood from the fact that the photon field induces an attractive delta potential for an electron-hole pair through dipole interaction. In two or three dimension, the lowest bound state energy becomes negative infinity in the continuum. This is the reason why we need the introduction of a short-range cutoff for convergence of the energy.

4. Conclusion and remarks
The mean-field ground state of a microcavity polariton system is determined by an interpolating variational method based on the Comte-Nozières [14, 15]. Polariton condensation changes the energy and the wavefunction from those of excitons to photons. When the lattice constant is much smaller than the exciton Bohr radius i.e. the momentum cutoff is large, sudden change from excitonic to photonic condensation can occur. Although the calculation presented here is for three dimension, the same scenario applies to two-dimensional systems. Results for two dimension will be shown elsewhere.

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