The Bose-Einstein condensation (BEC) of two-dimensional excitons in a ring: Necklace-like modulation of order parameter

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We have studied theoretically the Bose-Einstein condensation (BEC) of two-dimensional excitons in a ring with small random width variation. We derive a nonlinear Gross-Pitaevskii equation (GPE) for such a condensate. Our numerical solution of the ground state of the GPE displays a necklace-like structure in the presence of small random variation of ring width. This is a consequence of the interplay between random potential and the nonlinear repulsive term of the GPE. Our result suggests that the formation of ring and necklace-like structures observed recently in the photoluminescence of quantum wells may be stable even in the BEC phase.

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Recent advances in the Bose-Einstein condensation (BEC) of atoms were made possible by exploring the confinement of atomic gases within potential traps. In semiconductor physics, the possibility of exciton BEC has been explored for a long time [2, 3]. In the dilute limit \( na_B^2 << 1 \) (\( a_B \) is the exciton Bohr radius, \( D \) the dimensionality, and \( n \) is the exciton density) excitons are expected to undergo the BEC [4]. Recently, the possibility of BEC of excitons in potential traps of semiconductor quantum wells has been explored [5, 6, 7, 8, 9, 10]. The quantum degeneracy temperature is expected to be about 1K, much higher than that of atoms due to the small mass of the exciton. Butov et al. [8, 9], Snoke et al. [10], and Rapaport et al. [11] have observed a circular ring in exciton photoluminescence (PL) from these quantum wells, where the radius of the ring (typically 10 \( \mu \text{m} \) to 100\( \mu \text{m} \)) depends on the laser excitation intensity. A mechanism for the formation of the ring is proposed that involves carrier imbalance, transport, and recombination [2, 11]. In addition, Butov et al. [8] have observed that, as temperature decreases, the exciton PL fragments suddenly into a macroscopically ordered state of nearly necklace-like structure: they observed that minimum and maximum positions of PL intensity vary nearly periodically along the ordered ring, although the intensity of minimum and maximum values are non-periodic. The distance between peak positions deviate from the mean period roughly about 20 percent. (For a typical large ring observed in Ref. [5], the distances between peak positions vary roughly between 14 – 22\( \mu \text{m} \)). These random variations are not understood yet.

In this Letter, we derive a nonlinear Gross-Pitaevskii equation (GPE) of exciton BEC in the presence of small random variation of ring width, and show that the ground state displays a necklace-like structure. Following the experimental observation of Butov et al. [8] and Snoke et al. [11] we assume that electrons and holes are confined to move in a ring. The observed ring radius and width vary locally [12]. For simplicity we will model this randomness through a random variation of ring width as excitons move along the circumference of the ring with a constant radius. This implies that excitons experience a random potential as they move along the circumference (smaller width gives larger in-plane exciton potential energy). In this paper we assume that excitons form a Bose-Einstein condensate at temperatures below the quantum degeneracy temperature and explore the nature of such a condensate in the presence of a random potential. We employ a mean field approach [8, 11], which is exact both in the low and high density limits. We derive in the low density limit a nonlinear Gross-Pitaevskii equation (GPE) for excitons and solve it numerically for the ground state using the imaginary time evolution method. We find that the order parameter of exciton BEC displays a necklace-like structure. This is a consequence of a nontrivial interplay between a repulsive nonlinear term of GPE and random potential. Our result suggests that the formation of a necklace-like structure observed recently in the PL of quantum wells may be stable even in the BEC phase at lower temperatures.

We derive an effective theory of the BEC of two-dimensional excitons in a potential trap, which will lead to the GPE. We perform a model calculation in which the electron-hole interaction to be \( -g \delta(x - x') \), \( g > 0 \). We only consider optically active s-wave excitons and ignore heavy and light hole coupling in the valence band [13]. We replace the quartic electron-hole interaction in the Hamiltonian involving the electron and hole operators, \( \psi_e(x) \) and \( \psi_h(x) \), with those containing the pairing averages, \( g \langle \psi_h(x) \psi_e(x) \rangle \), and \( g \langle \psi_h^\dagger(x) \psi_e^\dagger(x) \rangle \) denoted respectively by the gap functions, \( \Delta(x) \) and \( \Delta^*(x) \).
The system is described by the finite-temperature Green’s functions defined by
\[ G_0(x, x') = -(T_x\psi_e(x, \tau)\psi_e^\dagger(x', \tau')), \]
where the gap function \( \Delta(x) = gF(x, x') \) is obtained from the Green’s function self-consistently. Here \( V_{e,h}(x) \) is the external potential for the electrons and holes set by the potential trap as well as by the random disorder. In this model, we also consider a simple situation where the effect of the electron-electron and the hole-hole interactions can be included in \( V_{e,h}(x) \). Note the presence of the magnetic field represented by the vector potential \( A(x) \).

The coupled differential equations can be written as integral equations using the noninteracting Green’s functions, \( \tilde{G}_e,0, \) that are obtained for the case where \( \Delta = 0 \). Iterating the integral equations and keeping up to, say, the third order in \( \Delta \), we find
\[
\begin{align*}
 g^{-1}\Delta^*(x) & \approx \int d^2y \ Q(x, y) \Delta^*(y) \\
 & + \sum_{i=1}^3 d^2y_i \ R(x, y_1, y_2, y_3) \Delta^*(y_1) \Delta(y_2) \Delta^*(y_3),
\end{align*}
\]
where \( Q(x, y) = (\beta\hbar)^{-1} \sum_n \tilde{G}_e^n(y, x, -\omega_n) \tilde{G}_e^n(y, x, \omega_n) \) and \( R(x, y_1, y_2, y_3) = -(\beta\hbar)^{-1} \sum_n \tilde{G}_e^n(y_1, x, -\omega_n) \times \tilde{G}_e^n(y_1, y_2, \omega_n) \tilde{G}_h^n(y_3, y_2, -\omega_n) \tilde{G}_h^n(y_3, x, \omega_n) \) with the fermionic Matsubara frequency \( \omega_n \). The higher order terms in the expansion are given in a similar way. The magnitude of the higher order terms will be estimated below. It turns out that it is sufficient to keep only up to \( O(\Delta^3) \) in the present problem.

Unlike in the derivation of the Ginzburg-Landau equations, our GPE is valid in the so-called strong coupling regime \( 10^{-4} \) \[10^{-4} \] , which is characterized by the negative chemical potential \( \mu = \mu_e + \mu_h < 0 \) near \( T = 0 \), or \( \beta\mu \to -\infty \). We assume that the effect of the magnetic field can be included as a phase factor as \( \tilde{G}_e,0(x, y, \omega_n) = \exp(-i\phi_{e,h}(x, y)) \tilde{G}_e,0(x, y, \omega_n) \), where \( \phi_{e,h}(x, y) = \exp(\pm\frac{\text{sign}^2(|A(x) + A(y)|^2 - (x - y))^2}{\beta\hbar}) \) with the plus (minus) sign corresponding to the electrons (holes) and \( \tilde{G}_e,0 \) are the noninteracting Green’s function in the absence of the magnetic field. This approximation is exactly the eikonal approximation made by Gorkov in the weak coupling limit \[19\]. This is reasonable in this case since, \( A(x) \) can be considered constant over the size of the exciton. It neglects, however, the terms of order \( A^2 \) \[10\], thus not suitable for the strong field regime. Within this approximation, the effect of the magnetic field disappears in the expressions of \( Q \) and \( R \) in the resulting GPE. Note that, for \( V_{e,h}(x) = 0 \), \( G_{e,h}(x, y, \omega_n) \sim \exp(\sqrt{2m_{e,h}(|\mu_{e,h}| + i\omega_n)|x - y|}) \), which decays within the length scale \( \sqrt{\hbar^2/(2m_{e,h}(|\mu_{e,h}|))} \). The presence of an external potential such as \( V_{e,h}(x) \) in the strong coupling limit was studied in Ref. \[17\]. As long as the external potentials vary slowly over the Bohr radius and they are much smaller than the binding energy \( \epsilon_0 \), one can replace \( \mu_{e,h} \) by \( \mu_{e,h} - (V_{e,h}(x) + V_{e,h}(y))/2 \) in the Green’s functions.

Now, since \( Q \) and \( R \) are rapidly decaying functions of their arguments, we may approximate the first term on the right hand side of Eq. \( 2 \) as
\[
\Delta^*(x) \int d^2y \ Q(x, y) \Delta^*(y) + \frac{1}{4} \left[ \nabla^2 \Delta^*(x) \right] \int d^2y \ Q(x, y)(x - z)^2,
\]
and the second term as
\[
\Delta^*(x)|\Delta(x)|^2 \int d^2y_i \ R(x, y_1, y_2, y_3).
\]

The above integrals are evaluated in the strong coupling limit at \( T = 0 \) with the assumption \( \mu_{e,h} < 0 \). In our model, excitons move in a Mexican hat potential in addition to a random potential represented by \( V_D(r) \). The resulting GPE is conveniently expressed in terms of the pair wavefunction \( \Phi(x) = \sqrt{2m/\pi}\Delta(r) \) where \( D = \frac{m}{2\pi\hbar^2} \) is the two-dimensional density of state per spin for the reduced mass \( m^* \) given by \( 1/m^* = 1/m_e + 1/m_h \). The evaluation of higher order coefficients in the GPE is straightforward.
Here we present the GPE up to $O(\Phi^7)$ as follows:

$$\mu_B \Phi(r) = -\frac{\hbar^2}{2M} \nabla^2 \Phi(r) + \frac{1}{2} \alpha (r^2 - R^2)^2 \Phi(r) + V_D(r) \Phi(r) + \frac{1}{2D} |\Phi(r)|^2 \Phi(r) + \frac{3}{8|\mu|D^2} |\Phi(r)|^4 \Phi(r) + \frac{1}{12|\mu|^2D^3} |\Phi(r)|^6 \Phi(r),$$

(3)

where $R$ is the radius of the ring, $M = m_e + m_h$ and $\alpha$ determines the strength of the confinement potential. Note that the present GPE is obtained up to $O(\Phi^7)$ in contrast to the conventional one $[1]$, which contains only $O(\Phi^3)$ nonlinear term. The $O(\Phi^4)$ term has the opposite sign to the $O(\Phi^3)$ term and can become important when $\mu$ is small. This is, however, not the case in the present problem as can be seen below. In general, the magnitude of a higher order nonlinear term may be estimated by multiplying the previous lower order term by $\frac{\mu}{M}$. The relative importance of each nonlinear term will be discussed below. The condensate wavefunction is normalized to the electron density, given by $n(x) = |\Phi(x)|^2$. From the kinetic term of the GPE, we note that the effective mass of an exciton is $M = m_e + m_h$, as expected. Note that the coefficient of the cubic term in $\Phi$ is independent of the binding energy, which is special to two dimensions. The microscopic parameters appear in the energy $\mu_B$, which is evaluated to be $\mu_B = |\mu| (\ln \frac{\mu}{|\mu|} - \frac{1}{3}) = |\mu| (\frac{\Lambda}{|\mu|})$, where $\epsilon_0 = \epsilon_D e^{-\frac{\mu}{\mu_D}}$ is the binding energy of the electron-hole pair and $\epsilon_D = \frac{\Lambda^2 e^{\mu_D}}{\mu_D}$ with the ultraviolet cutoff $\Lambda$ used to regularize the delta-function interaction of the electrons and holes. This expression for the binding energy can be derived $[13]$ from the Schrödinger equation for the particle with reduced mass $m^*$ and energy $-\epsilon_0$ interacting with the delta function potential of strength $-g$. The strong coupling limit is defined by the chemical potential $\mu = \mu_e + \mu_h \rightarrow -\epsilon_0$. In the limit $\mu \rightarrow -\epsilon_0$, $\mu_B \approx \epsilon_0 + \mu$. This is in contrast with the weak coupling BCS limit where $\mu$ is approximated by the Fermi energy.

We rescale the wavefunction $\Phi = A\Psi$ and the position coordinate $x = r/a$ using a length scale $a$. We define $\hbar \Omega$ by the energy scale associated with the length scale $a$: $a^2 = \frac{\hbar \Omega}{\mu m}$. The energy scale of the confinement potential is $\hbar \omega = \alpha a^4$. Note that this confinement potential alone does not fix the width of the ring since the width depends also on the third order coefficient in $\Phi$ (see below). Since the number of exciton is $\int |\Phi(r)|^2 d^2r = N$, the normalization constant is $A = N^{1/2}/a$. The number of excitons may be estimated from $N = (2\pi RD_e)\epsilon_F D_c$, where $d \approx 1 \sim 10\mu m$ is the width of the ring, and $D_c$ and $\epsilon_F$ are the electron density of states and the Fermi energy respectively. It is useful to write the GPE in a dimensionless form:

$$-\frac{1}{2} \nabla^2 \Psi(x) + \frac{1}{2} \eta_0 (x^2 - x_0^2)^2 \Psi(x) + V_D(x) \Psi(x) + \eta_1 |\Psi(x)|^2 \Psi(x) - \eta_2 |\Psi(x)|^4 \Psi(x) + \eta_3 |\Psi(x)|^6 \Psi(x) = \beta \Psi(x).$$

(4)

Here $\eta_0 = \omega/\Omega$, $x_0 = R/a$, and $\beta = \mu_B/\hbar \Omega$. The coefficients of the nonlinear terms are $\eta_1 = \frac{\alpha^2}{\mu_D m} \approx \pi \left( \frac{\Omega}{\alpha a^4} \right) \frac{\hbar \Omega}{\mu m}$. $\eta_2 = \frac{3\alpha^2}{4} \frac{\hbar \Omega}{\mu m} (\frac{\mu_D^2}{m^*})^2 (\frac{\hbar \Omega}{\mu m})^2$, and $\eta_3 = \frac{3\alpha^3 e}{4} \frac{\hbar \Omega}{\mu m} (\frac{\mu_D^3}{m^*})^3$. We use $a = 10\mu m$, which gives $\hbar \Omega \approx 10^{-6}\text{meV}$. For exciton densities between $10^9 \sim 10^{10}\text{cm}^{-2}$ we estimate $\eta_1 \approx 10^4 \sim 10^5$. These large values will have important consequences (see below). Since $|\mu|$ is comparable to the indirect exciton binding energy of few meV we get $\epsilon_F/|\mu| < 0.01$. From these considerations, we conclude that the nonlinear terms, except the third order term, may be neglected. Note that the parameter $\beta$, i. e., the binding energy $\epsilon_0$ is determined from the solution of the GPE.

We now solve the dimensionless GPE for the ground state using the imaginary time evolution method. The
two-dimensional space is discretized using $512 \times 512$ grid points on a square of area $10a \times 10a$. The random potential is simulated by 250 Gaussian potentials placed randomly on the ring: $V_D(r) = \frac{1}{\sqrt{2\pi w^2}} e^{-\frac{(r-R_i)^2}{2w^2}}$, where $R_i$ are random position vectors on the ring with radius $R$ and $w = \frac{\sqrt{2\pi}}{\langle x^2 \rangle} \sim 1 \mu m$. The strength of the random potential is taken to a fraction of the strength of the confinement potential $V = 0.25 h \omega$. The correlation function of the random potential is $V_D(x)V_D(x') \propto e^{-\frac{|x-x'|}{2w^2}}$. We find numerically that the average distance between the peaks in $|\Psi(x)|^2$ is roughly the correlation length of the random potential $w$. The upper left panel of Fig. 1 displays how $|\Psi(x)|^2$ varies on the circumference of ring for $\eta_1 = 10^5$ and $\hbar \omega = 2 \times 10^5 \hbar \Omega$. A two-dimensional contour plot of $|\Psi(x)|^2$ displays a necklace-like structure as shown in the upper right panel of Fig.1. Positions of modulation maxima are nearly periodic while the values of modulation maxima are non-periodic. The angular distances between peak positions are given roughly as $12 - 20^\circ$, which shows a deviation from the mean period roughly about 20 percent. These results are in qualitative agreement with the experimental data (see Fig.3c of Butov et al.). The width of the ring increases with increasing coefficient of the non-linear repulsive term $\eta_1$. In the lower panels of Fig. 1, the solution to GPE is displayed when the repulsive third order term is present while the disorder potential is present. We observe that the modulation maxima fluctuate much more than those of $\eta = 10^5$, and that periodic modulation is absent in a two-dimensional contour plot of $|\Psi(x)|^2$. Comparing $|\Psi(x)|^2$ with the shape of the random potential in the left panels of Fig. 1, we can conclude that, as the repulsive third order term increases, the peak values of $|\Psi(x)|^2$ in the local minima of the potential fluctuate less from each other. We have also solved the GPE when the repulsive third order term is present while the disorder potential is absent. In this case, $|\Psi(x)|^2$ is uniform along the center of the ring, which implies that the uniform ring state represents a stable BEC of excitons in the absence of disorder.

We have derived a nonlinear Gross-Pitaevskii equation (GPE) of exciton BEC in the presence of small random variation of ring width, and have shown that the ground state displays a necklace-like structure. Our results demonstrate that the interplay between random potential and the nonlinear repulsive term of the GPE plays an important role in understanding necklace-like structures. Since the observed fragmented structure appears suddenly at low temperature, a collective mechanism of quantum origin may be involved, such as the BEC. Since we assumed a BEC phase of excitons in our derivation our results may be especially relevant in the low temperature regime of the phase diagram of the ordered state proposed by Butov et al. We believe more experiments at lower temperature are needed that would elucidate the interplay between the non-linear repulsive term and random potential in the formation of the fragmentation.

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