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# Magnetic field dependence of the exciton energy in type I and type II quantum disks

K.L. Janssens\*, F.M. Peeters, V.A. Schweigert<sup>1</sup>, B. Partoens*Departement Natuurkunde, Universiteit Antwerpen (UIA), Universiteitsplein 1, B-2610 Antwerpen, Belgium*

## Abstract

The influence of an externally applied magnetic field on the properties of an exciton in a quantum disk is studied. As a type I system, we investigated  $\text{In}_{0.55}\text{Al}_{0.45}\text{As}$  dots embedded in  $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$  and calculated the diamagnetic shift. Similar calculations are presented for the type II system of vertically coupled InP dots embedded in GaInP. © 2001 Elsevier Science B.V. All rights reserved.

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## 1. Introduction

Self-assembled quantum dots (for a recent review, see, e.g., [1]) have gained much interest over the last decade, due to their expected importance in applications such as quantum dot lasers [2]. The dots are formed by the Stranski–Krastanow growth mode, which requires two semiconductor materials with a substantially different lattice parameter. Due to the lattice mismatch, typically about 4% [3], small islands are formed when one material is deposited on top of the other. The density, size and shape of the dots are strongly dependent on the materials being used and on the growth conditions.

Typical sizes of dots vary between a basis size of 7–20 nm and a height of a few nanometers [2].

In the first part of this paper, we study  $\text{In}_y\text{Al}_{1-y}\text{As}$  quantum dots, embedded in an  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  matrix. We approximate the quantum dots by a quantum disk with a hard-wall confinement of finite height, and we include the mass-mismatch between the dot and the barrier material. We study theoretically, the effect of an externally perpendicular applied magnetic field on the properties of an exciton, confined in the quantum disk. We fully take into account the Coulomb interaction between the electron and the hole and the three-dimensional (3D) nature of the problem. The diamagnetic shift and the effect of different disk radii and effective masses on this shift are studied. We compare our results with the experimental data of Wang et al. [4] for the case of  $\text{In}_{0.55}\text{Al}_{0.45}\text{As}$  dots. In the second part, we consider InP/GaInP quantum dots. Because InP is a type II system, the holes will be located in the barrier material. We studied the diamagnetic shift for two and three vertically

\*Corresponding author. Fax: + 32-3-820-22-45.

E-mail addresses: karenj@uia.ua.ac.be (K.L. Janssens), peeters@uia.ua.ac.be (F.M. Peeters).

<sup>1</sup>Permanent address: Institute of Theoretical and Applied Mechanics, Russian Academy of Sciences, Novosibirsk 630090, Russia.

coupled dots and compared our results with the experimental results of Hayne et al. [5].

## 2. Theoretical model

The Hamiltonian, which describes our system, is given by

$$H = \sum_{j=1}^2 H_j(\mathbf{r}_j) + V_c(\mathbf{r}_1 - \mathbf{r}_2) \quad (1)$$

with

$$H_j = \left( \mathbf{p}_j - \frac{q_j}{c} \mathbf{A}_j \right) \frac{1}{2m_j(\mathbf{r})} \left( \mathbf{p}_j - \frac{q_j}{c} \mathbf{A}_j \right) + V_j(\mathbf{r}_j), \quad (2)$$

where the indices  $j = 1, 2$  correspond to the electron and the hole with masses  $m_1$  and  $m_2$ , respectively.  $V_j(\rho_j, z_j) = 0$  ( $\rho_j < R, |z_j| < d/2$ ),  $V_{j,o}$  (otherwise) is the confinement potential, with  $R$  the radius of the quantum disk and  $d$  its thickness;  $\rho_j = \sqrt{x_j^2 + y_j^2}$ ,  $V_c(\mathbf{r}) = -e^2/\varepsilon|\mathbf{r}|$  and  $q_j = \mp e$ . We take a difference in mass between the dot region and the region outside the dot into account:  $m_j(\mathbf{r}) = m_{w,j}$  inside the dot and  $m_j(\mathbf{r}) = m_{b,j}$  outside the dot. Using cylindrical coordinates  $\mathbf{r}_j = (\rho_j, \phi_j, z_j)$ , the one-particle Hamiltonian takes the form

$$H_j = -\frac{\hbar}{2} \left( \frac{\partial}{\partial z_j} \frac{1}{m_j} \frac{\partial}{\partial z_j} + \frac{1}{\rho_j} \frac{\partial}{\partial \rho_j} \frac{\rho_j}{m_j} \frac{\partial}{\partial \rho_j} + \frac{1}{\rho_j^2 m_j} \frac{\partial_j^2}{\partial \phi_j^2} \right) \mp \frac{i}{2} \hbar \omega_{c,j} \frac{\partial}{\partial \phi_j} + \frac{1}{8} m_j \omega_{c,j}^2 \rho_j^2 + V_j(z_j, \rho_j). \quad (3)$$

where  $\omega_{c,j} = eB/m_j c$  are the electron and hole cyclotron frequencies and the vector potential is taken in the symmetrical gauge  $\mathbf{A} = (\frac{1}{2})B\rho\mathbf{e}_\phi$ . As a consequence of the axial symmetry of our problem, there is no coupling between the wave functions with different values of the  $z$ -component of the total angular momentum  $L$ . Therefore, the exciton wave function  $\Psi_L$  with fixed total momentum  $L$ , can be constructed as the linear combination

$$\Psi_L(\mathbf{r}_1, \mathbf{r}_2) = \sum_{l=-l_m}^{l_m} \psi^l(\chi) e^{i(l/2)(\phi_1 - \phi_2) + i(L/2)(\phi_1 + \phi_2)}, \quad (4)$$

where the function  $\psi^l(\chi)$  obeys the Schrödinger equation

$$\sum_{j=1}^2 H_j^l \psi^l(\chi) + \sum_{l'=-l_m}^{l_m} V_c^{l-l'}(\chi) \psi^{l'}(\chi) = E \psi^l(\chi) \quad (5)$$

with  $E$  the eigenenergy,  $\chi$  denotes the coordinates  $(z_1, z_2, \rho_1, \rho_2)$ ,  $V_c^l$  is the matrix element of the Coulomb interaction

$$V_c^l(\chi) = -\frac{e^2}{\varepsilon} \frac{1}{2\pi} \int_0^{2\pi} d\phi \frac{e^{-il\phi}}{\sqrt{(z_1 - z_2)^2 + \rho_1^2 + \rho_2^2 - 2\rho_1\rho_2 \cos \phi}} \quad (6)$$

and  $L_m = 2l_m + 1$  is the total number of angular harmonics in the expansion. To solve this problem, we use the finite difference scheme as presented in Ref. [6].

## 3. Results

First, the results for the  $\text{In}_{0.55}\text{Al}_{0.45}\text{As}$  dots are discussed, where we used the following parameters:  $d = 3.22$  nm and  $R = 8.95$  nm,  $\varepsilon = 12.71$ ,  $m_{w,e} = 0.076m_0$ ,  $m_{b,e} = 0.097m_0$ ,  $m_{w,h} = m_{b,h} = 0.45m_0$ ,  $V_{e,0} = 258$  meV, and  $V_{h,0} = 172$  meV.

The groundstate energy and binding energy of the exciton in the disk were investigated. This groundstate energy is given by

$$E = E^e + E^h - E_{\text{exc}}, \quad (7)$$

where  $E^e$  and  $E^h$  are the single particle energies of, respectively, electron and hole, and  $E_{\text{exc}}$  is the exciton binding energy, which is the Coulomb interaction energy. From the calculation of the exciton groundstate energy as a function of a magnetic field, we deduce the exciton diamagnetic shift through the following formula:

$$\Delta E = E(B) - E(B = 0). \quad (8)$$

In Fig. 1, this diamagnetic shift is shown by the solid curve. The squares indicate the experimental data of Wang et al. [4]. For low magnetic fields, our theoretical result agrees well with the experimental result. For higher fields, however, the theoretical result substantially underestimates the

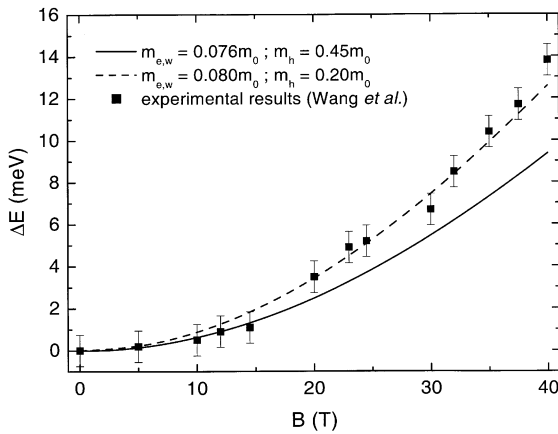


Fig. 1. The diamagnetic shift for different masses, as indicated. The squares are the experimental data of Wang et al. [4].

diamagnetic shift. In Ref. [7], it was argued that for a magnetic field normal to the sample plane, the light hole mass should be used. Using their values for InAs and combining them with values for AIAs of Ref. [8], we find by linear interpolation to the material  $\text{In}_{0.55}\text{Al}_{0.45}\text{As}$ , values of  $0.08m_0$  and  $0.2m_0$  for the electron and the hole mass, respectively. The result for the diamagnetic shift in this case is shown by the dashed curve in Fig. 1 and we find a much better agreement with the experiment, in particular in the high magnetic field region.

In Fig. 2, the dependency of the exciton binding energy on the disk radius is depicted for  $B = 0\text{ T}$  and  $40\text{ T}$ . We used the original values for the masses of the particles. Starting from large  $R$ , we find an increase of the binding energy with decreasing radius, which continues up to  $R \approx 3\text{ nm}$ . The reason for this increase can be attributed to the fact that the particles are pushed closer together for smaller disks, and therefore, they will be more tightly bound. However, with further decreasing disk radius, we find a sudden strong decrease of the exciton binding energy. This is a consequence of the spill-over of the wave function into the barrier material, indicating that the dot is in fact too small to confine the exciton. This is confirmed by the inset of Fig. 2, where the percentage of the electron and hole wave function inside the disk is shown as a function of the disk radius. Notice the strong decrease of this percentage for  $R \leq 3\text{ nm}$ . The effect

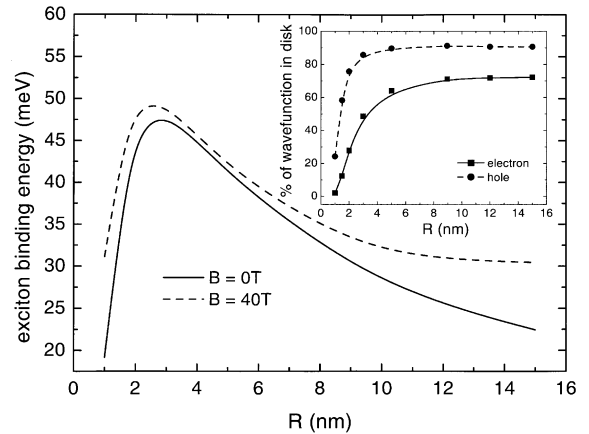


Fig. 2. The exciton binding energy as a function of the disk radius. The inset shows the percentage of the wave function as a function of the disk radius.

of the magnetic field on the dot size dependence of the exciton binding energy is depicted by the dashed curve in Fig. 2, where the result is plotted for  $B = 40\text{ T}$ . Notice that the largest  $B$ -dependence compared with  $B = 0\text{ T}$  is found for very small and very large  $R$ , where the exciton is less confined and therefore a magnetic field will have a larger influence.

Furthermore, we considered type II quantum dots, namely the InP/GaInP dots as studied experimentally in Ref. [5]. In type II systems, the dots actually form an antidot for the holes, which are located in the barrier material. However, due to the Coulomb interaction and strain effects, the holes will still be confined close to the dots. For the case of vertically coupled quantum disks, we expect that, for very closely stacked disks, the hole will actually be located between the disks in the vertical direction. In this case the total system of stacked disks, electron and hole can even be considered as one large disk, with the stack height as disk thickness and both the electron and the hole located in the disk. We will study such a simplified model for the case of very closely stacked dots under the influence of a perpendicular applied magnetic field for, respectively, two and three coupled disks, and we compare our results with the experimental data of Hayne et al. [5]. For our study, we consider the stacked disks as one entity, where both electron and hole are confined in the stack and therefore, we

can still apply the same model as for the type I disks, with now the stack height as disk thickness.

For this study, the following parameters were used:  $R = 8$  nm,  $\varepsilon = 12.5$ ,  $m_{w,e} = m_{b,e} = 0.077m_0$ ,  $m_{w,h} = m_{b,h} = 0.6m_0$ ,  $V_{e,0} = 250$  meV, and  $V_{h,0} = 50$  meV. In Fig. 3, the diamagnetic shift for the case of two vertically coupled disks is shown. From Ref. [5], we know that the single disk height of the studied InP disks is about 2 nm, and the separation between the disks for the case of the double layer is about 4 nm, which leads to a total stack height  $d = 8$  nm. The solid curve represents our theoretical result, whereas the squares indicate the experimental data of Hayne et al. [5]. Notice that our results compare very well with the experimental results for magnetic fields, up to 30 T. For higher fields however, the agreement is not as good. This can be attributed to the fact that a separation of 4 nm between the disks is too large to consider the total stack as one dot. The dashed curve shows the result for a disk diameter  $R = 10$  nm.

Fig. 4 depicts the diamagnetic shift for a system of three vertically coupled disks. In this case the separation between the disks is 2 nm, leading to a total stack height of 10 nm. Again, the solid and dashed curves indicate our theoretical results for  $R = 8$  and 10 nm, respectively, and the squares are the experimental results of Hayne et al. [5]. The result for  $R = 8$  nm only gives good agreement for

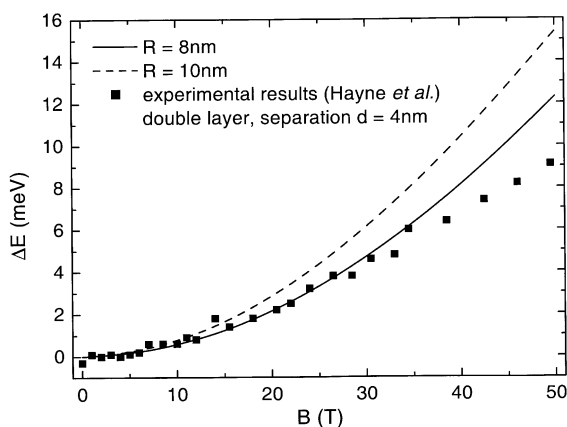


Fig. 3. The exciton diamagnetic shift for two vertically coupled InP dots. The curves are the theoretical results for a single disk of height  $d = 8$  nm for two different disk radii, whereas the squares indicate the experimental results of Hayne et al. [5].

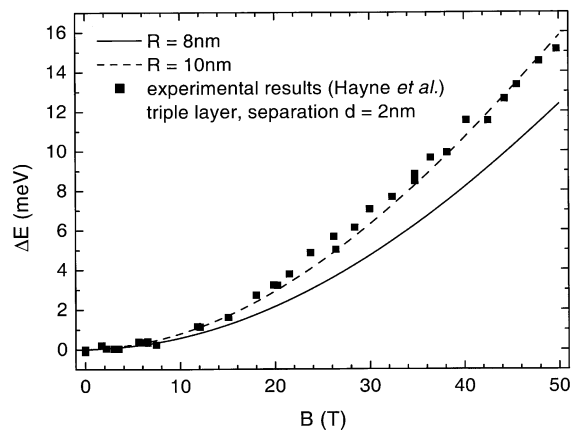


Fig. 4. The same as Fig. 3, but now for three vertically coupled dots (the single disk height is 10 nm).

very low fields, up to  $B = 10$  T, while for higher fields, the theoretical result underestimates the experimental data. For  $R = 10$  nm, however, we find a very good agreement with the experiment along the whole  $B$ -region. For a larger disk, the exciton wave function is more extended and will therefore be more strongly influenced by a magnetic field, resulting in an enhanced diamagnetic shift.

#### 4. Conclusions

We calculated the diamagnetic shift of an exciton in a type I quantum disk with radius  $R$  and thickness  $d$  for a hard wall potential of finite height, using finite difference techniques. Comparing our results with experimental results, we found better agreement when using the light hole mass. The influence of the disk radius on the exciton binding energy was studied. For small  $R$ , we found a strongly decreased exciton binding energy due to a spill-over of the wave function into the barrier material. This is corroborated by a study of the percentage of the wave function in the disk, as a function of  $R$ .

Furthermore, we considered coupled type II quantum disks, where the holes are located in the barrier material. For the studied case of very closely stacked dots, we approximated the system of coupled disks by one large disk, containing both the electron and the hole inside the disk. We

compared our theoretical calculation of the diamagnetic shift, with experimental results of Hayne et al. [5], and found that our approximation works surprisingly well for the system of three coupled disks (a separation of 2 nm), but fails in the high magnetic field region for the case of two coupled disks, where the separation is 4 nm.

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