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CONFINED TRANSMISSION RESONANCES IN MULTIPLE QUANTUM WELL SYSTEM

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ABSTRACT

An investigation of the confined transmission resonances in multiple quantum wells has been carried out using modified envelope function approximation including the $\Gamma 6$, $\Gamma 7$, and $\Gamma 8$ host bands. The theoretical results are compared with the results of experimental excitation spectroscopy. Both symmetric and anti-symmetric confined levels have been observed. While the first symmetric confined level exists for all values of the well-width, all others disappear for well-width less than 5.0nm.

INTRODUCTION

The possibilities of growing high Heterostructures with the help of such crystal growth techniques like molecular bean epitaxy (MBE) and matal organic chemical vapour deposition have offered important opportunity for both the development of novel devices and also for the advancement of fundamental solid state science. When the thickness of the layers of these structures is smaller than the de Broglie wavelength (i.e. $L_z \sim \lambda$) of the electronic particles (i.e. electrons and holes) confined in the Heterostructures, the properties of the structure are dominated by quantum size effects (QSE) (*Adelabu 1996a).* The electronic states from the two-dimensional (2D) sub-bands of the structures with the corresponding rise in energy due to the confinement depend primarily on the layer thickness, the particle effective mass, and the depth of the potential wells (*Dingle et al 1974, Dingle 1975).* Thus, studies of the electronic and optical properties of these super structures can provide information on most of the fundamental characteristics of the semiconductor heterojuntions.

Most of these investigations have focused on properties associated with the direct band – gap (r). This paper reports on the results of investigation on the confined transmission resonances in MQW. A modified enveloped function approximation of Bastard (1982, 1984) including $\Gamma 6$, $\Gamma 7$, and $\Gamma 8$ host bands has been used. In addition to the theoretical work the results of excitation spectroscopy experiment on these structures are presented. One of the observed lines corresponds to an optical transition which involves a light hole state.

THEORETICAL CONSIDERATIONS AND CALCULATIONS.

Most of the theoretical investigations like those by Bastard (1981, 1982, 1984) and by White and Sham (1981) have been devoted to the calculation of the dispersion relations along the growth axis. Unfortunately the properties of the heterostructures wave function that are of major reference when evaluating the strength and shape of the absorption and recombination spectra have received little attention.

Assuming perfect lattice matching between the host materials, a superlattice crystal displays two periodicities: the natural periodicity (d_o) and the artificial periodicity (d). Usually, the situation of concern is the case of $\mathbf{d >> d_o}$. The Superlattice (SL) and multiple quantum well (MQW) electronic states have been calculated by such approximations as the tight binding approximation (TBA) by Schulman and Chang (1985) and the envelope Function Approximation (EFA) by Bastard (1981,1982, 1984) and also by Bastard et al (1984). Each of these approximations has its own merits and demerits. The TBA focuses the attention on atomic-like properties (i.e. at the d_o scale) and builds the SL and MQW states from host atomic site to host atomic sites. The calculations are exact in essence but to be accurate, they require more elaborate computational efforts. On the other hand, the envelope function approximation takes the natural periodicity d_o, into account by means of an effective – mass approximation with the superperiodicity, d, acting upon the envelope functions which are slowly varying at the scale of d_o. In the envelope function scheme, some microscopic information (i.e. at the scale of d_o) is lost. In particular, the details of the interfaces between consecutive layers and the exact chemical nature of actual layers, which are the chemical elements of the two terminating planes of a given layer are left undefined. In this coarse-grained description, which is reasonable only for sufficiently thick host layers with each layer being an effective medium of only some gaps and interband matrix elements are known. The electronic dynamic in the SL and MQW is described

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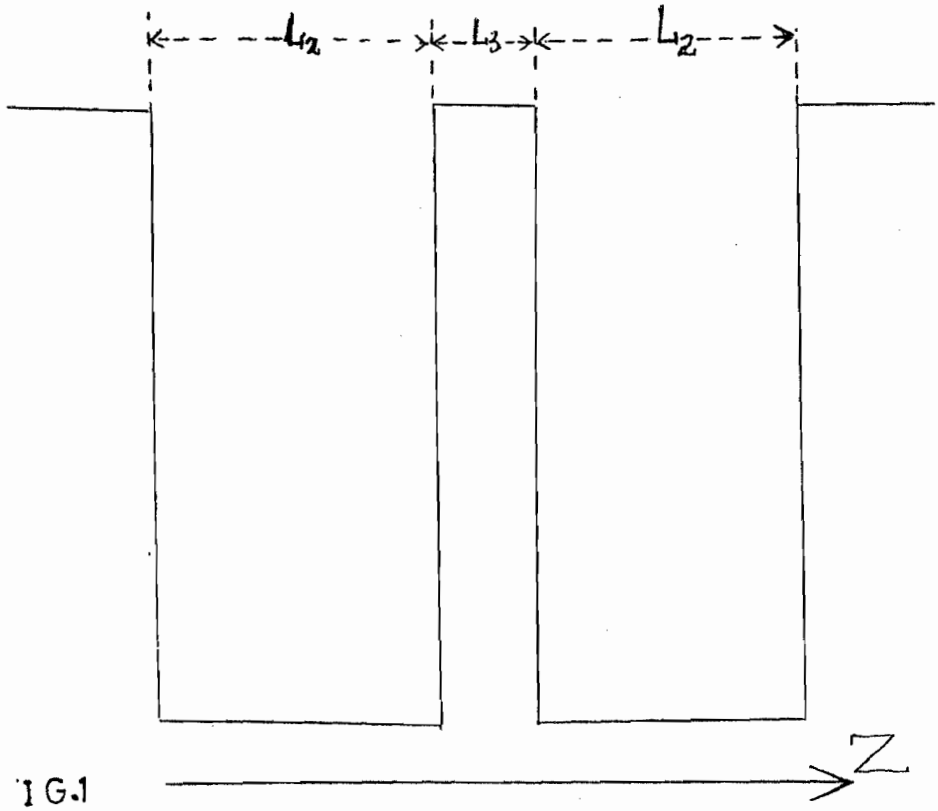


Fig. 1. Schematics of the assumed structure

(Bastard et al 1984) by the envelope functions which are eigenstates of an effective Hamiltonian. The only microscopic information which has survived in the envelope function scheme is embodied into a few parameters (in practice Γ gaps, Γ spin – orbit and Kane matrix element) which are known from experiments on bulk materials. The EFA (Bastard et al 1984) is in excellent agreement with experiment for both the type I and the type II SL and MQW systems *(Adelabu 1996a)* as long as the experiments have been performed on crystals with $d>>d_o$ for which the interface planes represent a relatively minor detail compare with the "bulk" of each host layers.

For the study here, a binary SL and MQW obtained by alternatively stacking layers of A material (thickness L_2), and layers of B materials (thickness L_3) (Fig. 1.) is considered. Here, the same layers (e.g. the A layers) are quantum wells for both the conduction and valence states. This situation is met within the so called type I structures such as the GaAs/AlGaAs and GaInAs/AlInAs systems. In this case the corresponding wave functions are mostly localized in the A layers.

In this work, the basic assumptions are that the A and B materials are direct-gap materials, typically III-V and II-VI compounds. Furthermore, it is assumed that only the usual Γ6, Γ7 and Γ8 host band edges significantly contribute to the SL and MQW wave function. The r point-periodic parts of the host Bloch functions are assumed identical in the A and B layers. Any inversion asymmetry effect associated with the Zincblende lattice is neglected. All the above assumptions are adequate since the object is to calculate SL and MQW states which are close enough from the host Γ-points.

In the considerations, just like Bastard et al (1984), a symmetric double well is assumed. Here there are two wells of material A, say (thickness L_A) clad by an infinitely extended barrier of material B and separated by a barrier of material B of thickness L_B. To exploit the symmetry of the structure, the mid-point of the central barrier is taken as the origin. Since the A and B layers are III-IV compounds previous analyses *(Bastard 1981, White and Sham 1981)* can be drawn upon which have shown *(Adelabu 1993)* how to include band discontinuities at the A-B interfaces in the Kane model *(Kane 1957)* for the Γ related bound SL and MQW states. The envelope-function scheme which takes into account band non-parabolicity, rests ultimately on a reasonable approximation that the Γ6, Γ7 and Γ8 period parts of the Bloch functions are the same in both materials A and B. The matrix element:

$$P=(1/m_o < s / p_x / x>$$

Is constant throughout the whole structure. In addition to p, the parameters of the model are the band gaps

($E_{g\,A}$ and $E_{g\,B}$), and the Γ spin – orbit energies (Δ_A and Δ_B) of the host materials.

For zero wave vector, K_l in the layer planes (where the onset of interband absorption occurs), the energy E of a carrier is related to the wave vector K_A and K_{Bl} in each layer by:

$$E(E+E_{gn})(E+E_{gn}+\Delta_A)= P^2\hbar^2k^2_A(E+E_{gA}+2\Delta_A/3) \qquad \ldots(1)$$

$$(E-V_s)(E-V_s+E_{gB})(A-V_s+E_{gB}+\Delta E_B)= P^2\hbar^2k_B^2(E-V_s+E_{gB}+2\Delta_B/3) \qquad \ldots(2)$$

where V_s is the shift in the Γ6 edge when going from material A and B. The bottom of the Γ6 band of material A is taken as the energy Zero.

By considering the appropriate boundary conditions (Bastard 1981, White and Sham 1981) at the A-

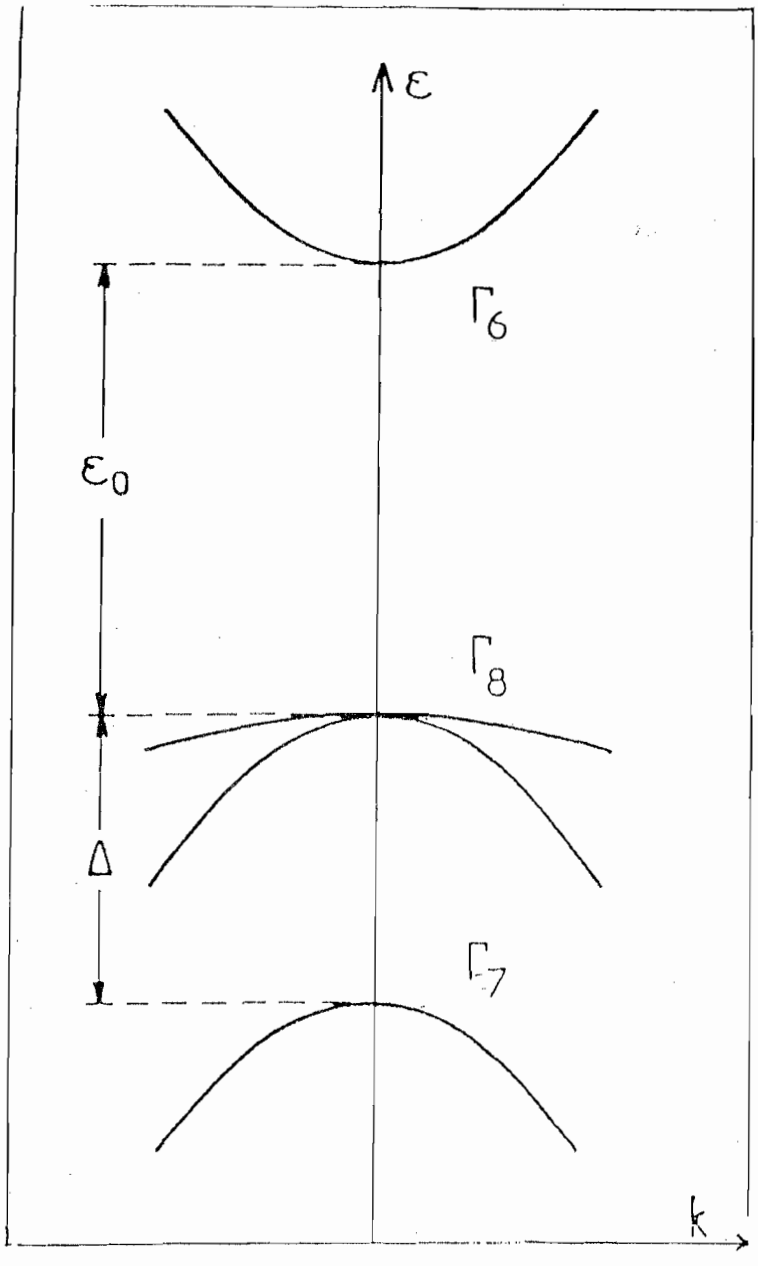


Fig. 2. Decoupling of the Γ8 heavy hole from the light hole at K = 0.

B interfaces the dispersion relation for the SL and MQW system is given by:

$$2Cosk_A l_z + \left(\frac{1}{\zeta} - \frac{1}{\zeta}\right) \sin Kal_z \pm \left(\frac{1}{\zeta} + \frac{1}{\zeta}\right) \sin K_A l_2 \, exp(-k_{B1} l_3) = 0 \qquad \ldots(3)$$

$$\zeta = K_{B1}/K_A(2/E\text{-}V_s+E_B + 1/E\text{-}V_s + E_B + \Delta_B)(2/E+E_A + 1/E+E_A+\Delta_A)^{-1} \qquad \ldots(4)$$

The minus sign refers to the symmetric (S_n) states with respect to Z=O while the plus sign refers to the anti symmetric (As_n) states.

$$T(E) = \{1+1/4(\square\text{-}1/\square)^2 \sin^2 k_A l_2[2Cosk_A l_2 Cosk_B l_3 - (\square\text{-}1/\square) sink_A l_3]\}^{-1}$$

Where K_B replaces K_{B1} of equation (3) and all other symbols are as have already been defined.

If L_3=0, and bound structure effects are not considered ($\zeta = k_A k_B$), the familiar expression for a single well with width $L_w = 2l_2$ is obtained.

Similarly,

$$K_A(E)l_2 = p\Pi, \text{ p is an integer} \qquad \ldots (5)$$

and

$$Cosk_A(E)l_z \, Cosk_B(E)l_3 - \frac{1}{2}(\zeta_{(E)}) + \frac{1}{\zeta}(E)\text{Sin } k_A(E)l_z \text{ Sin } k_B(E) L_3 = 0 \qquad \ldots(6)$$

The above situations refer to the electrons and light holes. As for the ⌈8 heavy holes, they are totally decoupled (Bastard 1981, White and Sham 1981) from the light particle state since K_i=0 (Fig. 2). In the energy range of interest, the heavy hole bands are parabolic with masses m_A and m_B in the respective host layers. The same analysis that led to equations (3) to (6) are repeated for the heavy hole as was done by Bastard et al (1984). The same equations are obtained except that:

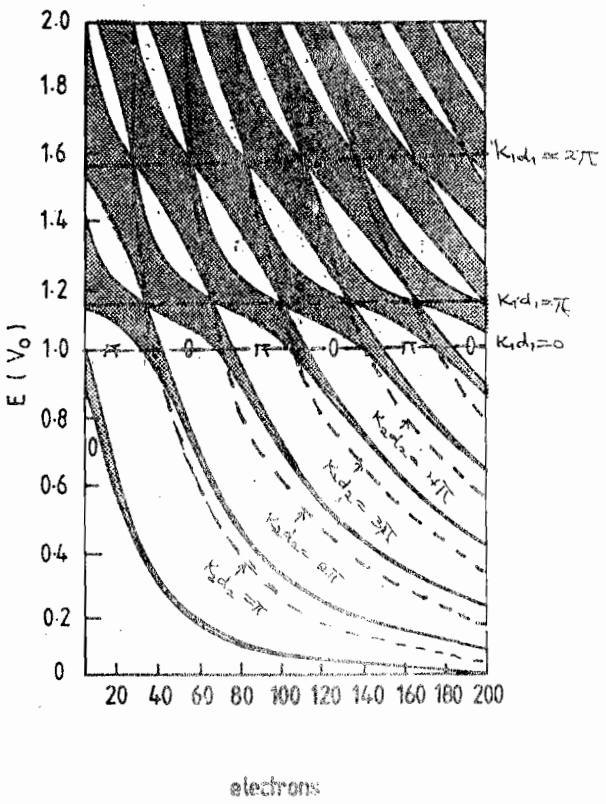
$$\square = (k_A m_B) / (m_A k_B) \qquad \ldots(7a)$$

and

$$E = -E_A - (\hbar^2 k^2_A)/2m_A = Vs - E_B - (\hbar^2 k^2_B)/2m_B \qquad \ldots(7b)$$

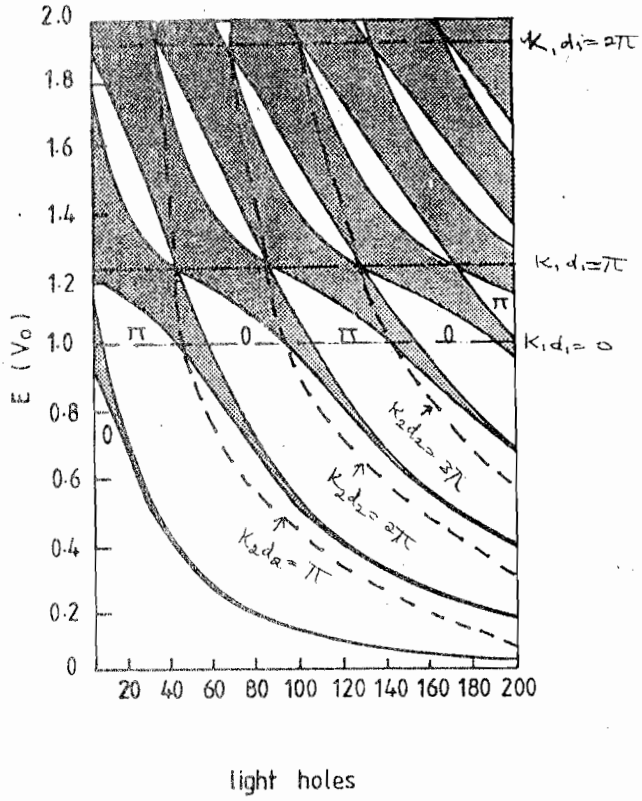
RESULTS AND DISCUSSION

Figs. (3) and (4) present typical results. For the bound states, K_{Bl} in eqn(2) is imaginary. This corresponds to an evanescent state in the barrier. For this, one simply lets $K_B = iK_{Bl}$ in the equation to obtain the appropriate dispersion relations. Since the system has minor symmetry with respect to Z=0, the bound state envelope functions are even or odd in Z. They decay like $exp(-K_{B1}/z)$ at large Izl. The symmetric (S_n) (solid line) and the antisymetric (As_n) broken line levels, (where n=1,2,3,... are integers) are degenerate for an infinitely-thick barrier. The first symmetric confined level S_1 exists for all values of the well – width L_z while all others disappear for well width less than 5nm. The first antisymmetric level, AS_1 will be bound, for all barrier – width L_3, if the single well of width $2L_2$ admits two bound levels. This according to equations (1) to (3) is the case for electrons but not for light holes in the system with L_2 = 4.5nm. The dissymmetry is due to the relative magnitude of the valence and conduction barriers, the former being much smaller than the latter in this system.



electrons

Fig. 3. Results for the levels in the electrons



light holes

Fig. 4 Results for the levels in the holes.

The continuum levels are each twice degenerate, corresponding to a wave traveling either towards increasing Z or towards decreasing Z. Suppose a wave coming from Z= ∞ is impinging on the double well structure. At X = -L_2, L_3 / 2, it is partly transmitted and partly reflected. Inside the structure, similar reflection – transmission phenomena occur at each interface. Finally, a part of incident wave is transmitted by the entire double well structure.

A characteristic feature of eqn (4) present also in the single quantum well case is that T(E) goes to zero at the onset of the continuum in the general case, which means that the carrier actually avoids the quantum well under this condition. This repulsion disappears deep in the continuum. However, T(E) may actually equal unity for some discrete energies. These energies are solutions of eqn (4).

The solutions of eqns. (5) and (6) are scattering resonances. Equivalently they may be viewed as virtual bound states (Adelabu 1996b) characterized by an accumulation of electron wave function inside double well structure. Eqn. (5) is the same as that for single wells of width l_2. Were the basis l_2 and l_3 infinitely repeated, eqn. (6) would be the equation of a SL and MQW state with wave Vector $\pi/2\,(l_2 + l_3)$ (Bastard 1981). The double well structure exhibits resonances which are either characteristic of single wells or are the precursors of SL and MQW bands. When $E \sqsupset V_s$ $(or\ V_s - E_B\ or\ V_s - E_B\ \Delta_B)$ and the conditions in eqns. (5) and (6) are fulfilled, the virtual bound levels match the true bound level determined by eqn. (3). The delocalized resonance, of eqn (6) converges towards the anti-symmetric bound states As_n at $E = V_s$ $(V_s - E_B\ or\ V_s - E_B - \Delta_B)$ whereas the isolated resonances of eqn (5) converge towards the symmetric states S_n in the same limit. When a resonant level approaches $V_s or (V_s - E_B\ or V_s - E_B - \Delta_B)$ the transmission ceases to be low and for energies within the resonance width the probability of being in the well is significantly increased over the value found at the same energy in the non-resonant situation.

The extended states, i.e. those states with energy E larger than V_b, the height of the confining barrier, have been marginally neglected. However, it is of interest to understand how a bound state evolves when its confinement energy exceeds V_b. Moreover, low-lying barrier states ($E \geq V_b$) may play a significant role in carrier capture by a quantum well. This has been made possible by the high quality of the present day quantum well structures (i.e. the existence of sharp interfaces) which leads to pronounced oscillatory pattern of the electron transmission coefficients across the quantum wells. Under the condition of constructive interference, the electron is captured by the quantum well for a reasonably long time. During this capture time the carrier can easily relax towards the true bound states where radiative recombination

becomes efficient. This resonant capture can alternatively be viewed as virtual bound states. When the parameters of the structure (V_b and the well-width thickness L_w) are varied, the bound levels evolve continuously towards virtual bound states (Bastard et al 1984).

CONCLUSION

Bound and virtual bound states in SL and MQW using the double coupled quantum well structures arrangements have been considered. Based on the results of the calculations, it is concluded that, under certain circumstances virtual bound states do not participate in optical transmission within the type I SL and MQW structures.

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