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# Depolarization and exciton-like shifts in modulation-doped single rectangular and diffusion-modified quantum wells under uniform electric fields

S Fung, S Panda and B K Panda

Department of Physics, The University of Hong Kong, Hong Kong, People's Republic of China

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**Abstract.** Energy levels in the modulation-doped single rectangular and diffusion-modified quantum wells  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  are obtained using the Kohn and Sham density functional theory (DFT). The generalized DFT which uses a screened exchange potential in the local density approximation has been used to improve the accuracy of the energies and wavefunctions in these wells. The energy difference between the first excited state and the ground state has been studied in the presence of combined photon and electric fields for two wells with well widths of 70 Å and 100 Å. The energy difference is found to increase as a result of the depolarization and exciton-like shifts when there is no external bias. Under the electric field the shift in the energy difference decreases due to the vanishing of the exciton-like effect. The results obtained within the conventional Kohn and Sham DFT and within the generalized DFT are found to be the same for the well with a width of 100 Å. However, the results obtained from these two schemes are found to be different when the well width is 70 Å.

## 1. Introduction

The optical absorption technique has been used to characterize quantum wells in view of the potential applications of optoelectronic devices, such as in photodetectors, modulators and lasers [1]. A full understanding of the optical properties of quantum wells will require a knowledge of the details of the electronic structures of the subband levels under a uniform electric field. For an undoped sample, the electronic levels are obtained from the single-band effective-mass equation with the confinement potential [2]. In a modulation-doped quantum well, the electrons flow from the barrier region into the well to bring the system to equilibrium. As a result of the higher density of electrons in the well, the Coulomb interaction between electrons becomes very important, with the result that a complete many-body approach is needed to solve this problem [2]. The density functional theory (DFT) based on the Kohn–Sham scheme has been successful in treating the many-body effects in a single-particle formalism [3]. In this scheme, the complicated many-body processes are included in the exchange–correlation potential in a local density approximation (LDA) method. This method has been applied to solve the single-band effective-mass equation for the modulation-doped quantum well [4]. Although the LDA is a good approximation for calculating ground-state energies, the excited-state energies are underestimated in this method. Tomita has shown that the subband energies are well estimated by including a self-energy correction in the  $GW$ -approximation [5]. This formalism has been applied by Huang and Manasreh to obtain the subband energy levels in quantum wells accurately [4]. While this procedure has been quite successful in improving the

subband energies, the wavefunctions, which are needed for the calculation of the dipole matrix elements in the absorption spectra, are not determined in a self-consistent manner. Bylander and Kleinman [6] and later Seidl *et al* [7] have generalized the Kohn–Sham scheme to include the screened non-local exchange potential in the *sx*-LDA method; they calculated the energies and wavefunctions in a self-consistent way.

When an electron is excited to the higher subband upon absorbing the energy of an incident photon, it creates a hole state in the initial occupied subband. This will lead to an excitonic interaction between the excited electron and the hole state. This has been incorporated in the vertex correction by Huang and Manasreh [4]. Ando has included the excitonic and depolarization effects in the time-dependent single-band effective-mass equation and shown that these two effects broaden the calculated energy separation between the ground and first excited states by a substantial amount [8]. The theoretical absorption spectra agree very well with the experiment when these effects are taken into account. Karunasiri, Wang and Park have applied this scheme to study the parabolic SiGe/Si quantum wells, and found that the depolarization and excitonic effects are quite important in interpreting optical absorption spectra [9].

In order to understand the operating principles of biased quantum wells, it is necessary to study the depolarization and excitonic effects under an electric field. In our previous work we have studied the Stark shift and mean tunnelling lifetimes in the single rectangular and diffusion-modified quantum wells [10]. In the present work we will study these effects under a uniform electric field; to the best of our knowledge, this has not been done before.

## 2. Theory

The self-consistent Kohn–Sham equation for calculating the energy levels  $E_n$  and wavefunctions  $\Psi_n(z)$  within the effective-mass approximation is given by

$$\left[ -\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m^*(z)} \frac{\partial}{\partial z} + V_{qw}(z) + V_H(z) + V_{xc}(z) + eFz \right] \Psi_n(z) = E_n \Psi_n(z) \quad (2.1)$$

where  $V_{qw}$ ,  $V_H$  and  $V_{xc}$  are the quantum confined potential, the Hartree potential and the exchange–correlation potential respectively. The Hartree potential is obtained from the Poisson equation as follows:

$$\frac{\partial}{\partial z} \epsilon_r(z) \frac{\partial}{\partial z} V_H(z) = 4\pi e^2 \rho(z) \quad (2.2)$$

where  $\epsilon_r(z)$  is the relative dielectric constant along the  $z$ -direction and  $\rho(z) = [N_D^+(z) - n(z)]$  with  $n(z)$  and  $N_D^+(z)$  the carrier density and the ionized dopant density respectively. The carrier charge density at some finite temperature is given as

$$n(z) = \sum_{i=1}^{n_b} n_i^{2D}(z) |\Psi_n(z)|^2. \quad (2.3)$$

The two-dimensional occupation probability which includes the position dependence of the effective mass is given by

$$n_i^{2D}(z) = \frac{k_B T m^*(z)}{\pi \hbar^2} \ln \left[ 1 + \exp \left( \frac{\mu - E_i}{k_B T} \right) \right] \quad (2.4)$$

where  $\mu$  is the chemical potential.

Integrating equation (2.2) twice, we obtain the Hartree potential as

$$V_H(z) = 4\pi e^2 \int_{-\infty}^z \frac{dz'}{\epsilon_r(z')} \int_{-\infty}^{z'} \rho(z'') dz''. \quad (2.5)$$

The boundary condition applied to this equation is that  $V_H(\pm\infty) = 0$ . The exchange potential is given by [11]

$$V_x(z) = -2 \left[ \frac{9}{4\pi^2} \right]^{1/3} \frac{1}{r_s} R_y. \quad (2.6)$$

Here,

$$\begin{aligned} r_s &= [3/4\pi a_0^3(z)n(z)]^{1/3} & a_0(z) &= \epsilon_r(z)/m_r^*(z)a_B \\ R_y &= m_r^*(z)/\epsilon_r^2(z) \text{ Ryd} & m_r^*(z) &= m^*(z)/m_0 \end{aligned}$$

where  $a_B$  and Ryd are the Bohr radius and the Rydberg respectively. The correlation potentials for the low-density and high-density limits are of the Ceperley–Alder [12] and Gell-Mann–Bruckner [13] types respectively. We have used the following parametrized form given by Perdew and Zunger [14]:

$$V_c(z) = \begin{cases} -\frac{0.2864}{1 + 1.0529\sqrt{r_s} + 0.3334r_s} \left[ 1 + \frac{0.5264\sqrt{r_s} + 0.3334r_s}{3(1 + 1.0529\sqrt{r_s} + 0.3334r_s)} \right] R_y & r_s > 1 \\ [0.062 \ln(r_s) - 0.1166] R_y & r_s < 1. \end{cases} \quad (2.7)$$

The chemical potential ( $\mu$ ) is obtained from the charge-neutrality and depletion approximation conditions [15].

### 2.1. The generalized Kohn–Sham scheme

The generalized Kohn–Sham density functional scheme, as shown by Seidl *et al* [7], is given as

$$\begin{aligned} \left[ -\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m^*(z)} \frac{\partial}{\partial z} + V_H(z) + V_{xc}^{sx}(z) + eFz \right] \Psi_n(z) - \int dz' V_x^{sx,NL}(z, z') \Psi_n(z') \\ = E_n \Psi_n(z) \end{aligned} \quad (2.8)$$

where

$$V_x^{sx,NL}(z, z') = - \sum_n \frac{\Psi_n(z) e^{-q_{TF}|z-z'|} \Psi_n^*(z')}{|z-z'|}. \quad (2.9)$$

The local exchange potential is screened by the Thomas–Fermi wave vector  $q_{TF}$  [16] as follows:

$$V_x^{sx}(z) = V_x(z) G(q_{TF}/k_F) \quad (2.10)$$

where

$$G(\gamma) = 1 - \frac{4}{3}\gamma \arctan \frac{2}{\gamma} - \frac{\gamma^2}{6} \left[ 1 - \left( \frac{\gamma^2}{4} + 3 \right) \ln \left( 1 + \frac{4}{\gamma^2} \right) \right]. \quad (2.11)$$

We have adopted the Fourier series method [17] to solve equations (2.1) and (2.8).

### 2.2. Excitonic and depolarization effects

It is known that the photon-induced many-body contributions, such as the depolarization and exciton-like interaction between the ground and excited states, shift the calculated energy position by a substantial amount. These two effects come about as a result of the dependence of the plasma frequency on the charged sheet, which results due to excitation of the electron upon absorbing the photon. For the two-dimensional gas, such effects are estimated by solving

the time-dependent Schrödinger equation self-consistently using the Hartree and exchange–correlation potentials [8]. The intersubband transition energy is shifted by the depolarization and exciton-like effects as follows:

$$\tilde{E}_{10}^2 = E_{10}^2(1 + \alpha - \beta) \quad (2.12)$$

where  $E_{10}$  is the difference ( $E_1 - E_0$ ) between the subband energy levels calculated by using equations (2.1) and (2.8) self-consistently. Here,  $\alpha$  and  $\beta$  are the depolarization and exciton-like shifts respectively. The depolarization shift  $\alpha$  for the transition between the ground state and the first excited states is given by

$$\alpha = 2\hbar^2 \frac{4\pi e^2}{E_{10}} \int_{-\infty}^{\infty} dz \frac{n_{01}^{2D}(z)}{2m^*(z)\epsilon_r(z)} \left[ \Psi_1(z) \frac{d\Psi_0(z)}{dz} - \Psi_0(z) \frac{d\Psi_1(z)}{dz} \right]^2 \quad (2.13)$$

where  $n_{01}^{2D}(z) = n_0^{2D} - n_1^{2D}$ . Using equation (2.4), we evaluate  $n_{01}^{2D}$  as

$$n_{01}^{2D}(z) = \frac{k_B T m^*(z)}{\pi \hbar^2} \ln \left[ \frac{1 + \exp\left(\frac{\mu - E_0}{k_B T}\right)}{1 + \exp\left(\frac{\mu - E_1}{k_B T}\right)} \right]. \quad (2.14)$$

The exciton-like shift  $\beta$  is defined as

$$\beta = \frac{2}{E_{10}} \int_{-\infty}^{\infty} dz n_{01}^{2D}(z) \Psi_1^2(z) \Psi_0^2(z) \frac{\partial V_{xc}[n(z)]}{\partial n(z)}. \quad (2.15)$$

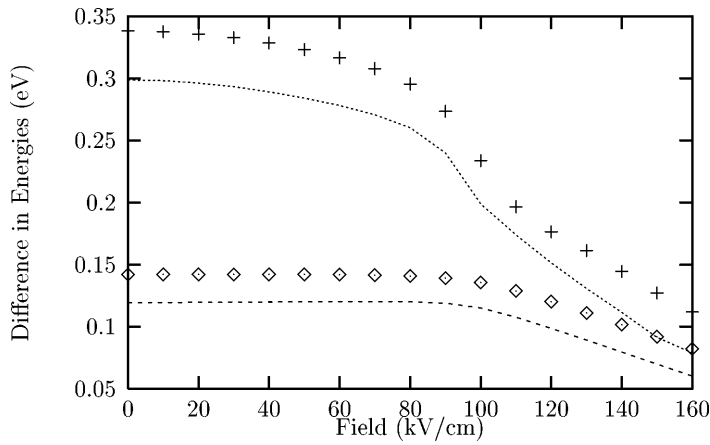
### 3. Results and discussion

The potential profile for the single rectangular quantum well (RQW) and the diffusion-modified quantum well (DMQW) formed by  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$  in the barrier region and GaAs in the well region have been described in our earlier work [10]. The barriers are doped with Si donors with binding energy 20 meV and concentration  $2 \times 10^{18} \text{ cm}^{-3}$ . We have used the Fourier series method to obtain the energies and wavefunctions [10]. The method of Ben Jazia *et al* is followed to obtain faster convergence in energy eigenvalues [18]. We need six iterations to achieve convergence in eigenvalues. We have considered the ground and first excited states in order to study the depolarization and exciton-like shifts in all wells. The temperature is taken to be 300 K.

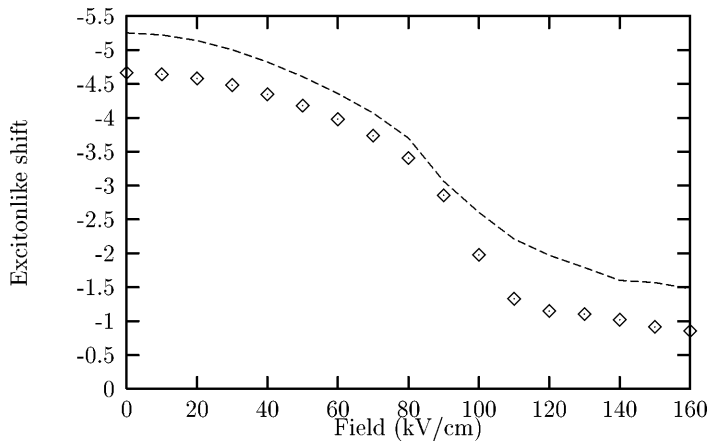
#### 3.1. The single rectangular quantum well

We first consider the RQW with the well width of 70 Å. The chemical potential is found to be situated at 118 meV in this well. The ground-state and first-excited-state energy levels are found to be 55 meV and 197 meV respectively in the LDA scheme. The energy levels obtained in the generalized Kohn–Sham scheme are 55 meV and 175 meV respectively. The effect of the screened exchange is found to affect the excited state only. In the bulk semiconductors, the energy levels in the conduction bands are increased by this correction [7], whereas in the present case, the first excited state is decreased by this correction. Since the chemical potential is close to the first excited state, the effect of the screened exchange might be different in this case to that for bulk semiconductors. The screened exchange has no effect on the ground-state energy level, as the chemical potential is well above it.

In figure 1 we have shown  $E_{10}$  and  $\tilde{E}_{10}$  as a function of the applied uniform electric field. We observe that the effect of the screened exchange is prominent at all field strengths. The depolarization and excitonic effects are found to reduce with increasing electric field and completely disappear at high electric field. In order to understand this effect, we have checked the individual depolarization ( $\alpha$ ) and excitonic shift ( $\beta$ ) terms. We have observed that both



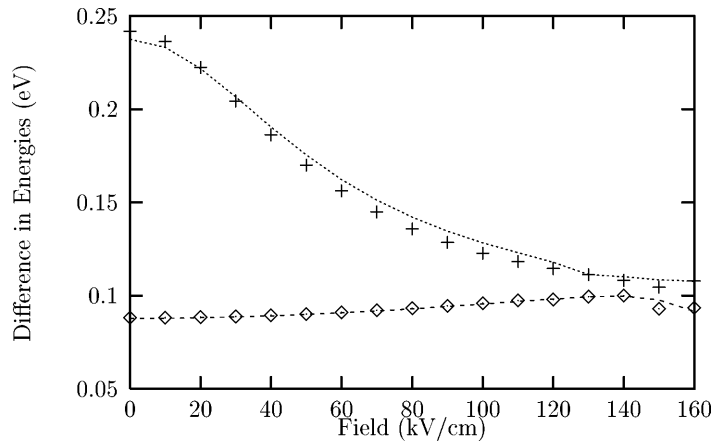
**Figure 1.** The differences between the ground-state and first-excited-state energies with and without depolarization and excitonic effects in the  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  rectangular single quantum well with a well width of  $70 \text{ \AA}$ . The crosses and squares correspond respectively to the energy difference with and without depolarization and exciton-like shifts in the LDA scheme. The dotted and dashed curves correspond respectively to the energy differences with and without depolarization and exciton-like shifts in the sx-LDA scheme.



**Figure 2.** The exciton-like shift in the single rectangular quantum well with a well width of  $70 \text{ \AA}$ . The dashed curve and squares correspond to the excitonic shifts calculated in the LDA and sx-LDA schemes respectively.

terms decrease with increasing electric field. However, the exciton-like shift term is more dominant than the depolarization term. Hence, we have shown the excitonic shift term as a function of the electric field in figure 2. We observe that the overall behaviour of this term with electric fields is quite similar to that of the energy separation term  $\tilde{E}_{10}$ . The electric field induces the tunnelling of the electrons out of the well by destroying the excitonic effects.

In order to see the effect of this correction, we have studied the same well but with a well width of  $100 \text{ \AA}$ . In the LDA formalism the energy levels are found to be  $38 \text{ meV}$  and  $126.5 \text{ meV}$  with the chemical potential at  $7.58 \text{ meV}$ . In the generalized Kohn–Sham scheme the ground-state and first-excited-state energy levels are found to be  $41.30 \text{ meV}$  and  $129.35 \text{ meV}$  respectively. The effect of the screened exchange is found to increase both the ground state

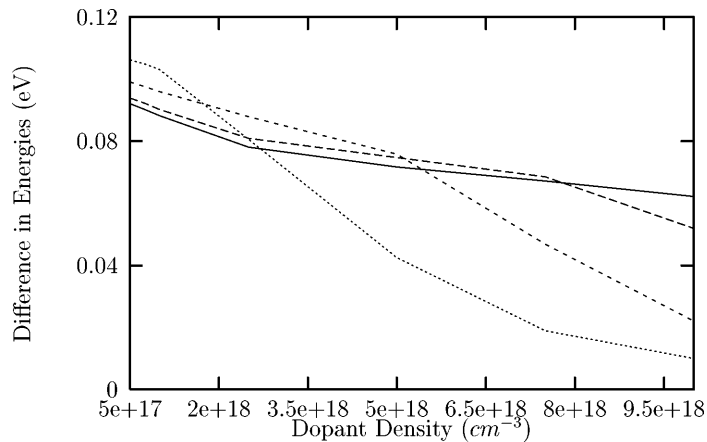


**Figure 3.** The differences between the ground-state and first-excited-state energies with and without depolarization and excitonic effects in the  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  rectangular single quantum well with a well width of  $100 \text{ \AA}$ . The notation is the same as for figure 1.

and the first excited states by  $3 \text{ meV}$ . Since the Fermi level lies well below the ground-state level, both the ground and first excited states are affected by the screened exchange term.

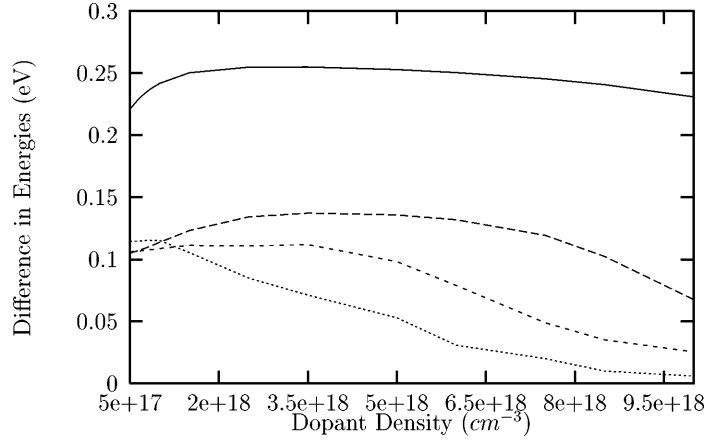
In figure 3 we have shown  $E_{10}$  and  $\tilde{E}_{10}$  as a function of the applied electric field. In this case the contribution of the screened exchange term to the energy difference is found to be negligibly small. Both the ground state and the excited state are increased by  $3 \text{ meV}$  at all field strengths according to the screened exchange method. The depolarization and excitonic effects are found to reduce with increasing electric field and completely disappear at electric fields higher than  $150 \text{ kV cm}^{-1}$ . We have examined the effect of the electric field on  $\beta$  and found that there is no difference between the LDA and sx-LDA calculations for this well.

The energy difference  $E_{10}$  under the electric field was calculated for different conc-



**Figure 4.** The differences between the ground-state and first-excited-state energies in the  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  rectangular single quantum well with a well width of  $100 \text{ \AA}$  with different dopant concentrations. The solid, long-dashed, short-dashed and dotted curves correspond to the fields at  $0 \text{ kV cm}^{-1}$ ,  $50 \text{ kV cm}^{-1}$ ,  $100 \text{ kV cm}^{-1}$  and  $150 \text{ kV cm}^{-1}$  respectively. The depolarization and excitonic shifts are not considered here.

entrations of Si donors in the RQW with well width 100 Å and is shown in figure 4. Since there is no difference between the results from the LDA and sx-LDA schemes for this well, we have used the LDA scheme to calculate the energy levels. We find that the effects of the electric field on  $E_{10}$  are different at low and high dopant concentrations. With the low dopant concentration,  $E_{10}$  is found to increase slightly with the electric field, whereas with high dopant concentration,  $E_{10}$  behaves in the opposite manner. The chemical potential at  $5 \times 10^{17} \text{ cm}^{-3}$  is found to be 3 meV and it increases monotonically with dopant concentration to a value of 21 meV at  $1 \times 10^{19} \text{ cm}^{-3}$ . The difference between the behaviours of the energy differences at low and high dopant concentrations might have resulted from the chemical potential.



**Figure 5.** The differences between the ground-state and first-excited-state energies with the depolarization and excitonic effects in the  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  rectangular single quantum well with a well width of 100 Å with different dopant concentrations and applied electric fields. The solid, long-dashed, short-dashed and dotted curves correspond to the fields at  $0 \text{ kV cm}^{-1}$ ,  $50 \text{ kV cm}^{-1}$ ,  $100 \text{ kV cm}^{-1}$  and  $150 \text{ kV cm}^{-1}$  respectively.

The effect of the depolarization and excitonic shifts on the energy difference is shown in figure 5. At zero electric field the energy difference is found to increase with dopant concentration slightly and then decrease in the high-concentration region. The effect of the electric field is only to decrease the energy difference, as already discussed. At low dopant concentrations, the energy differences at low and high electric fields are found to be nearly the same, whereas with high dopant concentrations, the effect of the electric field on the energy difference is quite significant for different field intensities.

### 3.2. The diffusion-modified quantum well

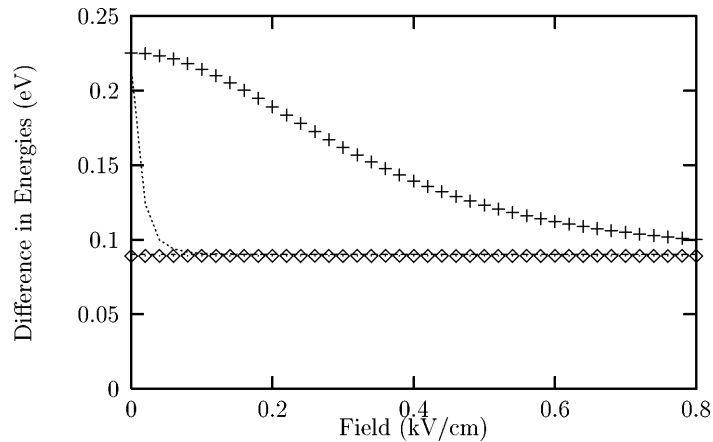
When the single RQW is subject to annealing above  $800 \text{ }^\circ\text{C}$ , intermixing starts at the heterojunction, and the formation of the Ga vacancy induces Al atoms to diffuse into the GaAs layer from the AlGaAs barrier. The interdiffusion process is therefore characterized by the Al diffusion length ( $L_d = \sqrt{Dt}$ ) which can be obtained from the diffusion constant ( $D$ ) at a given annealing temperature and annealing time ( $t$ ). Taking the diffusion constant to be isotropic, the position-dependent Al concentration is found from the diffusion equation to be [19, 20]

$$w(z) = x \left[ 1 - \frac{1}{2} \left\{ \text{erf} \left( \frac{L+2z}{4L_d} \right) + \text{erf} \left( \frac{L-2z}{4L_d} \right) \right\} \right] \quad (3.1)$$

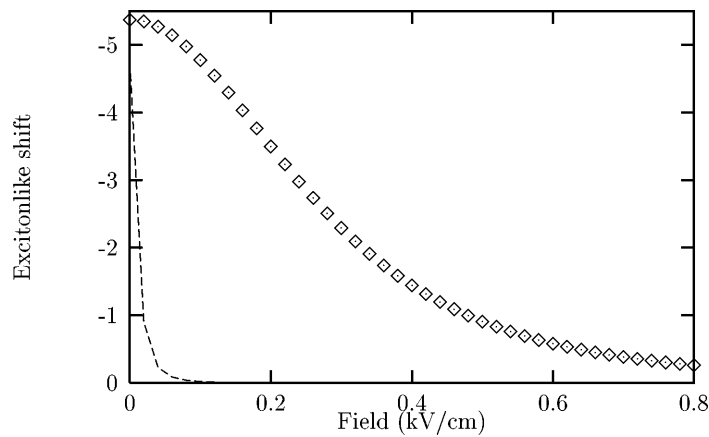
where erf is the error function [21] and  $L$  is the width of the single RQW. We have taken the diffusion length as  $L_d = 20 \text{ Å}$ .



We have studied the diffusion-modified well with well width  $70 \text{ \AA}$ . In the LDA method we find the energies of the ground and first excited states to be  $61 \text{ meV}$  and  $150 \text{ meV}$  respectively with the chemical potential at  $125.7 \text{ meV}$ . As in the RQW with the same well width, the chemical potential in this well also lies close to the first excited state. On the other hand the ground-state and first-excited-state energy levels in the sx-LDA scheme are found to be  $61 \text{ meV}$  and  $151 \text{ meV}$  respectively with the same chemical potential as in the LDA scheme. We find that in addition to having no effect on the ground state, the screened exchange also has no effect on the first excited state.



**Figure 6.** The differences between the ground-state and first-excited-state energies with and without depolarization and excitonic effects in the diffusion-modified quantum well with a well width of  $70 \text{ \AA}$ . The notation is the same as for figure 1.

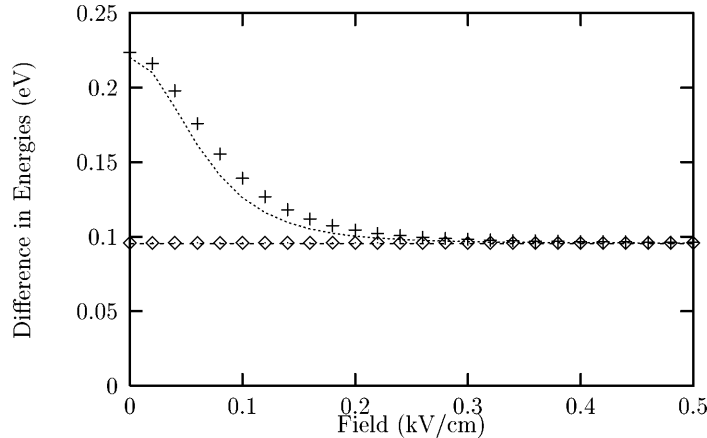


**Figure 7.** The exciton-like shift in the single rectangular quantum well with a well width of  $70 \text{ \AA}$ . The notation is the same as for figure 2.

The effects of the electric field on both  $E_{10}$  and  $\tilde{E}_{10}$  are shown in figure 6. We observe that the sx-LDA scheme predicts a rapid decrease of the energy difference with electric field. In figure 7,  $\beta$  shows similar behaviour with the electric field. Since the barrier height in this well is much smaller than that in the RQW, the effect of the low electric field on the excitonic and depolarization shifts is also quite significant.

We then calculated the energy levels for a well width of 100 Å. The energy levels of the ground state and first excited state in the LDA scheme are found to be 59.4 meV and 155.5 meV respectively. The chemical potential is found to be 8.25 meV. In the sx-LDA scheme the ground-state and first-excited-state energy levels are increased by 1 meV. As for the well with width 70 Å, the screened exchange correction has a smaller effect on the energy levels than on those in the RQW.

The energy differences with the applied electric fields are shown in figure 8. We observe no significant difference between the LDA and sx-LDA schemes for in the RQW with the same well width.



**Figure 8.** The differences between the ground-state and first-excited-state energies with and without depolarization and excitonic effects in the diffusion-modified quantum well with a well width of 100 Å. The notation is the same as for figure 1.

#### 4. Conclusions

In the present work we have calculated the energy levels in the modulation-doped single rectangular and diffusion-modified quantum wells using the conventional and generalized DFT methods in order to study the effect of the electric field on the depolarization and excitonic effects in these wells. The effect of the electric field is found to reduce the depolarization and excitonic effects when dopant concentrations are large. The details of the calculation show that the exciton-like shifts are reduced when an electric field is applied.

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