Ground state of excitons and charged excitons in a quantum well

C. Riva and F. M. Peeters

Departement Natuurkunde, Universiteit Antwerpen (UIA), B-2610 Antwerpen.

K. Varga

Physics Department, Argonne National Laboratories, Argonne, 60439 Illinois.

(December 26, 2021)
I. ABSTRACT

A variational calculation of the ground state of a neutral exciton and of positively and negatively charged excitons (trions) in a single quantum well is presented. We study the dependence of the correlation energy and of the binding energy on the well width and on the hole mass. Our results are compared with previous theoretical results and with available experimental data.

II. INTRODUCTION

Negatively (X\textsuperscript{−}) and positively (X\textsuperscript{+}) charged excitons, also called trions, have been the object of intense studies in the last years, both experimentally and theoretically. The stability of charged excitons in bulk semiconductors was proven theoretically by Lampert \[1\] in the late fifties, but only recently they have been observed in quantum well structures: first in CdTe/CdZnTe by Kheng \textit{et al.} \[2\] and subsequently in GaAs/Al\textsubscript{x}Ga\textsubscript{1-x}As \[3–5\].

The calculation we present in this paper, of the ground state energy for the exciton (X) and the charged exciton, fully includes the Coulomb interaction among the particles, i.e. no approximated average potential is assumed in any of the three spatial directions and the correlation among the particles is fully taken into account.

The Hamiltonian of a negatively charged exciton (X\textsuperscript{−}) in a quantum well is in the effective mass approximation given by

\[ \hat{H} = T_{1e} + T_{1h} + T_{2e} + V_C + V_{1e} + V_{2e} + V_{1h}, \]

where 1\textit{e}, 2\textit{e} indicate the electrons and 1\textit{h} the hole; \textit{V}_{1\textit{e}}, \textit{V}_{1\textit{h}} are the quantum well confinement potentials; \textit{T}_i = \frac{p^2_i}{2\textit{m}_i} is the kinetic operator for particle \textit{i}, with \textit{m}_i the corresponding mass; \textit{V}_C is the sum of the Coulomb electron-electron and electron-hole interactions,

\[ V_C = \frac{e^2}{\varepsilon} \left( \frac{1}{|\vec{r}_1e - \vec{r}_2e|} - \frac{1}{|\vec{r}_2e - \vec{r}_1h|} - \frac{1}{|\vec{r}_1e - \vec{r}_1h|} \right), \]

(2)
with $e$ the elementary charge and $\varepsilon$ the static dielectric constant. In the present work the heights of the square well confinement potentials are $V_{ie} = 0.57 \times (1.155x + 0.37x^2)$ eV for the electrons and $V_{ih} = 0.43 \times (1.155x_0 + 0.37x^2)$ eV for the holes for the GaAs/Al$_x$Ga$_{1-x}$As quantum well system.

The Hamiltonian is then solved using the stochastic variational method [6]. The trial function is taken as a linear combination of correlated Gaussian functions,

$$
\phi_0(\vec{r}_{1e}, \vec{r}_{2e}, \vec{r}_{1h}) = \sum_{n=1}^{K} C_{n0} \Phi_{n0}(\vec{r}_{1e}, \vec{r}_{2e}, \vec{r}_{1h}), \quad (3)
$$

$$
\Phi_{n0}(\vec{r}_{1e}, \vec{r}_{2e}, \vec{r}_{1h}) = \mathcal{A} \left\{ \exp \left[ -\frac{1}{2} \sum_{i,j \in \{1e,2e,1h\}} \sum_{k \in \{x,y,z\}} A_{nijk} r_{ik} r_{jk} \right] \right\}, \quad (4)
$$

where $r_{ik}$ gives the positions of the $i$th particle in the direction $k$; $\mathcal{A}$ is the antisymmetrization operator and $\{C_{n0}, A_{nijk}\}$ are the variational parameters. The dimension of the basis, $K$, is increased until the energy is sufficiently accurate.

III. THE RESULTS

The correlation energy of a charged exciton is defined as

$$
E_C(X^-) = E_T(X^-) - 2E_e - E_h, \quad (5)
$$

$$
E_C(X^+) = E_T(X^+) - 2E_h - E_e, \quad (6)
$$

with $E_T(X^\pm)$ the energy level of the charged exciton and, $E_e$ and $E_h$ the energy levels of the free electron and hole, respectively, in the quantum well. We discuss here the results obtained for a GaAs/Al$_x$Ga$_{1-x}$As quantum well with $x = 0.3$. The values of the GaAs masses used are $m_e = 0.0667m_0$, $m_{hh} = 0.34m_0$, which results into $2R_y = \hbar/m_ea_B = 11.58$ meV and $a_B = \hbar^2\varepsilon/m_e e^2 = 99.7$ Å.

Our numerical results for the correlation energy are shown in Fig. [1] and are compared with the results of Ref. [7]. For the X we find that the magnitude of the correlation energy...
is larger than the one obtained in Ref. [7] while for the X\(^-\) our approach gives a 5\% smaller magnitude for the correlation energy. The reasons for the difference are: 1) in Ref. [7] the Coulomb potential along the \(z\)-direction was approximated by an analytical form, see Appendix in Ref. [7]. This approximation leads, as the authors already noted, to an error in the X correlation energy of approximately 5\%; 2) for the X\(^-\) energy the authors of Ref. [7] did not report an estimate of the error introduced by the approximations made. However we find a decrease of the absolute value of the correlation energy by about 5\%. We think that this result is not in conflict with the one obtained for the X. In fact if in Ref. [7] for the X case the intensity of the attractive interaction between the electron and hole (e-h) was underestimated, for the X\(^-\) case also the intensity of the repulsive interaction between the electrons (e-e) is underestimated which leads to a less negative \(E_C\).

We also report the correlation energy for the X\(^+\) in Fig. 1. Note that the correlation energy of the X\(^+\) is practically equal to the one of X\(^-\). This is in perfect agreement with recent experimental data [8] where the binding energy of the X\(^+\) is found to be equal to the one of the X\(^-\).

Next we take into account, for the narrow well regime, the difference in mass of the particles in the well (GaAs) and in the barrier (Al\(_x\)Ga\(_{1-x}\)As) material. The values for the GaAs-masses, i.e. the masses for the electron and the hole, are taken equal to the one used in the previous calculation. The values for the masses in Al\(_x\)Ga\(_{1-x}\)As are \(m^*_{eb} = 0.067+0.083x\), \(m^*_{hhb} = 0.34+0.42x\), where \(x\) indicates the percentage of Al present in the alloy. If we assume, as a first approximation, that the electron and the hole have part of their wave function in the quantum well and the rest in the barrier we may take the total effective mass of the electron and the hole as given by

\[
\frac{1}{m_i} = \frac{P_{iw}}{m_{iw}} + \frac{P_{ib}}{m_{ib}}, \tag{7}
\]

where \(m_{iw}, m_{ib}\) are the masses of the \(i\)-th particle in the barrier and in the well, and \(P_{iw}, P_{ib}\) are the probabilities of finding the \(i\)-th particle in the well or in the barrier, respectively.

The results of this calculation are shown in Fig. 2. We observe that the effect of the mass
mismatch is important only in the narrow quantum well regime, i.e. \( L < 40 \) Å, where it leads to a substantial increase of the energy.

The dependence of the total energy on the hole mass for a 200 Å wide quantum well is shown in Fig. 3. The energy of the negatively charged exciton becomes equal to the D\(^-\) energy [8] for \( m_h/m_e > 16 \). Note that the X\(^+\) energy is for large values of the hole electron mass ratio parallel to the one of the X\(^-\). For a large hole mass its contribution to the total energy in terms of confinement energy is negligible, and the difference between the total energy of the positively and the negatively charged exciton is just due to the confinement energy of one electron, which does not depend on the hole mass.

Experimental data were reported for the binding energy of the X\(^-\) in zero magnetic field for a 200 Å [3], a 220 Å [9] and a 300 Å [9] quantum well. The binding energy is defined as \( E_B = E_T(X) + E_e - E_T(X^-) \). The experimental results are shown in Fig. 4 together with our theoretical calculation, where the shaded band indicates the estimate accuracy of our variational procedure. Notice that the experimental results give a larger binding energy as compared to the theoretical estimate and this discrepancy increases with decreasing well width. This may be a consequence of the localization [10] of the trion due to well width fluctuations which become more important with decreasing \( L \).

Last we study the wave function of the X\(^-\). In Fig. 5(a) we show the contour plot of \( |\phi_0(\vec{r}_{1e}, \vec{r}_{2e}, \vec{r}_{1h})|^2 \) for a X\(^-\) in a quantum well of width 100 Å. We fix the hole in \( \vec{r}_{h} = (0, 0, 0) \) and one of the two electrons in \( \vec{r}_{e} = (-0.25a_B, 0, 0) \) and calculate the probability to find the other electron in the \( \hat{x}y \)-plane. Notice that the second electron sits far from the hole and the fixed electron and behaves like an electron weakly bound to a polarized exciton. If now we fix the hole in \( \vec{r}_{h} = (2a_B, 0, 0) \) and the electron in \( \vec{r}_{e} = (0, 0, 0) \), see Fig. 5(b), we observe that the second electron is completely localized around the hole and the configuration that we obtain is the one of an exciton plus an extra electron.
IV. CONCLUSION

In this paper a new calculation for the exciton and the charged exciton energy in a quantum well was presented which is based on the stochastic variational method. To our knowledge, this is the first time, that a calculation fully includes the effect of the Coulomb interaction and the confinement due to the quantum well. The results obtained do not show a big qualitative difference from the one already present in the literature, however a sensible quantitative difference is observed. This difference leads to an improvement of the agreement with available experimental data for the binding energy.

V. ACKNOWLEDGMENT

Part of this work is supported by the Flemish Science Foundation (FWO-Vl) and the ‘Interuniversity Poles of Attraction Program - Belgian State, Prime Minister’s Office - Federal Office for Scientific, Technical and Cultural Affairs’. F.M.P. is a Research Director with FWO-Vl. Discussions with M. Hayne are gratefully acknowledged.
REFERENCES

* Electronic address: riva@uia.ua.ac.be.

◦ Electronic address: peeters@uia.ua.ac.be.

[1] M. A. Lampert, Phys. Rev. Lett. 1, 450 (1958).

[2] K. Kheng, R. T. Cox, Y. Merle d’Aubigné, F. Bassani, K. Saminadar, and S. Tatarenko, Phys. Rev. Lett. 71, 1752 (1993).

[3] G. Finkelstein, H. Shtrikman, and I. Bar-Joseph, Phys. Rev. B 53, R1709 (1996); G. Finkelstein, H. Shtrikman, and I. Bar-Joseph, Phys. Rev. B 53, 12593 (1996).

[4] A. J. Shields, J. L. Osborne, D. M. Whittaker, M. Y. Simmons, M. Pepper, and D. A. Ritchie, Phys. Rev. B 55, 1318 (1997); A. J. Shields, F. M. Bolton, M. Simmons, M. Pepper, and D. A. Ritchie, Phys. Rev. B 55, R1970 (1997).

[5] M. Hayne, C. L. Jones, R. Bogaerts, C. Riva, A. Usher, F. M. Peeters, F. Herlach, V. V. Moshchalkov, and M. Henini, Phys. Rev. B 59, 2927 (1999).

[6] Y. Suzuki and K. Varga, Stochastic Variational Approach to Quantum-Mechanical Few-Body Problems (Springer, Berlin-Heidelberg, 1998).

[7] B. Stébé, G. Munsch, L. Stanuffer, F. Dujardin, and J. Murat, Phys. Rev. B 56, 12454 (1997).

[8] C. Riva, V. Schweigert, and F. M. Peeters, Phys. Rev. B 57, 15392 (1998).

[9] A. J. Shields, M. Pepper, D. A. Ritchie, M. Y. Simmons, and G. A. C. Jones, Phys. Rev. B 51, 18049 (1995).

[10] O. Mayrock, H.-J. Wünsche, F. Henneberger, C. Riva, V. A. Schweigert, and F. M. Peeters, Phys. Rev. B 60, 5582 (1999).
FIGURES

FIG. 1. The correlation energy vs. the quantum well width for the heavy hole exciton and charged exciton.

FIG. 2. The correlation energy of the negative charged exciton vs. the quantum well width. For the case of constant masses, in the hole and in the barrier, and for the the case of different masses.

FIG. 3. The total energy of the negative charged exciton and the positive charged exciton vs. $m_h/m_e$ for a quantum well of width 200 Å. The total energy of a $D^-$ in the same quantum well is shown (dotted line) for comparison.

FIG. 4. The theoretical and experimental binding energies of the negatively charged exciton vs. the well width.

FIG. 5. Contour maps for the conditional probability of the electron in $X^-$. The symbols indicate the position of the fixed particles.
$E_C$ (meV) vs. $L$ (Å)

constant mass case

different mass case
$E_B$ (meV) vs. $L$ (Å)
