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Transverse Stark effect of electrons in GaAs semiconducting quantum boxes

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Abstract. The transverse Stark shift of the electronic energy levels in GaAs semiconducting quantum box is investigated by the use of variational solutions to the effective-mass approximation. It is found an interesting phenomenon that the largest Stark shift is obtained for the electric field directed along the diagonal in cross section of a quantum box, while for a rectangular one, the shift reaches peak value for the low field directed along a side of cross section and for the high field along the diagonal. Likewise, the conclusion is shown that the transverse Stark shift in a quantum box depends highly on the ratio of cross sectional sides while is irrelevant to itsheight. The large Stark shift of the electron and hole trapped in a quantum box leads to an obvious reduction of the interband recombination and wide irradiance spectrum.

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Key words: Stark effect, quantum boxes, electric field, variational method, quantum sizes

1 Introduction

In recent several decades, low-dimensional semiconductor quantum dots (QDs), with zero-dimensional electronic properties, have stimulated great interest due to their important roles in fundamental physical research and for developing novel devices, and has potential applications in the 21st century nanoelectronics. It has been one of frontier topics of materials science to study the characterization of self-organized quantum dots and device applications. The study of energy shifts of particles in semiconductor nanostructures of different geometries turns out to be a very important task since the shifts are associated with the spatial separation between electrons and holes in these structures which induces a reduction of interbandrecombination.The Stark effect significantly changes the optical absorption, reflection,

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and photoluminescence properties. It is useful to understand quantum lasers and application of quantum dot fluorescence in the biology field. Consequently, the quantum confined Stark effect of low-dimensional system has attracted considerable attention recently. There has been quite a bit of work on the Stark effect in quantum wells, quantum wires, and spherical quantum dots when an electric field is applied along the direction of carrier confinement in the system [1–10]. There has been less work concerning the Stark effect in quantum boxes. Mendoza *et al.* [11] have calculated the Stark shift of the energies of impurities in a cubical quantum box. Spector *et al.* [12] have calculated the effect of a transverse electric field on the ground and the first few excited states of the electrons confined in a cubical quantum box. Li *et al.* [13] have calculated the Stark effect of the energy of a hydrogenic donor impurity in a rectangular parallelepiped-shaped quantum dot in the framework of effective-mass envelope-function theory using the plane wave basis.

In previous paper [14], we have given the Stark effect in a rectangular quantum boxes in the present of spatial electric field by means of variational calculation method and effective-mass approximation. In this paper, we use the same method to calculate the energy shift in a quantum box in the presence of a transverse electric field. The dependences of the shift in a quantum box upon the ratio of cross sectional sides and the transverse electric field directions are studied. It is necessary to investigate the transverse Stark effect in a quantum box which is very promising for the realization of fast optical switches and modulators. These results are relevant to any optical processes, such as emission and absorption. This feature is important for application of the nanostructures to optical modulators with lower voltage operation and quantum dot fluorescence in the biology field.

2 Theory

The Hamiltonian of a charged particle in a quantum box in the presence of a transverser electric field applied to the center axis of the box is

$$H=\frac{\vec{p}^2}{2m^*}+V(\vec{r})-q(Fx\cos\phi+Fy\sin\phi), \tag{1}$$

where $F>0$ is electric field, $\vec{p}$ is the carrier momentum, m^* and q are the carrier effective mass and charge respectively, the orientations of the transverser electric field $\vec{F}$ in cross section is specified by the angle ϕ between the positive direction of x-axis and the electric field direction. $\vec{r}$ is the position vector of the carrier. Confining potential $V(r)$ is given by

$$V(\vec{r})=\begin{cases} -\frac{L}{2}<x<\frac{L}{2}, \quad -\frac{W}{2}<y<\frac{W}{2}, \quad \text{and} \quad -\frac{H}{2}<z<\frac{H}{2}, \\ \text{elsewhere}, \end{cases} \tag{2}$$

using the infinite well model. Here, L, W and H are the length, width and height of the quantum box in the x, y and z directions respectively. We take the variational wave function as

$$\Psi(x,y,z)=N(\alpha,\beta)\cos\frac{\pi x}{L}\cos\frac{\pi y}{W}\cos\frac{\pi z}{H}e^{(\alpha x/L)}e^{(\beta y/W)}, \tag{3}$$

where α, β are the variational parameters which depend upon the electric field F and φ, $N(\alpha,\beta)$ is the normalization constant of the wave function, which is the function of α, β. Using the normalization condition

$$\int \psi^*\psi dr=1, \tag{4}$$

the normalization constant is obtained by

$$N^{-2}(\alpha,\beta)=\frac{HWL\pi^4 \sinh(\alpha)\sinh(\beta)}{8\alpha\beta(\alpha^2+\pi^2)(\beta^2+\pi^2)}. \tag{5}$$

A straightforward calculation yields the following expression for the expectation value of the Hamiltonian given by Eq. (2) using the variational wave function given in Eq. (3)

$$\begin{aligned} E(\alpha,\beta)=E_0+\frac{\hbar^2\alpha^2}{2m^*L^2}+\frac{\hbar^2\beta^2}{2m^*W^2}+qLF\cos\varphi\left(\frac{\alpha}{\alpha^2+\pi^2}+\frac{1}{2\alpha}-\frac{\coth\alpha}{2}\right) \\ +qWF\sin\varphi\left(\frac{\beta}{\beta^2+\pi^2}+\frac{1}{2\beta}-\frac{\coth\beta}{2}\right), \end{aligned} \tag{6}$$

where E_0 is the ground-state energy at zero field,

$$E_0=\frac{\hbar^2\pi^2}{2m^*L^2}+\frac{\hbar^2\pi^2}{2m^*W^2}+\frac{\hbar^2\pi^2}{2m^*H^2}. \tag{7}$$

From Eq. (6), the Stark shift, which is defined as the difference between the energy of the carrier with the electric field and without the electric field, can obtain by minimizing $E(\alpha,\beta)$ with respect to α and β. It is given by

$$\begin{aligned} \Delta E=E(\alpha,\beta)-E_0=\frac{\hbar^2\alpha^2}{2m^*L^2}+\frac{\hbar^2\beta^2}{2m^*W^2}+qLF\cos\phi\left(\frac{\alpha}{\alpha^2+\pi^2}+\frac{1}{2\alpha}-\frac{\coth\alpha}{2}\right) \\ +qWF\sin\phi\left(\frac{\beta}{\beta^2+\pi^2}+\frac{1}{2\beta}-\frac{\coth\beta}{2}\right). \end{aligned} \tag{8}$$

The variational parameters α and β in Eq. (8) are determined by the following the following equations,

$$qLF\cos\phi=\frac{\hbar^2\alpha}{m^*L^2\left(\frac{1}{2\alpha^2}-\frac{1}{\pi^2+\alpha^2}+\frac{2\alpha^2}{(\pi^2+\alpha^2)^2}-\frac{1}{2\sinh^2\alpha}\right)}, \tag{9}$$

$$qWF\sin\phi=\frac{\hbar^2\beta}{m^*W^2\left(\frac{1}{2\beta^2}-\frac{1}{\pi^2+\beta^2}+\frac{2\beta^2}{(\pi^2+\beta^2)^2}-\frac{1}{2\sinh^2\beta}\right)}. \tag{10}$$

From Eq. (8), the transverse Stark shift is only dependent on the cross-setion sizes of the quantum dot while is irrelevant to the height.

3 Results and discussion

By solving numerically Eqs. (8)-(10) for different sizes of the quantum box at various electric fields, we can study the Stark shift which is dependence of the sizes of the quantum box and transverse electric field direction and intensity. In the following discussion, the energies are measured in effective electron Rydberg units $Ry = e^2/2\kappa a$, the sizes of the quantum box are measured in effective electron Bohr radii $a = \hbar^2\kappa/m^*e^2$ and the electric field is measured in atomic units $F_0 = e/\kappa a^2$, here κ is the dielectric constant of the semiconductor. In GaAs the electron effective mass is $m^* = 0.0665m_0$, the hole effective mass is $m_h^* = 0.46m_0$, where m_0 is the fee electron mass and $\kappa = 13.1$. With this set of parameters, the effective units correspond to $a^* \approx 100$ Å, $Ry \approx 5.7$ meV and $F_0 \approx 11.5$ KV/cm.

In Fig. 1, for various transverse fields, $-\Delta E$ is shown as a function of the angle ϕ. Figs. 1(a) and (b) are for the square and rectangular boxes respectively. The typical symmetry is shown in Fig. 1(a). And we can see that $-\Delta E$ always reaches a peak value when $\phi_m = \frac{\pi}{4}$, namely the electric field $\vec{F}$ is along the direction of the diagonal line of the cross section, this feature is independent of the field intensity. For the field directed along a side of the cross section, $-\Delta E$ is the smallest. However in Fig. 1(b), due to the change of the cross section, the symmetry is broken. Electric intensity has an important role. From Fig. 1(b), one can see that the angle ϕ_m varies obviously with various field intensities for the rectangular one. For the low field directed along a side of the cross section, $-\Delta E$ is the largest. Let the angle between the direction along the diagonal line of the cross section and the positive direction of x-axis is ϕ_0, with the field intensity the angle ϕ_m approaches toward the angle ϕ_0, that is, for the high field directed along the diagonal $-\Delta E$ reaches the maximum. These phenomena can be obtained from the theoretical calculation. Using the Eq. (8), in the lower field [14], the expression can be obtained,

$$\Delta E = -\frac{q^2F^2m^*}{2\hbar^2}\left(L^4\cos^2\phi + W^4\sin^2\phi\right)\left(\frac{1}{6} - \frac{1}{\pi^2}\right)^2. \qquad (11)$$

By minimizing ΔE with respect to ϕ, the equations are obtained as follow

$$\sin 2\phi\,(W^4 - L^4) = 0. \qquad (12)$$

From Eq. (12), when the cross section is square, the largest shift is independent of the direction of the electric field. Take one closer see the Fig. 1(a) for the weak field $F = 10$, the difference between the maximum of the Stark shift and its minimum is about 0.002 Ry, very tiny. It is indicated that $-\Delta E$ hardly depends upon the direction of the electric field for the very low fields as it is obtained theoretically. For the rectangular cross section, the maximum of the Stark shift is found when the direction of the electric field is along sides of the section.

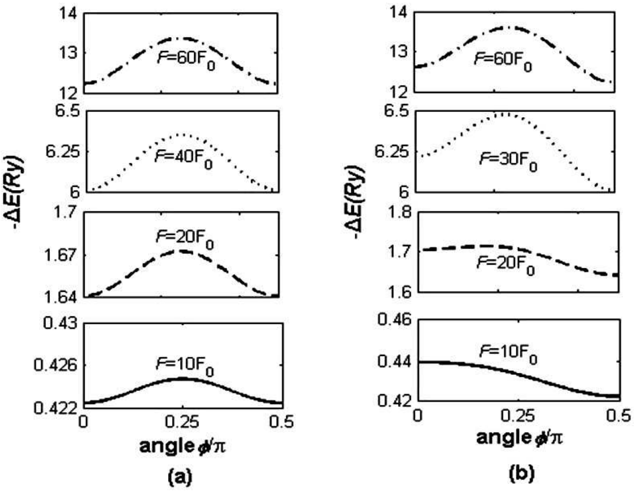

Figure 1: $-\Delta E$ in a quantum box is shown as a function of the angle φ for various electric field intensities. (a) For $W=L=1a$. (b) For $W=1a$, $L=1.01a$.

In the higher field [14], we can obtained

$$\Delta E = -\frac{qE}{2}(L\cos\phi + W\sin\phi). \tag{13}$$

Similarly, by minimizing ΔE with respect to ϕ, we can obtain

$$\tan\phi = \frac{W}{L}. \tag{14}$$

That is

$$\phi = \phi_0. \tag{15}$$

From Eq. (15), the biggest shift can be obtained when the electric field is directed along the diagonal line of either the rectangular section or square one.

In Fig. 2, when $\phi = \frac{\pi}{4}$ and $W+L=4a$, $-\Delta E$ is plotted as function of electric field for the different ratio of cross section sides. From this figure, we can clearly that $-\Delta E$ depends highly on L/W. For a given electric field, $-\Delta E$ increases as L/W becomes large. When the cross section is square, $-\Delta E$ is minimum.

These upper features can be also seen in Fig. 3 which plots $-\Delta E$ as a function of the electric field directed along the diagonal of the box or along its length. For the square section, at low fields the Stark shift is almost independent of the two orientations of the electric field, the depicted curves overlap together. However, a completely different behavior takes place for high fields at which the Stark shift for the field directed along the diagonal is much larger than that for the field directed along the length. For the rectangular one, at low fields the Stark shift for the field directed along the length is larger; at high fields the feature seen in the figure is same as that for the square section. In addition, as it is pointed out in Fig. 2, we can see that $-\Delta E$ increases with the increasing L/W.

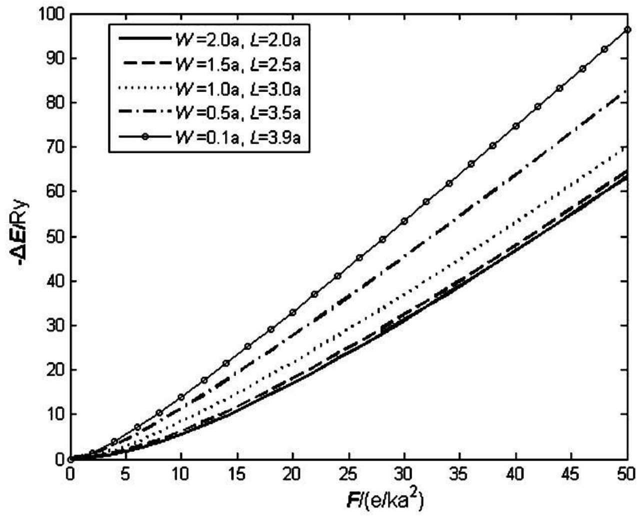

Figure 2: When $\varphi=\pi/4$ and $W+L=4a$, $-\Delta E$ is shown as a function of the electric field F for various ratio of the cross-sectional sides.

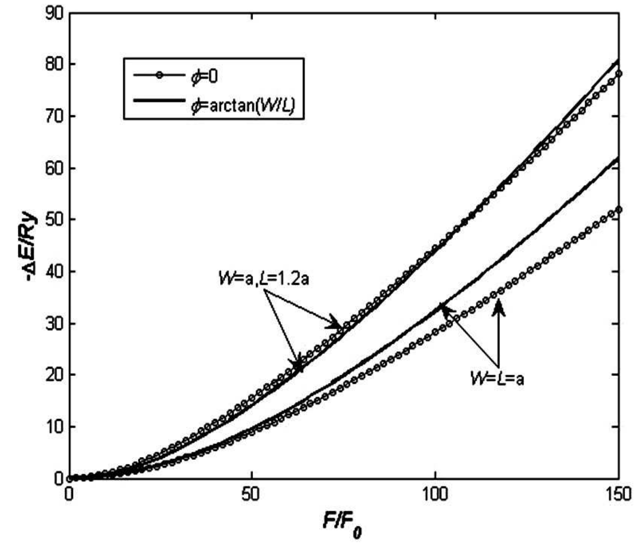

Figure 3: $-\Delta E$ is as a function of the electric field directed along the diagonal of the cross section or along its length.

In many photoluminescence experiments, one is concerned with the recombination rate between the spatial confined electron and hole in an electric field, which is very significant. the overlap integral M_{eh} is defined as [10,14]

$$M_{eh}=\int_{-\infty}^{\infty} dxdydz\psi_e(x,y,z)\psi_h(x,y,z).$$

In GaAs with the hole effective mass is $m_h^* = 0.46m_0$. The recombination rate is proportional to ${M_{eh}}^2$ in Fig. 4, ${M_{eh}}^2$ is shown as a function of the transverse electric field directed along the diagonal of the cross section or along its length. The particles are trapped in the square box for $W = L = 1a$ and in the rectangular one for $W = 1a,\ L = 1.5a$ respectively. From this figure, ${M_{eh}}^2$ decreases with the increasing L/W. As it is pointed out before, increase of L/W leads to the large shift of particles, which induce spatial separation of the electron and hole in the GaAs quantum box. So The polarization effect in the box depends highly on the ratio of cross section sides. Likewise, we can see that ${M_{eh}}^2$ for the field directed along the diagonal decreases much faster than that for the field directed along the length for the square box„ especially at high fields. For the rectangular box, at low fields the decrease of ${M_{eh}}^2$ is more for the direction of the filed along the length of the cross section; at high fields the feature is identical to that for the square box. These features stem from the field-induced spatial separation of the electron and hole in the GaAs quantum box. The polarization effect in the box depends also highly on the orientation of an transverse electric field. For the square box, the polarization effect is the most obvious for the field directed along the cross-section diagonal. However, for the rectangular one, the effect is the most pronounced for the low field directed along the length and for the high field directed along diagonal.

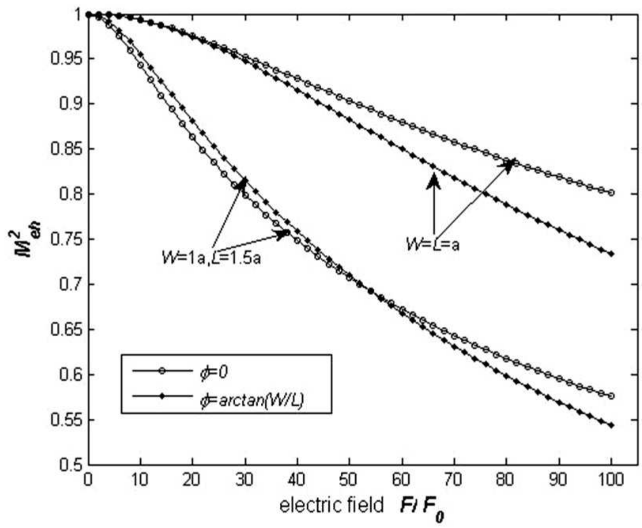

Figure 4: ${M_{eh}}^2$ is as a function of the transverse electric field directed along the diagonal of the cross section or along its length.

4 Conclusions

In the presence of the transverse electric field, the Stark shift of electronic energies in a semiconducting quantum box has been investigated using variational calculation method and effective-mass approximation.

The largest Stark shift in a quantum box can be found by means of changing the ratio (L/W) of cross sectional sides and the direction of an external electric field. When (L/W) increases, the $-\Delta E$ will increases, and ${M_{eh}}^2$, which is proportional to the recombination rate between the spatial confined electron and hole, will decraese. For a square box, when the field is directed along the diagonal, the Stark shift is largest. For a rectangular one, the largest Stark shift can be obtained when the field is applied along a side of cross section at low fields and applied along the diagonal at high fields. An obvious reduction of interband recombination is also yielded due to the large Stark shift of the electron and hole confined in a quantum box. Finally, we believe our results can provide an indication for design of some photoelectric devices constructed based on GaAs quantum box structures.

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