Electron energy levels for a finite elliptical quantum wire in a transverse magnetic field

Abstract: We investigate the electron ground state energy, the first excited energy and the electron density of probability within the effective-mass approximation for a finite strain elliptical wire. A magnetic field is applied perpendicular to the wire axis. The results are obtained by diagonalizing a Hamiltonian for a wire with elliptical edge. The electron levels are calculated as functions of the ellipse parameter of the wire with different values of the applied magnetic field. For increasing magnetic field the electron has its energy enhanced. The electron energy has decreased as the elliptical wire size increasing. The density of probability distribution in the wire with different size in the presence of a magnetic field has been calculated also. The smaller elliptical wire size can effectively draw electron deviation from the axis.

Key Words: energy levels, electron density of probability, magnetic field, elliptical wire

I. INTRODUCTION

In the past 40 years, modern growth techniques like molecular beam epitaxy, chemical vapour deposition metal organic chemical vapour deposition and advanced lithography techniques have made the realization of high quality semiconducting heterostructures possible. The peculiar optical and electronic properties of nanometric systems with quantum-confined electronic states are promising for uses in devices. Low-dimensional quantum nanostructures such as quantum wires and quantum dots have attracted considerable attention in view of their basic physics and potential device applications.[1-2] Quantum wire nanostructures can be fabricated now with monolayer precision, with dimensions of a few nanometers, free from damage due to lithographic processing, and in high density by the use of all-growth fabrication processes based on epitaxial techniques. One of the most successful all-growth techniques for fabricating wires has been cleaved edge overgrowth.[3-5] In this approach, elliptical wires are created. Because of size quantization, the physical properties of charge carriers in quantum structures strictly depend on external shape of the system under investigation.

Recently, considerable effort was devoted to the achievement of self-assembled quantum wires, which can be formed under certain growth conditions by solid source molecular beam epitaxy. In this case the wires are formed by the Stranski-Krastanow growth mode, in which the materials that are deposited on top of each other have a substantially different lattice parameter. Spontaneous formation of self-assembled InAs quantum wires on InP (001) substrate, having 3.2% lattice mismatch, has been recently demonstrated.[6-7] These nanostructures are promising candidates for light-emitting devices for wavelengths 1.30 μm and 1.55 μm[8-9]

In the theoretical works, it is customary to assume a circular, rectangular, V-groove and T shape for quantum wire. Considerable experimental and theoretical attention has also been devoted to elliptical quantum wire and ellipsoidal quantum dot. There are many investigations focus on the quantum wires and quantum dots.[10-21] The scattering matrix and Landauer-Buttiker formula within the effective free-electron approximation has been used to investigate theoretically the electron transport properties of a quantum wire.[20] The effects of strong coupling magnetopoiaron in quantum dot has been studied by using variational method.[21] III-V semiconductor is investigated particularly.[22-26] In addition, quantum ring has been studied also. [27-30] A two-electron system of a quantum ring under the influence of a perpendicular homogeneous magnetic field has been investigated.[30] Among the papers, electron energy spectrum in quantum wire has been studied. Electronic states in quantum dots have been calculated. Binding energy in quantum ring has been studied using variational method.

In this paper, we present a diagonalization technique (within the effective-mass approximation) for obtaining the electron energy levels and wave functions in a finite potential wire of elliptical dimensions. Then we have the electron ground states and the first excited states varied with transverse magnetic field and the ellipse eccentricity of the wire considering the lattice mismatch of the wire. We have calculated the density of probability distribution also. In Sec.II we set up our model and Hamiltonian. In Sec.III we present our numerical results. We offer conclusions in Sec.IV. We expect that these conclusions will be useful in perfecting the understanding of the growth process.

II. THEORY

We note first of all that the shape of the wire is ellipse. Let us consider an electron moving in a quantum wire of elliptical shape. We consider the geometry of InAs/InP QWR as a two-dimensional (2D) elliptical quantum box with the major axis a along the x direction and semi-major axis b along the y direction. Different effective masses are assumed inside and outside the wire. Schematic illustration of a 2D elliptical quantum box is given in figure 1.

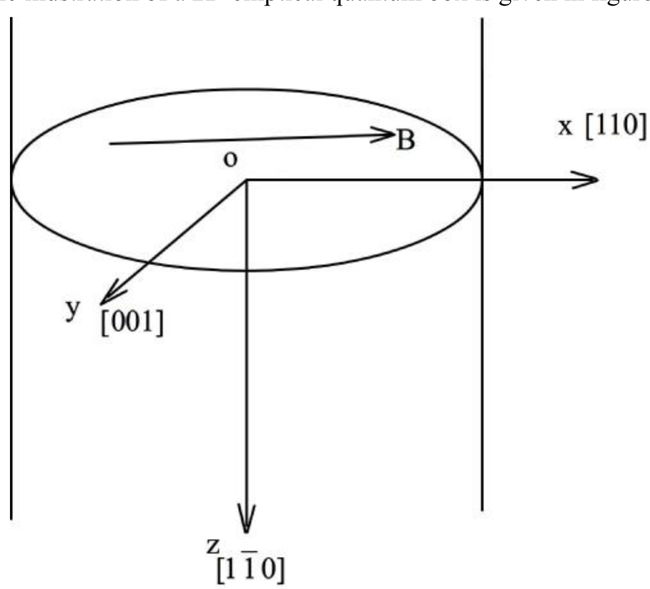

FIG. 1. The cross-section and the characteristic dimensions of the elliptical quantum wire.

In our work, the uniform magnetic field is perpendicular to the axis of the wire and is assigned by the vector potential

$$\vec{A} = By\hat{z} \tag{1}$$

Electron is confined in the x- and y- directions and can move freely along the wire direction because of the strong confinement in the x-y plane. Within the effective mass approximation, the Hamiltonian of the electron in a quantum wire is given by

$$\hat{\vec{H}} = (\hat{\vec{P}} - \frac{e}{c}\vec{A})\frac{1}{2m^*(x,y)}(\hat{\vec{P}} - \frac{e}{c}\vec{A}) + V(x,y) \quad (2)$$

where $m^*(x,y)$ is the electron effective mass, $V(x,y)$ is the strained conduction band offset, and $\hat{\vec{P}} = -i\hbar\nabla$ is the momentum. $m^*(x,y)$ and $V(x,y)$ in the wire and barrier can be written as

$$m^*(x,y) = \begin{cases} m_1^*, & x^2/a^2 + y^2/b^2 \le 1 \\ m_2^*, & x^2/a^2 + y^2/b^2 > 1 \end{cases} \quad (3)$$

$$V(x,y) = \begin{cases} 0, & x^2/a^2 + y^2/b^2 \le 1 \\ V_0, & x^2/a^2 + y^2/b^2 > 1 \end{cases} \quad (4)$$

where a and b are the ellipse semiaxes. The total Hamiltonian (with the confinement) still commutes with p_z, and therefore the wave function in the z direction can still be taken as a plane wave. The energy can be obtained for $p_z = 0$. Therefore, the problem is still 2D.

$$V_0 = E_{ce}(x,y) + a_c \varepsilon_{hyd} \quad (5)$$

$E_{ce}(x,y)$ is the unstrained conduction band offset, a_c is the hydrostatic deformation potential for the conduction band, and $\varepsilon_{hyd} = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$ denotes the hydrostatic strain. The formation of self-assembled InAs/InP quantum wire is based on the strain-relaxation effect. It is therefore interesting and important to consider the influence of strain on the electronic properties of the quantum wire. It is well known that ε_{xx} and ε_{yy} are determined as a function of the size of the wire, while ε_{zz} is equal to the misfit strain $\varepsilon_0 = (a_{0InAs} - a_{0InP})/a_{0InP}$ within the strained QWR and equal to zero in the barrier. Therefore, the expression ε_{hyd} in the case of hydrostatic strain for the electron depends only on the x- and y coordinates. It should be noted that in our strain calculation model this value is independent of the size of the quantum wire, because the sum of the normal strain components ε_{hyd} is constant. For the electron, the edge of the conduction band is shifted down by the hydrostatic strain $a_c \varepsilon_{hyd}$, which is $144 MeV$ for InAs/InP quantum wire.

We have used the effective electron Bohr radius in InAs, $a_0^* = \dfrac{\varepsilon_0 \hbar^2}{m_1^* e^2}$, as the unit of length and the effective electron Rydberg, $Ry^* = \dfrac{m_1^* e^4}{2\hbar^2 \varepsilon_0^2}$, as the unit of energy. We have also used the quantity $\gamma = \dfrac{e\hbar B}{2m_1^* c Ry^*} = \dfrac{\hbar^3 \varepsilon_0^2 B}{m_1^{\circ 2} c e^3}$. The Hamiltonian inside and outside the wire are different. The Hamiltonian in the wire can be given as

$$\hat{H}_1 = \left[-\frac{\hbar^2}{2m_1^*} \frac{1}{a_0^{*2}} \nabla^2 + \frac{e^2 B^2}{2m_1^{*2} c^2} a_0^{*2} y^2 \right] \Big/ Ry^* = -\nabla^2 + \gamma^2 y^2 \tag{6}$$

The Hamiltonian in the barrier can be given as

$$\hat{H}_2 = \left[-\frac{\hbar^2}{2m_2^*} \frac{1}{a_0^{*2}} \nabla^2 + \frac{e^2 B^2}{2m_2^{*2} c^2} a_0^{*2} y^2 + V_0 \right] \Big/ Ry^* = -\frac{m_1^*}{m_2^*} \nabla^2 + \frac{m_1^{*2}}{m_2^{*2}} \gamma^2 y^2 + \frac{V_0}{Ry*} \tag{7}$$

We investigate the elliptical quantum wire in elliptic coordinates system. In the elliptic coordinates ξ and θ bound to the Cartesian by the relationships

$$x = h \cosh \xi \cos \theta \; ; \qquad y = h \sinh \xi \sin \theta \tag{8}$$

where h is half of the distance between the foci of the ellipse. We expand the electron wave function in terms of confluent hypergeometric function basis set because of a magnetic field is perpendicular to the axis of the wire,

$$\psi(\xi, \theta) = \sum_{n,m} a_{nm} \varphi_{nm}(\rho(\xi, \theta), \theta) \tag{9}$$

where, a_{nm} is the coefficient of the expansion and $\varphi_{nm}(\rho(\xi,\theta),\theta)$ is the orthogonal basis we have chose.

$$\varphi_{nm}(\rho(\xi,\theta),\theta) = \frac{\alpha^{|m|+1}}{|m|!} \sqrt{\frac{(n+|m|)!}{\pi n!}} \rho^{|m|}(\xi,\theta) F(-n, |m|+1, \alpha^2 \rho^2(\xi,\theta)) e^{-\frac{\alpha^2 \rho^2(\xi,\theta)}{2}} e^{im\theta} \tag{10}$$

where, α is a parameter and F is a confluent hypergeometric function.

Inserting Eq. (9) into Eq. (2), we obtained the secular equation

$$\left| H_{nm,n'm'} - E \delta_{nn'} \delta_{mm'} \right| = 0 \tag{11}$$

The elements of the Hamiltonian matrix can be given as

$$\begin{aligned} H_{nmn'm'} &= \iint \varphi_{nm}^*(\rho(\xi,\theta),\theta) \hat{H} \varphi_{n'm'}(\rho(\xi,\theta),\theta) dS \\ &= \int_0^{2\pi} d\theta \int_0^{\xi_0} d\xi a^2 \left(sh^2 \xi + \sin^2 \theta \right) \varphi_{nm}^*(\rho(\xi,\theta),\theta) \hat{H}_1 \varphi_{nm}(\rho(\xi,\theta),\theta) + \\ &\int_0^{2\pi} d\theta \int_{\xi_0}^{\infty} d\xi a^2 \left(sh^2 \xi + \sin^2 \theta \right) \varphi_{nm}^*(\rho(\xi,\theta),\theta) \hat{H}_2 \varphi_{nm}(\rho(\xi,\theta),\theta) \end{aligned} \tag{12}$$

After obtaining the eigenvalues (the ground states and the excited states) and the wave functions of the electron, we can get the energy levels when the magnetic field fixed and the electron density of probability distribution.

III. NUMERICAL RESULTS AND DISCUSSIONS

In order to study the electron energy levels and the influence of a transverse magnetic field, the ground state energy, the first excited state energy and the density of probability distribution have been calculated for different magnetic fields. Several different size elliptical quantum wires have been investigated in this paper.

The parameters we used in this paper are list in Table 1. [31] For these values of the parameters, the units of length and energy are respectively, $1a_0^* = 349.3\,\mathring{A}$, $1Ry^* = 1.36meV$, $1\gamma = 1.8517B(T)$. The conduction band offset of the wire is $513meV$ when the strain is considered.

Table 1. The electron energy and the density of probability distribution are calculated using these parameters.

Material	m_e	ε	a_0(Å)	E_g(eV)	A_c
InAs	0.023	15.15	6.058	0.417	-5.08
InP	0.077	12.5	5.869	1.424	---

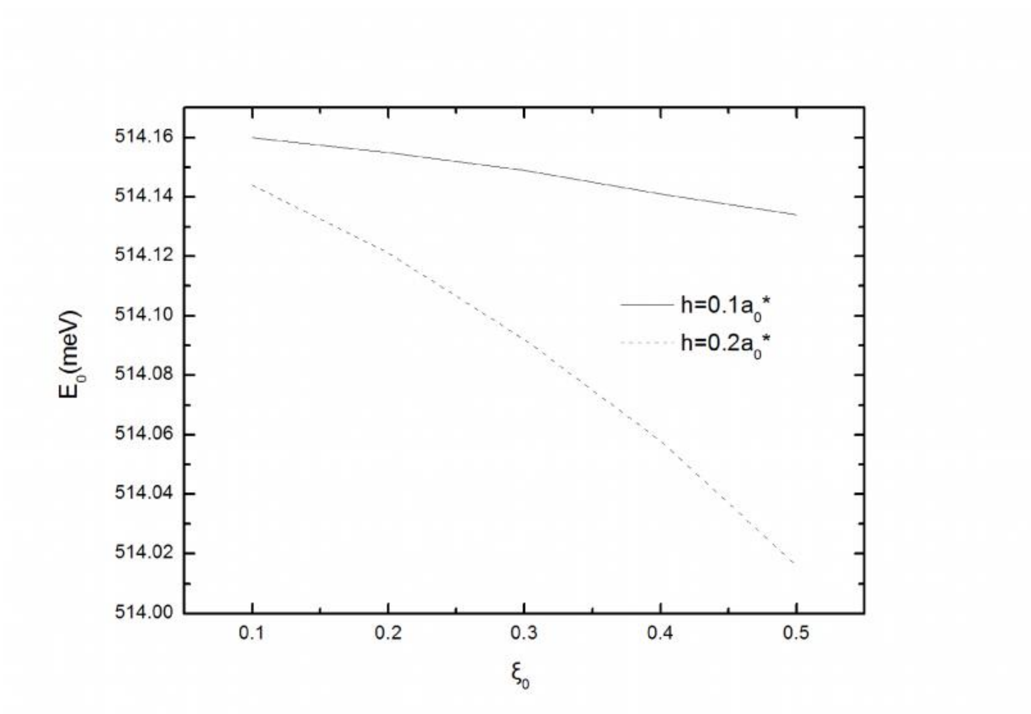

FIG. 2. The ground state energy of electron for a transverse magnetic field of 0.5T.

Figure 2 shows the ground state energy of electron in elliptical quantum wire in a transverse magnetic field equal to 0.5T as a function of ξ_0. It is observed that for elliptical quantum wires where $0.1 < \xi_0 < 0.5$ the ground state energy of electron decreases rapidly as the parameter ξ_0 increases, especially for $h = 0.1a_0^{\bullet}$ and the energy value of the wire for $h = 0.1a_0^{\bullet}$ is bigger than for $h = 0.2a_0^{\bullet}$ when the ξ_0 is fixed. That's because the ground state energy of electron is determined by the magnetic field applied on the x-axis and the size of the elliptical quantum wire when the magnetic field is fixed. The difference of the two curves is due to the different size of the wire. In small size wire, the confinement is much stronger than in big size wire. Therefore the effect of the magnetic field on the energy of the electron becomes strong as the wire size increases. The size of elliptical quantum wire becomes big as the parameters h and ξ_0 increases.

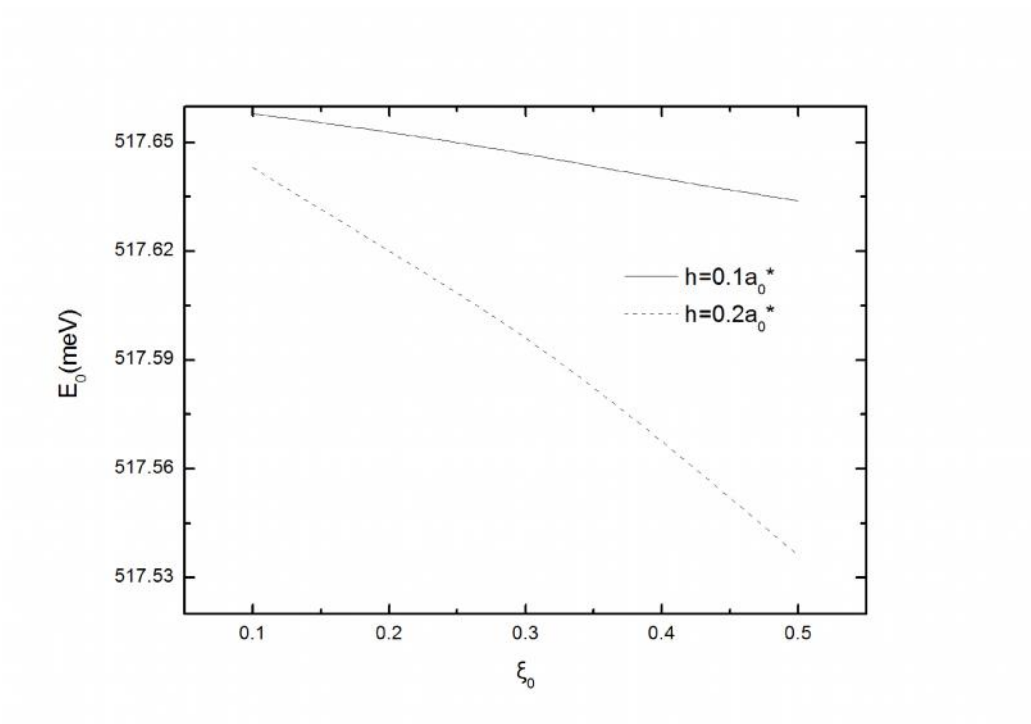

FIG. 3. The ground state energy of electron for a transverse magnetic field of 1.0T.

Figure 3 represents the parameter ξ_0 dependence of the ground state energy of electron in elliptical quantum wire in a transverse magnetic field equal to 1.0T. The results are similar to the case of the transverse magnetic field equal to 0.5T. The value of the ground state energy of the electron decreases as the parameter ξ_0 increases. The difference between the two energy values for the wires with $h = 0.1a_0^{\bullet}$ and $h = 0.2a_0^{\bullet}$ becomes small as the ξ_0 increases. From figure 2 and figure 3, it can be seen that the energy value in the wire when the magnetic field equal to 1.0T is bigger than that of 0.5T because of large magnetic field effects.

In Fig. 4, we plot the fist excited energy of electron versus the parameter ξ_0 for different elliptical quantum wires as the parameter $h = 0.1a_0^{\bullet}$ and $h = 0.2a_0^{\bullet}$ in a transverse magnetic field equal to 0.5T. As can be seen, the fist excited energy decreases as ξ_0 increases and the energy in the wire for $h = 0.2a_0^{\bullet}$ is smaller than the energy for $h = 0.1a_0^{\bullet}$. That is because the spatial confinement caused the results when the magnetic field is fixed. The spatial confinement is determined by the size of elliptical quantum wire, which becomes big as the parameters h and ξ_0 increases. In comparing the results in figure 4 to the data in figure 2, we can find that the first excited energy is bigger than the ground state energy of the electron in the elliptical quantum wire.

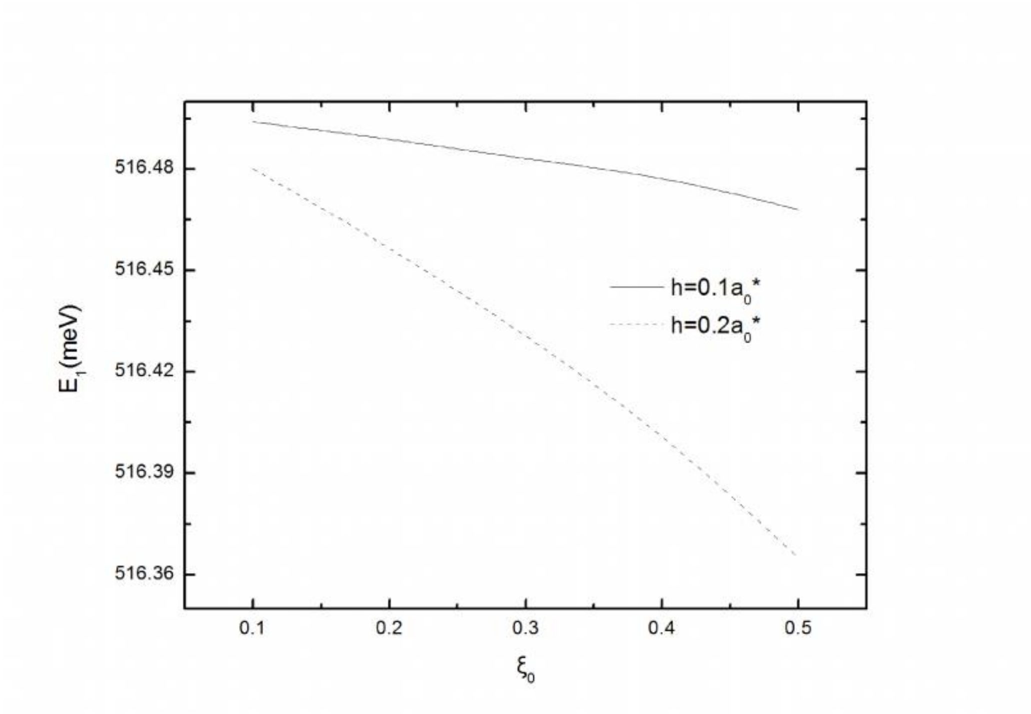

FIG. 4. The first excited energy of electron for a transverse magnetic field of 0.5T.

For the wires with the parameter $h = 0.1a_0^{\bullet}$ and $h = 0.2a_0^{\bullet}$, the fist excited energy of electron as a function of the parameter ξ_0 in elliptical quantum wire for a transverse magnetic field equal to 1.0T is shown in figure 5. The energy decreases with the parameter ξ_0 increasing. The difference between the curves of the first excited energy for the wires given ξ_0 with the parameter $h = 0.1a_0^{\bullet}$ and $h = 0.2a_0^{\bullet}$ increases as the ξ_0 increases. The results are similar to the case of the transverse magnetic field equal to 0.5T. From figure 4 and figure 5, we obtain that the first excited energy of the electron in a magnetic field equal to 1.0 T is bigger than the energy in a magnetic field equal to 0.5 T when the size of the wire is fixed. That is because when the wire size is fixed, the value of the first excited energy of the electron with the bigger applied magnetic field becomes more big due to the energy comes both from the spatial confinement and the magnetic field confinement. From Figs. 3 and 5, we can conclude that the first excited energy is bigger than the ground state energy in a wire with a fixed magnetic field.

We can also calculate the electron ground state energy and the first excited energy when the magnetic field varies or the value of the magnetic field equal to zero using this method. For a given wire, the ground state energy and the first excited energy of electron increase as the applied magnetic field increases in the elliptical quantum wire.

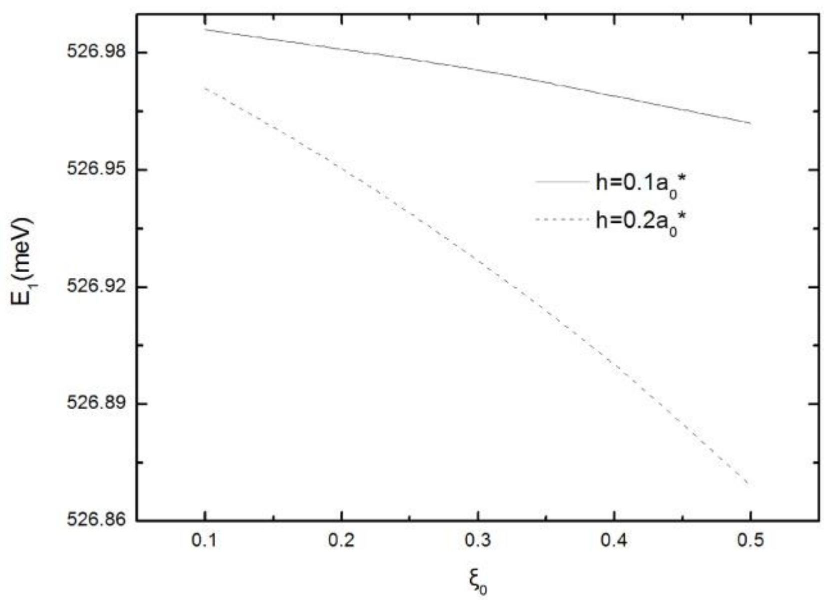

FIG. 5. The first excited energy of electron for a transverse magnetic field of 1.0T.

To further confirm the size of quantum wire effect, the electron density of probability distribution $|\psi|^2$ in the wire with h=0.10 a_0^*, h=0.15 a_0^*, h=0.20 a_0^* for $\theta = \pi/2$ and $\xi_0 = 0.1$ in the presence of a magnetic field equal to 1.0T is shown in Fig. 6. After calculating the wave functions of the electron, we obtained the density of probability of the electron. It can be clearly seen that the electron density of probability $|\psi|^2$ increases with ξ increases, reaching a maximum value between 0.35 and 0.38 and then decreases rapidly. After comparing the three curves, we have got that the smaller size elliptical quantum wire tends to shift the electron wave function away from the wire center. The smaller size wire can effectively draw electron deviation from the axis, so the electron energy is become bigger correspondingly.

We can calculate the density of probability distribution in other region of the wire, such as $\theta = \pi/6$, $\pi/4$, $\pi/3$ and so on. We can also get the density of probability distribution in other elliptical quantum wires.

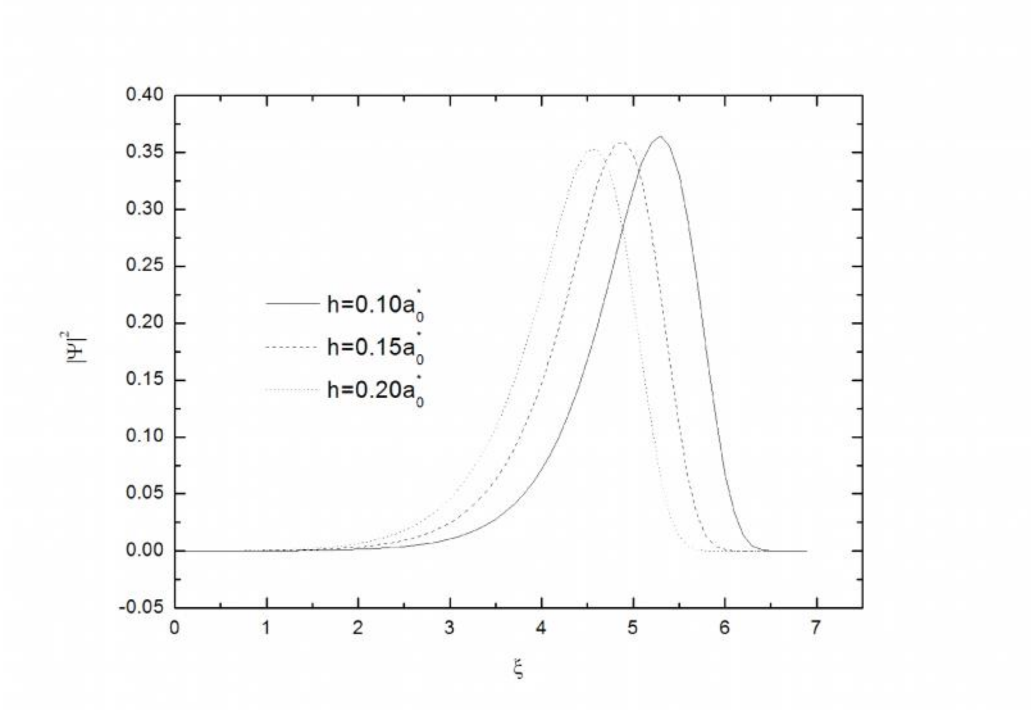

FIG. 6. $|\psi|^2$ for a electron in wire with h=0.10 a_0^*, h=0.15 a_0^*, h=0.20 a_0^* for B=1.0T as $\theta = \pi/2$ and $\xi_0 = 0.1$

IV. CONCLUSIONS

In summary, considering the hydrostatic strain, through investigating a self-assembled InAs/InP finite elliptical quantum wire in a transverse magnetic field by a diagonalized method within the effective-mass approximation, we have obtained that the ground and first excited state energies and the density of probability distribution.

The main results are that the ground state energy and the first excited state energy are become small as ξ_0 varies from 0.1 to 0.5 with $h = 0.1a_0^{\bullet}$ and $h = 0.2a_0^{\bullet}$ in the presence of a fixed transverse magnetic field when the applied magnetic value equal to 0.5T and 1.0T. The electron ground state energy and the first excited energy with the magnetic field varies or the value of the magnetic field equal to zero by diagonalizing a Hamiltonian for a wire with elliptical edge. The ground state energy and the first excited energy of electron increase as the applied magnetic field increases. We obtained the density of probability distribution in the wire with h=0.10 a_0^*, h=0.15 a_0^*, h=0.20 a_0^* for $\theta = \pi/2$ and $\xi_0 = 0.1$ in the presence of a magnetic field equal to

1.0T. The smaller size elliptical quantum wire tends to shift the electron wave function away from the wire center with a fixed magnetic field, so the electron energy is become bigger in a smaller size wire.

The numerical calculations reveal that the influences of the magnetic field and the barrier on the electron energy levels are considerable. It is shown that the energy depends on the magnetic field strength and the dimensions, whereas their competition determines the energy levels. The electron energy levels for the narrow elliptical wire are more sensitive to the applied magnetic field and for the bigger magnetic field are sensitive to the elliptical wire size.

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