

Magnetoexciton states and diamagnetic shifts in GaAs–Ga_{1–x}Al_xAs quantum dots/ultrathin quantum wells under growth-direction magnetic fields

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Abstract

A theoretical study of the exciton diamagnetic shifts in GaAs–Ga_{1–x}Al_xAs quantum dots (QDs) and ultrathin quantum wells (QWs), under growth-direction applied magnetic-fields, is performed. We work in the effective-mass approximation and take into account nonparabolicity effects for the effective masses of both the conduction and valence bands. Calculated results for the diamagnetic shifts of the $m = 0$ ground-state, $m = -1$ and -2 excited states of the heavy-hole exciton, within a simple “QD + ultrathin QW” model heterostructure, are found in overall agreement with recent experimental measurements by Schildermans et al. (Phys. Rev. B **72** (2005) 115312) and Sidor et al. [Phys. Rev. B **73** (2006) 155334].

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Due to their possible applications in a variety of optoelectronic and spintronic devices, semiconductor quantum dots (QDs) have been the subject of considerable work in the last decade or so [1,2]. Here we are concerned with GaAs–Ga_{1–x}Al_xAs QDs and ultrathin quantum wells (QWs). Recently, Rastelli et al. [3] have been able to obtain 3D unstrained GaAs–Ga_{1–x}Al_xAs QDs and performed photoluminescence (PL) spectroscopy measurements with very narrow inhomogeneous broadening and clearly resolved excited states. Further studies of the optical properties of unstrained GaAs–Ga_{1–x}Al_xAs QD/ultrathin QW systems were also made by Schildermans et al. [4] and Sidor et al. [5].

The purpose of the present work is to theoretically study the growth-direction magnetic-field effects on the exciton states in GaAs–Ga_{1–x}Al_xAs QDs and ultrathin QWs, and compare calculated results and corresponding exciton

diamagnetic shifts with the measurements by Schildermans et al. [4] and Sidor et al. [5]. We first note that magneto-photoluminescence data by Schildermans et al. [4] in GaAs–Ga_{1–x}Al_xAs QD/ultrathin QW systems reveal well-resolved QW and QD PL peak energies. We choose therefore a simple theoretical modelling [6] of the GaAs–Ga_{1–x}Al_xAs semiconductor heterostructure which is loosely depicted in Fig. 1, and should be compared with the insets in Fig. 2 of Rastelli et al. [3] or in Fig. 1 of Schildermans et al. [4]. In the present calculations, we follow Schildermans et al. [4] and ignore spin effects. Moreover, we assume that the relative motion of the carriers and that of the center of mass (CM) are independent. With these assumptions, the exciton envelope wave function may be taken as $\Psi_{\text{exc}}(\vec{\rho}, z_e, z_h)$, where $\vec{\rho}$ is the relative e – h in-plane vector position for motion parallel to the heterostructure interfaces and on carrier coordinates z_e and z_h along the growth-direction.

In the calculation of the QD exciton PL peak energies [or electron–hole (e – h) correlated transition energies], we

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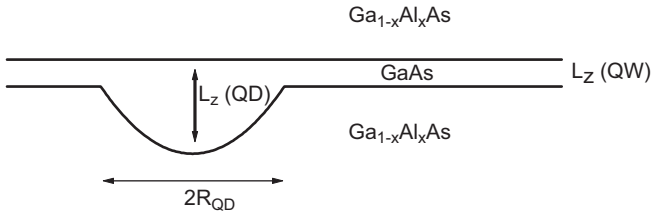


Fig. 1. Pictorial view of the “QD + ultrathin QW” model heterostructure used in the present work.

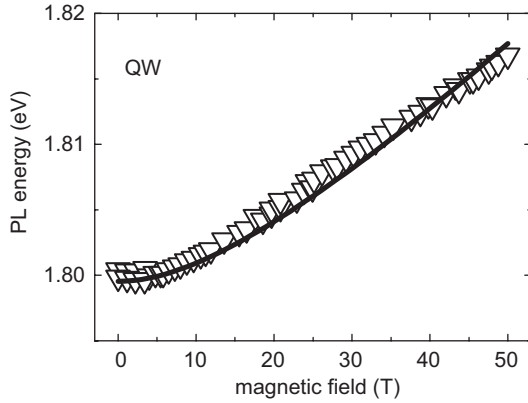


Fig. 2. Growth-direction magnetic-field dependence of the heavy-hole exciton peak energies (or ground-state correlated $e-h$ transition energies) for a symmetric ultrathin $L_z(\text{QW}) = 1.6 \text{ nm}$ GaAs–Ga_{0.65}Al_{0.35}As QW. Experimental data (down triangles) are from Schildermans et al. [4] and present theoretical results (full curve) are obtained by taking into account nonparabolicity effects for both the GaAs conduction and valence bands [10–12].

consider the Hamiltonian

$$\begin{aligned}
 H = & -\frac{\hbar^2}{2m_e^*} \frac{\partial^2}{\partial z_e^2} + \frac{1}{2m_e^*} \left[-i\hbar(\nabla_e)_\parallel + \frac{e}{c} \mathbf{A}_e \right]^2 \\
 & -\frac{\hbar^2}{2m_{h_\perp}^*} \frac{\partial^2}{\partial z_h^2} + \frac{1}{2m_{h_\parallel}^*} \left[-i\hbar(\nabla_h)_\parallel - \frac{e}{c} \mathbf{A}_h \right]^2 \\
 & + V_{\text{QD}} + V_C,
 \end{aligned} \quad (1)$$

where we take into account growth-direction applied magnetic-field effects, m_e^* is the electron effective mass, and $m_{h_\perp}^*$ and $m_{h_\parallel}^*$ are the hole effective masses. The V_{QD} confinement potential of the QD is given by $V_{\text{QD}} = V_e(z_e) + V_h(z_h) + V_\rho$, i.e., it is modelled by the sum of electron and hole one-dimensional z -direction $L_z(\text{QD})$ square-well barrier potentials and a lateral in-plane parabolic confinement potential taken as $V_\rho = \frac{1}{2}\mu_x\omega^2\rho^2$, where $\mu_x = m_e^*m_{h_\parallel}^*/(m_e^* + m_{h_\parallel}^*)$ is the heavy-hole exciton in-plane effective mass, $\hbar\omega$ is a measure of the strength of the in-plane confinement potential, and ρ is the $e-h$ in-plane coordinate (it is convenient to define a lateral QD radius as $R_{\text{QD}} = \sqrt{\hbar/\mu_x\omega}$). The $e-h$ correlation is taken into account through $V_C = -(e^2/\epsilon r)$, a Coulomb potential screened by the dielectric constants of the barrier or well materials, where r is the $e-h$ distance.

In order to calculate the QW exciton PL peak energies for a ultrathin QW, we ignore the QD (see Fig. 1) and consider a thin isolated QW, with $H = H_e + H_h + V_{\text{QW}} + V_C$, and the electron and hole confinements in the z -direction modelled by the $L_z(\text{QW})$ square-well $V_e(z_e)$ and $V_h(z_h)$ barrier potentials $V_{\text{QW}} = V_e + V_h$, respectively. The vector potential is chosen in the symmetric gauge as $\mathbf{A} = (B/2)(-y, x, 0)$. The z -dependent $V_i(z_i)$ ($i = e, h$) confinement potential is invariant under the transformation $z \rightarrow -z$. Therefore, one may assign a definite parity for the e or h QW wave function. As the $e-h$ Coulomb interaction is invariant under the simultaneous inversion of the electron and hole positions, the exciton envelope wave function will therefore have a well-defined parity (i.e., parity is a good quantum number), and the excitonic envelope function may be expanded as products of QW electron and hole eigenfunctions preserving the parity. Details of the calculation procedure may be found elsewhere [7].

In what follows, relevant material parameters were initially taken, at low-temperature, within the parabolic effective-mass approach, as in Li [8]. For simplicity, we have used the GaAs values of the effective masses and dielectric constant throughout the heterostructure. One must, however, take into account the effects of nonparabolicity both in the conduction [9,10] and valence [11,12] bands, which result in changes in the values of both the GaAs conduction-band electronic effective mass as well as in the GaAs valence-band effective mass. In the case of nonparabolicity effects on the GaAs valence-band effective mass, we refer to the theoretical work by Pacheco et al. [11] and Ekenberg and Altarelli [12], from which one may estimate the ground-state heavy-hole effective mass to be $0.47m_0$ and $0.55m_0$, where m_0 is the free-electron mass, for GaAs QWs of widths equal to 4 and 7 nm, respectively.

Fig. 2 shows experimental and calculated results for the growth-direction magnetic-field dependence of the heavy-hole exciton peak energies, for a symmetric ultrathin $L_z(\text{QW}) = 1.6 \text{ nm}$ GaAs–Ga_{0.65}Al_{0.35}As QW. Calculations are performed with the GaAs conduction-band m_e effective mass chosen by taking into account nonparabolicity effects as calculated by de Dios-Leyva et al. [10] (i.e., $m_e = 0.10m_0$), and a heavy-hole effective mass chosen as $m_{hh\parallel} = 0.35m_0$ [13]. Calculated results are in nice agreement with the measured PL exciton peaks by Schildermans et al. [4], as is apparent from the full theoretical curve in Fig. 2. Notice that the 1.6 nm QW width (which is in good agreement with the value of 1.8 nm for the Sample 2 in the experiment) was chosen in order to fit the zero magnetic-field experimental result by Schildermans et al. [4].

Theoretical calculations, with nonparabolicity effects both for the conduction and valence effective masses, are then performed for the magnetic-field dependence of the diamagnetic shifts of the $m = 0$ ground-state, $m = -1$ and -2 excited states of the heavy-hole exciton for a GaAs–Ga_{0.65}Al_{0.35}As QD of thickness $L_z(\text{QD}) = 4.7 \text{ nm}$ and lateral dimension $2R_{\text{QD}} = 16 \text{ nm}$; we take into account

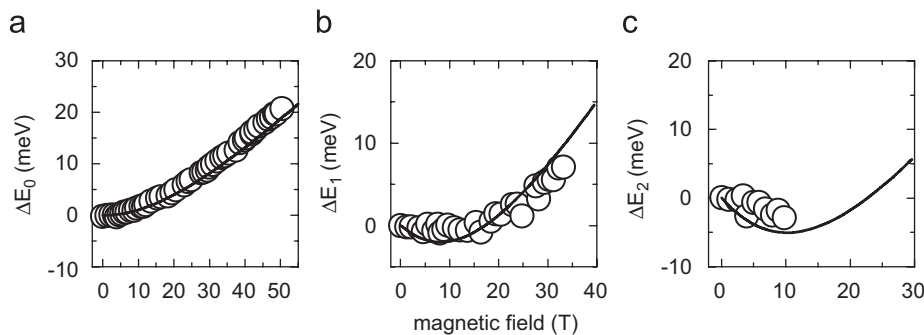


Fig. 3. Experimental [4,5] diamagnetic shifts of the (a) ground-state, (b) first, and (c) second excited states of the heavy-hole exciton, in the case of growth-direction applied magnetic fields, for a GaAs–Ga_{0.65}Al_{0.35}As QD, are shown as open dots whereas theoretical results for the $m = 0$ ground-state, $m = -1$ and -2 excited states of the heavy-hole exciton appear as full curves.

nonparabolicity effects for the GaAs conduction [10] band, i.e., $m_e = 0.084 m_0$, where m_0 is the free-electron mass, and for the GaAs valence band [11,12], with $m_{hh} = 0.35 m_0$. Theoretical results are compared, in Fig. 3, with the experimental measurements by Schildermans et al. [4] and Sidor et al. [5]. One notices that the $L_z(\text{QD}) = 4.7 \text{ nm}$ QD thickness is in fair agreement with the 5.96 nm value quoted, for Sample 2, in Table I by Schildermans et al. [4]. Present theoretical calculations indicate that a choice of $2R_{\text{QD}} = 16 \text{ nm}$ for the lateral size of the QD, or $\hbar\omega = 17.5 \text{ meV}$ ($\hbar\omega = \hbar^2/\mu_x R_{\text{QD}}^2$), provides a quite good description of the experimental diamagnetic-shift data.

It is of interest to comment that Schildermans et al. [4] have “measured” the exciton in-plane effective masses through a fitting procedure of the PL exciton energy, and obtained values two times larger than the bulk GaAs exciton mass. In the present calculation, however, we have obtained agreement with experimental data by including realistically both $e-h$ Coulomb interaction and nonparabolicity effects [9–12] with a conduction-band mass $m_e \approx 0.08-0.10 m_0$ and a valence-band mass $m_{hh} = 0.35 m_0$. This indicates that the values obtained by Schildermans et al. [4] for the exciton in-plane effective masses should be viewed with caution. The present calculation ignores effects of interdiffusion by taking a QD in-plane confinement-potential profile defined by a lateral QD radius instead of an asymmetric profile as in Figs. 4(b) and (c) by Rastelli et al. [3]. We do believe, however, that an isotropic in-plane confinement potential preserves the essential physics of the QD-exciton problem, and that a calculation with a more elaborated profile of the confinement potential would not change the overall conclusions of the present work.

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