Optical Characterizations of Quantum Structure Family of Infrared Photo Detectors.

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خصائص عائلة الكواشف الضوئية ذات التركيب الكمى
للأشعة تحت الحمراء

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ملخــص

ان عملية حصر الإلكترونات أو الثقوب داخل طبقة رقيقة من مواد أشباه الموصلات تؤدى إلى التغيير الجذرى فى سلوك كل من الإلكترونات والثقوب. ولعل هذا المبدأ يمكن تطويرة والإستفادة منه بتقليل عدد الإتجاهات أو المحاور التى يمكن للإلكترونات أو الثقوب الحركة خلالها. وذلك ابتداءً من تقييد حركة الإلكترون (أو الثقب) فى اتجاة واحد والسماح له بالحركة فى الإتجاهين الآخرين فيما يعرف بالمستوى الكمى، أو عن طرق السماح له بالحركة فى اتجاة واحد وتقييد حركتة فى الإتجاهين الآخرين وهذا مايعرف بالخط الكمى، وفى نهاية المطاف فإنة بإمكاننا تقييد حركته فى جميع الإتجاهات فيما يعرف بالنقطة الكمية.

مانود التركيز عليه فى هذا البحث هو إيضاح ماسبق عن طريق الإستنتاج الرياضى ورسم منحنيات كلاً من مستويات الطاقة ودالة الموجة وكثافة المستويات (the energy levels, the wave function and the density of states) لكل من المستوى الكمى والخط الكمى والنقطة الكمية.

Abstract

The reduction in dimensionality produced by confining electrons (or holes) to a thin semiconductor layer leads to a dramatic change in their behavior. This principle can be developed by further reducing the dimensionality of the electron's environment from a two-dimensional quantum well to a one-dimensional quantum wire and eventually to a zero-dimensional quantum dot. The dimensionality refers to the number of degrees of freedom of the electron momentum, so the electron is confined across two directions within a quantum wire, rather than just the one in a quantum well. In a quantum dot the electron is confined in all three-dimensions, thus reducing the degrees of freedom to zero. Our scope in this paper is to drive and plot the theoretical formulation of the energy levels, the wave function and the density of states of each quantum well, wire and dot structures.

Keywords

I. Introduction

To generate or receive an infrared wavelength it is important to have an infrared device that has energy levels with a difference that equals of the energy of the desired infrared wavelength. Because the energy levels of the natural atoms have certain differences while the infrared band has a continuous wide range of wavelengths, it should search for another physical technique to allow us to detect or generate any infrared wavelength. This technique is called "quantum structure".

Semiconductor quantum structures of different shapes, e.g. well, wire and dot have been grown and a shift in the energy level due to the dimensional quantization has been found from photoluminescence measurements. A heterojunction results in a sudden jump in the value of the band-gap energy at the interface between the two semiconductor materials. Such a jump corresponds to a potential barrier, which can block the movement of charge carriers through the junction. This allows the possibility of creating regions in the semiconductor where one or both charge

carriers can be confined. Two heterojunctions may be located side by side to confine the carriers to a specific region of the material. These are called double heterostructures. Energy levels in such structures may be easily calculated if the potential barriers are of infinite height and the structures have simple geometry such as cubes, wells, cylinders or spheres. The barrier height is about 250 meV in most cases, since the well material is covered by the barrier material. Actual energy levels are, therefore, very different from those obtained by assuming the barrier potential to be infinite. However, for the design of lasers and other electro-optical devices using dimensional quantum-confinement structures, the energy levels will be required to be known properly. To find the energy levels for wells with finite barrier height, the Schrodinger equation must be solved by satisfying the boundary conditions imposed by the geometry of the structure [1]. The rapid changes in the number of carriers leads to electron transport phenomena due to which stimulated emission and electromagnetic radiations are occurred [2]. The semiconductor structures whose sizes are small enough that their quantum effects may be significant are called quantum structures [3]. The energy distribution of the electrons in the quantum structures is narrower than that in the bulk structures. Therefore, the optical gain concentrates on certain energy (wavelength). As a result, in the quantum structure lasers, a low threshold current, a high speed modulation, a low chirping, and a narrow spectral linewidth are expected [3]. The infrared detection mechanism is based on the intraband photoexcitation of electrons from confined states in the conduction band wells or dots into the continuum. The emitted electrons drift towards the collector in the electric field provided by the applied bias, and photocurrent is created [4].

II. Model description and theoretical background

In the next sections, a theoretical comparison between different quantum structures (well, wire and dot) is presented by using constant quantum parameters such as quantum dimensions, effective mass, etc... The theoretical calculations of energy levels of quantum structures are determined using time independent Schrodinger equation. In quantum well structure, Schrodinger equation is solved in one dimensional only while the other two dimensions are still unchanged as in bulk structure. On the other hand, the contrary in the case of quantum wire structure; i.e. the Schrodinger equation must be solved in two dimensions only leaving the other dimension unchanged as in bulk structure. Additionally, in quantum dot structure, it is solved in all three dimensions. In the following, our scope is to briefly outline the basic characteristics of each one of the quantum family of optical devices.

II.1- Structure of quantum well

In this category of optical devices, the active layer takes the structure of quantum well. If the underlined device contains one potential well, it is called single quantum well device (SQW), while that has plural QWs is known as multiple quantum well (MQW) as shown in Fig. (1) [3, 5].
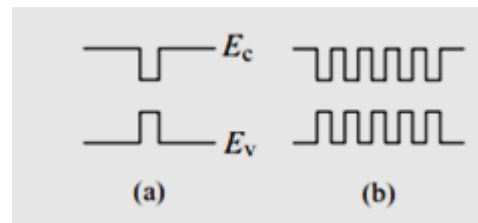

Figure 1 (a) SQW, (b) MQW

II.1.1-   The infinite potential quantum well

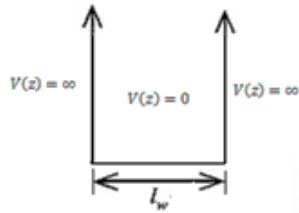It is assumed that a carrier exists in a square potential well, as shown in Fig. (2).

Figure 2 one-dimensional infinite potential quanta well

By restricting the Schrodinger equation of this square potential well to the one-dimensional potential of interest here (z-dimensional), then the Schrodinger equation for a particle of mass **m** in a potential well aligned along the z-axis (as in Fig. (2)) [3, 5, 6] would be:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi(z) + V(z)\psi(z) = E\psi(z) \quad (1)$$

Outside of the well, the potential energy $V(z) = \infty$, and hence the only possible solution of the wave function outside of the well is $\psi(z) = 0$. So $\psi(z)$ inside the well will be

$$\psi_n(z) = \sqrt{\frac{2}{l_w}}\sin(kz) \quad , \quad k$$

$$= \frac{n\pi}{l_w} \qquad (2)$$

k : denotes the wave vector while **n** stands for an integer representing a series of solutions. The energy of the confined states is given by [7]:

$$E_n$$
$$= \frac{\hbar^2\pi^2 n^2}{2ml_w^2} \qquad (3)$$

Figs (3 & 4) display the results of calculations of the lowest three energy states of an electron in a GaAs well of width l_w surrounded by hypothetical infinite barriers.

Figure 3 Solution of one-dimensional infinite potential quantum well
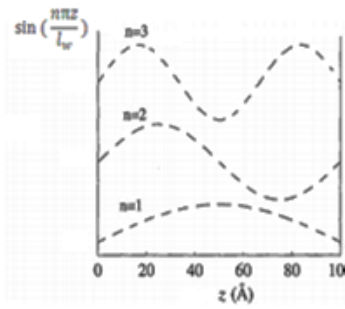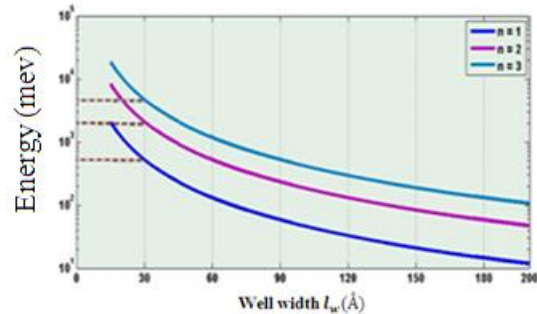

Figure 4 First three energy levels versus well width for an electron in a GaAs infinite potential well

II.1.2- The finite potential quantum well

Suppose a single particle of mass m^* confined within a region $0 < z < L$ with potential energy $V(z) = 0$ bounded by potential barriers $V(z) = V$ as shown in Fig.(5). By solving the time independent Schrodinger equation for this potential system, the obtained three solutions are

$$\psi(z) = Be^{\alpha z} \qquad z \leq 0 \qquad (4)$$
$$\psi(z) = P\cos(kz) + Q\sin(kz) \quad 0 < z < L \qquad (5)$$
$$\psi(z) = Ce^{-\alpha z} \qquad z \geq L \qquad (6)$$

$$k = \sqrt{\frac{2m^*E}{\hbar^2}} \quad \text{and} \quad \alpha$$

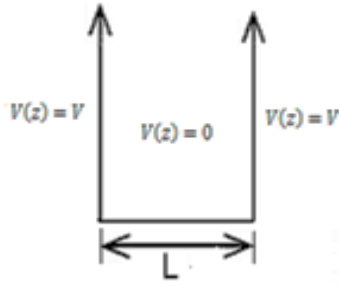$$= \sqrt{\frac{2m^*(V-E)}{\hbar^2}} \qquad (7)$$

Figure 5 one-dimensional finite potential quanta well

In the above expressions B, P, Q and C are some constants and the relations among them can be obtained through the boundary conditions at z=0 and z=L. This means that the first two solutions; i.e. Eqs.(4 & 5), along with their first derivatives must be the same at $z = 0$, while the second, Eq.(5), and third, Eq.(6), solutions along with their derivatives must be the same at $z = L$. The result of this equating gives us a homogeneous system of equations that has solutions, only if the determinant of the system vanishes

$$\begin{vmatrix} \alpha & -k \\ \alpha\cos(kL) - k\sin(kL) & \alpha\sin(kL) + k\cos(kL) \end{vmatrix} = 0 \quad (8)$$

This condition leads to

$$\tan(kL) = \frac{2\alpha k}{k^2 - \alpha^2} \quad (9)$$

Solving this equation as a function of k will give the allowed values of k for which the particle in this finite potential well has available energy states. The corresponding energies become

$$E = \frac{h^2 k^2}{2m^*} \quad (10)$$

Eq. (9) can be rewritten in the form

$$\tan(kL) = \frac{2(\frac{\alpha}{k})}{1 - (\alpha/k)^2} \quad (11)$$

Comparing the last equation with the two trigonometric formulae given by:

$$\tan 2\theta = \frac{2\tan\theta}{1 - \tan^2\theta} \quad \text{and} \quad \tan 2\theta = \frac{2\cot(-\theta)}{1 - \cot^2(-\theta)}$$

The two following conditions can be obtained as,

$$\tan\left(\frac{kL}{2}\right) = \frac{\alpha}{k} \;,$$
$$-\cot\left(\frac{kL}{2}\right) = \frac{\alpha}{k} \quad (12)$$

This leads to get:

$$\frac{\alpha}{k} = \sqrt{\frac{V - E}{E}} = \sqrt{(\frac{k_0}{k})^2 - 1} \quad (13)$$

Where

$$k_0 = \sqrt{\frac{2m^*V}{\hbar^2}} \quad (14)$$

To plot those formulas as a function of $\left(\frac{kL}{2}\right)$, it is useful to rewrite the above expression for α /k as
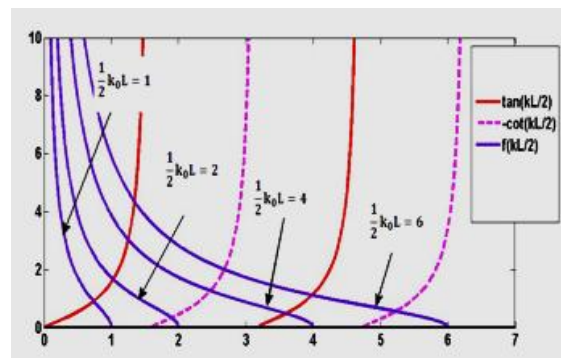
$$\frac{\alpha}{k} = \sqrt{(\frac{\frac{1}{2}k_0 L}{\frac{1}{2}kL})^2 - 1} = f(\frac{1}{2}kL) \quad (15)$$

Where,

$$\tan\left(\frac{kL}{2}\right) = f\left(\frac{1}{2}kL\right) \text{ and } -\cot\left(\frac{kL}{2}\right)$$
$$= f\left(\frac{1}{2}kL\right) \quad (16)$$

Now, one can plot $\tan\left(\frac{kL}{2}\right), -\cot\left(\frac{kL}{2}\right)$ and $f\left(\frac{1}{2}kL\right)$ as a function of $\frac{1}{2}kL$ for various values for k_0.

Figure 6 Graph to determine bound states a finite potential quantum well

The points of intersection of the curve $f\left(\frac{1}{2}kL\right)$ with the tan and −cot curves will then give the kL values for an allowed energy levels of the particle in this potential [7]. This is illustrated in Fig. (6) Where

there are four curves given for different values of V. The important feature of these curves is that the number of points of intersection is finite, there are only a finite number of values of k that solve Eq. (16). Correspondingly, there will only be a finite number of allowed values of **E** for the particle, and there will always be at least one allowed value. To determine the corresponding wave functions is a straight forward. The first step is to show, by using Eq. (16) and the equations for B , C , P and Q that

$$\psi(z) = Be^{\alpha z} \qquad z \le 0 \tag{17}$$

$$\psi(z) = B(\cos(kz) + \frac{\alpha}{k}\sin(kz)) \qquad 0 < z < L \tag{18}$$

$$\psi(z) = Be^{-\alpha(z-L)} \qquad z \ge L \tag{19}$$

The constant B is determined by

$$\int_{-\infty}^{\infty} |\psi(z)|^2 \ dz = 1 \tag{20}$$

The result found is that

$$B = \frac{k}{k_0} \sqrt{\frac{\alpha}{\frac{1}{2}\alpha L + 1}} \tag{21}$$

Figure (7) summaries the application of the method to a GaAs single quantum well, surrounded by barrier of height 100 meV.
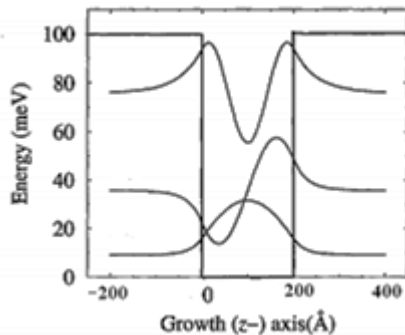

Figure 7 Eigen functions $\psi(z)$ for the first three energy levels of the $200A^0$ GaAs well with constant effective mass $m^* = .067m_0$ and V=100meV

II.1.3- Density of States of Quantum Well Structure

The density of states is defined as the number of states per energy per unit volume of real space:

$$\rho(E) = \frac{dN}{dE} \tag{22}$$

In k−space, the total number of states N is equal to the volume of the sphere of radius k, divided by the volume occupied by one state and divided again by the volume of real space, so

$$\frac{dN}{dk} = 2\frac{4\pi k^2}{(2\pi)^3} \quad , \quad \frac{dk}{dE}$$

$$= (\frac{2m^*}{\hbar^2})^{\frac{1}{2}} \frac{E^{-\frac{1}{2}}}{2} \tag{23}$$

This finally gives the density of states in bulk as:

$$\rho(E) = \frac{1}{2\pi^2}(\frac{2m^*}{\hbar^2})^{\frac{3}{2}} E^{\frac{1}{2}} \tag{24}$$

The density of states in quantum well systems follows analogously; however this time, as there are only two degrees of freedom, successive states represented by values of n_x and n_y fill a circle in k−space, as illustrated in Fig. (8).
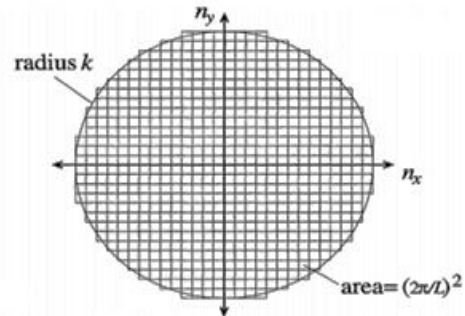

Figure 8

The total number of states per unit cross-sectional area is given by the spin degeneracy factor, multiplied by the area of the circle of radius k, divided by the area occupied by each state, and divided by the area in real space.

$$N^{2D} = 2\pi k^2 \frac{1}{(2\pi/L)^2} \frac{1}{L^2}$$

$$= \frac{2\pi k^2}{(2\pi)^2} \tag{25}$$

$$\therefore \frac{dN^{2D}}{dk}$$

$$= \frac{k}{\pi} \qquad (26)$$

Now, the density of states in (2D) can be defined as

$$\rho^{2D}(E) = \frac{dN^{2D}}{dE}$$

$$= \frac{dN^{2D}}{dk}\frac{dk}{dE} \qquad (27)$$

As the in-plane dispersion curves are still described by parabolas, then reuse can be made of equation (23), as follows:

$$\rho^{2D}(E)$$

$$= \frac{k}{2\pi}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{1}{2}} \quad E^{-\frac{1}{2}} \qquad (28)$$

By substituting for k in terms of the energy E, using equation (7), the density of states for a single subband in a quantum well system can be obtained as,

$$\rho^{2D}(E)$$

$$= \frac{m^*}{\pi\hbar^2} \qquad (29)$$

If there are many (n) confined states within the quantum well system then the density of states ρ^{2D} at any particular energy is the sum over all subbands below that point, which can be written succinctly as:

$$\rho^{2D}(E) = \sum_{i=1}^{n} \frac{m^*}{\pi\hbar^2} \Theta (E - E_i) \qquad (30)$$

Where, Θ is the unit step function [5, 7, 8, 9, 10, 11]. Fig. (9) gives an example of the two-dimensional density of states for a particular quantum well with L = 3nm showing the first three confined levels that have energies values of Fig. (4).
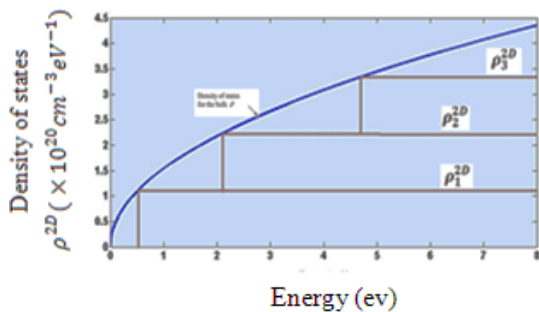

Figure 9 Density of states for the one-dimensional quantum well for $L_z = 3nm$ and

$m^* = 0.08m_0$ (brown line) and that for the bulk structures (blue line)

II.2-   Structure of Quantum Wire

Fig. (10) gives a simple outline of how quantum wires might be fabricated. Any charge carriers are still confined along the heterostructure growth (z-) axis, as they were in the quantum well, but they are now confined along an additional direction y-axis.
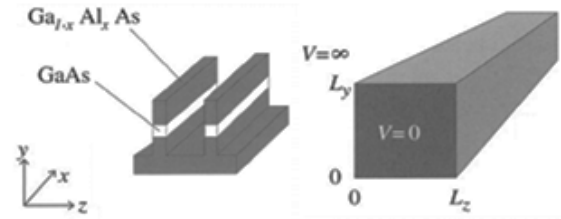

Figure 10 Structure of quantum wire

II.2.1-   The Infinite Potential Quantum Wire

By considering the case of an infinite potential at the sides of the wire with
-        The wire having zero potential, and
-        The wire running in the X- direction as shown in Fig. (10), the Schrodinger equation can be written as,

$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V_1 + V_2(y)\right.$$
$$\left. + V_3(z)\right]\psi_1(x)\psi_2(y)\psi_3(z)$$
$$= E\psi_1(x)\psi_2(y)\psi_3(z) \qquad (31)$$

Where V1=0. This equation can be decomposed into the following three equations (a, b and c):

a) $-\dfrac{\hbar^2}{2m^*}\dfrac{\partial^2}{\partial x^2}\psi_1(x)$
$= E_1\psi_1(x) \qquad (32)$
$\therefore \psi_1(x) = e^{ik_x x}$ with E_1
$$= \frac{\hbar^2 k_x^2}{2m^*} \qquad (33)$$

b) $\left[-\dfrac{\hbar^2}{2m^*}\dfrac{\partial^2}{\partial y^2} + V_2(y)\right]\psi_2(y)$
$$= E_2\psi_2(y) \qquad (34)$$

$$\therefore \psi_2(y) = \psi_n(y)$$

$$= \sqrt{\frac{2}{L_y}} \sin\left(\frac{n_y \pi}{L_y} y\right) \qquad (35)$$

c) $\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + V_3(z)\right] \psi_3(z)$

$$= E_3 \psi_3(z) \qquad (36)$$

$$\therefore \psi_3(z) = \psi_n(z)$$

$$= \sqrt{\frac{2}{L_z}} \sin\left(\frac{n_z \pi}{z} z\right) \qquad (37)$$

The confined states of a quantum wire are therefore described by the two principal quantum numbers n_y and n_z [4,6], which give the components of energy as:

$$E_2 = E_y$$
$$= \frac{\hbar^2 \pi^2 n_y^2}{2m^* L_y^2} \qquad (38)$$

$$E_3 = E_z$$
$$= \frac{\hbar^2 \pi^2 n_z^2}{2m^* L_z^2} \qquad (39)$$

Thus, the total energy due to confinement, $E_{y,z} = E_y + E_z$, is:

$$E_{y,z} = \frac{\hbar^2 \pi^2}{2m^*} \left(\frac{n_z^2}{L_z^2} + \frac{n_y^2}{L_y^2} \right) \qquad (40)$$

Fig. (11) displays the confinement energies $E_{y,z}$ for (n_z, n_y) equal to (1,1), (1,2),(2,1), and (2,2) as a function of the side length $L_z = L_y$. In the case of $L_z = L_y$ a square cross-sectional wire, the confinement energies of the (1, 2) and (2, 1) states are equal; however clearly this will not be the case for a rectangular cross-section wire, which has $L_z \neq L_y$.
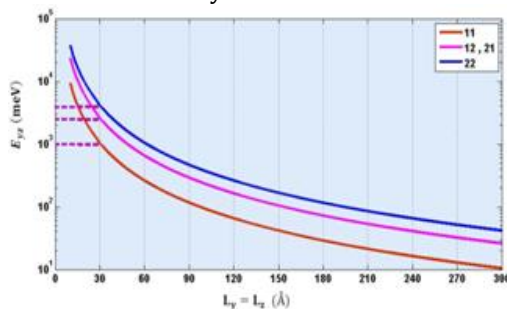

Figure 11 First three energy levels versus well width for an electron in a $GaAs$ infinite potential quantum wire

II.2.2- The finite potential quantum wire

Fig. (12) (a) illustrates the two-dimensional confinement potential $V(y, z)$. For this system, it is not possible to write the potential $V(y, z)$ as a sum of two independent potentials $V(y)$ and $V(z)$, and thus it is not possible to separate the y- and z-motions. However, a very loose approximation may be to write the potential as in Fig. (12) (b).
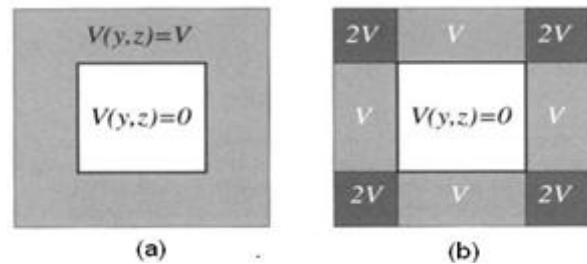

Figure 12 (a) Rectangular finite potential quantum wire, (b) approximate form for the potential

The approximation occurs in the 'corner regions' outside of the wire where the two quantum well potential barrier heights V sum to give 2V. So the Schrodinger equation for the y-z cross-sectional confined motion in a quantum wire is given by

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}\psi(z) + V(z)\psi(z) = E_z \psi(z) \qquad (41)$$

And

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}\psi(y) + V(y)\psi(y) = E_y \psi(y) \qquad (42)$$

The final outcome is the same, namely that as the independent potentials $V(y)$ and $V(z)$ are simply those of a finite quantum well, then the solutions for both the wave functions and the confinement energies follow as a finite quantum well.

II.2.3- Density of States of Quantum Wire Structure

In the bulk crystal, the three degrees of freedom for the electron momentum mapped out a sphere in k-space, while in a quantum well the electron momentum fill successively circles, continuing this argument for a quantum wire with just one degree of freedom, the electron momentum

then fill states along a line. Therefore, proceeding with the same argument as before, the total number of states N is then equal to the length of the line in k-space (2k), divided by the length occupied by one state ($2\pi/L$), and divided by the length in real space (see Fig. (13)).
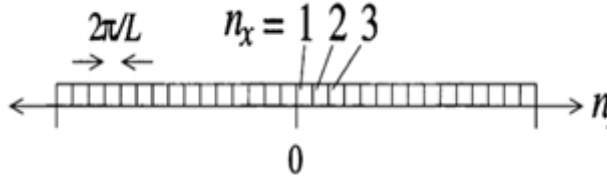

Figure 13 The occupation of states in k-space along a one-dimensional quantum wire

$$N^{1D} = 2 \times 2k\frac{1}{2\pi/L}\frac{1}{L}$$
$$= \frac{2k}{\pi} \qquad (43)$$

Where, the '2' factor accounts for spin degeneracy. Therefore:

$$\therefore \frac{dN^{1D}}{dk} =$$
$$\frac{2}{\pi} \qquad (44)$$

$$\therefore \rho^{1D}(E)$$
$$= \frac{1}{\pi}(\frac{2m^*}{\hbar^2})^{\frac{1}{2}} \quad E^{-\frac{1}{2}} \qquad (45)$$

If there are many (n) confined states within the quantum wire with subband minima E_i, then the density of states at any particular energy is the sum over all the subbands below that point [4, 7, 8], which can be written as:

$$\rho^{1D}(E) = \sum_{i=1}^{n}(\frac{2m^*}{\hbar^2})^{\frac{1}{2}} \frac{1}{\pi(E - E_i)^{\frac{1}{2}}}\Theta\,(E - E_i) \qquad (46)$$

Fig. (14) gives an example of the 1D density of states, for a square cross-section GaAs quantum wire surrounded by infinite barriers with $L_y = L_z = 3nm$ that has energy levels values of Fig. (11).
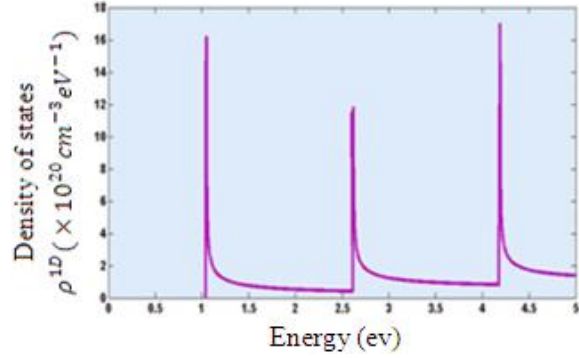

Figure 14 The density of state in one-dimensional infinite quantum wire

II.3- Structure of Quantum Dot

Cuboids quantum dots, perhaps more specifically designated as quantum boxes can be thought of as simply a generalization of the rectangular cross-section quantum wires, in which there is additional confinement along the remaining x-axis as shown in Fig. (15). This additional confinement removes the remaining degree of freedom in the particle's momentum.

Figure 15 Structure of quantum dot
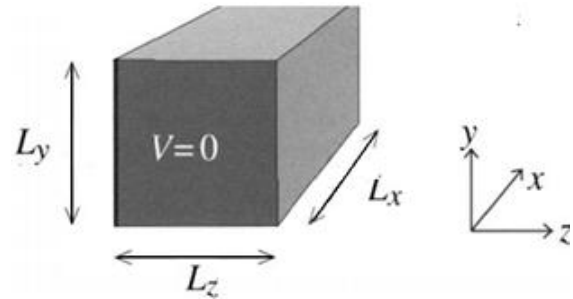
II.3.1- The Infinite Potential Quantum Dot

Considering the case of an infinite potential separating the inside of the box from the outside, then the Schrodinger equations within the box is given by:

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2}\psi(x)$$
$$= E_x\psi(x) \qquad (47)$$
$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}\psi(y)$$
$$= E_y\psi(y) \qquad (48)$$
$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}\psi(z)$$
$$= E_z\psi(z) \qquad (49)$$

The solutions are just the solutions to infinitely deep quantum wells, of widths L_x, L_y and L_z respectively.

The confinement energy within this quantum box follows as:

$$E_{x,y,z} = \frac{\hbar^2\pi^2}{2m^*}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right) \qquad (50)$$

The three-dimensional nature of the confinement thus requires three quantum numbers, n_x, n_y and n_z to label each state.

II.3.2- The finite Potential Quantum Dot

Finite-barrier quantum boxes could be gleaned from three decoupled one-dimensional quantum well calculations in a similar manner to the finite barrier quantum wire. However, in this case any perturbative correction would have to account for eight corner-cubes of additional potential 2V and twelve edge-cuboids of additional potential ′V′. Alternatively, a full three-dimensional solution can be constructed by expanding the wave function as a linear combination of infinite well solutions.

II.3.3- Density Of States Of Quantum Dot Structure

For brevity, by letting $L_x = L_y = L_z = L$, the energies are written as

$$E = E_x + E_y + E_z \qquad (51)$$

$$E_x = \frac{\hbar^2\pi^2}{2m^*}\left(\frac{n_x^2}{L^2}\right) \qquad (52)$$

$$E_y = \frac{\hbar^2\pi^2}{2m^*}\left(\frac{n_y^2}{L^2}\right) \qquad (53)$$

$$E_z = \frac{\hbar^2\pi^2}{2m^*}\left(\frac{n_z^2}{L^2}\right) \qquad (54)$$

It should be noted that the energies are completely discrete [5, 7, 8]. The density of states $\rho^{0D}(E)$ is a delta function, which is written as

$$\rho^{0D}(E) = 2 \sum_{n_x,n_y,n_z} \delta(E - E_x - E_y - E_z) \qquad (55)$$

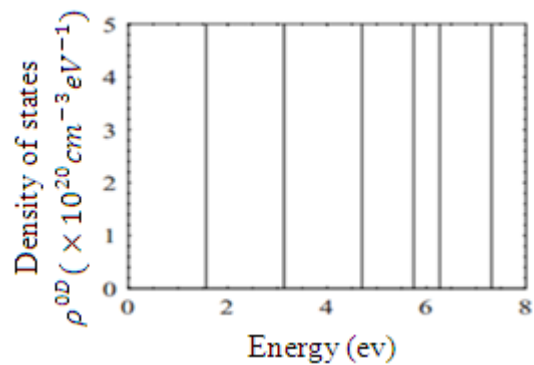Figure 16 shows the density of states in the three-dimensional quantum well (quantum box).

Figure 16 Density of states of quantum dot

Conclusions

Wave function and energy level equations of quantum well, wire, and dot are presented and plotted under specific parameters of quantum structures. After that the density of states of bulk, quantum well and wire structures are calculated. It can be seen that successive reductions in the degrees of freedom for the electron motion, lead to reductions in the functional form of p(E) by factor of $E^{1/2}$.

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