

QUANTIZATION IN TYPE I MULTIPLE QUANTUM WELL (MQW) AND SUPERLATTICE (SL) SYSTEMS.

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ABSTRACT

The paper presents briefly the developmental path in the research of semiconductor Multiple Quantum Well (MQW) and Superlattices (SL) systems which are generally called Low Dimensional structures (LDs) or Heterostructures in the past few decades. The presentation includes a general introduction which briefly touches on some characteristics of the systems, materials for the systems and the physics of the systems. Emphasis is then placed on the studies carried out on the band structure calculations in the systems within the limit of the parabolic band approximations.

Key words : Band, structure, Quantum, well, superlattices.

INTRODUCTION

An excellent prospect for new discoveries in physics lies in the establishment of a new programme of research in the area of Low Dimensional structures, LDs (Adelabu 1996a). The research on these structures was initiated with a proposal by Esaki and Tsu (1970). These structures are formed by the precise deposition of flat, well defined layers (typically only a few angstroms thick) of crystalline semiconductors and by the formation of narrow channels using lithographic techniques (Cho 1971, Cheng et al 1981, Gossard et al 1976).

In the LDs, nearly all physical properties are changed from those of bulk solids. Entirely new phenomena appear (Tsu and Esaki 1973; Chang et al 1974; Sollner et al 1983, 1984, 1985; Shewchuk et al 1985; Tsu et al 1975; Van der Ziel et al 1975; Chemla et al 1983; Miller (a) et al 1984a; Esaki and Chang 1974; Miller (b) et al 1980). The research programmes are leading to more important developments in condensed matter physics and technology. From the experience so far, it has been revealed that the variety of possible LDs far outplays their conventional bulk counterparts. The present understanding of physics of LDs is already pointing the way to new electronic devices (Dupius et al 1978, Mimura et al 1980, Tsang 1981, Wood et al 1983). Thus, our semiconductor industries will be able to draw on the results of fundamental researches in order to help develop devices which for example, are expected to form the basis of the next generation of computers and many more new

devices.

Among the peculiar features of the LDs is that they can be designed to emphasize and isolate the property of interest so allowing direct observations and measurements. Also, the study of LDs is of an interdisciplinary nature. Physicists, chemists, material scientists and device engineers all have essential roles to play. Chemists will lead research into improving sample growth techniques, material scientists will contribute much to the understanding of the properties of LDs using sophisticated characterization and microscopic techniques while close cooperation between physicists and device engineers will lead to the use of the novel results from the physics of LDs, for new device concepts. In the LDs, electronic transport (Esaki et al 1972; Chang et al 1974; Esaki and Chang 1974; Sollner 1983; Coon et al 1985; Luryi and Capasso 1985; Capasso et al 1986; Davis et al 1985) optical absorption and emission (Dingle et al 1974, 1975; Miller (b) et al 1980; Petroff et al 1981; Vočej et al 1980; Weisbuch et al, 1981), phonon interactions and structure stability (Colvard et al 1980; 1985; Narayanamurti et al 1979; Jusser and et al 1984, 1986; Sood et al 1985a, b, c) all take on new astonishing forms. The best known examples are the Quantum Hall and Fractional Quantum Hall effect (Laughlin 1983; Kawaji et al 1984; Mendez et al 1984a,b; Stormer et al 1986). These and other electronic properties are related to the very fundamental problems of disordered and interacting many body systems and thus offer a unique opportunity to investigate those problems. Ballistic behaviour of

electrons and phonons, cooperative phenomena, electronic transition processes and dielectric properties are all different from their bulk equivalent in ways which challenge experimental studies and theoretical analysis. The new physics arises because elementary concepts, some of which date back to the work of Boltzman, cannot be used in LDs where the sample size in at least one dimension is on the atomic scale. Typical direct consequences of this change are that electron mobilities at low temperature can be several orders of magnitude greater than can be obtained in bulk solids (Wang et al 1984; Mendez and Wang 1985; Mendez et al 1984c; Hirakawa et al 1985) and that systems can be made in which electrons traverse the entire sample without collision.

This paper discusses some of the basic principles of these structures. In addition, it presents the results of investigations carried out on the band structure and its variation with the well-width within the limit of parabolic band approximation.

CATEGORIES

Basically, there are three categories of LDs which are also called heterostructures.

Firstly, if tunneling through barriers is important, the structure is a superlattice (SL) (Esaki and Tsu 1970; Esaki et al 1970, 1972; Blakeslee and Alitotta 1970; Tsu and Esaki 1973; Chang et al 1974; Esaki and Chang 1974; Sollner et al 1983, 1984; Shewchuk et al 1985; Coon et al 1985; Luyi et al 1985). The idea of a SL is that the barrier layers are thin enough say 10 or 20Å, so that quantum mechanical tunneling through them can occur. As a result of the quantum mechanical tunneling, electronic motion perpendicular to the layers can manifest unusual properties because of the appearance of mini-gaps in the usual conduction band structure. Just below such mini-gaps, electrons behave dynamically as if they have negative mass and their resultant motion can consist of spatial oscillations. It is one of the most curious

features of solid state physics that the natural motion of an electron in a conduction band in response to a steady electric field is not to flow steadily in the direction of the electric force but to oscillate in space. This is referred to as ZENER BLOCH OSCILLATIONS (Mendez and Bastard 1993).

Secondly, if the barriers are too thick for tunneling, but the wells are still thin enough to exhibit quantum mechanical effects, we have Multiple Quantum Wells (MQW) (Dingle 1975; Dingle et al 1974, 1975, Weisbuch et al 1980, 1981).

Thirdly, if the wells and the barriers are both thick, the situation is simply referred to as multiple layers.

MATERIALS

The first team of the eleven semiconductors that nature has given us is of the elemental semiconductors: Silicon and Germanium and the nine binary compounds formed from groups III and V of the periodic table. Apart from this first team, there are other dozen compounds formed out of the group II and IV on one hand and lead or tin (group IV) plus group VI on the other hand. These vigorously compete in their own spheres. These materials, which are 26 in number and are tabulated in Table 1, exhibit a wide range of semiconductor properties. However, this range is not wide enough. Part of this insufficiency is being filled by forming alloys out of these binary compounds. Examples of these are $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and $\text{Ga}_{1-x}\text{In}_x\text{As}$. The former has an energy gap intermediate between that of gallium arsenide and that of aluminum arsenide while the optical properties of the latter, when x (the mole fraction) is about 0.5, are exactly right for exploitation in optical fibre communications (Cho 1971; Razeghi and Duchemin 1983, 1984; Cheng et al 1981; Petroff et al 1979; Chang et al 1981). Despite all these provisions, the range of available semiconductor materials is still limited.

Table 1: Semiconductor Area of the Periodic Table

| | | | | |
|----|-----|----|----|----|
| II | III | IV | V | VI |
| | Al | Si | P | S |
| Zn | Ga | Ge | As | Se |
| Cd | In | Sn | Sb | Te |
| Hg | | Pb | | |

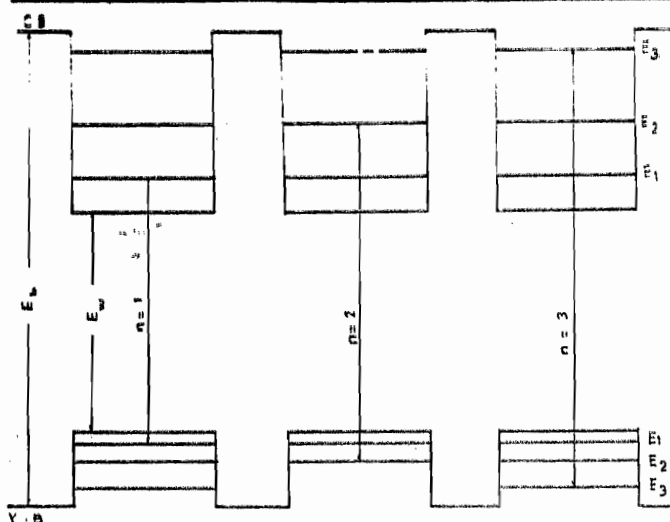


Fig. 1: Schematic representation of the quantum well energy band discontinuities in real space. The arrows in the wells show the $n = 0$ selection rule E_b is the energy gap of barrier material E_w is the energy gap of well material.

The search for the lifting of these limitations has led to the discovery of these new synthetic semiconductor materials, which are called LDs or heterostructures. The III-V semiconductor compounds, which are made from group III and group V elements have the basic properties necessary for fabricating LDs. These semiconductors have a direct band-gap. That is, they can emit or absorb light without the help of lattice vibrations, and thus are very efficient absorbers and emitters. They can form various solid solutions with identical crystal structures and well-lattice matched parameters but with different energy gaps and refractive indices.

PHYSICS OF LDs/HETEROSTRUCTURES

Electrons and holes can propagate freely in the periodic potential of semiconductors (Dingle 1975; Dingle et al 1974; Weisbuch et al 1980, 1981). The dynamics of the charge carriers caused by the semiconductor environment cause the replacement of both the free electron masses by much smaller electron and hole effective masses and a substantial increase in the dielectric constant. As a consequence of these changes, basic physical quantities such as the Bohr radius and the Rydberg constant are drastically modified in semiconductors. The change of scale in these natural units causes a number of processes

involving electrons and holes in semiconductors to be different from the free space atomic processes that they parallel. Thus, carriers in semiconductors are more sensitive to small perturbations. In the LDs, modifications of free particle behaviours due to Quantum Size Effect (QSE), which arise when the dimensions of a quantum system become comparable to the Bohr radius are very important. It is established (Dingle et al 1974) that QSE can be observed in semiconductor microstructures that have dimensions on the order of 100\AA as was initially proposed by Esaki and Tsu (1970).

The simplest examples of systems where size produces fundamental modifications of the optical and electronic properties are quantum well structures (Dingle et al 1974). These structures consist of ultrathin layers of two or more compounds grown one on another periodically (i.e. epitaxially) through various methods (Cho 1971; Neave et al 1983; Razeghi and Duchemin 1984; Tsang 1984a). Because the layers have different band gaps, the energy bands present discontinuities in real space (Dingle et al 1974) as schematically shown in Fig. 1. Quantization of carrier motion in the direction perpendicular to the layers produces a set of discrete energy levels (Dingle 1975). If the energy discontinuities are large enough and the layers with the large band-gap (i.e. the barriers) are wide enough (i.e. MQW systems) there will be little interaction between adjacent low-gap layers (i.e. the well). The confined carriers will behave almost independently (Dingle et al 1974, 1975). However, when the barriers are narrow, or the energy of a state is comparable to the energy discontinuity (i.e. SL system), the interaction between layers is important. The wave functions of the carriers are extended perpendicular to the layers, so that the behaviour of the carriers is modified by the long range modulation superimposed upon the crystalline potential (Adelabu 1996a).

In quantum well structures, electrons and holes do not move with their usual degrees of freedom. They show one-dimensional behaviour normal to the layers and two-dimensional behaviour in the plane of the layers. This reduced dimensionality induces drastic changes in the electric and optical properties of quantum well materials. For example, one can introduce impurities into the barriers in such a way that the impurity nuclei will be trapped while the carriers that are introduced can migrate towards the wells and form two-dimensional gases at the interfaces. This produces a physical separation

between impurities and carriers and leaves the carriers highly mobile. This, illustrated in Fig. 2, is referred to as modulation doping (*Dingle et al 1978; Stormer et al 1980, 1981, 1984*).

For undoped quantum well structures, excitonic effects are further modified by the confinement of carriers. Optical effects associated with excitons have been found (*Dingle et al 1974, 1975*) to be playing crucial roles in many opto-electronics applications of these man-made semiconductor structures (*Van der Ziel et al 1975; Dupius et al 1978; Holonyak Jr. et al 1978; Tsang 1981, 1984b; Dutta et al 1985; Wood et al 1983; Miller (a) et al 1984b*). Usually when a high purity bulk semiconductor absorbs a photon, the electron that is promoted to the conduction band interacts with the hole left in the valence band. Thus, the electron and hole can form a bound-state analog of the hydrogen atom called an exciton. This final state interaction produces a set of discrete and very strong emission and absorption lines just under the band-gap. Because the binding energy of the exciton is very small, excitons are very fragile and thus they are very sensitive to any kind of defect with the consequences that they can only be observed at low temperature since they are easily broken apart at other temperatures by thermal phonons. However, in quantum well structures which have layer thicknesses smaller than the Bohr radius, the exciton modifies its structure to fit into the low-gap layers. Thus it contracts and shrinks. The electrons and holes are forced to orbit closer to each other, while the binding energy increases by a factor of two or three. This added stability makes the excitons

resonances observable at room temperature. In the emission and absorption spectra, one can always see the steps associated with the transitions between sub-bands with the exciton peaks coming before each step (*Dingle et al 1974, 1975; Miller (b) et al 1980; Petroff et al 1981; Vojak et al 1980; Weisbuch et al 1980, 1981*). The peaks are very apparent in quantum well structures because of the increased exciton binding energy and also because the confinement strongly enhances the contrast with the continuum.

ENERGY BAND CALCULATIONS IN LDs

In this section, is presented an aspect of investigations in this field. Some other investigations have been the subjects of some earlier publications among which are those by *Adelabu (1993; 1995a,b,c; 1996b,c,d,e; 1998a,b,c)*, *Adelabu and Abdullahi (1997)*; *Adelabu and Akande (1997)* and *Adelabu et al (1988, 1989, 1997)*. The energy band structure calculations are intended to establish the key features of the electronic structures of solids. Thus, a proper understanding of it is needed to provide a basis for the quantitative interpretations of numerous experimental results and to guide further investigations. The more the knowledge of the features of a band structure, the better the analysis thereof.

Using the structural parameters as listed in table II, one may calculate the band structure (*Adelabu 1993*) and confinement energies for the electrons (E) the heavy hole (HH) and the light holes (LH) by applying any of the available models among which are:

- i. The Kronig - Penney model KPM, (*Kronig and Penney 1930*) which approximates the periodic potential by periodic square wells.
- ii. The envelope - function approximation model, EFAM (*Bastard 1981*) which takes the SL and MQW wave function as a linear combination of plane waves inside layers of each component materials.
- iii. The Kane model, KM (*Bastard 1982; 1984; Bastard et al 1984*) which is due to Bastard and which uses a Kane type envelope function description involving eight bands including spin.

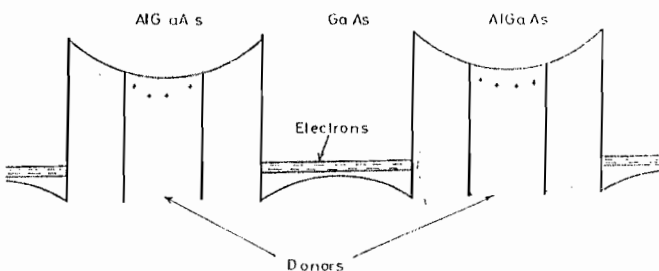


Fig. 2: Modulation doping. Electrons donated by impurities deliberately introduced only in the central region of the barrier layer fall into the well. Being spatially separated from their parent atoms, the electrons are only weakly scattered by them and so the mobility is enhanced.

- iv. The tight-binding model, TBM (*Schulman and Chang 1985*) which considers the mixing of the light and heavy holes.

A careful study of these models reveals that (ii) and (iii) above are not very different as far as the type I SL and MQW materials (*Adelabu 1996a*) are concerned, most especially for the lower transitions, which are the subjects of experimental concerns. There is evidence (*Schuermans and Hooft 1985*) that there is an excellent agreement between the two which is hereby referred to as modified Kronig-Penney model (MKPM). Thus, there are basically three models: KPM, MKPM and TBM apart from the simple "particle-in-a-box" model used by Dingle et al (*1974*) but which is now outdated in view of the real structure of the system.

The KPM, though has been used by many investigators to explain their experimental observations, also has its own limitations. The model assumes the same masses for the charge carriers (electron, heavy hole and the light hole) in both the well and the barrier whereas these particles have their respective masses in the well different from those in the barrier (*Adelabu 1993*).

For the work reported here, the MKPM has been adopted. This model ensures the continuity of the wave function as well as that of the probability current and consequently guarantees that the eigenstates are stationary (*Bastard 1981, White and Sham 1981*). The model, in addition yields the electronic band structure of the SL and MQW system and also gives the energies above the confining barrier (*Adelabu 1994, 1996b,d; Babiker 1986, Bastard et al 1984; Brum and Bastard 1986; Jaros and Wong 1984; Zucker et al 1984*). In the work reported here, the following assumptions have been made in a fashion similar to that by *Adelabu (1993, 1998b)*:

- i. The band structures of the host materials, in the vicinity of the centre of the Brillouin zone, are quite similar.
- ii. The interface potentials are strongly localised in the vicinity of the barrier/well interfaces with spatial localisation such that at the scale of the variation of the slowly varying envelopes, the interfaces reduce to the plane.
- iii. No charge redistribution exists at the interfaces.
- iv. The interface potentials do not mix but only shift the S- and P-like band edge states.

In the model (*Adelabu 1993, 1994, 1996b,d*), the SL and MQW wave functions have been taken as a linear combination of plane waves inside layers of each component material while the usual effective mass boundary conditions at the two successive SL and MQW interfaces (*Bastard 1981; White and Sham 1981*) have been adopted, using Bloch's theorem. These led to the dispersion relations now well documented (*Adelabu 1993, 1995a, 1996b,c,d; 1998a, b,c; 1999; Adelabu and Abdullahi 1997*) and given by:

$$\text{Cos}QD = \text{Cos}k_1d_1 \text{Cos}k_2d_2 - \frac{1}{2} (Z + 1/Z) \text{sin}k_1d_1 \text{sin}k_2d_2$$

where

$$k_1 = (2m_1^*E/\hbar^2)^{1/2}$$

$$k_2 = [2m_2^*(E-V_0)/\hbar^2]^{1/2}$$

and

$$Z = m_1^*k_2/m_2^*k_1$$

$D = (d_1 + d_2)$ is the periodicity length, V_0 is the barrier height, E is the energy eigen-value, d_1 and d_2 are the layer thicknesses, $m_i^* (i = 1, 2)$ are the corresponding effective-masses. The subscript 1 refers to GaAs while 2 refers to AlGaAs. The above equations differ from those of KPM in that Z in the present equations contains m_i^* . These equations were collectively

Table II: MATERIAL PARAMETERS USED IN CALCULATIONS

| Parameter | Material | |
|-----------------|-------------|-------------|
| | GaAs | AlGaAs |
| Energy gap | 1.42eV | 1.79eV |
| Electron mass | 0.067 m_0 | 0.069 m_0 |
| Heavy hole mass | 0.45 m_0 | 0.51 m_0 |
| Light hole mass | 0.082 m_0 | 0.102 m_0 |

used to calculate the band structures for the charge carriers using the various parameters in Table II.

m_0 is the free electron mass while the values of the parameters were from Casey and Panish (1978).

The variation of the band structure with the well-width for electrons, heavy hole and light hole calculated in a similar manner for the GaInAs/AlInAs SL and MQW systems (Adelabu 1996b, 1998c) are respectively presented in Figs. 3, 4 and 5.

The same expressions were used to calculate the figures, however, with the various values of the individual parameters in the well and barrier used. This procedure is adopted because of the following:

- i The confinement potential step of the light-hole is considerably smaller than the spin-orbit splittings. Consequently, the confinement energies are also smaller than the spin-orbit splittings. This gives the chance of being able to treat the light-hole in a similar way as the electron.
- ii Owing to the complete decoupling between heavy-hole on one hand and the electron and light-hole on

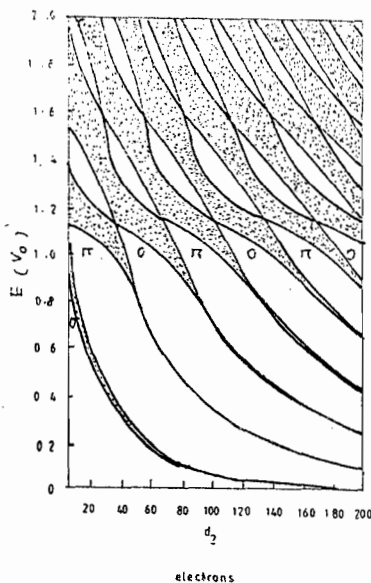


Fig. 3: Variation of the band structure with the well-width for the electron in GaAs/AlGaAs SL and MQW system within parabolic band approximation. The barrier width is kept constant at 100Å.

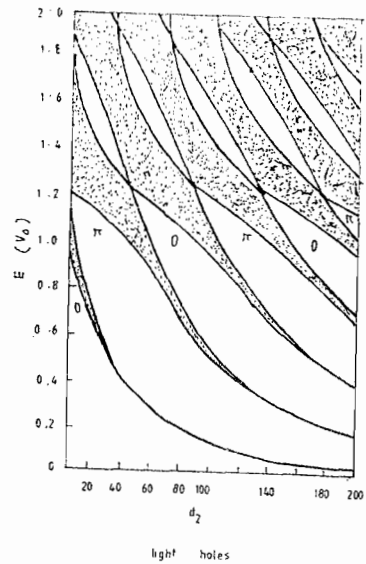


Fig. 4: Variation of the band structure with the well-width for the light hole in GaAs/AlGaAs SL and MQW system within parabolic band approximation. The barrier width is kept constant at 100Å.

the other hand. Fig. 6, the heavy-hole SL and MQW bands can be calculated exactly in the same way as of the electron and the light-hole.

- iii The use of a unified expression for the three particles eliminates the chances of parameters having to be separately adjusted and consequently leading to bad transition energy.

The figures clearly illustrate some of the important features characterising the quantum mechanical calculations in LDs. These are the discrete nature of the carrier states within the well discussed in section IV, and the existence of discrete transmission resonances with energies just above the barrier (Bastard 1984, Bastard et al 1984; Jaros and Wong 1984; Zucker et al 1984, Babiker 1986; Adelabu 1994, 1996b, 1998c).

For Figs 3, 4 and 5, the barrier width is kept constant at 100Å. The band edges are such that $QD=0$ and π in the dispersion relation. The region of the figures below $E(V_0)$ equal 1 are those within the wells while those for $E(V_0)$ greater than 1 are those above the barriers. The wave function of the quantum well

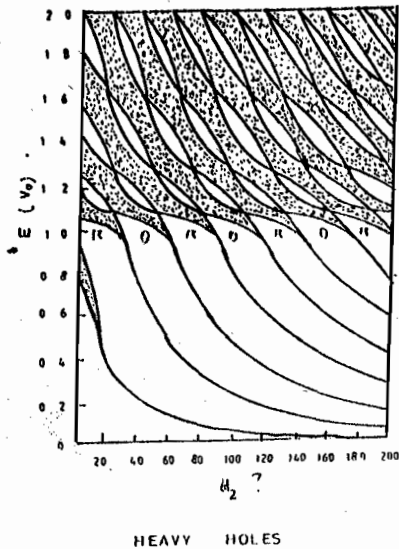


Fig. 5: Variation of the band structure with the well-width for the heavy hole in GaAs/AlGaAs SL and MQW system within parabolic band approximation. The barrier width is kept constant at 100\AA^0

continuum states along the z-axis are linear combinations of plane waves, either in the well or in the barrier. These wave vectors are normalized over the length L_z of the structure. For a given energy and a given wave vector, there exist two degenerate continuum states which correspond to a carrier moving along the z-axis either from the left to the right or vice versa. When the n^{th} quantum well bound state has popped in the continuum to become a transmission resonance and when this resonance is narrow enough, the virtual bound state largely retains the parity property of the original bound state.

As evident from the figures, the bottom of the lowest sub-band above the barrier enters the well. In addition, the figures show that at least one energy level or state exists for each of the three particles. The inclusion of band structure effects (band non-parabolicity and others) as has been done for the GaInAs/AlInAs SL and MQW systems (Adelabu 1996b,c; 1998c) will not qualitatively alter the results presented and conclusions arrived at here which are ultimately based on the existence of two genuine quantum well features: the bound and virtual bound states.

The model used in obtaining the figures reported here has been in part used to fit theory to experiment in some of the previous work on the GaInAs/AlInAs SL and MQW system (Adelabu et al 1998, 1989). A comparison of the present work with the previous ones on GaInAs/AlInAs system reveals that there are more levels in the GaInAs/AlInAs system than in the GaAs/AlGaAs system. This is in part due to the shallower wells in the GaAs MQW system than in the GaInAs MQW system, and the lower effective masses of the carriers in the GaInAs MQW system which consequently lead to better confinement in the GaInAs MQW system.

SUMMARY/CONCLUSION

Progress in crystal growth techniques has made feasible the realisation of periodic semiconductor structures composed of ultrathin layers. The structures consist of periodic sequence of two different semiconductor materials with lattice matching. Here, a potential is induced in the conduction and valence band by the periodic variation of the energy gap in the direction of growth (i.e., discontinuities exist). The existence of discontinuities results in the electrons and holes in the well experiencing

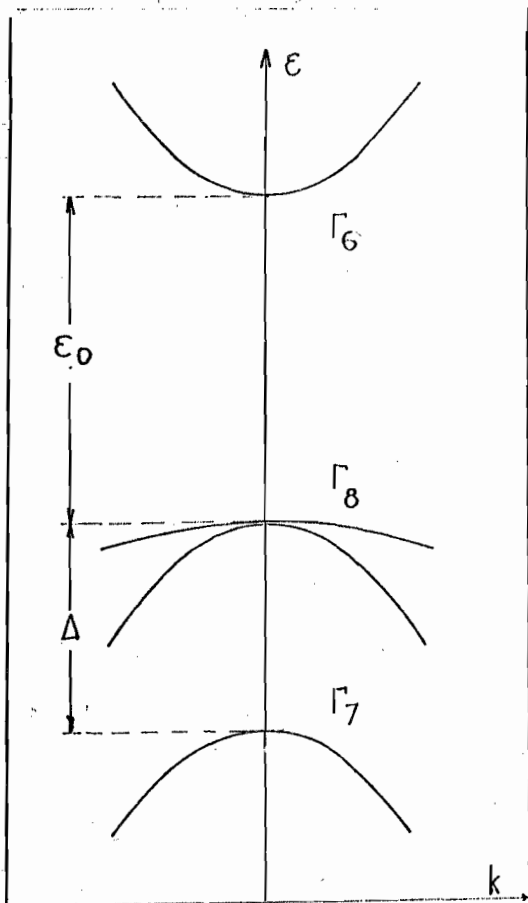


Fig 6: Decoupling of the heavy hole electron and light hole states.

confinement and consequently lead to quantization. Each quantized level in both the valence band (for holes) and the conduction band (for electrons) defines respectively the maximum and the minimum of two-dimensional energy band. The confinement energies in both depend inversely on the square of the well width. Adopting the MKPM, the calculation of the energy band structure and its variation with the well width reveal boundedness within the well and discrete resonances out of the well.

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