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The Ben Daniel-Duke Model Applied to Semiconductor Hetero-structure - Part 2

We investigate the semiconductor heterostructure with the Ben Daniel-Duke model applied for the lowest conduction states Ga As-Ga (1) as and for the heavy levels at $k_\perp = 0$ *in any heterostructures (1). In a quantic level we obtained the familiar staircase density of states (2). In (3) we calculated the incrgy position of the interface state in a single HgTe-CdTe heterojonction. We also obtained the existence of the interface state relies only on the relative position of the* Γ_8' *edges of HgTe and CdTe, their actual energy position, as well as their behavior at* $k_\perp \neq 0$ *.*

Keywords: *Ben Daniel-Duke model, heterostructure, quantum well, Ben Daniel-Duke quantum well*

Equation(19) defines the in-plane effective mass of the n^{th} sub band in the vicinity of $k_\perp$=0. It may be remarked that if $m_B > m_A$, as is the case in GaAs-Ga(Al)As or $Ga_{0.47}In_{0.53}As - InP$,this in-plane mass m_n will increase with increasing sub band index n

Using the approximately parabolic in-plane dispersion laws (equation (14)) it is very easy to calculate the density of states $p(\varepsilon)$ associated with the bound states E_n. Proceeding exactly as in chapter I we obtain:

$$p(\varepsilon) = \sum_n p_n(\varepsilon) \tag{20a}$$

$$p_n(\varepsilon) = \frac{m_n S}{\pi \hbar^2} Y(\varepsilon - E_n) \tag{20b}$$

where Y(x) is the step function. We recover the familiar staircase density of states.

The properties of a Ben Daniel-Duke quantum well are summarized in figure 4.

From the left to the right: conduction band edge profile, energy levels $E_1 and E_2$ and their associated envelope functions; in-plane dispersions of the E_1 and E_2 sub bands; energy dependence of the heterostructure density of states $p(\varepsilon)$.

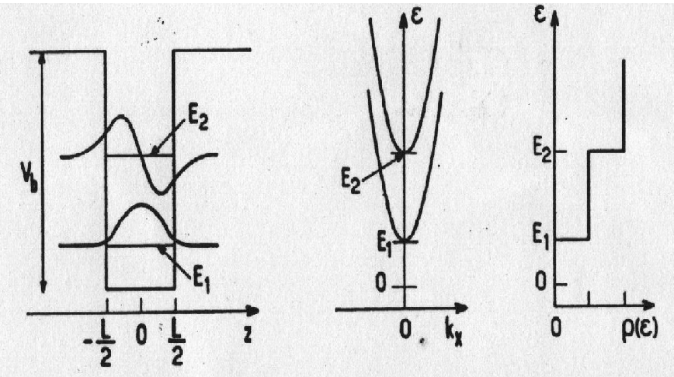

Figure 4. - A recollection of the main properties of the quantum well bound states, solutions of a Ben Daniel-Duke Hamiltonian.

3.Interface states of Ben Daniel-Duke quantum wells $(m_A m_B < 0; k_\perp = 0)$

The case $m_A m_B < 0$ is practically realized in HgTe-CdTe heterostructures [20] (see Fig. 5). CdTe is a conventional open gap semiconductor whose level ordering is the same as is found in GaAs. HgTe is a symmetry-induced zero gap semiconductor. The Γ_6 band, which is a conduction band in most III-V and II-VI semiconductors, is a light hole band in HgTe. The Γ_6 edge lies ~ 0.3 eV below the Γ_8 edges. As the Γ_8 light band Γ_6 band are nearly mirror-like, the Γ_8 light band is a conduction band in HgTe, degenerate at the zone centre with Γ_8 heavy hole band(inversion asymmetry splitting having been neglected).

Ignoring the absence of centro-symmetry of the zinc-blade lattice, the light particle and heavy hole states decouple at .

We can thus treat the problem of the light particle states associated with a Γ'_8 edge as if we were considering a single band. The interesting feature of the HgTe-CdTe heterostructures is that the light particle changes the sign of its effective mass across the interfaces, being electro-like in the HgTe layer and light hole-like in the CdTe layers. To be specific, let us consider a CdTe-HgTe-CdTe double heterostructures.

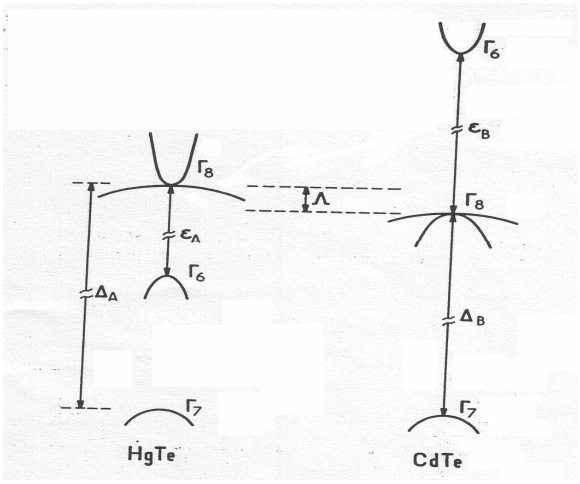

Figure 5.- Band structures of bulk HgTe (left panel) and CdTe (right panel) in the vicinity of the I′ point (schematic).

According to [27] the bottom of the HgTe I'_8 conduction band lies at an $\Lambda \sim$ 40 meV above the top of the CdTe I'_8 valence band. Thus, bound states of the heterostructures only exist if $\varepsilon \geq -\Lambda$ (the energy zero being taken at the I'_8 edge in HgTe). If $-\Lambda \leq \varepsilon \leq 0$, the states are evanescent in both kinds of layers while if $\varepsilon \geq 0$, the carrier wave vector is real (imaginary) in the HgTe (CdTe) layers. Clearly, bound states of positive energies will exist (an infinite number in the one-band description of each host layer). Proceeding as in section 1. their energies will fulfil

$$\cos\varphi_A + \frac{|m_B|}{m_A}\frac{k_A}{k_B}\sin\varphi_A = 0 \qquad \textit{for even states} \tag{21}$$

$$\cos\varphi_A - \frac{m_A}{|m_B|}\frac{k_B}{k_A}\sin\varphi_A = 0 \qquad \textit{for odd states} \tag{22}$$

$$\varphi_A = \frac{1}{2}k_A L_A \tag{23}$$

$$k_A = \sqrt{\frac{2m_A}{\hbar^2}\varepsilon}; \qquad k_B = \sqrt{\frac{2|m_B|}{\hbar^2}(\varepsilon + \Lambda)} \tag{24}$$

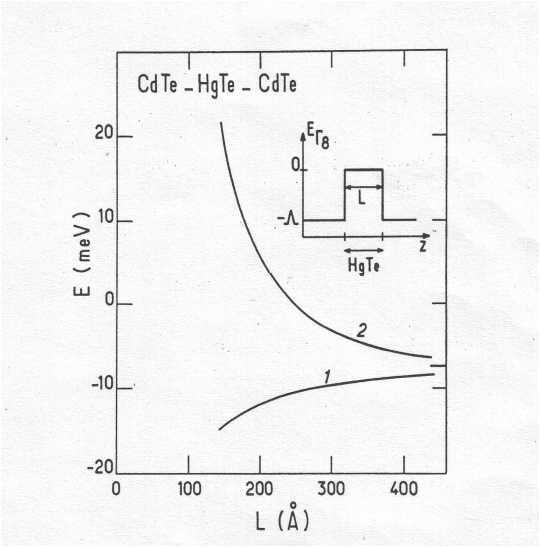

Figure 6.- Evolution of ground and first excited bound states (labeled 1 and 2 respectively) versus the HgTe slab thickness in a CdTe-HgTe-CdTe double heterostructure.

The bound state wave functions are all characterized by cusps at the interfaces due to the change in the carrier effective mass at the hetero-interfaces. This sign reversal also implies that equation (22) can be fulfilled at $\varepsilon = 0$ for a certain L_A while equation (21) can not. This means that at least one state (even in z) should lie below the bottom of the HgTe conduction band edge. This state is an interface level, built from evanescent states in *each* of the host layers, whose wave function peaks at the interface. More precisely, we can write:

$$\chi_1(z) = A\cos(k_A z) \qquad |z| \le \frac{1}{2}L_A \tag{25}$$

$$\chi_1(z) = B\exp\left[-k_B\left(z - \frac{1}{2}L_A\right)\right] \qquad z \ge \frac{1}{2}L_A \tag{26}$$

$$\chi_1(-z) = \chi_1(z) \tag{27}$$

with:

$$k_A = \sqrt{\frac{2m_A}{\hbar^2}(-\varepsilon)}; \quad k_B = \sqrt{\frac{2|m_B|}{\hbar^2}(\varepsilon + \Lambda)} \tag{28}$$

By matching $\chi_1(z)$ and $\mu^{-1}(z)\frac{d\chi_1}{dz}$ at $z=\frac{1}{2}L_A$, we find that ε should be the root of the implicit equation

$$\tanh\left(\frac{1}{2}k_A L_A\right)=\frac{m_A}{|m_B|}\frac{k_B}{k_A} \tag{29}$$

It is very easy to check that equation (29) always admits one solution E_1(and only one) which extrapolates to – Λ when $L_A \to 0$. A second state may actually exist in the energy segment [-Λ,0] if the HgTe layer is thick enough. It corresponds to an odd envelope function:

$$\chi_2(z)=A\sinh(k_A z); \qquad |z|\le\frac{1}{2}L_A \tag{30}$$

$$\chi_2(z)=B\exp\left[-k_B\left(z-\frac{1}{2}L_A\right)\right]; \qquad z\ge\frac{1}{2}L_A \tag{31}$$

$$\chi_2(-z)=-\chi_2(z) \tag{32}$$

The E_2 energy is the solution of the implicit equation:

$$\cot anh\left(\frac{1}{2}k_A L_A\right)=\frac{m_A}{|m_B|}\frac{k_B}{k_A} \tag{33}$$

which admits a solution if

$$L_A>\frac{2|m_B|}{m_A}\sqrt{\frac{\hbar^2}{2|m_B|\Lambda}} \tag{34}$$

Again, the solution of equation (33), if it exists, is unique. When L_A becomes very large the energies E_1 and E_2 converge to the value:

$$E_\infty=-\frac{\Lambda}{1+\frac{|m_B|}{m_A}} \tag{35}$$

which is the energy position of the interface state in a single HgTe-CdTe heterojunction [3, 4].

Clearly, at large L_A (i.e. $k_A L_A>1$) the two states E_1 and E_2 are very well approximated by the symmetric and antisymmetric combinations of the two interface states centred at $\pm\frac{1}{2}L_A$ respectively. The behavior of E_1 and E_2 versus

L_A presented in figure 6 to illustrate the previous discussion. In figure 7 we show the calculated $\chi_1(z)$ envelope functions in $Hg_{1-x}Cd_xTe$-HgTe-$Hg_{1-x}Cd_xTe$ quantum wells to illustrate the interface nature of the E_1 state. Although the existence of the interface state relies only on the relative position of the I'_8 edges of HgTe and CdTe, their actual energy position, as well as their behavior at $k_\perp \neq 0$ (where they strongly couple to the heavy hole states), remains a subject of active research.

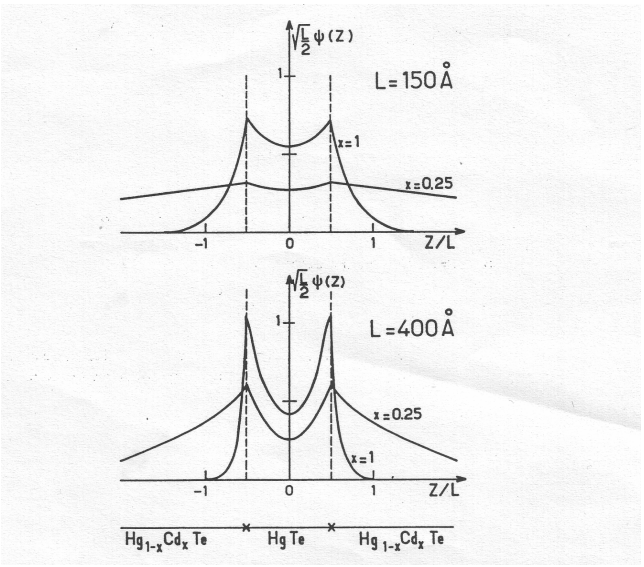

Fig. 7. – Dimensionless envelope functions of the ground states in $Hg_{1-x}Cd_xTe$-HgTe-$Hg_{1-x}Cd_xTe$ double heterostructures (x=1 and x=0.2) for two different HgTe slab thicknesses.

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