The effects of the carrier interaction and electric fields on subband structures of selectively–doped semiconductor quantum wells

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(August 3, 2018)

Abstract

We investigate the ground–state electronic properties of the symmetrically–doped semiconductor quantum well in the presence of a homogeneous electric field. In this paper we examined the effect of the electric field and carrier interaction on the subband structure as a function of the field strength and carrier concentration. The many–body effects are evaluated using a local density functional exchange–correlation potential. We find that the electron subband energy is reduced as the magnitude of the electric field is increased, but it is increased as the surface carrier density is increased. However, the separation of the electron subband energies is reduced for the increase in both the electric field and surface carrier density. On the other hand, the energy separation of the hole subbands is increased as the carrier density and field strength are increased. Effect of the exchange–correlation potential on the subband structure is found negligibly small in this calculation. The subband energies are reduced slightly, increasing their separations little in the presence of the local exchange–correlation potential.

PACS: 73.20.Dx, 73.40.Kp
1. INTRODUCTION

In recent years extensive efforts have been devoted to investigating the electronic properties of semiconductor quantum well structures [1]. These studies were motivated by the improvements in the crystal growth techniques, such as molecular beam epitaxy and metal organic chemical vapor deposition. These growth methods are capable of producing ultrathin layers of semiconductor heterostructures with sharp interfaces of high quality. A high–mobility semiconductor quantum well structures can be realized with a use of the modulation–doping technique [2]. In modulation–doping technique, for example, only the AlGaAs layers are doped with impurities and the GaAs layers are undoped. Doped impurities (donor impurities in our case) in the AlGaAs layers are ionized and electrons transfer to the GaAs layers. In this case one needs to examine the subband structures self–consistently taking into account the effects of charge transfer from AlGaAs to GaAs layers and of the band bending.

In the presence of an external d. c. electric field, new structures and phenomena were predicted and observed experimentally [3,4]. In particular, the tunability of the optical properties of the structure in the presence of an external electric field were studied considerably in detail [5,6]. Far infrared intraband absorption [7,8] was also observed in GaAs/AlGaAs layers with high detectivity approaching that of HgCdTe [9]. The quantum well high–electron–mobility transistor has also been studied [10]. Most of these studies involve some form of modulation of the quantum well eigenenergies and eigenfunctions in the presence of an electric field for their principal mode of operation.

Previous investigations have been focused in understanding the effects of the electric field and carrier interaction separately employing methods of either variational or perturbation calculations in a frame of the single-particle picture. The variational method, although computationally the simplest, has drawback of not knowing the accuracy and region of validity [11]. Bloss investigated only the electric field effects by solving differential equation numerically and neglecting the effects of carrier interaction [12]. Ando investigated only the
effect of carrier interaction in the absence of the electric field \[ R \]. However, in practical devices, one should take both of these two effects, self-consistently, into account on an equal footing.

In this paper, we investigate the effects of the carrier interaction and electric field on the electronic properties of symmetrically-doped GaAs/AlGaAs single quantum well (SQW) structures. We evaluate the electron and hole subband structures self-consistently within a Hartree approximation in the presence of a d.c. external electric field perpendicular to the interfaces. Also, a simplified local density functional exchange–correlation potential is employed to include the many–body effects such as exchange and correlation interactions in the calculation. In section 2, we describe a self–consistent numerical calculation of subband structures of the SQW in the presence of a d. c. electric field and carrier intercation. In section 3, we present the numerical results of GaAs/AlGaAs system. The subband energies are presented as a function of surface carrier density for several different values of the field strength. Finally, we conclude the work in section 4.

2. THEORY

We consider a symmetrically–doped GaAs/AlGaAs SQW structure in the presence of an external d. c. electric field within the effective mass approximation \[ 14 \]. Here we assume that the effective mass encounters the effect of bulk band structure and we ignore the mismatch of effective masses in the well and barrier regions. The motion of carriers (electrons or holes) in the \( z \) direction, which is the growth direction of the SQW and is perpendicular to the interface, is quantized due to the one–dimensional confining potential well. And, hence, the carriers possess only two degrees of freedom along the \( x \) and \( y \) directions. Therefore, the single–particle wave function describing the motion in the \( xy \)–plane is simply plane wave like and the wave function in the \( z \) direction is the solution of a one–dimensional Schrödinger equation

\[
\left[ -\frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + V_i(z) \right] \psi(z) = E \psi(z).
\] (1)
Here \( m^* \) is the effective mass of a carrier in the quantum well and the effective potential energy function \( V_l(z) \) subjected to a single particle in the system is given by

\[
V_l(z) = V_w(z) + V_F(z) + V_{s.c.}(z).
\] (2)

In equation (2) \( V_w(z) \) is the rectangular well potential energy associated with the band–gap mismatch at heterointerfaces and \( V_F(z) \) is the linear potential energy due to the constant electric field applied along the growth direction. And \( V_{s.c.}(z) \) is the energy of a given carrier due to the interactions with ionized impurities doped in the barrier material and with the other remaining carriers in the quantum well. The interaction potential energy \( V_{s.c.}(z) \) should be determined self–consistently.

If one simply replaces the wide band–gap material (AlGaAs layer) with a simple potential barrier of height \( V_o \), \( V_w(z) \) is written by [see figure 1]:

\[
V_w(z) = \begin{cases} 
0, & |z| < L/2 \\
V_o, & |z| > L/2
\end{cases}
\] (3)

where \( L \) is the width of the gap region (GaAs layer) i.e., the width of the quantum well. In this work the band–gap mismatch \( V_o \) is assumed to be 60\% (or 40\%) of the band–gap mismatch of AlGaAs and GaAs for the conduction (or valence) band \[12\]. In the presence of an external d.c. electric field \( F \) in the \( z \) direction, the motion of the electrons are further confined in addition from that in the absence of the field. The potential energy due to the electric field is given by

\[
V_F(z) = \mp eFz
\] (4)

where \(- \) is for an electron and \(+ \) is for a hole. In this paper the electronic charge is \(-e \) \((< 0)\). As one increases \( F \), carriers confined initially by \( V_w(z) \) would tunnel out of the well and therefore lowering their potential energy. If, however, the electric field is not extremely strong, the quantum–confined states would have a long lifetime and can therefore be considered as quasi–bound \[11\].
In modulation–doped SQW structures of GaAs/AlGaAs, electrons are transferred from the impurities doped AlGaAs to the GaAs region so as to lower the potential energy of electrons. As electrons transfer to the well region, the conduction and valence band edges are modified from the flat ones. This band–bending effect is to be included in the calculation by solving the Schrödinger equation with a use of a self–consistent potential energy $V_{s.c.}(z)$,

$$V_{s.c.}(z) = V_H(z) + V_{xc}(z).$$

Here $V_H(z)$ is the Hartree interaction energy, which is the sum of two contributions; the electrostatic interaction of a given carrier with the other carriers in the quantum well and that with ionized impurities remaining in the barrier region. $V_{xc}(z)$ is a single particle version of the exchange–correlation energy, which is not included in $V_H(z)$. In the Hartree approximation one only considers $V_H(z)$ and neglects $V_{xc}(z)$ in $V_{s.c.}(z)$. The Hartree term $V_H(z)$ is a solution of a Poisson equation. In this work, we consider the case that impurities are doped symmetrically with a bulk density $N_d$ in each barrier region on both sides of a SQW [see figure 1]. Therefore, the Poisson equation is written by [13]

$$\frac{d^2V_H(z)}{dz^2} = \mp \begin{cases} 
\frac{4\pi e^2}{\epsilon} [n(z) - N_d], & L/2 < |z| < L/2 + d_b \\
\frac{4\pi e^2}{\epsilon} n(z), & \text{otherwise}
\end{cases}$$

where the upper (lower) sign refers to electrons (holes). In equation (6) $n(z)$ is the carrier density of the SQW and $d_b$ is the width of the impurity–doped region in the barrier. The total effective width of the SQW is $d = L + 2d_b$ [see figure 1]. The static dielectric constant of the quantum–well material $\epsilon$ is assumed to be the same in both the barrier and well region. The average two–dimensional (2D) carrier density $N_s$ of the well is given by $N_s = 2N_dd_b$. In this paper, we confine ourselves to the ground–state, zero–temperature limit of the problem. Hence the volume density distribution $n(z)$ is written by

$$n(z) = \sum_i N_{si} |\psi_i(z)|^2$$

where $N_{si}$ is the 2D density of carriers in the $i$th subband (i.e., $\sum_i N_{si} = N_s$). If the electrons occupy only the ground subband ($i = 1$), $N_s = N_{s1}$ [which is the case of weakly–doped samples in experiment], and we can rewrite equation (7) by
\[ n(z) = N_s|\psi_1(z)|^2. \] (8)

The Hartree approximation is, in general, known to overestimate the Coulomb repulsive force of other electrons in the short range, and, in real system, many–body effects such as the exchange–correlation interaction could become important in the study of subband structures or intersubband resonance absorption \[15\]. We include the exchange–correlation effects in our calculation by introducing a simplified local exchange–correlation potential \( V_{xc}(z) = V_{xc}[n(z)] \equiv \mu_{xc}[n(z)] \) within the local density–functional approximation (LDA) \[16\] \[18\]. Here \( \mu_{xc} \) is the chemical potential of an inhomogeneous electron gas, which is obtained from that of a homogeneous electron gas by replacing the uniform electron density by the local electron density \( n(z) \) of the inhomogenous system. Several different forms of \( V_{xc}(z) \) are proposed by a number of people \[19\]. In our work, we use a simple form suggested by Gunnarson and Lundqvist \[20\],

\[ V_{xc}[n(z)] = -\frac{2}{\alpha r_s} \left[ 1 + 0.0545 \ln(1 + \frac{11.4}{r_s}) \right] \frac{m^* e^4}{2 \epsilon^2 \hbar^2} \] (9)

where \( \alpha = (4/9\pi)^{1/3} \) and \( r_s \) is defined in term of \( n(z) \) by \( n(z) = [\frac{4\pi}{3}(a_B^* r_s)^3]^{-1} \) with \( a_B^* = e\hbar^2/m^*e^2 \), the effective Bohr radius. Therefore, the Schrödinger equation for a single particle of the potential energy \( V_{s.c.}(z) \) given by equations (6) and (9) becomes the ‘so–called’ Kohn–Sham equation.

In actual numerical calculation, one first needs to introduce impenetrable potential barriers at the positions sufficiently far from both sides of the SQW in such a way that the positions of the barriers do not affect the solutions of the problem. In our calculation, we assume these barriers of infinite height at \( x = \pm L_B \approx \pm 2.5L \) \[12\] where \(-L/2\) and \(L/2\) are the edges of the finite SQW [see figure 1]. We, then, write, within the central difference approximation \[21\], the second–order differential equation, equation (1) by a difference equation of unknown \( \psi(z_i) \) for each point \( z_i \), a point of the \( i \)th subdivision of the interval \([-L_B, L_B]\). Therefore, we replace the ordinary differential equation, equation (1) by a finite difference equation;
In equation (10), \( \Delta \) is the grid spacing, which is the length of each subinterval and \( n \) is the number of subintervals. The boundary conditions require \( \psi_o(z_o) = \psi_{n+1}(z_{n+1}) = 0 \), where \( z_n = z_o + n\Delta \). Writing equation (10) in a matrix form, we get an \( n \) by \( n \) tridiagonal matrix eigenvalue equation. This eigenvalue equation is solved by diagonalizing the matrix. In this work, we solve this problem self-consistently with an accuracy such that the difference in the Hartree potential energies of the \( i^{th} \) and \((i+1)^{th}\) iterations is less than \( 10^{-3}\)meV. The matrix-size dependence of the eigenvalues is given in figure 2, as an example. It shows the electron subband energies in the absence of the field within a single-particle scheme, that is, \( N_s = 0 \); the solution of equation (10) with \( V_i(z) = V_w(z) \). Rapid convergence is observed in the eigenenergies as we increase the size of the matrix in solving the equation (10). We choose, in the rest of this paper, 500 by 500 as a relevant size of the matrix in actual numerical calculations. In this case, the discrepancy in eigenenergies obtained by the shooting and finite difference methods is not greater than 0.1meV.

3. RESULTS AND DISCUSSION

The subband energies of an electron and a hole in GaAs/AlGaAs SQW are evaluated and the effects of carrier interaction and electric field are examined. The physical quantities used in obtaining numerical results are listed in table I. In this paper, we ignore the variation of the effective masses in the well and barrier regions of the SQW. And we consider the case that the bulk impurity density \( N_d = 10^{18}/\text{cm}^3 \) in the rest of the paper.

3.1. Self-Consistency Effects

The potential profiles of the modulation-doped SQW in the presence of an external d. c. electric field \( F = 30\text{kV/cm} \) are shown in figure 3 for three different surface carrier densities \( N_s \). In the figure, the vertical axis, especially the energy gap in the well is not drawn in
scale. In the well region, the bottom of the conduction band moves upwards as one include the Hartree potential \( V_H(z) \), i.e., the interaction of a given electron with other electrons in the quantum well and also with the ionized impurities doped in the barrier region. Hence, the electron subband energies are also expected to increase due to the Hartree correction. In the valence band, however, the holes are more confined by the Hartree potential than electrons in the conduction band. This effect could cause a reduction of the hole subband energies. On the other hand, in modulation–doped SQW structures, there occurs a band–bending effect due to the dipoles formed between the plus (ionized donors) and the minus (electrons) charges and this effect would modify the subband energies. The effects of doped ionized impurities on the electron and hole subbands are different because of the opposite sign of the electric charges of an electron and a hole.

Figure 4 shows electron subband energies \( E_{en} \) as a function of the carrier density \( N_s \) for four different values of the electric field strength \( F \). The ground \((n = 1)\) and first excited \((n = 2)\) subband bottom energies are displayed, respectively, in the figure 4(a) and (b). The insets indicate that the electron subband energies are measured upwards from the bottom of the conduction band of the well with \( F = 0 \) and \( N_s = 0 \), which is taken the same as the midpoint of the conduction band bottom of the well in the presence of the field within a single-particle scheme; with \( N_s = 0 \). The \( E_{en} \) decreases as one increases the magnitude of the electric field \( F \). The reduction of the subband energies under the electric field is in agreement with observations of quantum confined Stark effect [22].

The \( N_s \) dependence of the subband energies is different in magnitude for different subbands. The subband energy \( E_{e1} \) increases monotonically as \( N_s \) increases. [figure 4(a)] However, the first excited subband energy \( E_{e2} \) shows different behavior.[figure 4(b)] The \( E_{e2} \) increases initially as \( N_s \) increases. For a given value of \( F \), beyond a certain density \( N_s^{th} \), \( E_{e2} \) decreases until the subband \( n = 2 \) becomes quasi–bound to tunnel out the barrier located at the right–hand side. The ground subband energy \( E_{e1} \) increases more rapidly than that of the first excited subband \( E_{e2} \). This different behavior is related to the effect of band–bending on the barrier region. Figure 5 shows the probability density \( |\psi_e(z)|^2 \) of the ground\((n = 1)\)
and first excited \((n = 2)\) electron subbands for \(F = 30\text{kV/cm}\) and \(N_s = 0.9 \times 10^{12}/\text{cm}^2\) and \(1.7 \times 10^{12}/\text{cm}^2\). In the well region, as the surface carrier density \(N_s\) increases, the magnitudes of both \(|\psi_e(z)|^2\) for both \(n = 1\) and \(2\) decrease. On the other hand, the probability densities increase in the barrier region as the \(N_s\) increases. The reduction of the \(|\psi_e(z)|^2\) in the well region results from the fact that the Hartree potential tends to locate the electrons near the interfaces, raising the corresponding confinement energies. However, the effect of band bending reduces the effective width of the potential barrier [see figure 3] and causes penetration of wave functions into the barrier region. The wave function penetration is more pronounced for the first excited subband than the ground subband. For the first excited subband, most of the electrons remain near the edges of the well for \(F \leq 50\text{kV/cm}\) even in the absence of the Hartree potential. But, the electrons in the ground subband, if \(F\) is not extremely large, such as, \(F \leq 150\text{kV/cm}\), are well localized inside the quantum well by the confining potential \(V_t(z)\), in which the Hartree potential \(V_H(z)\) is excluded.

Figure 6 shows the energy separation \(E_{e2-e1}\) of the ground and first excited electron subbands as a function of \(N_s\) for \(F = 0, 30, 50,\) and \(70\) \text{kV/cm}. The separation of electron subband energies decreases as \(N_s\) increases because the effect of band bending is more pronounced in the first excited subband than in the ground subband. This result differs from the cases of Si inversion layers [23] or GaAs single heterostructures [24]. In the cases of Si inversion layers and GaAs heterostructures, subband energy separations are observed to increase with increasing surface carrier density. This difference is conjectured to be related with the different boundary conditions and the effective potentials \(V_t(z)\). For the case of Si inversion layers, the potential barrier at the interface of Si and SiO\(_2\) is well approximated to be infinitely high so that the wave functions vanish at the interface. For the case of single heterojunction interface, the barrier height is finite. The potential functions \(V_t(z)\) in both cases are of triangular shape and infinite number of subbands are expected to be bound. However, in the SQWs, two heterojunction boundaries exist and the shape of potential function is rectangular one with finite depth, hence, allowing only a few subbands to be bound.
The ground hole subband energies $E_{h1}$ and first excited hole subband energies $E_{h2}$ are shown, respectively, in figure 7(a) and (b) as a function of $N_s$ for various electric fields $F$. The hole subband energies are measured down from the midpoint of the valence band top of the well region with $N_s = 0$, as is indicated in the insets of figure 7(a) and (b). From the carrier-density dependence of the potential energy profile of the valence band [see figure 3], the confinement of the holes is expected to increase as $N_s$ increases. As one increases the carrier concentration of the SQW, the top of the valence band moves up so that the holes are more tightly bound. Hence, hole subband energies decrease with increasing surface carrier density. The electric–field dependences of $E_{h1}$ and $E_{h2}$ are opposite to each other. The first excited hole subband is less bound for higher electric fields[see figure 7(b)].

Figure 8 shows the probability densities $|\psi_h(z)|^2$ of the ground($n = 1$) and first excited($n = 2$) hole subbands in the presence of an electric field $F = 30$ kV/cm for two different surface carrier densities $N_s = 0.9 \times 10^{12}$/cm$^2$ and $1.7 \times 10^{12}$/cm$^2$. We observe that the wave functions are more confined near the center of the well for higher $N_s$ and this confinement is more pronounced for the case of the ground subband. The first excited hole subband energies increase as $F$ increases as is shown in figure 7(b). This peculiar behavior is caused by the fact that the first excited wave function is more confined to the center of the well as the electric field increases [25]. Figure 9 shows the energy separation of the ground and first excited hole subband energies $E_{h2−h1}$ as a function of $N_s$ for four different values of the electric field strength $F$. We observe that the hole subband energies separation increases as one increases either $N_s$ or $F$. This observation differs from the case of electron subbands [see figure 6] because of the different potential profiles[see figure 3]. In the zero–field case, the first excited hole subband energy ($\approx 33$ meV) is relatively small compare to the valence band offset ($\approx 160$ meV). Therefore, the effect of the Hartree potential on the first excited hole subband is much less than that on the corresponding electron subband.
3.2. Many–Body Effects

We include the effects of exchange and correlations in our calculation by employing a simple local exchange–correlation potential energy $V_{xc}(z)$ given by equation (9). Strictly speaking, the density–functional formulation is good only for the calculations of the ground state energy and electron density distribution [16–18]. However, it has been used, in a good approximation, for the subband structure calculation [23]. The potential energy profiles of the conduction and valence bands of a SQW are shown, respectively, in figure 11(a) and (b) in the presence of an external d. c. electric field with (solid line) and without (dotted line) the exchange–correlation potential. The exchange–correlation potential slightly reduces the Coulomb repulsive force and electrons are pushed further toward the interface [13]. However, in this work, we observe that $V_{xc}(z)$ lowers the conduction and valence band profiles of the SQW by negligibly small amount. The magnitude of the $V_{xc}(z)$ is so small, compared to other terms in $V_t$, that its effect on the total potential energy profiles is quite small. This result differs from the cases of Si inversion and accumulation layers [23,24].

The subband energy separations of $E_{e2-e1}$ and $E_{h2-h1}$ are shown, respectively, in figure 11 (a) and (b) as a function of the surface carrier density $N_s$ with (solid line) and without (dotted line) the exchange–correlation potential. The effect of the exchange–correlation potential is not significant and is only to increase subband energy separations slightly as is shown in the insets of figure 11(a) and (b). This increase comes from the fact the ground subband energy is lowered slightly more than that of the excited subbands, in agreement with the cases of Si layers [23]. The negligible effect of the exchange–correlation potential on the subband structure of the SQW system is conjectured to the relatively large (kinetic) confinement energy of the system, as compared with the cases of the single heterostructures [24] or Si space charge layers [23].
4. CONCLUSIONS

We investigated the electronic properties of symmetrically–doped GaAs/AlGaAs single quantum wells in the presence of an external d. c. electric field perpendicular to the system and examined the effects of the field and carrier interactions on the system.

We summarize the results as follows. First, we evaluated the subband energies and wave functions as a function of surface carrier density. A self–consistent calculation within a Hartree approximation shows that, as the surface carrier density increases, the ground electron subband energy increases monotonically, but the first excited subband energy starts to decrease beyond a certain density. However, the energy separation of the lowest two electron subbands is reduced as the surface carrier density increases. For the hole subbands, as the surface carrier density increases, individual subband energy decreases, but their energy separation increases. This different behavior in the carrier–density dependence of the electron and hole subbands results from the different confinement effects for two different charge carriers. Second, the exchange–correlation effect is examined within a local density–functional approximation. A small reduction of the subband energies and an slight enhancement of the subband energy separation is observed. However, the many–body effect is found not so significant. This result is different from the cases of the Si inversion layers or GaAs single heterostructures.

ACKNOWLEDGMENTS

This work was supported in part by the BSRI–94–234 program of the Ministry of Education, Korea and in part by 1994 program of Korea Research Foundation (project number 02-D-0141).
REFERENCES

[1] G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures* (Halsted Press, New York, 1988).

[2] R. R. Dingle, H. L. Stömer, A. C. Gossard, and W. Wiegmann 1978 Appl. Phys. Lett. 33 665.

[3] D. A. B. Miller, D. S. Chemla, T. C. Damen, A. C. Gossard, W. Wiegmann, T. H. Wood, and C. A. Burrus, 1984 Phys. Rev. Lett. 53 2173.

[4] D. A. B. Miller, D. S. Chemla, T. C. Damen, A. C. Gossard, W. Wiegmann, T. H. Wood, and C. A. Burrus 1985 Phys. Rev. B 32 1043.

[5] W. T. Tsang, C. Weisbuch, R. C. Miller, and R. Dingle 1979 Appl. Phys. Lett. 35 673.

[6] T. H. Wood, C. A. Burrus, D. A. B. Miller, D. S. Chemla, T. C. Damen, A. C. Gossard, and W. Weigmann 1984 Appl. Phys. Lett. 44 16.

[7] L. C. West and S. J. Eglash 1985 Appl. Phys. Lett. 46 1156.

[8] B. F. Levine, K. K. Choi, C. G. Bethea, J. Walker, and R. J. Malik 1987 Appl. Phys. Lett. 50 1092.

[9] B. F. Levine, C. G. Bethea, G. Hasnain, J. Walker, and R. J. Malik 1988 Appl. Phys. Lett. 53 296.

[10] U. K. Mishra, A. S. Brown, L. M. Jelloian, L. M. Hackett, and M. J. Delaney 1988 IEEE Electron Dev. Lett. EDL9 41.

[11] G. Bastard, E. E. Mendez, L. L. Chang, and L. Esaki 1983 Phys. Rev. B 28 3241 and the references therein.

[12] W. L. Bloss 1989 J. Appl. Phys. 65 4789.

[13] T. Ando and S. Mori 1979 J. Phys. Soc. Jpn. 47 1518.
[14] D. S. Bendaniel and C. B. Duke 1966 Phys. Rev. 152 683.

[15] R. Dingle, W. Weigmann and C. H. Henry 1974 Phys. Rev. Lett. 33 827.

[16] P. Hohenberg and W. Kohn 1964 Phys. Rev. 136 B864.

[17] W. Kohn and L. J. Sham 1965 Phys. Rev. 140 A1133.

[18] L. J. Sham and W. Kohn 1966 Phys. Rev. 145 561.

[19] A. A. Katsnelson, V. S. Stepanyuk, A. I. Saasz, and O. V. Farberovich, Computational Methods in Condensed Matter : Electronic Structure (translated by Kevin Hendzel, Am. Inst. of Phys., New York, 1992).

[20] O. Gunnarson and B. I. Lundquist 1976 Phys. Rev. B 13 4274.

[21] C. F. Gerald and P. O. Wheatley, Applied Numerical Analysis, 4th edition (Addison–Wesley Publ. Co., New York, 1989).

[22] L. Vina, E. E. Mendez, W. I. Wang, L. L. Chang, and L. Esaki 1987 J. Phys. C : Solid State Phys. 20 2803.

[23] For example, T. Ando 1976 Phys. Rev. B 13 3468; K. S. Yi and J. J. Quinn 1983 Phys. Rev. B 27 2396; K. S. Yi 1993 New Physics 33 641.

[24] F. Stern and S. D. Sarma 1984 Phys. Rev. B 30 840.

[25] M. Matsuura and T. Kamizato 1986 Phys. Rev. B 33 8385.
Figure Captions

Figure 1. Schematic diagram of an idealized quantum well structure of width $L$ and barrier height $V_o$ in the presence of an external d. c. electric field $F$. The wave functions are to vanish at $-L_B$ and $+L_B$ for the convenience of a calculation. The width of symmetrically doped region is indicated by $d_b$ in the barrier regions.

Figure 2. The variation of the electron subband energies as a function of the size of matrix. The results are the case of undoped SQW in the absence of the electric field. The width of the well is 85Å.

Figure 3. The potential energy profiles of modulation–doped SQW in the presence of an electric field $F = 30kV/cm$ for different surface carrier densities $N_s$. The width of the well is 85Å. The vertical axis, especially, the energy gap in the well region is not drawn in scale.

Figure 4. The electron subband energies as a function of the surface carrier density $N_s$ for various electric fields $F$. The inset indicates that the energy is measured up from the midpoint of the conduction band bottom in a single–particle scheme in the presence of the fields. (a). the ground electron subband. (b). the first excited electron subband.

Figure 5. The probability density of the ground and first excited electron subbands under an electric field $F = 30kV/cm$ for two different surface carrier concentrations $N_s$. The width of the well is 85Å.

Figure 6. The energy separation of the ground and first excited electron subbands as a function of the surface carrier density $N_s$ for four different values of electric field strength.
Figure 7. The hole subband energies as a function of the surface carrier density $N_s$ for various electric fields $F$. The inset indicates that the hole subband energies are measured down from the midpoint of the valence band top in the well region in a single–particle scheme in the presence of the fields. (a). the ground hole subband. (b). the first excited hole subband.

Figure 8. The probability density of the ground and first excited hole subbands under an electric field $F = 30kV/cm$ for two different surface carrier concentrations $N_s$. The width of the well is 85Å.

Figure 9. The energy separation of the ground and first excited hole subbands as a function of the surface carrier density $N_s$ for four different values of electric field strength $F$.

Figure 10. The potential energy profiles with (solid line) and without (dotted line) the exchange–correlation potential in the presence of an electric field $F = 30kV/cm$ for a constant surface carrier density $N_s = 1.7 \times 10^{12}/cm^2$. The width of the well is 85Å. (a). the bottom of the conduction band. (b). the top of the valence band.

Figure 11. The energy separation of the lowest two subbands with (solid line) and without (dotted line) the exchange–correlation potential as a function of the surface carrier density $N_s$ for an electric field $F = 30kV/cm$. The solid and dotted lines are superposed nearly on top of each other. (a). the electron subband energy separation. (b). the hole subband energy separation.
TABLE I. Physical quantities used in numerical calculation

\((m_o : \text{free electron mass})\)

| Quantum Well Material | GaAs/AlGaAs SQW |
|-----------------------|-----------------|
| Well width            | 85Å             |
| Electron effective mass | 0.067\(m_o\)   |
| Hole effective mass   | 0.45\(m_o\)    |
| Conduction band offset | 240meV         |
| Valence band offset   | 160meV          |
| Background dielectric constant | 13.1          |
| Doped impurity density, \(N_d\) | \(1.0 \times 10^{18}/\text{cm}^3\) |