International Journal of Physics and Mathematical Sciences ISSN: 2277-2111 (Online)
An Online International Journal Available at http://www.cibtech.org/jpms.htm
2013 Vol. 3 (1) January-March, pp.7-12/Arulmozhi
Research Article

ELECTRON-HOLE TRANSITION ENERGIES IN $|Z|^{2/3}$ QUANTUM WELL – MATCHING IN THE MIDDLE METHOD

***M. Arulmozhi**
Department of Physics, Jayaraj Annapackiam College for Women (Autonomous), Periyakulam–625 601
Theni District, Tamilnadu, India
**Author for Correspondence*

ABSTRACT
Energy levels of an electron, a heavy hole and a light hole in a quantum well with potential shape proportional to $|z|^{2/3}$ are calculated as a function of the wellwidth and the barrier height, using "matching in the middle" method combined with Runge-Kutta method. The energies decrease as the wellwidth increases and increase as the barrier height increases. The transition energies E_{nm} are obtained between the n^{th} electron state and the m^{th} heavy hole or light hole state. The results agree well with the available theoretical and experimental values. The earlier conclusion that the energy levels in a quantum well with graded interfaces are the same as those in a quantum well whose effective thickness is slightly larger than that of the nominal QW, is confirmed for the present case.

Key Words: *Nanomaterials, Schrodinger Equation, Runge Kutta Method, Quantum Wells, Energy Levels*

INTRODUCTION
Low dimensional systems such as quantum wells, quantum dots and quantum dots and quantum wires are produced from semiconductor nanomaterials by crystal growth techniques. Quantum wells (QW) are grown with various shapes as rectangular quantum wells (RQW) (Greene and Bajaj, 1983; Miller *et al.*, 1984), parabolic quantum wells (PQW) (Merlin, 1987; Brey *et al.*, 1989-II), triangular quantum wells (TQW) (Jiang and Wen, 1994-II), $|z|^{2/3}$ QW (Sputz and Gossard, 1988-I; Arulmozhi and Balasubramanian, 1995 and Arulmozhi and Balasubramanian, 1996) etc. Calculation of electron and hole energy levels and hence the transition energies in such quantum wells will be useful for many advanced studies on them. The intersubband transitions and impurity binding energy in differently shaped semiconductor quantum wells under a magnetic field are calculated by Yesilgul *et al.*, (2011) using a variational method within the effective mass approximation. The effects of nitrogen and indium mole concentration on the intersubband optical absorption for (1-2) transition and the binding energy of the shallow-donor impurities in a $Ga_{1-x}In_xN_yAs_{1-y}/GaAs/Al_{0.3}Ga_{0.7}As$ quantum well under the electric field is theoretically calculated by Ungan *et al.*, (2012).

Villamil *et al.*, (2005) have studied the behaviour of the binding and transition energies of a donor shallow impurity in a cylindrical $GaAs\text{-}Ga_{0.6}Al_{0.4}As$ quantum well wire (QWW) as a function of the wire radius, the impurity position and the applied magnetic field. Eseanu (2010) has investigated the intersubband transitions in square and parabolic quantum wells under simultaneous action of the hydrostatic pressure and high-frequency laser field. The simultaneous effects of hydrostatic pressure and magnetic field applied along the quantization direction on intersubband optical transitions in Pöschl-Teller quantum well are investigated by Hakimyfard *et al.*, (2009).

The dependences of intersubband transitions on well width and nitrogen (N) content in n-type $In_{0.23}Ga_{0.77}As_{1-x}N_x/GaAs$ quantum wells (QWs) are investigated by Liu *et al.*, (2008) using a ten-band k.p model. The effects of hydrostatic pressure on the correlated e-h transition energies in single $GaAs\text{-}Ga_{1-x}Al_xAs$ quantum wells are calculated by Raigoza *et al.*, (2006) via a variational procedure, in the framework of the effective-mass and non-degenerate parabolic-band approximations. Various methods have been followed for finding the energy levels of electron and hole by solving Schrödinger equation and this paper follows a refined procedure called "matching in the middle" method combined with the conventional Runge Kutta method.

International Journal of Physics and Mathematical Sciences ISSN: 2277-2111 (Online)
An Online International Journal Available at http://www.cibtech.org/jpms.htm
2013 Vol. 3 (1) January-March, pp.7-12/Arulmozhi
Research Article

THEORY

The potential profile for a $|z|^{2/3}$ QW is taken to be of the form (along z-axis)

$$V(z) = \begin{cases} V_o \left| \frac{z}{L/2} \right|^{2/3} \ldots\ldots\ldots\ldots\ldots\ldots |z| \le L/2 \\ V_o \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots |z| > L/2 \end{cases} \quad (1)$$

where L is the wellwidth and V_o is the barrier height which depends on Aluminium composition x. $V_o = 0.65\Delta E_g$ for the electron (Leavitt, 1987-I) and $V_o = 0.35\Delta E_g$ for the hole (Leavitt, 1987-I), ΔE_g is the variation in bandgap difference between the conduction band and valence band with x.

$\Delta E_g = 1.55x + 0.37x^2$ eV (2)

The unit of energy is the effective Rydberg and the unit of length is the effective Bohr radius given by the following expressions respectively.

$$R^* = \frac{m^* e^4}{2\hbar^2 \varepsilon_0^{\,2}} \text{ and } a^* = \frac{\hbar^2 \varepsilon_0}{m^* e^2} \quad (3)$$

where ε_0 is the static dielectric constant of GaAs and m* is the effective mass of the electron or the heavy hole or the light hole, as the case may be. The Hamiltonian for an electron or a hole in a bare quantum well is given in the effective mass approximation as

$$H = -\frac{d^2}{dz^2} + V(z) \quad (4)$$

The Schrödinger equation for such a system is given by $H\psi = E\psi$, which is a second order differential equation

$$\frac{-d^2\psi}{dz^2} + V(z)\psi = E\psi \quad (5)$$

where E is the energy eigenvalue. This equation is solved by a refined procedure called "Matching in the middle" method combined with the conventional Runge-Kutta method used by Neethiulagarajan and Balasubramanian (1989).

Runge-Kutta method

Equation (5) can be represented as system of two simultaneous first order differential equations as

$$\frac{d\psi}{dz} = y \text{ and } \frac{dy}{dz} = \left[V(z) - E\right]\psi . \quad (6)$$

The Runge-Kutta method is used to integrate these equations simultaneously and determine the value of the function and its derivative at a point (z + h), if the value of the function and its derivative at a point z are known, with h being the stepsize of the integration. The computation formulae are given below.

- $\psi(z+h) = \psi(z) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$
- $y(z+h) = y(z) + \frac{1}{6}(l_1 + 2l_2 + 2l_3 + l_4)$

where

- $k_1 = hy(z)$
- $l_1 = h\left[V(z) - E\right]\psi(z)$
- $k_2 = h\left[y(z) + \frac{l_1}{2} \right]$

- $l_2 = h\left[V\left(z+\frac{h}{2}\right)-E\right]\left[\psi(z)+\frac{k_1}{2}\right]$
- $k_3 = h\left[y(z)+\frac{l_2}{2}\right]$
- $l_3 = h\left[V\left(z+\frac{h}{2}\right)-E\right]\left[\psi(z)+\frac{k_2}{2}\right]$
- $k_4 = h\left[y(z)+l_3\right]$
- $l_4 = h\left[V(z+h)-E\right]\left[\psi(z)+k_3\right]$

Matching in the middle method

In this procedure, equation (5) is integrated forward from the origin in the direction of increasing z and integrated backward from the distance $\frac{L}{2}(a^*)$ in the direction of decreasing z. The forward solution ψ_f and its derivative y_f and the backward solution ψ_b and its derivative y_b, thus obtained are matched at the middle point $\frac{L}{4}(a^*)$ called the matching point.

For the forward solution, the initial conditions are at z = 0, ψ = 1, y = 0 and for the backward solution, the conditions are at z = L/2, $\psi = e^{-\beta L/2}$, y = t (arbitrary). The two adjustable parameters E and t are calculated in the iterative process that attempts to match the solution ψ_f and ψ_b at the matching point $\frac{L}{4}(a^*)$. Matching conditions are $\psi_f = \psi_b$ and $y_f = y_b$ at z = $\frac{L}{4}(a^*)$. When the effective mass mismatch is included, the matching conditions are $\psi_f = \psi_b$ and $m_2{}^* y_f = m_1{}^* y_b$ at z = $\frac{L}{4}(a^*)$, where $m_1{}^*$ and $m_2{}^*$ are the effective masses in GaAs and $Ga_{1-x}Al_xAs$ respectively.

Iterative process is started with some arbitrary values of E and t and adjusted with the following expressions until the matching conditions are ultimately satisfied.

$$\Delta E = \frac{\left[\psi_b(y_f - y_b) - y_b(\psi_f - \psi_b)\right]}{\left[y_b(U_f - U_b) - \psi_b(W_f - W_b)\right]}$$

$$\Delta t = t\frac{\left[(U_f - U_b)(y_f - y_b) - (W_f - W_b)(\psi_f - \psi_b)\right]}{\left[y_b(U_f - U_b) - \psi_b(W_f - W_b)\right]}$$

Where $U = \frac{\partial\psi}{\partial E}$ and $W = \frac{\partial^2\psi}{\partial E^2}$, which are calculated during the course of the program..

RESULTS AND DISCUSSION

The experimental sample used by Sputz and Gossard (1988-I) has L = 1024 Å and x= 0.27. The effective masses and the dielectric constant in $Ga_{1-x}Al_xAs$ are calculated as given by Adachi (1985).

$$m^*\left(Al_xGa_{1-x}As\right) = m^*\left(GaAs\right) + x\left[m^*\left(AlAs\right) - m^*\left(GaAs\right)\right]$$

$$\varepsilon_0\left(Al_xGa_{1-x}As\right) = \varepsilon_0\left(GaAs\right) + x\left[\varepsilon_0\left(AlAs\right) - \varepsilon_0\left(GaAs\right)\right]$$

The material parameters used are listed in Table – 1. These give a* = 105 Å and R* = 5.19 meV for electron in the GaAs region. The effective masses and also the dielectric constants are different in the well region and the barrier region. The dielectric constant mismatch is ignored in the present work. The small difference in the dielectric constants would give rise to image potentials which are generally weak for the semiconductor systems considered in our present work except for extremely narrow wells.

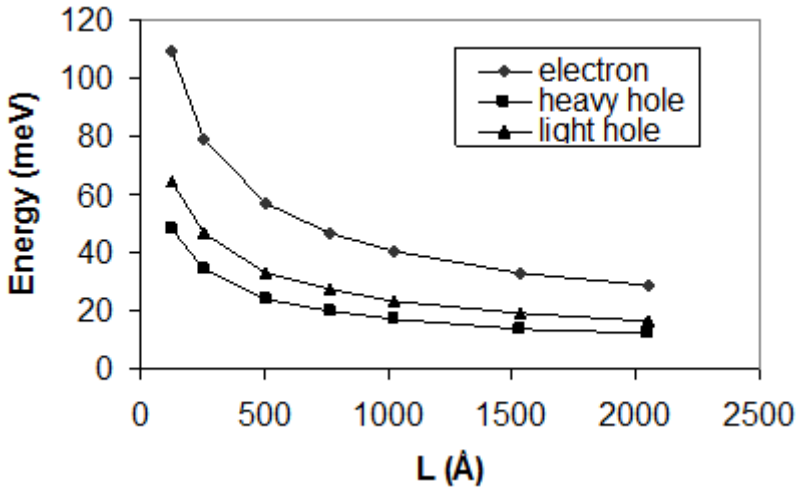

Figure 1: Variation of the ground state energies of an electron, a heavy hole and a light hole in a $|z|^{2/3}$ quantum well (with effective mass mismatch included) as a function of the wellwidth

The energies of the electron and hole states are obtained by solving equation (5) numerically. The effective mass mismatch for the conduction electron is considered, in the calculations. For the holes, the problem is more complicated since the valence bands are not spherical and there is also the spin-orbit splitting. However, the simplified picture with similar continuity condition, as for the electron state, is used. The same formula for the effective masses of the holes in $Ga_{1-x}Al_xAs$ is used, as for the electrons.

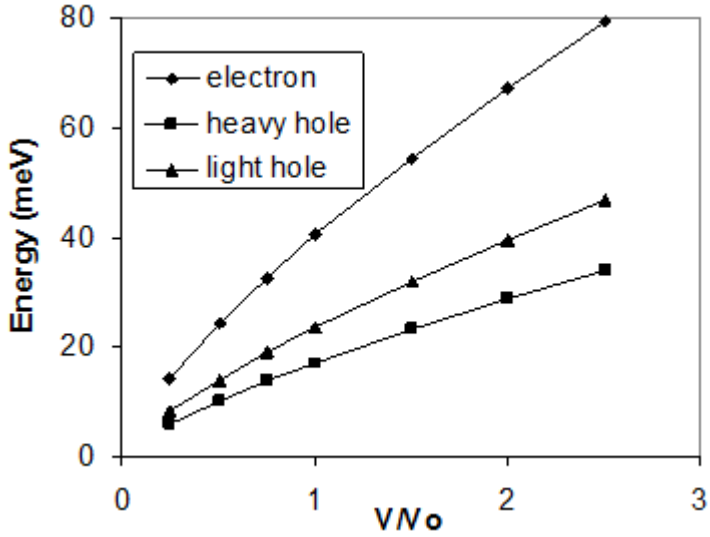

Figure 2: Variation of the ground state energies of an electron, a heavy hole and a light hole in a $|z|^{2/3}$ quantum well (with effective mass mismatch included) as a function of the barrier height. V_o for electrons = 220.23 meV. V_o for holes = 118.59 meV

Figure - 1 shows the ground state energies of the electron, heavy hole and light hole as a function of the wellwidth and Figure – 2 as a function of the barrier height. It is noted that the light hole energies are higher than that of the heavy hole energies and lower than that of the electron. This is expected because $m_e^* < m_{lh}^* < m_{hh}^*$. The energies decrease as the wellwidth increases and increase as the barrier height increases. This behavior is the same as in other quantum wells.

Table 1: The material parameters used in the calculations x = 0.27

Parameters	**GaAs [19]**	**AlAs [19]**	**$Ga_{1-x}Al_xAs$**
m_e^*	0.0665 m_0	0.15 m_0	0.09 m_0
m_{hh}^*	0.34 m_0	0.40 m_0	0.36 m_0
m_{lh}^*	0.094 m_0	0.18 m_0	0.12 m_0
ε_0	13.2	10.1	12.26

The transition energies E_{nm} are obtained between the n^{th} electron state and the m^{th} heavy hole or light hole state. The results are listed in Table – 2, which also shows the experimental results of Sputz and Gossard (1988-I). There has been a discrepancy between their theoretical estimates of the electron and the hole state energies and their experimentally measured values from photoluminescence data in $|z|^{2/3}$ QW. The average difference between the theoretical transition energies and the experimental ones has been attributed to the binding energy of an exciton.

Table 2: Transition energies E_{nm} between n^{th} electron state and m^{th} heavy hole or light hole state. x = 0.27, V_0 = 220.23 meV for electrons and V_0 = 118.59 meV for holes.

Transition	**Transition energy (meV)**				
	Without effective mass mismatch L = 1024 Å	**With effective mass mismatch L = 1024 Å**	**L = 1224 Å**	**Theoretical results [6]**	**Experimental results [6]**
E_{11h}	64.01	57.43	52.56	52.6	46.0
E_{11l}	71.16	63.88	58.44	58.4	52.0
E_{13h}	87.33	82.34	75.35	75.4	72.8
E_{22h}	110.86	109.78	101.07	101.4	94.1
E_{22l}	123.25	122.98	111.36	113.3	108.4
E_{24h}	128.10	125.47	114.20	117.6	111.9
E_{33h}	143.12	139.97	128.27	130.4	123.2
E_{35h}	157.54	154.50	141.56	144.1	138.9

The values calculated including the effective mass mismatch are found to be systematically higher then the experimental results by an average value of 13.6 meV for the case of L = 1024 Å. This large difference is mainly due to two reasons.

Correction due to exciton binding energy should be applied to the theoretical values.

The experimental sample of Sputz and Gossard (1988-I) has graded interfaces and this has not been taken into account in the present work.

The energy levels in a rectangular quantum well with narrow graded interfaces have been discussed by Bastard (1981). His main conclusion is that the energy levels in a quantum well with graded interfaces are the same as those in a rectangular quantum well whose effective thickness is slightly larger than that of the nominal QW. In order to check this for the present case with potential profile proportional to $|z|^{2/3}$, calculations are repeated by varying the well thickness. The results for L = 1224 Å and x = 0.27 are also given in the Table – 2, without correcting for the exciton binding energy. The values agree well with the experimental results of Sputz and Gossard (1988-I) after correcting for the exciton binding energy estimated by Arulmozhi and Balasubramanian (1995).

REFERENCES

Adachi S (1985). GaAs, AlAs, and $Al_xGa_{1-x}As$@B: Material parameters for use in research and device applications. *Journal of Applied Physics* **58** R1.

Arulmozhi M and Balasubramanian S (1995). Binding energy of a hydrogenic donor and of a Wannier exciton in the $|z|^{2/3}$ quantum well *Physical Review B* **51**(4) 2592-2595.

Arulmozhi M and Balasubramanian S (1996). Effect of magnetic field on the binding energy of a hydrogenic donor in a $|z|^{2/3}$ quantum well. *Physica Scripta* **54** 651-656.

Bastard G (1981). Hydrogenic impurity states in a quantum well: A simple model. *Physical Review B* 24 4714-4722.

Brey L, Johnson NF and Halperin BI (1989-II). Optical and magneto-optical absorption in parabolic quantum wells**.** *Physical Review B* **40**(15) 10647-10649.

Eseanu N (2010). Simultaneous effects of laser field and hydrostatic pressure on the intersubband transitions in square and parabolic quantum wells. *Physics Letters A* **374**(10) 1278-1285.

Greene RL and Bajaj KK (1983). Energy levels of hydrogenic impurity states in GaAs-$Ga_{1-x}Al_xAs$ quantum well structures. *Solid State Communications* **45**(9) 825-829.

Hakimyfard Alireza, Barseghyan MG and Kirakosyan AA (2009). Simultaneous effects of pressure and magnetic field on intersubband optical transitions in Pöschl–Teller quantum well. *Physica E* **41**(8) 1596-1599.

Jiang GZ and Wen CZ (1994-II). Donors and excitons in triangular GaAs-$Ga_{1-x}Al_xAs$ quantum wells. *Physical Review B* **50**(4) 2689-2692.

Leavitt RP (1987-I). Binding energies of hydrogenic impurities in parabolic quantum wells**.** *Physical Review B* **36** 7650-7652.

Liu W, Zhang DH, Fan WJ, Hou XY and Jiang ZM (2008). Intersubband transitions in GaAsN/GaAs quantum wells. *Journal of Applied Physics* **104**(5) 8.

Merlin R (1987). Subband-Landau-level coupling in tilted magnetic fields: Exact results for parabolic wells. *Solid State Communications* **64**(1) 99-101.

Miller RC, Gossard AC, Kleinman DA and Munteanu O (1984). Parabolic quantum wells with the GaAs-$Al_xGa_{1-x}As$ system**.** *Physical Review B* **29**(6) 3740.

Neethiulagarajan A and Balasubramanian S (1989). On numerical solutions of the radial Schrodinger equation. *European Journal of Physics* **10** 93.

Nelson DF, Miller RC, Tu CW and Sputz SK (1987-II). Exciton binding energies from an envelope-function analysis of data on narrow quantum wells of integral monolayer widths in $Al_{0.4}Ga_{0.6}As$/GaAs**,** *Physical Review B* **36** 8063-8070.

Raigoza N, Duque CA, Reyes-Gómez E and Oliveira LE (2006). Hydrostatic-pressure effects on the correlated electron-hole transition energies in GaAs-$Ga_{1-x}Al_xAs$ semiconductor quantum wells. *Physica Status Solidi B* **243**(3) 635-640.

Sputz SK and Gossard AC (1988-I). Potential-well shape $U(z)=U_0|z/(L_z/2)|^{2/3}$ with the GaAs/$Al_xGa_{1-x}As$ system. *Physical Review B* **38** 3553-3555.

Ungan F, Yesilgul U, Kasapoglu E, Sari H and Sokmen I (2012). Optical intersubband transitions and binding energies of donor impurities in GaInNAs/GaAs/AlGaAs quantum well under the electric field. *International Journal of Modern Physics B* **26**(06) 1-11.

Villamil Pablo, Cabra Carlos and Porras-Montenegro N (2005). Shallow impurity states and transition energies in cylindrical GaAs–$Ga_{0.6}Al_{0.4}As$ quantum well wires under applied magnetic fields, *Journal of Physics: Condensed Matter* **17**(33) 5049-5058.

Yesilgul U, Ungan F, Kasapoglu E, Sari H and Sökmen I (2011). The intersubband transitions and binding energy of shallow donor impurities in different shaped quantum wells under the magnetic field. *Modern Physics Letters B* **25**(32) 2451-2459.