Shallow donor impurities in different shaped double quantum wells under the electric field

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The binding energy of the donor impurity in double triangle quantum well (DTQW), double graded (DGQW) and double square (DSQW) GaAs–(Ga,Al)As quantum wells under the electric field is calculated by using a variational approach. The results have been obtained in the presence electric field applied along the growth direction as a function of the impurity position, barrier width and the geometric shape of the double quantum wells.

1 Introduction

A double-quantum well (DQW) structure incorporating a two-dimensional electron gas (2DEG) in each quantum well is a unique system from the viewpoint of both device applications and fundamental physics. One feature making this system particularly interesting is the ability to manipulate the electron wave functions using gates. That is, when the gate biases are turned in such a way that the eigenstates of the two quantum wells are aligned in energy, the electronic states initially localized in the individual quantum wells are quantum mechanically coupled, thus forming delocalized states extending over the two quantum wells.

In recent years, a considerable amount of work has been devoted to the study of artificial low-dimensional systems, such as semiconductor heterostructures due to their interesting basic physical properties and the possible technological applications as in photodetector and optoelectroical devices. Among the various systems under current investigation, the quantum wells (QWs) have attained considerable theoretical experimental attention. The QWs are commonly taken to be symmetric, but the asymmetric QWs give new tunable properties, which are very important for device applications [1–6]. Within the last few years, there has been great interest in the electronic properties in the asymmetric quantum well (AQW) structures because they are the ideal systems for the study of terahertz electromagnetic radiation from semiconductor heterostructures [7–14]. This interest is mainly due to the possible applications of quantum devices high-speed electronics and to the generation and detection of terahertz bandwidth signals. In order to get sufficient tuning range, different QW structures such as stepped QW and asymmetric coupled double QW have been tried [15–17]. Various QW structures such as graded-gap, two-step, and coupled asymmetric QW have been investigated in an effort to enhance the electric-field-induced changes ([8] and references therein). In these structures, the Stark shifts, the changes in oscillator strengths and absorption coefficients were predicted theoretically and confirmed experimentally to be larger than changes that occur in conventional square potential QWs [8].
In this work, we calculate the binding energies for shallow donor impurities in double graded, triangle and square GaAs/Ga$_{1-x}$Al$_x$As quantum wells under the parallel-applied electric field to the growth direction using a variational technique. These potential profiles and the amplitude of the normalized subband wave function of electron $|\psi(z)|$ versus the normalized position $\tilde{z} = L/a_0$ are given in Figs. 1, 2 and 3 for cases a) $F = 0$ and b) $F \neq 0$.

**Fig. 1** Potential profile of DGQW and amplitude of the normalized subband wave function of electron $|\psi(z)|$ versus the normalized position $\tilde{z} = L/a_0$ for cases a) $F = 0$ and b) $F \neq 0$.

**Fig. 2** Potential profile of DTQW and amplitude of the normalized subband wave function of electron $|\psi(z)|$ versus the normalized position $\tilde{z} = L/a_0$ for cases a) $F = 0$ and b) $F \neq 0$. 

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Graded potential profile is obtained by changing linearly from zero to 0.3 the aluminium concentration $x$ in the Ga$_{1-x}$Al$_x$As layer. As known, one important aspect of electronic band structure engineering is the realization of graded heterostructures, in which the composition is varied continuously in space. Electronic and optoelectronic devices which exploit these effects include, to date; graded-base heterostructure bipolar transistors which promote the egress of carriers through the base; graded separate confinement heterostructure laser active regions which not only confine light to the quantum wells, but may also promote transport within the active region and increase device bandwidth.

2 Theory

In this study, we focus our attention a double graded quantum well (DGQW), double triangle quantum well (DTQW) and double square quantum well (DSQW) structures depicted in Figs. 1, 2 and 3, consisting of two graded quantum well separated by a thin potential barrier, subject to an electric field applied parallel to the growth direction (chosen as the $z$ direction). The Hamiltonian of a donor impurity in the presence of the electric field may be written as,

$$
H = -\frac{\hbar^2}{2m^*} \left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \Phi^2} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \Phi^2} \right) + \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial \rho^2} + V(z) + \left| e \right| F z - \frac{e^2}{\varepsilon_0 \sqrt{\rho^2 + (z - z_i)^2}}
$$

(1)

where $m^*$ is the electron effective mass, $\varepsilon_0$ is the static dielectric constant, $r$ is the distance between the carrier and the donor impurity site ($r = \sqrt{\rho^2 + (z - z_i)^2}$) and $\rho (= \sqrt{\rho^2 + y^2})$ is the distance between the electron and impurity in the $(x-y)$ plane, $F$ is the electric field strength, $V(z)$ are the finite confinement potentials in the $z$-direction. The functional forms of the DGQW, DTQW and DSQW are, respectively,

$$
V(z)^{DGQW} = \begin{cases} 
V & z < -b \\
\frac{V}{2L} & -b < z < -a \\
V & -a < z < a \\
\frac{V}{2L} & a < z < b \\
V & z > b
\end{cases}
$$

(2a)
Using the variational method, it is possible to associate a trial wave function, which is an approximated eigenfunction of the Hamiltonian described in Eq. (1). The ground-state wave function of the impurity is given by

\[ \psi(r) = \psi(z) \Phi(\rho, \alpha) \]  

where the wave function in the \((x–y)\) plane is chosen to be the wave function of the ground state of a two-dimensional hydrogen-like atom [18, 19]:

\[ \Phi(\rho, \alpha) = \frac{1}{\alpha} \left( \frac{2}{\pi} \right)^{1/2} \exp \left( -\rho/\alpha \right) \]

in which \(\alpha\) is a variational parameter. The ground-state impurity energy is evaluated by minimizing the expectation value of the Hamiltonian \(\langle \psi(r)|H|\psi(r) \rangle\) with respect to \(\alpha\).

The ground-state donor binding energy is given by [7, 20]

\[ E_b = E_i - \min_\alpha \langle \psi(r)|H|\psi(r) \rangle \]

where \(E_i\) is the ground state energy of the electron obtained from the Schrödinger equation in the \(z\)-direction without the impurity.

### 2 Results and discussion

The values of the physical parameters used in our calculations are \(m^* = 0.0665m_e\) (where \(m_e\) is the free electron mass), \(\varepsilon_0 = 12.58\) (static dielectric constant is assuming to be same everywhere), \(V_0 = 228\) meV and the distances are given in units of the effective Bohr radius \(a_0 = \varepsilon_0\hbar^2/m^*e^2\).

The variations of the ground state impurity binding energy of DGQW, DTQW and DSQW structures as a function of the normalized impurity position \((z_e/a_0)\) for barrier width-\(L_b = 10\) Å are given in Figs. 4a and b for \(F = 0\) and \(F = 50\) kV/cm electric field values, respectively. In Fig. 4a, the maximum binding energy is observed in DTQW for the impurity located in the barrier center and than for DGQW and DSQW, respectively due to the geometric confinement. When the electric field is applied, the Coulombic interaction between the electron and a donor impurity located in the barrier center decreases since
the electrons shift to the left side of the wells, and the binding energy of a donor impurity located in the center of left well or in the outer edge of the left well increases. As seen in this figure, DTQW structure is very sensitive to the electric field with respect to the other structures, and the impurity binding energy for DSQW is greater than the others structures.

For see the effects of the coupling between the wells on donor impurity binding energy, the variations of the ground state impurity binding energy of DGQW, DTQW and DSQW structures as a function of the normalized impurity position ($z_i = z/a_0$) for barrier width $L_b = 10 \, \text{Å}$ are given in Figs. 5a and b for $F = 0$ and $F = 50 \, \text{kV/cm}$, respectively. When we compare the obtained results for $L_b = 40 \, \text{Å}$ with previous results ($L_b = 10 \, \text{Å}$), as the coupling between the well decreases we see that the impurity binding energy decreases. As known, as the barrier width increases the effective length $L_{\text{eff}} = L_b + L_0 + L_2$; ($L = L_0 = L_2$) increases and the Coulombic interaction between the electron and a donor impurity decreases, for $F = 0$ the probability of finding of the electrons in both of the wells is the same and so, impu-
The impurity binding energy is minimum for donor impurity located in the barrier center. In Fig. 5b, the probability of finding of the electrons in the left wells increase with the effect of the electric field. When the coupling between the wells becomes weak, all of the structures with different potential profile begin to become sensitive to the electric field. 

For different geometric confinement potentials, the variation of the binding energy as a function of the electric field is given in Fig. 6 for different impurity positions. The barrier width is taken as $L_b = 10 \text{Å}$ which provides significant coupling of the adjacent wells. As the electric field increases, the Coulombic interaction between the electron and a donor impurity located in the barrier center (bc) or right well center (rwc) decreases and so, impurity binding energy decreases while it increases for impurity located left well center, since the electrons shift to the left side of the structure. The decrement in the binding energy for impurity located in the barrier center or the left well center is very weak for DTQW. DTQW has a stable character with respect to the other structures. As the well dimension increases, the wave function of the electron becomes strongly localized in the DTQW and DGQW with respect to the DSQW, and so the impurity binding energy of DTQW and DGQW are greater than DSQW, respectively.

In the large electric field values, electrons are localized in the left well for all structures. At a critical field value, graded quantum well is completely leveled of and it behaves like a single asymmetric quantum well because of electrons are localized in the left well. After a critical electric field values, graded quantum well behaves like a single triangle quantum well. This behavior is observed in Fig. 4 for large electric field values.

In summary, we have studied the binding energy of the hydrogenic impurities of different shaped double quantum wells (graded, triangle or full graded and square quantum wells) under the electric field. The calculations were performed within the effective-mass approximation and by using a variational method. The dependence of the ground state impurity binding energy on the applied electric field, geometric shapes of the wells and barrier width was discussed. To the best of our knowledge, this is the first study for hydrogenic donor impurities in double graded and triangle shaped quantum wells. We expect that this method will be of great help for theoretical studies of the physical properties of graded and triangle shaped quantum wells. Furthermore, the simplicity of the method might be useful for describing the correct behavior of shallow-donor impurities in double quantum-wells with different shapes in the external fields, and for designing some devices in the future.
References