U.P.B. Sci. Bull., Series A, Vol. 68, No. 4, 2006

ELECTRON EIGENSTATES IN MAGNETOELECTRONIC SUBBANDS

Ecaterina NICULESCU*

În lucrare sunt calculate stările uniparticulă pentru electroni şi goluri grele într-un fir cuantic cilindric din GaAs, în prezenţa unui câmp magnetic extern paralel cu axa firului. Metoda originală propusă conduce la valori ale energiei stării fundamentale şi ale extinderii radiale a funcţiei de undă care sunt în bună concordanţă cu cele obţinute prin metoda variaţională, utilizată uzual în astfel de calcule. Metoda necesită un timp de calcul redus şi poate fi extinsă pentru studierea stărilor excitate în heterostructuri semiconductoare sub acţiunea unor câmpuri externe

The single-particle states of electron and heavy-hole in a quantum wire in the presence of an axial magnetic field are calculated by an analytical method introduced herein. The quantum wire is assumed to be a cylinder of GaAs material surrounded by $Al_{0.3}Ga_{0.7}As$*, with finite confinement potentials. It is significant that a comparison of the ground-state energies and of the radial widths of the wave function with those computed by a variational method shows good quantitative agreement for varying wire radii and magnetic field strengths. The method is fast computationally and can be readily extended to calculate energies of higher excited states.*

Introduction

In recent years, there has been great interest in investigating quantum-well wires (QWWs) both theoretically and experimentally. In such systems, the electron is confined to move along the length of the wire while the motion is quantised in the two transverse directions. Due to the strong confinement of QWW's, the optical and electron transport characteristics are quite different from those of 3D and 2D systems, leading to novel optoelectronic devices.

This has motive extensive research in nanowire technology [1-3] and in study of their electronic properties [4-9]. The optical spectra of semiconductor quantum wires can be dramatically modified by the application of external static electric and / or magnetic fields**.** In particular, the magnetic field modifies the symmetry of the electronic states and increases the confining energies of the carriers.

The first step towards understanding the optoelectronic properties of a quantum wire device is to calculate the quantum-confined electron and hole states

* Prof., Physics. Department, University "Politehnica" of Bucharest, ROMANIA

in the structure. Previously, Tsetseri *et al*. [8] reported a study of the ground state of quantum wires using the finite difference method, in the absence of the external fields. The energy levels of a shallow impurity in GaAs-AlGaAs QWWs under the action of the magnetic field were theoretically studied using variational methods for the infinite potential barriers [10,11].

In the present paper we investigate the effect of an axial magnetic field on the electron and heavy hole ground states in GaAs-AlGaAs QWWs with a finite height of the confinement potential.

Theory

We consider a cylinder of radius R, which is composed of GaAs embedded in $Al_xGa_{1-x}As$ under the action of a magnetic field applied in the axial direction, $\mathbf{B} = B\hat{\mathbf{z}}$. In the effective mass approximation, the Hamiltonian describing the electron (hole) motion is given by

$$H_i = \frac{1}{2m_i}\left(\mathbf{p}_i - q_i\mathbf{A}_i\right)^2 + V_i\left(\mathbf{r}_i\right) \tag{1}$$

Here i = (e,h) denotes electron and hole, respectively, $\mathbf{A}_i$ is the vector potential, and the confining potentials for the electrons (holes), $V_{e(h)}$, depend on the band offsets, taken here to be $Q_e = 0.57$, $Q_h = 0.43$. In cylindrical coordinates the components of the vector potential are $A_\rho = A_z = 0$, $A_\varphi = \frac{1}{2}B\rho$, (Landau gauge), and

$$V_i(\rho) = \begin{cases} 0, & \rho < R \\ V_{0i}, & \rho > R \end{cases}. \tag{2}$$

The eigenenergies and eigenstates of **the electron** confined in the quantum wire are obtained by solving the Schrödinger equation

$$-\frac{\hbar^2}{2m_e}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\Psi}{\partial\varphi^2} + \frac{\partial^2\Psi}{\partial z^2}\right] - \frac{ie\hbar B}{2m_e}\frac{\partial\Psi}{\partial\varphi} + \frac{e^2B^2}{8m_e}\rho^2\Psi + \\ + V_e(\rho)\Psi = E\,\Psi \tag{3}$$

In zero magnetic field case, the problem can be solved exactly. The electron wave function for a confined state $\Phi(\rho,\varphi,z)$ with corresponding energy eigenvalue E_0 is given by

$$\Phi(\rho,\varphi,z) = \begin{cases} A_m J_m(k_1\rho)e^{im\varphi}\,e^{ik_z z} & \rho < R \\ B_n K_n(k_2\rho)e^{in\varphi}\,e^{ik_z z} & \rho > R \end{cases} \tag{4}$$

where J is the Bessel function of the first kind and K is the modified Bessel function of the second kind,

$$k_1 = \left[\left(2m_e/\hbar^2\right)E_0 - k_z^2\right]^{1/2} \tag{5}$$

$$k_2 = \left[\left(2m_e/\hbar^2\right)\left(V_{0e} - E_0\right) - k_z^2\right]^{1/2}. \tag{6}$$

A_m and B_n are the normalization factors and the energy E_0 is get by applying the boundary conditions at $\rho = R$.

When a magnetic field is applied the problem can no longer be solved analitically. We will proceed by relying on a variational calculation of the energy. We propose the following variational wave function

$$\Psi(\rho,\varphi,z) = \Phi(\rho,\varphi,z)e^{-\alpha\rho^2} \tag{7}$$

where α is the variational parameter. For the ground state energy, $(m = 0, k_z = 0)$,

$$\Psi_0(\rho) = \begin{cases} A_0 J_0(k_1\rho)\, e^{-\alpha\rho^2} & \rho < R \\ B_0 K_0(k_2\rho) e^{-\alpha\rho^2} & \rho > R \end{cases} \tag{8}$$

and α is obtained by minimizing the energy

$$E = \frac{\langle \Psi_0 | H\, \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}. \tag{9}$$

The method presented above is also quite applicable to holes. For our analysis we used the simplest approximation of parabolic valence band, neglecting any mixing between heavy and light holes. This approximation is reasonable good for quantum wires in magnetic fields; as pointed out Goldoni *et al*. [12] and Vouilloz *et al*. [2] even in strongly confined two-dimensional systems the ground state in the valence band is almost a pure heavy hole (hh) state (92%). Thus, for the study of the hole's ground state the Hamiltonian can be obtained from (3) by exchanging the index $e \leftrightarrow h$, and changing the sign of the elementary charge (in Eq. (3), $e > 0$).

However, the calculation of the band structure of quantum wires in magnetic field can be done analitically if we use structures with infinite potential barrier heights and the effective radius, $R_{eff\ e}$, $R_{eff\ hh}$, so that we obtain the correct zero-field energies. Thus, R_{eff}'s are so chosen that for each i =(e, hh),

$$J_0\left(k_{10}\ R_{eff}\right) = 0 \tag{10}$$

so $k_{10}\ R_{eff}$ is the first zero of the spherical Bessel function with $k_{10} = k_1(k_z = 0)$. Of course, the effective radius, R_{eff}, are greater than the physical radius because in real structure there is significant penetration of the wave functions into the barriers.

For the infinite-barrier case,

$$V_i(\rho)=\begin{cases}0, & \rho < R_{eff\ i}\\ \infty, & \rho > R_{eff\ i}\end{cases}. \tag{11}$$

The Schrödinger equation for the ground *s*-like state of the electron is rewritten as

$$\frac{d^2\Psi_\infty}{d\rho^2}+\frac{1}{\rho}\frac{d\Psi_\infty}{d\rho}-\frac{1}{4}\gamma^2\rho^2\Psi_\infty(\rho)=\frac{2m\ E}{\hbar^2}\Psi_\infty(\rho) \tag{12}$$

with $\gamma=\frac{q\ B}{\hbar}$. By letting $\xi=\frac{1}{2}\gamma\rho^2$ and $\beta=\frac{mE}{\hbar qB}$, Eq. (12) becomes

$$\xi\frac{d^2\Psi_\infty}{d\xi^2}+\frac{d\Psi_\infty}{d\xi}+\left(-\frac{\xi}{4}+\beta\right)\Psi_\infty=0\ . \tag{13}$$

The eigenfunctions are written as follows

$$\Psi_\infty(\xi,\beta)=C\,e^{-\xi/2}F_1\left(-\beta+\frac{1}{2},1;\xi\right) \tag{14}$$

where $F_1\left(-\beta+\frac{1}{2},1;\xi\right)$ is the confluent hypergeometric function, which remains finite at $\xi=0$ and *C*, the normalization factor. The value of β is determined by the boundary condition

$$F_1\left(-\beta+\frac{1}{2},1;\ \frac{1}{2}\gamma\ R_{eff}^2\right)=0\,. \tag{15}$$

If $\left(-\beta_0+\frac{1}{2}\right)$ is the first zero of Eq. (15), the eigenvalue are given by

$$E(R_{eff},B)=\beta_0\frac{\hbar qB}{m}\,. \tag{16}$$

This effective infinite-barrier (**EIB**) model is also applicable to heavy (light)-holes.

Results and Discussion

We have studied the electron and heavy hole ground states in cylindrical GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wires in the presence of an axial uniform magnetic field. We assumed an electron (heavy hole) effective mass constant for the entire structure: $m_e=0.067m_0$ and $m_{hh}=0.34m_0$. The finite potential barriers are taken as

$$V_{0i}=Q_i\left(1.155x+0.37x^2\right)\ \text{(eV)},$$

where *x* is the Al concentration.

The single-particle confined wire states are calculated using our effective infinite-barrier model and compared with those obtained from the variational method. In Fig. 1. is plotted the energy shift, $\Delta E = E(B) - E(0)$, as a function of the magnetic field for electrons in QWW.

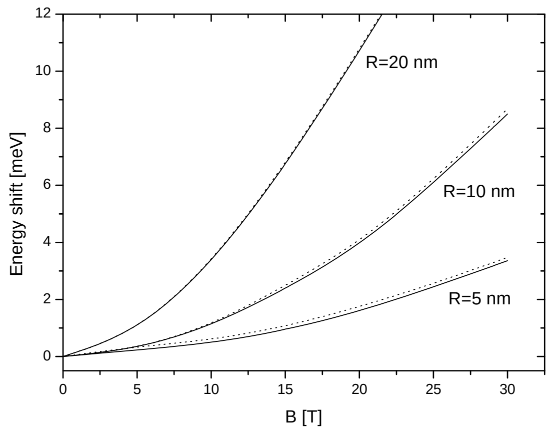

Fig. 1. The electron energy shift, $\Delta E = E(B) - E(0)$, as a function of magnetic field. Solid lines: EIB method; dotted lines: variational method.

It is significantly that there is a remarkably good agreement in the ground-state energies for all studied wire sizes and magnetic field strengths. Even for small values of the radius, when the geometric confinement determines the behavior of the electronic states and the difference $R_{eff} - R$ is appreciable (Table 1), the confining energies calculated with the infinite-model are less than 1% lower than the values obtained using the variational method. Similar results are obtained for heavy holes.

Table 1

R (nm)	$R_{eff\ e}$ (nm)	$R_{eff\ hh}$ (nm)
5	6.716	5.835
10	11.647	10.823
20	21.632	20.820

In Fig. 2 we present the single-particle energies obtained with EIB method as a function of the magnetic field for different values of the wire radius.

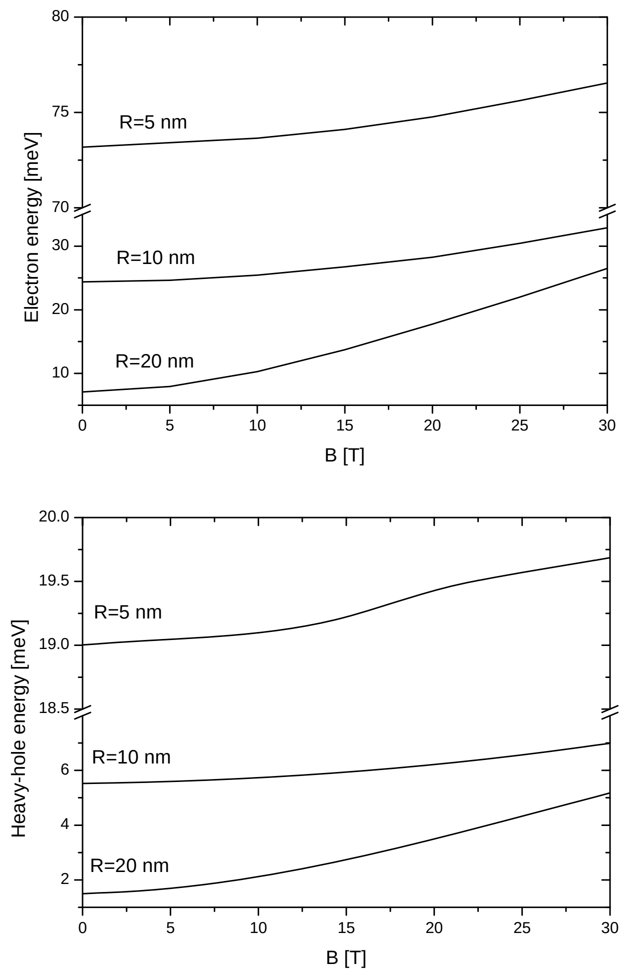

Fig. 2. Variation of single-particle 1s-energies with magnetic field in a GaAs QWW with different wire radii.

It is seen that for high magnetic fields such that the quantum confinement energy is smaller than the magnetic energy, the ground-state energies approach $\frac{1}{2}\frac{\hbar qB}{m_i}$, the n =0 Landau level. This high-field limit is reached if the wire effective radius, R_{eff}, exceeds the cyclotron radius, $R_c = \sqrt{\frac{1}{\gamma}}$, plotted in Fig. 3.

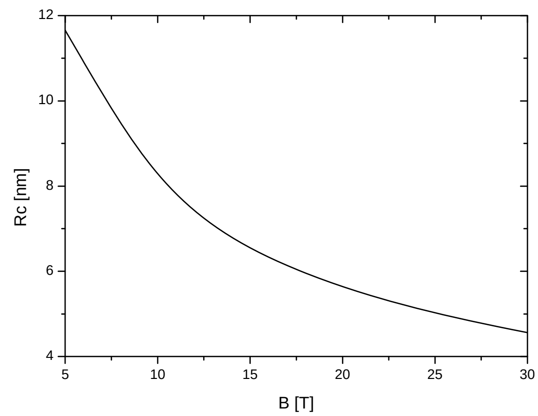

Fig. 3. Cyclotronic radius versus magnetic field

In the magnetic field presence, the wave functions become more compressed and the lateral width of the wave function, given by $\langle\rho\rangle = \langle\Psi_\infty | \rho\Psi_\infty\rangle$, is decreased. This is shown in Fig. 4, where the results scaled by the cyclotron radius are presented. The changeover from low-field to high-field behavior occurs when the average radial position $\langle\rho\rangle$ becomes comparable to R_{eff}, and in high-field limit the lateral width of the wave function approach R_c.

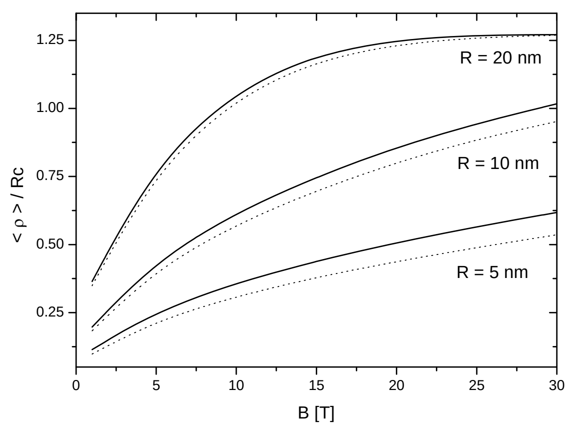

Fig. 4. Magnetic field dependence of average radial position scaled with the cyclotron radius. Electron: solid lines; heavy hole: dotted lines.

Note that the values obtained from the two methods are again in quantitative agreement, as observed in Fig. 5.

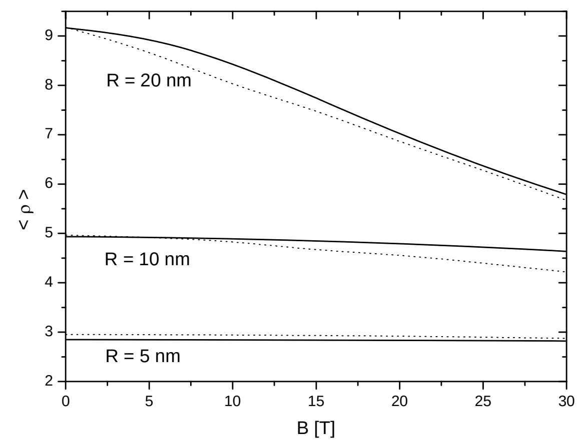

Fig. 5. The electron average radial position for different wire radii using EIB method (solid lines) and variational method (dotted lines).

Conclusion

We have been studied single-particle states of electron and heavy hole in a quantum wire with finite potential barrier in the presence of a uniform magnetic field. The calculation has been performed using an original analytical method, whose results agree fairly well with corresponding variational ones. As expected, in quantum wires with large radii at high magnetic fields the single-particle ground states go over into the $n = 0$ Landau levels.

REFERENCES

1. *J. Bellessa, V. Voliotis, R. Grousson, X. L. Wang, M. Ogura, and H. Matsuhata*, Appl. Phys. Lett. **71**, 2481 (1997).
2. *F. Vouilloz, D. Y. Oberli, M. A. Dupertuis, A. Gustafsson, F. Reinhardt, and E. Kapon*, Phys. Rev. B **57**, 12378 (1998).
3. *M. H. Szymanska, P. B. Littlewood, and R. J. Needs*, Phys. Rev. **B63**, 205317 (2001).
4. *F. Tassne and C. Piermarocchi*, Phys. Rev. Lett. **82**, 843 (1999).
5. *O. Mauritz, G. Goldoni, F. Rossi, and E. Molinari*, Phys. Rev. Lett. **82**, 847 (1999).
6. *S. Das Sarma and D. W. Wang*, Phys. Rev. Lett. **84**, 2010 (2000).
7. *T. G. Pedersen and T. B. Lynge*, Phys. Rev. B **65**, 085201 (2002).
8. *M. Tsetseri and G. P. Triberis*, Superlatt. Microstruct. **32**, 79 (2002).
9. *T. Y. Zhang and W. Zhao*, Phys. Rev. B **73**, 245337 (2006).
10. *P. Villamil, N. Porras-Montenegro, and J. C. Granada*, Rev. B **59**, 1605 (1999).
11. *E. C. Niculescu, A. Gearba, G. Cone, and C. Negutu*, Superlatt. Microstruct. **29**, 319 (2001).
12. *G. Goldoni, F. Rossi, E. Molinari, A. Fasolino, and R. Cingolani*, Appl. Phys. Lett. **69**, 2965 (1996).