The electronic structure of a quantum well under an applied electric field

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The effects of an applied electric field on quantum well subband energies are calculated variationally within the effective mass approximation for model potential profiles. The concept of a quasi-bound state is examined critically. For higher electric field values it is shown that the quasi-bound state approximation for the ground and first excited state of the electron, and for the ground state of the hole is valid.

1. Introduction

Technological exploitation of the quantum-well type of semiconductor structure requires the application of electric fields. The effects of an external electric field applied to such structures have been extensively studied [1–13]. Mendez and coworkers [1] have demonstrated that the electric field decreases and eventually quenches the luminescence of GaAs/n-AlGaAs quantum wells.

Theoretical attempts to study such systems began with the variational approach of Bastard [1]. Sing employed the Monte-Carlo approach [14], Austin and Jaros used the phase-shift analysis [15], Harwit and Harris [16], Miller et al. [17] and McIlroy [18] used the transmission resonance approach. All these different approaches to the same problem have their weaknesses and strengths. We are not going to reanalyze the situation, as it is amply discussed in the literature [17]. Recently a novel light emitting device has been proposed and demonstrated experimentally [19]. The device consists of a GaAs quantum well placed on the n-side of the depletion region of a Ga_{1-x}Al_{x} p-n junction, and the operation of the devices is based upon the accumulation in the quantum well, of excess hot electrons injected from the n region of the barrier via tunneling and thermionic emission. The potential profiles of this device and of our model under external electric field have similarities. In such a device the quasi-bound criterion is an important physical feature.

In this work, we use a simple approximation to the potential profile of a quantum well under an electric field. This enables one to study relatively easily the nature of the bound states. At higher electric field values the eigenstates may become completely delocalized and unbound, since the potential energy is arbitrarily large and negative at large and negative distances. Despite the lack of true bound states at moderate electric field values, in the continuous spectrum the carrier wave function gives maximum amplitude in the quantum well at some particular energies [1,20]. As is well-known from some experiments, over a significant field range ($F \leq 10^5$ V cm$^{-1}$) the quantum well
structures support states that behave as if they were truly bound which are called quasi-bound states. Our approach is especially suited to study this quasi-bound nature of the eigenstates.

The theoretical model used is described in Section 2 and the results and conclusion are presented in Section 3.

2. The theoretical approach

We consider a GaAs quantum well sandwiched between two semi-infinite Ga$_{1-x}$Al$_x$As slabs. The potential profile of such a configuration under an electric field of strength applied along the growth axis-z is shown in Fig. 1A. The origin of coordinates is chosen at the center of the well. To solve this problem we approximated this potential $V_a$ as,

$$V_a(z) = \begin{cases} V_0 - qFz & \text{I } (-L_B < z < -L/2) \\ -qFz & \text{II } (|z| < L/2) \\ V_0 - qFz & \text{III } (L/2 < z < L_B) \\ \infty & \text{IV } |z| > L_B/2 \end{cases}$$

and

$$V_c(z) = \begin{cases} V_0 + qFL_B & \text{I } (z < -L_B) \\ V_0 - qFz & \text{II } (-L_B < z < -L/2) \\ -qFz & \text{III } (|z| < L/2) \\ V_0 - qFz & \text{IV } (L/2 < z < L_B) \\ V_0 - qFL_B & \text{V } (z > L_B) \end{cases}$$

which are shown in Fig. 1B and C, respectively.

The Hamiltonians of a particle with charge $q$ and the effective mass $m^*$ in potentials $V_b$ and $V_c$ in terms of the normalized parameters are,

$$H_b = \begin{cases} -\frac{1}{\hbar^2} \frac{\partial^2}{\partial \tilde{z}^2} + [-\tilde{q}\tilde{F}\tilde{z} + \tilde{V}_0] & \text{I } (-\tilde{L}_B < \tilde{z} < -\tilde{L}/2) \\ -\frac{1}{\hbar^2} \frac{\partial^2}{\partial \tilde{z}^2} - [\tilde{q}\tilde{F}\tilde{z}] & \text{II } (|\tilde{z}| < \tilde{L}/2) \\ -\frac{1}{\hbar^2} \frac{\partial^2}{\partial \tilde{z}^2} + [-\tilde{q}\tilde{F}\tilde{z} + \tilde{V}_0] & \text{III } (\tilde{L}/2 < \tilde{z} < \tilde{L}_B) \end{cases}$$

$$H_c = \begin{cases} -\frac{1}{\hbar^2} \frac{\partial^2}{\partial \tilde{z}^2} + (\tilde{V}_0 + \tilde{q}\tilde{F}\tilde{L}_B) & \text{I } (\tilde{z} < -\tilde{L}_B) \\ -\frac{1}{\hbar^2} \frac{\partial^2}{\partial \tilde{z}^2} + (\tilde{V}_0 - \tilde{q}\tilde{F}\tilde{z}) & \text{II } (-\tilde{L}_B < \tilde{z} < -\tilde{L}/2) \\ -\frac{1}{\hbar^2} \frac{\partial^2}{\partial \tilde{z}^2} - (\tilde{q}\tilde{F}\tilde{z}) & \text{III } (|\tilde{z}| < \tilde{L}/2) \\ -\frac{1}{\hbar^2} \frac{\partial^2}{\partial \tilde{z}^2} + (\tilde{V}_0 - \tilde{q}\tilde{F}\tilde{z}) & \text{IV } (\tilde{L}/2 < \tilde{z} < \tilde{L}_B) \\ -\frac{1}{\hbar^2} \frac{\partial^2}{\partial \tilde{z}^2} + (\tilde{V}_0 - \tilde{q}\tilde{F}\tilde{L}_B) & \text{V } (\tilde{z} > \tilde{L}_B) \end{cases}$$
Fig. 1. A. Effective potential for electrons or holes in the GaAs Ga$_{1-x}$Al$_x$As QW under the electric field which is applied along the z-axes. B and C the approximated model potential profiles for the potential in case A.

respectively, where the normalized parameters are defined as,

\[
\tilde{E} = \frac{E}{E_0}, \quad \tilde{F} = \frac{qFL}{E_0}, \quad \tilde{Z} = \frac{Z}{L}, \quad E_0 = \frac{\pi^2 \hbar^2}{2m^* L^2}
\]

is the ground state energy of a infinite quantum well with a width \(L\) and the parameter \(\tilde{q}\) with the values \(+1(-1)\) represents electrons (holes). By using the transformations

\[
\tilde{Z}_1 = -\left[\frac{\pi}{\tilde{F}}\right]^{2/3} [(\tilde{E} - \tilde{V}_0) + \tilde{q} \tilde{F} \tilde{Z}]
\]

\[
\tilde{Z}_2 = -\left[\frac{\pi}{\tilde{F}}\right]^{2/3} [\tilde{E} + \tilde{q} \tilde{F} \tilde{Z}]
\]

one can obtain the Schrödinger equation for the Hamiltonian \(H_h\)

\[
H_h \psi(z) = \tilde{E} \psi(z)
\]
The solutions of the eqn (7) in different regions are given by

\[
\begin{align*}
\psi_1(\tilde{Z}_1) &= C_1 A i(\tilde{Z}_1) + C_2 B\tilde{i}(\tilde{Z}_1), \\
\psi_2(\tilde{Z}_2) &= C_3 A i(\tilde{Z}_2) + C_4 B\tilde{i}(\tilde{Z}_2), \\
\psi_3(\tilde{Z}_1) &= C_5 A i(\tilde{Z}_1) + C_6 B\tilde{i}(\tilde{Z}_1).
\end{align*}
\] (8)

The coefficients \(C_1, C_2, C_3, C_4, C_5, C_6,\) and eigenvalues to be determined from the normalization condition, the boundary conditions \(\psi_1(\tilde{Z}_1(\tilde{z} = -\tilde{L}_B)) = \psi_3(\tilde{Z}_1(\tilde{z} = \tilde{L}_B)) = 0\) and the continuity of the wave function \(\psi(\tilde{z})\) at \(\tilde{z} = \pm 1/2\). The eigenvalues \(\tilde{E}_i\) and the eigenvectors \(\psi_1(\tilde{Z})\) are to be determined from the master equation as follows:

\[
U(\tilde{E}_i) = \begin{bmatrix}
Ai(\tilde{Z}_1(-\tilde{L}_B)) & Ai(\tilde{Z}_1(-\tilde{L}_B)) & 0 & 0 & 0 & 0 \\
Ai(\tilde{Z}_1^+) & Bi(\tilde{Z}_1^+) & Ai(\tilde{Z}_2^+) & Bi(\tilde{Z}_2^+) & 0 & 0 \\
Ai(\tilde{Z}_1^-) & Bi(\tilde{Z}_1^-) & Ai(\tilde{Z}_2^-) & Bi(\tilde{Z}_2^-) & 0 & 0 \\
0 & 0 & Ai(\tilde{Z}_2^+) & Bi(\tilde{Z}_2^+) & Ai(\tilde{Z}_1^+) & Bi(\tilde{Z}_1^+) \\
0 & 0 & 0 & Ai(\tilde{Z}_2^+) & Bi(\tilde{Z}_2^+) & Ai(\tilde{Z}_1^+) & Bi(\tilde{Z}_1^+) \\
0 & 0 & 0 & 0 & Ai(\tilde{Z}_1(\tilde{L}_B)) & Ai(\tilde{Z}_1(\tilde{L}_B)) & 0 & 0 \\
\end{bmatrix} = 0 \] (9)

where

\[
\tilde{Z}_1^+ = -\left[\frac{\pi}{\tilde{F}}\right]^{2/3} \left[\tilde{E} - \tilde{V}_0 \mp \tilde{q}\tilde{F}\frac{1}{2}\right],
\]

\[
\tilde{Z}_2^+ = -\left[\frac{\pi}{\tilde{F}}\right]^{2/3} \left[\tilde{E} - \tilde{V}_0 \mp \tilde{q}\tilde{F}\tilde{L}_B\right] \] (10)

In a similar way the solutions of the Schrödinger equation for the Hamiltonian \(H_c\)

\[
H_c\psi(\tilde{z}) = \tilde{E}\psi(\tilde{z}) \] (11)

in different regions are given by,

\[
\begin{align*}
\psi_1(\tilde{z}) &= A \exp[K_1\tilde{z}], \\
\psi_2(\tilde{z}_1) &= B \ Ai(\tilde{z}_1) + C \ Bi(\tilde{z}_1), \\
\psi_3(\tilde{z}_2) &= D \ Ai(\tilde{z}_2) + E \ Bi(\tilde{z}_2), \\
\psi_4(\tilde{z}_1) &= F \ Ai(\tilde{z}_1) + G \ Bi(\tilde{z}_1), \\
\psi_6(\tilde{z}) &= H \ exp[-K_2\tilde{z}],
\end{align*}
\] (12)
Fig. 2. The variations of normalized eigenvalues for (A) the ground and (B) first excited states as functions of $\tilde{L}_B$ for a constant electric field.

Fig. 3. Electric field dependence of the normalized ground and first excited state energies of the electron.

where we have

$$\tilde{\lambda}_1 = -\left[\frac{\pi}{\tilde{F}}\right]^{2/3} \left[(\tilde{E} - \tilde{V}_0) + \tilde{q}\tilde{F}_z\right],$$

$$\tilde{\lambda}_2 = -\left[\frac{\pi}{\tilde{F}}\right]^{2/3} \left[\tilde{E} + \tilde{q}\tilde{F}_z\right],$$

(13)
Normalized energy ($E = E_0$) \sim V_0 = 4.41

Normalized field ($F = qFL / E_0$) \sim 

Fig. 5. Electric field dependence of the normalized ground state energy of the hole.

Fig. 4. The normalized electron probability density $|\psi(z)|^2$ versus the normalized distance $Z/L$. The normalized electric field is taken to be (A) $\tilde{F} = 0$, (B) $\tilde{F} = 2$, (C) $\tilde{F} = 6$, and (D) $\tilde{F} = 8$. 

\tilde{V}_0 = 4.41
Fig. 6. The normalized hole probability density $|\psi_1(z)|^2$ versus the normalized distance $Z/L$. The normalized electric field is taken to be (A) $\tilde{F}=0$, (B) $\tilde{F}=2$, (C) $\tilde{F}=4$, and (D) $\tilde{F}=6$, (E) $\tilde{F}=8$, and (F) $\tilde{F}=10$.

$$K_1 = \pi \tilde{V_0} + \tilde{q} \tilde{F} \tilde{L}_B - \tilde{E}_i,$$

$$K_2 = \pi \tilde{V_0} - \tilde{q} \tilde{F} \tilde{L}_B - \tilde{E}_i.$$  

$A$, $B$, $C$, $D$, $F$, $G$, and $H$ are constants to be determined from the normalization condition and the continuity of the wave function $\psi(\tilde{z})$ at $\tilde{z} = \pm \tilde{L}_B$ and $\tilde{z} = \pm 1/2$. The eigenvalues $\tilde{E}_i$ and eigenvectors $\psi_i(\tilde{z})$ are to be determined from the master equation as follows:

$$U(\tilde{E}_i) = \begin{vmatrix} 1 & W_{12} & W_{13} & 0 & 0 & 0 & 0 & 0 \\ K_1 & W_{22} & W_{23} & 0 & 0 & 0 & 0 & 0 \\ 0 & W_{32} & W_{33} & W_{34} & W_{35} & 0 & 0 & 0 \\ 0 & W_{42} & W_{43} & W_{44} & W_{35} & 0 & 0 & 0 \\ 0 & 0 & 0 & W_{54} & W_{55} & W_{56} & W_{57} & 0 \\ 0 & 0 & 0 & W_{64} & W_{65} & W_{66} & W_{67} & 0 \\ 0 & 0 & 0 & 0 & W_{76} & W_{77} & 1 \\ 0 & 0 & 0 & 0 & W_{86} & W_{87} & -K_5 \\ \end{vmatrix} = 0$$
where

\[
\begin{align*}
W_{12} &= Ai(\tilde{\chi}_1(\tilde{z} = -\tilde{L}_B)) , & W_{13} &= Bi(\tilde{\chi}_1(\tilde{z} = -\tilde{L}_B)), \\
W_{32} &= Ai(\tilde{\chi}_1(\tilde{z} = -1/2)) , & W_{33} &= Bi(\tilde{\chi}_1(\tilde{z} = -1/2)), \\
W_{34} &= Ai(\tilde{\chi}_2(\tilde{z} = -1/2)) , & W_{35} &= Bi(\tilde{\chi}_2(\tilde{z} = -1/2)), \\
W_{54} &= Ai(\tilde{\chi}_2(\tilde{z} = 1/2)) , & W_{55} &= Bi(\tilde{\chi}_2(\tilde{z} = 1/2)), \\
W_{56} &= Ai(\tilde{\chi}_1(\tilde{z} = 1/2)) , & W_{57} &= Bi(\tilde{\chi}_1(\tilde{z} = 1/2)), \\
W_{76} &= Ai(\tilde{\chi}_1(\tilde{z} = \tilde{L}_B)) , & W_{77} &= Bi(\tilde{\chi}_1(\tilde{z} = \tilde{L}_B)), \\
W_{22} &= W_{12}, & W_{23} &= W_{13}, \\
W_{64} &= W_{54}, & W_{65} &= W_{55}
\end{align*}
\]

In calculating the quasi-bound state energies we have ensured that the eigenvalues are independent of the choice of \(L_B\) and that the wave functions are localized in the well region.
3. Results and conclusion

Using the method described in Section 2, we calculated numerically the eigenvalues and eigenfunctions satisfying the quasi-bound criteria. The eigenvalues for the ground and first excited states as functions of $\tilde{L}_B$ are shown in Fig. 2. This figure clearly shows the asymptotic energy values for large enough $L_B$ which corresponds to localization, indicating the quasi-bound nature of the states. The values of the material parameters we used in the calculation are taken to be $L = 120 \text{Å}$, $\tilde{L}_B = 5L$, $m_e^* = 0.067 m_0$, $m_h^* = 0.45 m_0$, and $V_0 = 228 (176) \text{meV}$ for conduction (valence) band discontinuities respectively, where $m_0$ is the electron rest mass. These parameters are appropriate for electrons and heavy holes in GaAs/Ga$_{1-x}$Al$_x$As quantum wells. The variation of the ground and the first excited state energies as a function of applied electric field along the $z$-direction is given in Fig. 3. At the highest electric field value of $\tilde{F} \approx 10 (300 \text{kV cm}^{-1})$ the decrease in the ground state energy is approximately 35 meV. For the potential profile $V$, the normalized electron probability density $|\psi(z)|^2$ for different field values is given in Fig. 4. Here, the position of the QW is shown by vertical lines. The motion of the electron towards the left and the increase of the penetration of the wave function into the classically forbidden region under increasing $\tilde{F}$ field is clearly visible.

The hole ground subband energies as a function of $\tilde{F}$ are shown in Fig. 5. The largest shift in hole energy at the largest applied field is around 60 meV. The variation of the corresponding hole wave functions are shown in Fig. 6. From this variation one can observe a larger change for heavier holes.

At this point, we note that theoretical work done by Austin and Jaros [15] suggests a turn-around behavior at the critical field $F = 40.5 \text{kV cm}^{-1} (7.7 \text{kV cm}^{-1})$ for electrons (holes), respect-
ively. Whereas, our calculations show that no turnaround behavior is observed for even higher electric field values. Furthermore, our results show that holes are localized up to an electric field value of $\tilde{F} = 6$ (190 kV cm$^{-1}$), despite the conclusion of Sing whose work suggests that at an electric field value of 150–160 kV cm$^{-1}$ holes should be completely out of the quantum well via tunneling [14].

The first excited electron wave function under $\tilde{F}$ is shown in Fig. 7. For fields greater than $\tilde{F} = 3.5$ the quasi-bound state criteria is not satisfied for the excited state. This situation is also visible in the variation of corresponding wave function in Fig. 7. We have also calculated the dipole matrix element, which is the integral of the first and second wave function of the electron multiplied by $z$. As is well known that the dipole matrix element is an important quantity for infrared detectors. The variation of the dipole matrix element versus the normalized electric field is given in Fig. 8 which illustrates that after the critical field value $\tilde{F} = 3.5$, where the second state is not localized any more, the dipole matrix element decreases rapidly with increasing field. This behavior is indicated by an arrow in Fig. 8.

We have repeated the calculations summarized in previous sections for the potential profile $V_b$. The walls used in these models are placed to control the localization of the wave functions. For both of these potential ($V_b$ and $V_c$) profiles our calculations yield very similar results, proving the soundness of our conclusions summarized in this section.

References