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RELATIONSHIP BETWEEN THE GROUND ENERGY LEVEL AND THE WELL – WIDTH OF ONE – DIMENSIONAL KRONIG – PENNY MODEL OF GaAs/AlGaAs. FOR ELECTRON, LIGHT HOLE AND HEAVY HOLE USING POWER SERIES EXPANSION

D. A. AJADI, O. M. ONI & K. S. OLASUNKANMI

Department of Pure and Applied Physics, Ladoke Akintola University of Technology. Ogbomosho, Nigeria

ABSTRACT

Computational analysis of the dispersion equation of the simplest Kronig – Penney Model for a general one – dimensional periodic potential was analyzed using power series expansion. The resulting solution obtained when the first term of the expansion series was used, shows that the energy of a particle, Electron (E); Light Hole (LH) and Heavy Hole (HH) can never be zero as the well-width increases and that it has a minimum value at very large well-width.

The result also shows that the use of different effective mass of E, LH, and HH in the potential well and the barrier provide the distinct differences between their eignvalues even though they all obey the similar power law.

KEYWORDS: Kronig – Penney Model, GaAs/AlGaAs, Schrodinger Equation

INTRODUCTION

In the early1960's, germanium (Ge) was the major semiconductor material, however germanium proved unstable in many applications because its devices exhibited high leakage current at moderately elevated temperatures (Shockley, 2010).In addition, germanium oxide is water soluble and unsuited for devices fabrication. In quantum mechanics, the analogue of Newton's law is Schrodinger's equation for a quantum system, usually atoms, molecules and subatomic particle; free, bound, or localized. In quantum mechanics, the Schrodinger equation is a partial differential equation that describes how the quantum state of a physical system changes with time. In classical mechanics the equation of motion is Newton's second law, and equivalent formulations are the Euler – Lagrange equation and Hamilton's equation. In all these formulations, they are used to solve for the motion of a mechanical system, and mathematically predict what the system will do at any time beyond the initial settings and configuration of the system (Kollmitzer, et al. 2011). The one-dimensional motion of a particle subjected to a periodic step-like potential serves as a prototype for particle motions in the crystal. Many treatments begin with and dwell considerably on the problem of finding energies or eignvalues of one-dimensional systems. The simplest model of a one-dimensional periodic potential is provided by an array of rectangular wells and barriers, illustrated in Figure 1 as originally given by Kronig – Penney in 1931.

The model is of considerable importance because it interprets the main features of the band structures of metals. The increase in the capacity of micro electrons to fabricate smaller devices is giving birth to a new era in nano – science technology, where the quantum natures of particles (electron, light hole and heavy hole) are more increasingly revealed. The Kronig – Penney (K – P) model is a strongly simplified one dimensional quantum mechanical model of a crystal (Donald, 1996; Himpsel et al. 2001). In spite of the simplifications, the electronic band structure obtained from this model shares many features with band structures that result from more sophisticated models. Despite the simplification, the

electronic band structure obtained from this model, shares many features with band structures that result from more sophisticated models. A new formalism of the K – P model has been developed which is considerably simpler than the conventional one. It gives not only the carrier energy bands but also the wave functions at the edges of each band. Although it is formulated to be applied to supper lattices, it is also applicable to bulk materials. Band structures with multiple quantum wells have mini bands in the quantum wells and for symmetric reasons, also for holes in the quantum well along the valence band (Donald, 1996).

The physical properties of semiconductors in very thin layers of the order of 10 nm have attracted much international attention both for fundamental reasons and for their potential applications (Ajadi et al., 2009) There have been the establishment and development of nanostructures, which are called Super-lattices (SL) or Multiple Quantum Wells (MQW) depending on the width of the barrier layers or simply called Heterostructures (Adelabu, 2002). Electrons and holes can propagate freely in the periodic potential of semiconductors. The regions denoted I correspond to the positively charged ions of the crystal lattice, the regions denoted II represent the empty spaces between the ions (McKelvey et al. 2006) It is the choice of this oversimplified potential that makes an analytical solution possible. The lattice parameter is d = a + b. The K - P potential is defined by three parameters, V_o, a, and d. The choice of the zero on the energy axis has no influence on the physics of the problem (Soren, 2005). This periodic square well problem requires a tedious amount of algebra for its solution because of the repetitive calculations involved.

In this paper, power series expansion is applied in analyzing the dispersion equation of the K – P Model Equation to show the relationship between the lowest possible energy E_o and the variation of well width.

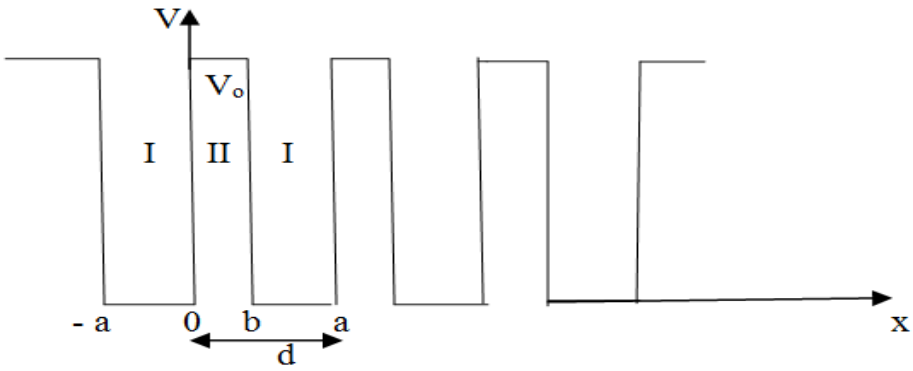

Figure 1: One – Dimensional Kronig - Penney Model, with d = a + b

Theoretical Background Calculation

Kronig – Penney generalized the double – well model to the N – well model (N → ∞) for the electron energies in meters. Each well represents the attractive potential due to an ion core seen by valence electron. If at time t = 0 the electron is localized in the well at one end, it propagates (tunnels) along the regularly spaced wells during its subsequent evolution. In the stationary state it has equal probability of being found in any of the wells. In this model the wave functions and their derivatives are matched at the material interfaces while a propagating solution through the whole crystal is sought using periodic boundary conditions (Adelabu, 1998). The periodic field assumed was in the form of potential wells of zero potential energy with width a, separated by rectangular barriers of width b, and height V_o as illustrated in Figure 1 above. The solution of one – dimensional time independent Schrodinger wave equation is determined in the regions I and II of Figure 1 above.

For region I, the Schrodinger wave equation is given as:

$$\nabla^2\Psi + k_1^2\Psi = 0 \quad (1)$$

For region II, the Schrodinger wave equation is given as:

$$\nabla^2\Psi + k_2^2\Psi = 0 \quad (2)$$

Where $k_1^2 = \frac{2m_1^* E}{\hbar^2}$; k_1 is real in the well and $k_2^2 = \frac{2m_2^*(E - V_o)}{\hbar^2}$ k_2 is real for $E < V_o$ and imaginary for $E > V_o$ in the barrier. E is the energy of the particle also called the eigenvalues (electron or hole) as the case may be; while V_o is the barrier energy or height (band edge discontinuity); k_1 and k_2 are the wave vectors in the well and the barrier respectively.

The solutions of the two equations above are given as:

For equation 1: $\Psi_1 = A \exp(ik_1x) + B \exp(-ik_1x)$ $(-a < x < 0, V(x) = 0)$ (3)

Where A and B are constant called incident and reflected wave amplitudes in the well respectively.

For equation 2: $\Psi_2 = C \exp(ik_2x) + D \exp(-ik_2x)$ $(0 < x < b, V(x) = V_o)$ (4)

Where C and D are constant called incident and reflected wave amplitudes in the barrier region.

For continuity, the boundary condition at x = 0 is applied,

$$\Psi_1(0) = \Psi_2(0) \text{ and } \left.\frac{d\Psi_1}{dx}\right|_{x=0} = \left.\frac{d\Psi_2}{dx}\right|_{x=0} \quad (5)$$

In a periodic lattice with V (x + a) = V (x), it is expected that the wave function will also exhibit this periodicity. Since the wave function must be a Bloch wave function, therefore the condition equation is given by: $\Psi_1(x + a + b) = \Psi_2(x) \exp[ik_2 (a + b)]$.

Incorporating this requirement at x = - b and x = a then: $\Psi_2 (-b) = \Psi_1 (a) \exp[ik_1 (a + b)]$; the boundary condition is applied thus:

$$\left.\frac{d\Psi_2}{dx}\right|_{x=-b} = \left.\frac{d\Psi_1}{dx}\right|_{x=a} \exp[-ik_2(a+b)] \quad (6)$$

It is necessary not to match the wave functions in the different regions of V(x) for all the wells in Figure 1 above. This reduces the arbitrarily large number of constants to just few. It is enough to consider just one of the regions say 0 < x < d. Applying all these boundary conditions, four equations in four unknown are obtained.

$A + B = C + D$

$ik_2 (A - B) = k_1 (C - D)$

$C \exp(ik_2b) + D \exp(-ik_2b) = \exp[ik_2(a + b)] \{ A \exp(ik_1a) - B \exp(-ik_1a) \}$

$k_1C \exp(ik_2b) + k_1 D \exp(-ik_2b) = \exp[ik_2(a + b)] ik_2\{A \exp(ik_1a) - B \exp(-ik_1a) \}$

For a nontrivial solution of the equations, the determinant of the coefficients of A, B, C, and D should vanish.

For $E < V_o$ the relation gives

$$\cos kd = \cos k_1 a \cosh k_2 b - \tfrac{1}{2}\left(c - c^{-1}\right) \sin k_1 \sinh k_2 \quad (7)$$

where $$c = \frac{m_2^* k_1}{m_1^* k_2}$$

so that the wave function is oscillating in the region I and eventually decaying in region II.

For $E > V_o$ the relation gives the value of ik_2 becomes k_2 and transforms the expressions of equation 7 to be

$$\cos qd = \cos k_1 a \cos k_2 b - \tfrac{1}{2}\left(z - z^{-1}\right) \sin k_1 a \sin k_2 b \quad (8)$$

where $$z = \frac{m_2^* k_1}{m_1^* k_2}$$

The band edge are such that $qd = 0$ and π in equation 8 above thus gives $\cos qd = \pm 1$. The dispersion relation of equation 8 shows that any rapidly varying term like the value of the periodic part of the Bloch function at the interface has disappeared. This result is coherent with the identification of the interface with planes. To avoid the edge effect at the two ends of the lattice, Born and von Karman assumed that the wave function has the same value at both ends (Adelabu).

Numerical Computation

Equation 8 above when solved using the power series expansion show the relationship between the energy and well width. In the model above the same masses for the charge carriers (electrons, light and heavy holes) in both the well and the barrier were used, whereas these particles have their respective effective masses in the well different from those in the barrier (Adelabu, 1993). For this work the following assumptions are used:

- The series expansion for cosine and sine functions are considered using only the first term only which is given as: $\sin x = x$ and $\cos x = 1$.
- Potential barrier width is fixed as b.
- Potential barrier height V_o is constant
- The values of effective masses of the electron (E), light holes (LH), and heavy hole (HH) for well and barrier of GaAs/AlGaAs materials used are shown in Table 1 below as given by Adelabu (1993).

Table 1: Effective Masses of Particles

Particles	Well (GaAs) m_1^*	Barrier (AlGaAs) m_2^*
Electron E	0.067 m_o	0.092 m_o
Light Hole LH	0.082 m_o	0.102 m_o
Heavy Hole HH	0.450 m_o	0.051 m_o

- The other constants values used in the computation are: $V_o = 0.374$eV; b = 10 nm;

$m_o = 9.1 \times 10^{-31}$ kg; and $\hbar^2 = 1.055 \times 10^{-34}$ all these values are adopted from Adelabu, 1993. Using equation 8, applying the condition $qd = \pi$, and $\cos qd = -1$; then the equation becomes

$$-1 = \cos k_1 a \cos k_2 b - \tfrac{1}{2}(z + 1/z) \sin k_1 a \sin k_2 b \quad (9)$$

Applying the power series expansion on equation 9 gives

$$4 = (z + 1/z)(k_1 a)(k_2 b) \quad 10$$

Substituting the values of z, k_1, and k_2 in equation 10, re-arrangement, the resulting equation and making E the subject of the equation gives:

$$E = \frac{F}{a} + G \quad 11$$

where F and G are constants depending on the particle under consideration and are given as:

$$F = \frac{4\hbar^2}{b\left(m_1^* + m_2^*\right)} \quad 12$$

$$G = \frac{m_1^* V_o}{\left(m_1^* + m_2^*\right)} \quad 13$$

Putting the constant values in equations 12 and 13 respectively for electron (E), light hole (LH) and heavy hole (HH) respectively the following equations are obtained from equation 11 as:

$$\text{For electron:} \quad E = \frac{2.916\times10^5}{a} + 0.158\times 10^{-19} \quad 14$$

$$\text{For light hole: } E = \frac{2.521\times10^5}{a} + 0.169\times 10^{-19} \quad 15$$

$$\text{For heavy hole: } E = \frac{0.926\times10^5}{a} + 0.335\times 10^{-19} \quad 16$$

Equations 14, 15 and 16 provide the simplest form of energy – well width relationship for computation and graphical analysis, varying the well width from 5nm to 500nm.

RESULTS AND DISCUSSIONS

From Equations 14, 15, and 16, there is a finite energy (E_o) at very large well width for each of the particle that is, as the well width turns to infinity the energy turns to infinity that is asymptotically to the well width.

The graphical illustration of figure 1 shows the compact results for range d between 5nm – 500nm. Energy increases near the zero point of the well and decreases exponentially along the well width. Thus energy curve is asymptotic to the well width axis. Hence both the energy and the well width cannot be zero which is shown clearly in the graph.

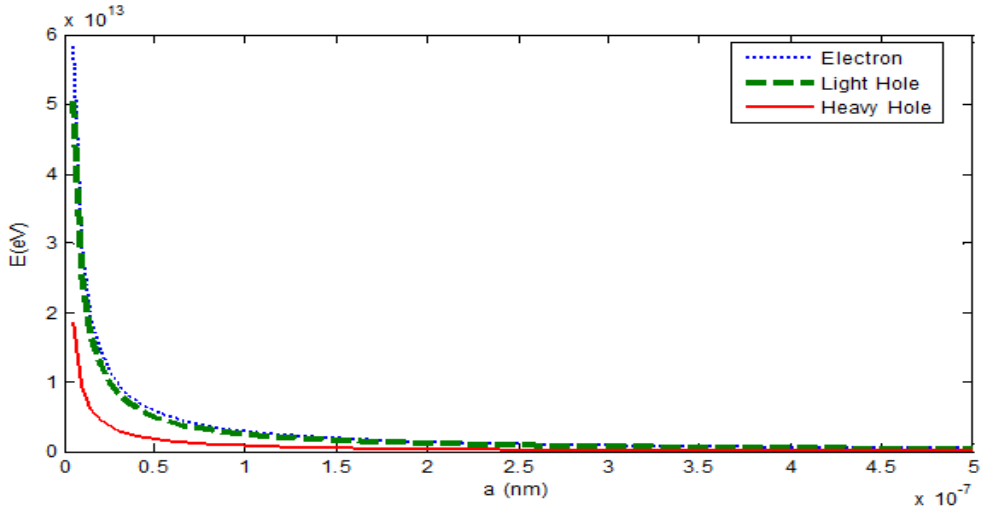

Figure 2: Variations in Ground Sate Energies of Particles with Well Width

CONCLUSIONS

It can be concluded that the method used in this work provided results that show that energy decreases exponentially with well – width, which is similar to the result of deep well potential obtained from the solution of a one – dimensional time independent Schrodinger Equation.

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