Applied electric field and hydrostatic pressure effects on quasistationary states in single and coupled GaAs–(Ga,Al)As quantum wells

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Abstract. We have studied the effects of hydrostatic pressure and an uniform electric field on the electron energy levels GaAs–(Ga,Al)As single quantum wells (QWs) and coupled double quantum wells (DQWs) by using the Enderlein’s method to solve exactly the Schrödinger equation. Numerical results were obtained using the density of states (DOS) as a function of the applied electric field, hydrostatic pressure, Al concentration, and the geometry as well. We found that the quasistationary ground and excited states energy diminish with and the applied electric field, increase with the confinement potential and the width of central barrier in the DQW. In the latter structure we observed the anti-crossing between the first and second quasistationary energy levels. We found that the applied electric field and the hydrostatic pressure modify the period of Pulsations in QWs.

1. Introduction
The physics of low dimensional semiconductor systems has been widely studied since the last century due to its potential application on the optoelectronic devices construction. Most of the studies on semiconductor systems have been carried out on GaAs–(Ga,Al)As heterostructure, especially single and multiple quantum wells, where GaAlAs is used as the barrier material and therefore the electron mobility is confined within the GaAs.

There have been several works devoted to the understanding the role of the applied electric field without considering the exactly solution of the wave function in the barrier regions [1–3] and others who have taken into account the influence of hydrostatic pressure on the electron states in these structures [4–9]. D. E. Aspnes [4], S. Adachi [5], B. Welber et al. [6] and R. C. Miller et al. [7] determined the carrier’s masses (electrons and holes), the height barriers, the bandgap and other properties of heterostructures experimentally as a function of hydrostatic pressure, besides adjusting the respective constants. In this paper, we used the exact solution proposed by R. Enderlein et al. [10,11] to calculate the effects of hydrostatic pressure and uniform electric fields on the electron energy levels in GaAs–(Ga,Al)As in QWs and DQWs.

2. Theoretical Framework
We performed the study of the effects of an electric field $F$ applied on the grown direction $-z$, as well as those of an applied hydrostatic pressure in QWs and DQWs. The DQW heterostructure
is compound by two GaAs wells, a central Ga$_{1-x}$Al$_x$As barrier, and by semi-infinite Ga$_{1-x}$Al$_x$As barriers in its extremes. The Schrödinger equation is given by

$$\left(-\frac{\hbar^2}{2m} \frac{d}{dz} \frac{1}{m^*(z)} \frac{d}{dz} - eFz + V(z)\right) \varphi_E(z) = E\varphi_E(z), \quad (1)$$

where $V(z)$ is the confinement potential for a QW or DQW, and the action of hydrostatic pressure is included in the electron effective-mass $m^*$. We will focus on theory corresponding to DQWs, considering the length of the DQW heterostructure is $L$, the electron wave function can be written as

$$\varphi_E(z) = \begin{cases} A_i \left(-\frac{z}{l_{bf}} + \frac{V_0 - E}{\hbar w_{bf}}\right), & z < -L/2, \\ \phi_E(z), & -L/2 \leq z \leq L/2, \\ a_3 A_i \left(-\frac{z}{l_{bf}} + \frac{V_0 - E}{\hbar w_{bf}}\right) + b_3 B_i \left(-\frac{z}{l_{bf}} + \frac{V_0 - E}{\hbar w_{bf}}\right), & z > L/2, \end{cases} \quad (2)$$

where $\phi_E$ is the solution to Schrödinger’s equation in $-L/2 < z < L/2$, $w_{bf},w_F = \left(\frac{\hbar^2}{2m_{bf}}\right)^{1/3}$, the subscripts $b$ and $w$ are for barrier and well, respectively. $\varphi_E$ can be written within each well or barrier, as a linear combination of Airy functions of first and second type. The interfaces of the heterostructure can be connected through the transfer matrix $S(E)$ [10,11] and the corresponding coefficients can be found using the continuity conditions of $\phi_E$ and $\phi_E/m^*$. From above, we can determine the DOS for a DQW under the action of an electric field [10,11].

$$\rho(E) = \frac{1}{\hbar w_{bf} l_{bf}} \frac{1}{|S_{11}|^2 + |S_{21}|^2}, \quad (3)$$

where $S_{11}$, $S_{21}$ are related with structural and energy parameters of the heterostructure. The energies are calculated finding the energy values which the denominator of Eq. 3 has a local minima.

The application of hydrostatic pressure modifies the lattice constants, barrier height, effective masses and dielectric constants. $m^*(P,T)$ is the pressure- and temperature-dependent electron effective-mass given by [5,12]. We use for the the pressure - and temperature - dependent energy gap for the GaAs the expression given by [9], also the gap differences between both semiconductors, and it dependence on $P$ and $x$ are given in reference [4,6]. Finally the hydrostatic pressure-dependent QW height is obtained from the fractional change in the volume of the zinc-blende structure as given in reference [13].

3. Results and Discussion

For a GaAs-(Ga,Al)As QW, the applied electric field makes the energy of the ground and excited states to decrease, being more notorious for ground and first excited state, even for weak electric fields, as it is shown in Fig. 2(a), the lines $E_g, E_{g'}, E_b$ and $E_{b'}$ are related with the points marked in the energy profile of the heterostructure as displayed in Fig. 1. The energy of ground, first, and second electron excited states as a function of the electric field for three values of the applied hydrostatic pressure is presented in Fig. 2(b). As expected, the energy of the ground and excited states diminishes with the well width and the applied electric field for a given value of $x$, as it is presented in Fig. 2(c). On the other hand, Fig. 2(d) presents the competition between the electric eld which makes the energy of the electron states to diminish and the confinement potential, which makes it to increase with the barrier width. As it is observed, both effects together make the energy of the ground state to stabilize, for $x$ values greater than a particular one, depending on the applied electric field. The behavior of the ground and first excited
Figure 1.
QW Energy Profile

Figure 2. Quasistationary ground and first excited states in a GaAs–Ga$_{1-x}$Al$_x$As QW as a function of (a) applied electric field, $F$, (b) applied electric field for different values of applied hydrostatic pressure, $P$ (c) well width, $L_W$, for different values of electric field (d) Al concentration, $x$, for different values of electric field.

Figure 3. Ground and first excited states in GaAs–(Ga,Al)As DQW as a function of (a) well widths,$L_{Ws}$ (b) Al concentration of the central barrier, $y$, (c) applied hydrostatic pressure, $P$, (d) electric field, $F$, the anti-crossing phenomenon is observed at $F_c=130.2$ kV/cm, (e) electric field, the anti-crossing phenomenon is observed at $F_c=149.3$ kV/cm

Figure 4. DOS in a QW (pulsation region) as a function of energy for different (a) applied electric fields with $x=0.3$, $L_W=10 nm$ and $P=0 kbar$ (b) well widths with $x=0.3$, $F=100 kV/cm$ and $P=0 kbar$ (c) Al concentrations with $F=100 kV/cm$, $L_W=10 nm$ and $P=0 kbar$, and (d) applied hydrostatic pressure, $P$ with $x=0.3$, $F=100 kV/cm$ and $L_W=10 nm$. 
state energy in a DQW as a function of the well width for \( x = 0.3 \) and \( y = 0.3 \), is presented in Fig. 3(a). Note as expected, that for both states diminish with the well width and for both states the energy is lower than in the QW due to the lower confinement the electron feels in the DQW, despite the presence of the central barrier. On the other hand, the height of the central barrier, which increases with \( y \), modifies the energy of the ground and excited states augmenting its value, as it is shown in Fig. 3(b), due to the increment of the confinement potential. The applied hydrostatic pressure makes the energy of the ground and excited states to decrease, as it is shown in Fig. 3(e). The anti-crossing between the first and second excited electron states is observed in Figs. 3(c) and 3(d), as a function of the applied electric field for two values of central barrier width, \( L_b = 4nm \) and \( L_b = 2nm \), respectively. Note that the anti-crossing strengthens for the case of smaller barrier width because the ground and excited states behave like they were QW states.

In Fig. 4 we present the DOS for a QW as a function of energy in the region of pulsations \((E > E_b)\), as displayed in Fig. 1). In panel (a) it is observed that the period of the fast oscillations increases with the applied electric field for a given well width. The number of nodes in a given energy region is proportional to the well width as it is shown in panel (b). However, panel (c) shows that while the number of nodes does not vary with \( x \), the DOS of the pulsations increases with it. On the other hand in panel (d) it is noted a tendency in increasing the number of nodes with pressure up to 50 kbar, but to diminish for pressures greater than this value. This result is related with the confinement potential with the applied hydrostatic pressure, as established in the work by Reyes et al[3]. As commented for QW the period of the fast oscillations increases with the applied electric field. These results can be used to interpret transitions between rotational and vibrational molecular states, which are in the energy range of the fast oscillations.

4. Conclusions

In summary, in this work by using the Enderlein’s method we have studied the effects of hydrostatic pressure and an uniform electric field on the electron energy levels in GaAs–(Ga,Al)As QWs and DQWs. We found that the applied electric field makes the energy of the quasistationary ground and excited states to decrease, being more notorious for the ground and first excited state, even for weak electric fields. The ground and excited states energy diminish with the well width and the applied electric field, increase with the confinement potential and width of the central barrier. In the latter structure we have found the anti-crossing phenomenon between the first and second quasistationary energy levels for a specific electric field, being more apparent for smaller central barrier width. We found that the period of Franz-Keldysh oscillation type in QWs increases with the applied electric field and that the number of nodes of pulsations augment with the well width.

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