"Dilute" excitons in a double layer system: single-exciton and mean-field approach

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Double layer systems where one layer has electrons and the holes are in a parallel layer a distance \( d \) away are expected to undergo excitonic condensation at low temperature. This excitonic condensate is traditionally described by a many-body wavefunction that encodes the coherence between electron and hole bands. Here we compare the mean-field ground state in the limit of dilute electron (hole) density with the ground state of a single electron-hole pair in double-layer system. As the interlayer distance \( d \) increases, we find that the excitonic size, characterized by the width of the momentum-space wavefunction, also increases. By comparing the single-exciton wavefunction with the mean-field analysis, we determine the \( d \)-dependence of the "diluteness" of the exciton gas in a balanced double-layer system with given electron (or hole) density.

I. INTRODUCTION

The Bose-Einstein condensation of excitons in double layer systems realized in semiconductor heterojunctions, where a macroscopic number of excitons occupy a single quantum state, has been a subject of intense research over the past decade.1,2 An exciton is a metastable bound state of an electron and a hole. In a balanced electron-hole system at low electron (hole) densities \( n_e = n_h = n_{2D} \), the distance between the excitons is much larger than the quantum exciton size and the excitons behave as weakly-interacting bosons.2,3,4 In a bulk semiconductor or a two-dimensional system, the internal state of the exciton is given by Hydrogenic wavefunctions2 that result from the Coulomb interaction \( V_A(r) = e^2/\epsilon r \). In this case, the wavefunction for the electron-hole separation decays exponentially with decay length \( a_{ex}/2 \) where \( a_{ex} = \hbar^2/\epsilon^2 m_r \) is the quantum size of the exciton. Here \( \epsilon \sim 10 \) is the dielectric constant of the semiconductor heterojunction, \( r_e (r_h) \) represents the electron (hole) position, \( m_r^{-1} = m_e^{-1} + m_h^{-1} \) is the (reduced) mass of exciton, and \( m_e (m_h) \) is the electron (hole) band mass. Note that for a symmetric electron-hole system that we consider in this paper, \( m_e = m_h = 2m_r \), the quantum size of carriers is half the exciton size, \( a_0 = \hbar^2/\epsilon^2 m_e = a_{ex}/2 \).

Therefore the dimensionless distance between excitons for a given carrier density \( n_{2D} \) is given by \( r_s/2 \) where \( r_s \), defined by \( \pi r_s a_0)^2 = 1/n_{2D} \) is the dimensionless distance between the carriers. Since the quantum size \( a_{ex} \) of the exciton is fixed by the semiconductor properties, it is possible to tune the interaction between excitons from weak \( (r_s \gg 1) \) to strong \( (r_s \sim 1) \).4 Note that for a bulk or planar system, as opposed to a double-layer system, the inter-exciton interaction and the formation of exciton are both governed by the same Coulomb interaction \( V_A(r) \).

In double-layer systems where carriers are in the top layer and holes are in the bottom layer, the formation of an exciton is determined by the attractive interlayer Coulomb interaction \( V_E(r) = -e^2/\epsilon \sqrt{r^2 + d^2} \) where \( d \) is the distance between the two layers and \( r \) denotes the two-dimensional position vector. Since the attractive interaction is \( d \)-dependent, the quantum size of exciton is not necessarily \( a_{ex} \) and, in fact, depends on the dimensionless ratio \( d/a_0 \). The interaction between the excitons, on the other hand, is also dependent on intralayer Coulomb repulsion \( V_A(r) \). Thus, in double-layer systems, the diluteness of excitons is a function of \( (d/a_0, r_s) \). In this paper, we quantitatively explore this issue. In the next section we present numerical solution to the single-exciton problem. We find that the exciton binding energy \( E_b \) decreases as \( d \) increases and concurrently the momentum-space ground state wavefunction sharpens. Thus, the quantum size of an exciton \( a_{ex}(d) \) increases with \( d \). In Sec. III, we complement the single-exciton results with mean-field analysis of the uniform excitonic condensate ground state for varying carrier density \( n_{2D} \). By comparing the exciton wavefunction obtained from the Wannier approximation with that in Sec. II, we obtain a quantitative criterion for the "diluteness" of an exciton gas. We conclude the paper with a remarks in Sec. IV.

II. SINGLE-EXCITON PROBLEM

Let us start with an electron and a hole in a double-layer system with \( d = 0 \). The eigenstates of this problem are obtained by solving the equivalent problem of a particle with mass \( m_r \) in a central attractive potential. Due to the rotational invariance in two dimensions5 and the existence of the conserved Runge-Lenz vector,6 the energy spectrum in the limit \( d = 0 \) is dependent only on the principle quantum number \( n \geq 1 \), \( E_n = -4E_0/(2n - 1)^2 \) where \( E_0 = e^2/\epsilon a_0 \) is the energy scale associated with the problem. (Note that typical parameters \( \epsilon \sim 10 \) and \( a_0 \sim 50 \text{ Å} \) imply \( E_0 \sim 30 \text{ meV} \).) The corresponding normalized ground-state wavefunction is given by \( \psi_0(r) = \sqrt{8/(\pi a_0^2)} \exp(-2r/\sqrt{a_{ex}}) = \sqrt{2/(\pi a_0^2)} \exp(-r/a_0) \).5 When \( d \neq 0 \), since the electron-hole interaction is given by \( V_E(r) = -e^2/\epsilon \sqrt{r^2 + d^2} \), the differential equation for the radial component of the ex-
citonic wavefunction that cannot be analytically solved. Instead, we use the momentum-space Schrödinger equation

$$\frac{\hbar^2 k^2}{2m_r} \psi_\alpha(k) + \int_{k'} V_E(|k - k'|) \psi_\alpha(k') = E_\alpha \psi_\alpha(k)$$ (1)

where $k$ is the two-dimensional wavevector, $\psi_\alpha(k)$ is the momentum-space eigenfunction with eigenvalue $E_\alpha$, and $V_E(q) = -V_A(q)e^{-q^2}$ where $V_A(q) = 2\pi e^2/\epsilon q$ is the Fourier transform of the intralayer Coulomb interaction in two dimensions. We focus on Eq.(1) projected onto the zero angular-momentum sector and obtain the eigenenergies and eigenfunctions by discretizing the integral equation and numerically diagonalizing the resulting matrix

$$H_{mn} = \frac{u_n^2}{2} \delta_{mn} + \frac{u_n \Delta u}{2\pi} \tilde{V}(u_m, u_n) = \frac{u_n}{u_n} H^*_{nm},$$ (2)

Here $\tilde{V}(u_m, u_n)$ is the angular-averaged dimensionless electron-hole interaction. Although the Hamiltonian (2) leads to bound and continuum states, since the excitonic internal states are only accessible at temperatures $T \geq E_0/k_B \sim 300$ K, in the following we only discuss the behavior of the ground state.

Figure 1 shows the numerically obtained ground-state energy of a single exciton as a function of interlayer distance $d$. At $d = 0$, the numerical result deviates from the well-known analytical answer by 10%; however, we have verified that this difference is solely due to discretization errors and can be systematically suppressed.\(^7\) When $d/a_0 \ll 1$ first-order perturbation theory implies that the change in the ground-state energy is linear, $\delta E_G = E_G(d) - E_G(0) = 4E_0(d/a_0)$. At large $d$ the excitonic binding energy is strongly suppressed; for example, when $d/a_0 = 10$ it is reduced to 10% of the binding energy at $d = 0$.

In Figure 2, we show the corresponding evolution of the ground-state wavefunction with increasing $d$. At $d = 0$ the normalized wavefunction is given by $\psi_G(k) = \sqrt{8\pi a_0^2/(1 + k^2 a_0^2)}^{3/2}$ and is reproduced by our numerical calculations. As $d$ increases, we see that the momentum-space wavefunction sharpens and shows that the single exciton size $a_{ex}(d)$ increases with $d$.

These results show that a single exciton in a double-layer system is increasingly weakly bound, and becomes larger as the interlayer distance $d$ increases. Therefore, although $r_s$ is a good measure of the diluteness of electrons or holes, it is not a good measure of diluteness for the excitonic gas. To quantify this observation, in the next section, we study the evolution of a uniform excitonic condensate state as a function of $(d/a_0, r_s)$.

III. MEAN-FIELD ANALYSIS

To explore the uniform excitonic condensate state, we start with a double-layer system with electrons in the top layer and holes in the bottom layer that is separated by distance $d$. The Hamiltonian for such a system is a sum of the kinetic energy for electrons and holes, as well as the intralayer Coulomb repulsion $V_A(q)$ and the interlayer Coulomb attraction $V_E(q)$. We use the standard mean-field approximation\(^8\) to obtain the mean-field Hamiltonian,

$$H = \sum_k (\epsilon_k \hat{h}_{-k}) \left( \begin{array}{c} \xi_k \\ \Delta_k \\ -\xi_k \end{array} \right) \left( \begin{array}{c} \epsilon_k \\ \Delta^*_k \\ -\xi_k \end{array} \right)$$ (3)
where $c_k^\dagger$ ($h_k^\dagger$) is the creation operator for an electron (hole) with two-dimensional momentum $\hbar \mathbf{k}$ in the top (bottom) layer, $\xi_k$ is renormalized electron (hole) dispersion that takes into account the interlayer capacitance and intralayer exchange energy, and $\Delta_k$ is the excitonic order parameter associated with the coherence between the electron and the hole bands in the two layers. We consider an isotropic excitonic-condensate order parameter and obtain the following self-consistent mean-field equations\cite{9,10}

\begin{align}
\xi_k &= \varepsilon_k + V_C - \mu - \int_{k'} V_A(\mathbf{k}-\mathbf{k'}) \langle c_k^\dagger c_{k'}^\dagger \rangle \\
\Delta_k &= \int_{k'} V_E(\mathbf{k}-\mathbf{k'}) \langle h_k c_{k'}^\dagger \rangle \\
n_{2D} &= \int (\varepsilon_k^2 + \varepsilon_k) = \frac{1}{2} \int_k \left( 1 - \frac{\xi_k}{E_k} \right) \tag{6}
\end{align}

where $\varepsilon_k = \hbar^2 k^2/2m_e = \hbar^2 k^2/2m_h$ denotes the electron (hole) band dispersion, $V_C = 2\pi e^2 n_{2D}/\varepsilon$ is the capacitive energy cost, and $\mu$ is the (electron and hole) chemical potential determined implicitly by Eq.(6). The self-consistent excitonic order parameter is determined by $\langle h_k c_k \rangle = \Delta_k/2E_k$, and $\pm E_k = \pm \sqrt{\xi_k^2 + \Delta_k^2}$ denote dispersion of the quasiparticle bands that result from Hamiltonian (3). We solve Eqs.(4)-(6) iteratively for a given $(d/a_0, r_s)$ to obtain the self-consistent order parameter $\Delta_k$ and quasiparticle energy dispersion $E_k$. To explore the dilute exciton limit, we recast Eq.(5) in terms of $\Phi(p) = \Delta_p/E_p$ and note that for $\Delta_p \ll \xi_p$, $\Phi(p)$ reduces to the single-exciton Schrödinger equation in momentum space, Eq.(1). This permits a quantitative comparison between the ground-state exciton wavefunction $\psi_G(p)$ and the Wannier exciton wavefunction $\Phi(p)$.

Figure 3 compares the Wannier wavefunction $\Phi(p)$ at $d/a_0 = 1$ for different values of $r_s$ with the single-exciton wavefunction $\psi_G(p)$. We see that $r_s$ increases the Wannier wavefunction approaches the single-particle result, as expected. Note that for small $r_s$, the Wannier exciton wavefunction $\Phi(p)$ is peaked at finite momentum because the excitonic order parameter $\Delta_p$ is maximum and $\xi_p$ is minimum at the Fermi momentum. However, as $r_s$ increases, for any given $d$, the peak in $\Delta_p$ shifts towards the origin and so does the maximum of the Wannier wavefunction.

To quantify the proximity between the Wannier and the single-exciton approach, we consider the overlap $\gamma(d/a_0, r_s)$ between the two (real) wavefunctions

$$\gamma(d/a_0, r_s) = \int \frac{dk}{(2\pi)^2} \Phi^*(k) \psi_G(k). \tag{7}$$

A high overlap value $\gamma(d/a_0, r_{sc}) \sim 1$, allows us to define a critical value of $r_{sc}(d/a_0)$ such that for $r_s \geq r_{sc}$ the single-exciton result provides an excellent substitute for the mean-field analysis. Figure 4 shows the critical $r_{sc}(d)$ obtained using $\gamma = 0.90$ and $\gamma = 0.95$. We see that for typical values of $d$ the critical $r_{sc}$ scales linearly with $d/a_0$. It implies, for example, that approaching the dilute-limit at $d/a_0 = 3$ will require reducing the carrier density by a factor of 5 from the corresponding value for the dilute limit at $d/a_0 = 1$.

**IV. DISCUSSION**

The subject of excitonic condensation in double-layer systems has been extensively explored in the literature; the properties of a single exciton in a double-layer system, however, have not been. In this paper, we have...
obtained the ground-state wavefunction and the ground-state energy for a single exciton as a function of interlayer distance \(d\). By comparing our results with those from a mean-field analysis of the uniform excitonic condensate, we have obtained the critical value \(r_{sc}(d)\) that is used to determine when the exciton gas for a given interlayer distance \(d\) is “dilute”.

Our analysis provides a quantitative picture of a single exciton in double-layer system with \(d \neq 0\) where analytical solution for the excitonic wave-functions is not possible. It shows that as \(d\) increases, due to the weakened electron-hole Coulomb interaction, the exciton size \(a_{ex}(d)\) increases.

We note that the Wannier approximation for excitonic wavefunction is based on a mean-field analysis that usually over-estimates\(^8\) the excitonic order parameter \(\Delta_k\). In particular, in double layer systems, it is known that the uniform condensate becomes unstable\(^11\) when \(d\) is larger than a critical layer separation \(d_c\). Thus, when fluctuations around the mean-field state are taken into account, the critical value of \(r_s\) for a given \(d \sim d_c\) will change substantially. Our mean-field analysis is based on a uniform excitonic condensate state. Due to dipolar repulsion between excitons, the uniform state is unstable towards formation of a crystalline excitonic condensate\(^12\) in the region \(\sqrt{r_s} \ll d/a_0 \ll r_s\). Since our calculations lie outside this parameter range, we have focused only on the uniform state; the question of a “dilute” exciton limit in a crystalline excitonic condensate, however, remains open.

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