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Abstract: The effects of lateral confinement and strong magnetic fields on the energy levels and optical spectra of magnetoexcitons in a disk-like parabolic quantum dot are considered. For a QD which in the absence of a magnetic field B is in the strong confinement regime, a crossover to the weak confinement regime can be realized when B is increased. Energy spectra and dipole matrix elements of optical transitions in different confinement regimes are found.

1. In recent years much attention has been paid to quasi-zero-dimensional quantum dots (QDs) and microcrystallites in which motions of electrons (e) and holes (h) are size-quantized in all spatial directions and energy spectra are completely discrete. In particular, considerable amount of work has been done on optical properties of these systems, which essentially differ from those of bulk 3D samples (e.g. [1–3] and the literature cited therein). When size quantization in a QD is weak, i.e. $L \gg a_B^{(e,h)}$ where L is the length scale of a lateral confining potential and $a_B^{(e,h)} = \varepsilon\hbar^2/m^*_{(e,h)}e^2$ are the effective electron (hole) Bohr radii, the interband optical excitation leads to a formation of an exciton whose center of mass motion is quantized. The oscillator strengths in this regime are concentrated mainly in the transition to the ground exciton s-state and are proportional to the volume of the system (e.g. [1,3]). When a strong confinement regime is realized, $L \ll a_B^{(e,h)}$, the motions of both electron and hole are strongly quantized with the interlevel spacing $\Delta E \sim 1/L^2$. This allows one to neglect the Coulomb interaction between particles $U \sim 1/L$. In this regime the absorption spectra are broadened and blue-shifted and the matrix elements of the optical transitions to different s-states of the e-h pair are practically equal and do not depend on the volume of the system (e.g. [1–3]).

When in addition to lateral confinement an external magnetic field is applied a new length scale, the magnetic length $l_B = (\hbar c/eB)^{1/2}$ enters the problem. In a strong magnetic field when $l_B \leq a_B^{ex} = \hbar^2\varepsilon/M_{ex}e^2$, the characteristic scale of the Coulomb interaction becomes $e^2/\varepsilon l_B$ (if there are no other lengths in the problem which are less than l_B) and the type of the exciton confinement (i.e. a strong or a weak) is determined by the relation between l_B and L. Therefore, for a QD which at the zero field B is in the strong confinement regime $L \ll a_B^{(ex)}$, a crossover to the weak confinement regime ($l_B \ll L$) can be realized when B is increased. As a consequence, the optimal field B_{opt} exists, at which non-linear effects are most strongly manifested (cf. [1]). In this paper, we obtain the energy spectra and consider the linear optical properties of excitons in a parabolic QD in quantizing magnetic fields $B > 6$T ($l_B < 100$Å).

2. It is important to indicate the difference between excitons and electrons in parabolic QDs in magnetic fields. In the Hamiltonian of an interacting one-component electron system in a magnetic field and in an (effective) parabolic potential, the center of mass motion is decoupled from the internal degrees of freedom. As a result, in the dipole approximation the energies of intraband magneto-optical transitions do not depend on the interparticle interactions and coincide with those in a one-particle system [4]. For a two-component e-h system containing charges of different sign, the center of mass motion in a magnetic field is coupled to the internal motion (even in the absense of external confining potential). Hence, a consistent treatment of interparticle correlations is needed for the calculation of the interband absorption spectra.

3. We assume a low level of excitation and consider only one e-h pair in a QD, neglecting the interaction between excitons. We also assume that the size quantization along the magnetic field direction is strong (i.e. that a QD width $d < a_B^{(e,h)}$) and consider strictly 2D problem neglecting the dependence of wavefunctions on z. We model lateral confinement in the QD by parabolic potentials for e and h with the effective frequencies ω_e, ω_h (assuming in general that $\omega_e \neq \omega_h$). We also adopt a simple two-band structure for the semiconductor.

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Within these approximations the Hamiltonian of the system is given by

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0^{(e)} + \hat{\mathcal{H}}_0^{(h)} + U(\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2) \tag{1}$$

where $\boldsymbol{\rho}$ is a 2D vector in the (x, y) plane, U is the interparticle interaction potential, $\hat{\mathcal{H}}_0^{(j)}$ is the Hamiltonian of a 2D particle in a magnetic field and in the parabolic confining potential

$$\hat{\mathcal{H}}_0^{(j)} = \frac{1}{2m_j^*}(-i\hbar\nabla - \frac{q_j}{c}\mathbf{A})^2 + \frac{m_j^*\omega_j^2(x^2+y^2)}{2} \tag{2}$$

here $j = e, h$ ($q_e = -e$, $q_h = e$), m_j^* are the effective masses, and $\mathbf{A} = \frac{1}{2}[\mathbf{B} \times \mathbf{r}]$ is the vector potential. Hamiltonian $\hat{\mathcal{H}}_0^{(e)}$ (2) is diagonal in the representation of the ladder operators (compare [5,6])

$$a_e^+ = -\frac{i}{\sqrt{2}}\left(\frac{\xi}{2R_e} - 2R_e\frac{\partial}{\partial\xi^*}\right), \quad b_e^+ = \frac{1}{\sqrt{2}}\left(\frac{\xi^*}{2R_e} - 2R_e\frac{\partial}{\partial\xi}\right), \tag{3}$$

where $\xi = x + iy$ is a complex variable. The effective length R_j in (3) is defined by

$$\frac{1}{R_j^4} = \frac{1}{l_B^4} + \frac{1}{l_j^4} \tag{4}$$

where the oscillator lengths of the confining potentials $l_j = (\hbar/2m_j^*\omega_j)^{1/2}$ are introduced. Operators (3) are the conventional ladder operators: $[a_e, a_e^+] = [b_e, b_e^+] = 1$, $[a_e, b_e] = [a_e, b_e^+] = 0$. The Hamiltonian of the hole $\hat{\mathcal{H}}_0^{(h)}$ has the same structure as $(\hat{\mathcal{H}}_0^{(e)})^*$, therefore the ladder operators diagonalizing it can be obtained from (3) by the complex conjugation and the substitution $R_e \to R_h$

$$a_h^+ = [(a_e^+)^*]_{R_e\to R_h}, \quad b_h^+ = [(b_e^+)^*]_{R_e\to R_h} \tag{5}$$

The single-particle Hamiltonian (2) written via the ladder operators (3),(5) becomes

$$\hat{\mathcal{H}}_0^{(j)} = \hbar\Omega_C^{(j)} a_j^+ a_j + \hbar\Omega_L^{(j)} b_j^+ b_j + \frac{1}{2}\epsilon_0^{(j)}. \tag{6}$$

In (6) the following notations are used

$$\Omega_{C(L)}^{(j)} = \frac{\hbar}{2m_j^*}\left(\frac{1}{R_j^2} \pm \frac{1}{l_B^2}\right) = \omega_c^{(j)}\frac{\sqrt{1+(l_B/l_j)^4} \pm 1}{2}, \tag{7}$$

$$\epsilon_0^{(j)} = \frac{\hbar^2}{m_j^* R_j^2} = \hbar\omega_c^{(j)}\sqrt{1+(l_B/l_j)^4}, \tag{8}$$

where $\omega_c^{(j)} = eB/m_j^*c$ is the cyclotron frequency. Note that $(l_B/l_j)^2 = 2\omega_j/\omega_c^{(j)}$, and in the strong magnetic fields when $l_B/l_j \sim B^{-1/2} \to 0$, we have $\Omega_C^{(j)} \to \omega_c^{(j)} \sim B$, $\epsilon_0^{(j)} \to \hbar\omega_c^{(j)} \sim B$, while the frequency $\Omega_L^{(j)} \to \omega_j^2/\omega_c^{(j)} \sim B^{-1}$ describes the fine structure of Landau levels (LLs).

Normalized eigenfunctions of the Hamiltonian (6) are

$$\psi_{nm}^{(j)}(\boldsymbol{\rho}) = \frac{(a_j^+)^n(b_j^+)^m}{\sqrt{2\pi R_j^2 n! m!}}\exp\left(-\frac{|\xi|^2}{4R_j^2}\right) \tag{9}$$

Eigenvalues n of the operator a^+a are numbers of LLs. The latter, in the absense of a confining potential, are degenerate in the oscillator quantum number m (which is the eigenvalue of the operator b^+b). The wavefunctions (9) describe localized states with fixed z-projection of the angular momentum ($m_z = n - m$ for e and $m_z = m - n$ for h). Mean squared distances from the origin at which the states are localized are $\langle\rho^2\rangle_{jnm} = 2(n+m+1)R_j^2$.

We expand the exciton wavefunction with the total angular momentum projection M_z over the complete orthonormal basis set of products of non-interacting wavefunctions (9)

$$\Phi_{M_Z}(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2) = \sum_{n_1 - m_1 + m_2 - n_2 = M_Z} A_{n_1 n_2 m_1 m_2}\psi_{n_1 m_1}^{(e)}(\boldsymbol{\rho}_1)\psi_{n_2 m_2}^{(h)}(\boldsymbol{\rho}_2) \tag{10}$$

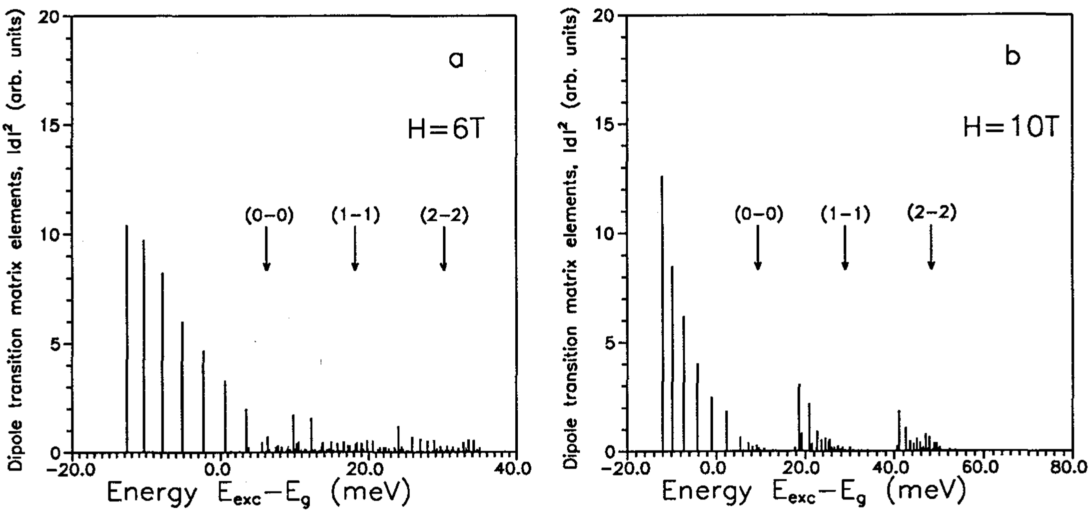

Figure 1: The dipole matrix elements $|d|^2 \sim |\sum_{n,m} A_{nnmm}|^2$ (see (11) with $R_e = R_h$) and the eigenenergies (shown relative to the band gap E_g at $B=0$) of the optically-active s-states of the magnetoexciton in the parabolic QD with the oscillator lengths $l_e = l_h = 150$Å at (a) $B = 6$T and (b) $B = 10$T. Vertical arrows show the edges of the allowed transitions (n-n) between Landau levels in the non-interacting QD.

Eigenenergies and eigenfunctions of Hamiltonian (1) are obtained from solving a secular equation (compare [7] and references therein). The matrix elements for the interband optical transitions are

$$d \sim \langle c|\mathbf{p}|v\rangle \int d\rho\, \Phi_{M_Z}(\rho,\rho)$$

i.e. are proportional to the probability amplitude of finding the electron and the hole at the same site. Since

$$d \sim \sum_{n_1-m_1+m_2-n_2=M_Z} A_{n_1n_2m_1m_2} \int d\rho\, \psi^{(e)}_{n_1m_1}(\rho)\psi^{(h)}_{n_2m_2}(\rho) \sim \delta_{M_Z,0} \tag{11}$$

only s-excitons are optically active, as it should be.

4. In numerical calculations we consider the Coulomb interaction $U = -e^2/\varepsilon r$ between the electron and hole neglecting image forces and use the values $m_e^* = 0.068$, $m_h^* = 0.34$ and $\varepsilon = 12.5$. Here we present the results for the oscillator lengths $l_e = l_h = 150$ Å and strong magnetic fields $B > 6$ T, when $l_B \le a_B^{(e)}$.

The matrix of the total Hamiltonian (1) is infinite (see (10)) even in the magnetic quantum limit when only the states from the zero Landau levels are taken into account (and hence $M_z = m_2 - m_1$). Physically, this is connected with the fact that when the confining potential is absent, the spectrum of the magnetoexciton is continuous. Mixing between the states within the same LL resulting from the Coulomb interactions can be characterized by the parameter

$$E_0/\hbar\Omega_L^{(e,h)} \sim \begin{cases} l_j^4/l_B^3 a_B^{(e,h)}, & \text{for } l_j > l_B \\ l_j/a_B^{(e,h)}, & \text{for } l_j < l_B. \end{cases} \tag{12}$$

where $E_0 \equiv e^2/\varepsilon R$ is the characteristic scale of the Coulomb interactions, $R = \sqrt{(R_e^2 + R_h^2)/2}$. The mixing between different LLs is small when $E_0 \ll \hbar\Omega_C^{(e,h)}$ which is equivalent to $l_B \ll a_B^{(e,h)}$ if $l_j > l_B$ (cf. [8]) and $l_j \ll a_B^{(e,h)}$ if $l_j < l_B$. In practice we truncate the initial matrix using the fact that, due to the proper choice of the basis set, the eigenvalues and eigenvectors of a truncated matrix converge to their exact values. We take into account 4 lowest LLs for e, 6 lowest LLs for h and 20 states in each LL, which allows us to obtain the energies and oscillator strengths of the low-lying exciton states with the accuracy about 5%.

In Fig.1,2 the calculated absorption spectra at different magnetic field strengths are shown. In lower fields, when l_B is of the order of l_j, the confinement is strong and the oscillator strengths are distributed

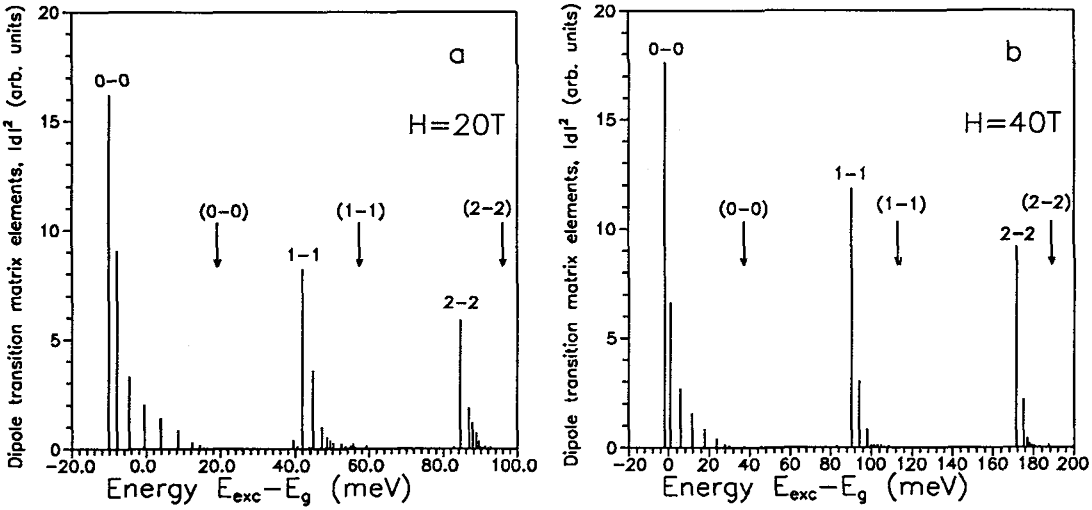

Figure 2: Same as in Fig.1 for (a) B = 20T and (b) B = 40T. Well-defined transitions between Landau levels (marked by n-n) are red-shifted from their positions (n-n) in the non-interacting QD.

between a number of exciton states and do not depend on the volume of the system. When the field B is increased, well-defined Landau-level transitions (marked as n-n in Fig2.) appear with additional lines due to the lateral potential. At the same time, the confinement in the QD becomes weaker and the oscillator strengths concentrate mainly at the transitions to the ground states of the magnetoexciton in each Landau level. The edge of the absorption spectrum shifts to higher energies (as $(\epsilon_0^{(e)}+\epsilon_0^{(h)})/2$, see (8)). In this regime the exciton center of mass motion is quantized. In the magnetic quantum limit ($n_1 = n_2 = 0$) the energy separation between the low-lying levels, ΔE, is determined by the effective mass of the magnetoexciton $M_{\rm eff} = \frac{2\hbar^2\epsilon}{e^2}\left(\frac{2eB}{\pi\hbar c}\right)^{1/2} \sim B^{1/2} \gg (m_e^* + m_h^*)$ which is entirely due to the e-h Coulomb interaction [8]. As a result, $\Delta E \simeq \hbar((m_e^*\omega_e^2 + m_h^*\omega_h^2)/M_{\rm eff})^{1/2} \sim B^{-1/4}$ and exceed the energies $\hbar\omega_j^2/\omega_c^{(j)} \sim B^{-1}$ defining the fine structure of the non-interacting LLs in the QD.

Note added. After this work had been completed, we became aware that very similar studies have been performed by V.Halonen, T.Chakraborty and P.Pietiläinen (Phys.Rev. B45, 5980 (1992)). We thank S.Glutsch for pointing this out to us.

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