



Influence of band non-parabolicity on electric field induced shifts in the bound states of a finite-barrier quantum well

Dibyendu Bala¹, Shubhasree Biswas Sett², Chayanika Bose¹

¹Department of Electronics and Telecommunication Engineering,
Jadavpur University,
Kolkata 700 032, West Bengal, India.

²The Institution of Engineers
8, Gokhale Road, Kolkata 700 020, West Bengal, India

Abstract: In this communication, electric field induced shifts in the energy levels, in presence of band non-parabolicity, are estimated by perturbation method for a finite-barrier quantum well. The band non-parabolicity induces lowering in all the bound states with greater influence on higher-lying levels. As the inter-subband separations are smaller in lower energy region, such downward shifts give rise to stronger overlapping of the neighbouring wave functions and thereby, greater field induced shifts. Thus, the energy lowering caused by the effect of band non-parabolicity enhances the electric field induced lowering in the ground state, while it partly compensates the field induced upward shifts in all other excited states.

Keywords: Band non-parabolicity, Electric field, Perturbation method, GaAs/Al_{0.4}Ga_{0.6}As quantum well

I. Introduction

The $\mathcal{E}$ - k dispersion relation of electrons in a semiconductor is nearly parabolic at the bottom of its conduction band and deviates more and more with increasing electron energy. In a square quantum well (SQW), the ground state itself lies above the band edge and the inter-subband separation increases with energy, placing the excited states away from the band edge. Consideration of band non-parabolicity thus becomes much more relevant in QWs, and is well investigated for such structures [1-3]. Under its influence, the energy levels are found to experience a downward shift. Further, application of an external electric field results in lowering of the ground state, while raising the excited states [4-8]. Therefore, the influence of band non-parabolicity on the energy levels, in presence of electric field, is worth investigating.

In this communication, we consider the effect of band non-parabolicity and determine energy of all the bound states in a finite SQW subjected to an electric field applied along its narrow dimension. In context of influence of band non-parabolicity on electric field induced shifts in ground state of an infinite-barrier SQW, we have seen earlier that perturbation method with the properly restricted electric field yields results as accurate as those obtained from variational method [9]. We, therefore, employ perturbation method to estimate the shifts in the bound state energies of a finite-barrier SQW due to incorporation of band nonparabolicities, both in absence and presence of external electric field.

II. Theory

To proceed, we first consider the Luttinger-Kohn equation [10], expressed as

$$\left[\mathcal{E} \left(-i \frac{d}{dx} \right) + V \right] \psi = E \psi, \quad (1)$$

where, $\mathcal{E} \left(-i \frac{d}{dx} \right)$ is the energy dispersion in the unperturbed periodic lattice, V is the potential that appears due to the discontinuity of band gap in heterostructure devices, E is energy of the quantum level in consideration and ψ is the corresponding wave function. $\mathcal{E}(k)$ is a function of wave vector k given by

$$\mathcal{E}(k) = a_2 k^2 + a_4 k^4 + a_6 k^6 + \dots \quad (2)$$

Ignoring the non-parabolic effect, this relation can be approximated as $\mathcal{E}(k) = a_2 k^2$. However in QW, the next higher order term should be retained reducing (2) to $\mathcal{E}(k) = a_2 k^2 + a_4 k^4$ [3].

We consider a SQW of width a , along x -direction, with potential energy barrier of height V_0 , originating from the conduction band offset of the well and the barrier materials. The $\mathcal{E}$ - k relation of electrons in the well region can be modelled as

$$\mathcal{E}(k) = \frac{\hbar^2 k_W^2}{2m_W^*} - \alpha \left(\frac{\hbar^2 k_W^2}{2m_W^*} \right)^2, \quad (3)$$

where, the parameter $\alpha = \left(1 - \frac{m_W^*}{m_0}\right)^2 \left(\frac{1}{E_{gW}}\right)$ and the only acceptable form of the wave vector k_W is $\sqrt{\frac{1-\sqrt{1-4\alpha E}}{2\alpha\beta_W}}$, with $\beta_W = \frac{\hbar^2}{2m_W^*}$, m_W^* and E_{gW} are respectively electron effective mass and band gap energy in the well region.

Thus (1) takes the form

$$-\beta_W \frac{d^2\psi}{dx^2} - \alpha\beta_W^2 \frac{d^4\psi}{dx^4} = E\psi \quad (4)$$

For the barrier material, bandgap is assumed to be wide enough to ignore band non-parabolicity and the $\mathcal{E}$ - k relation (2) reduces to its simplest form

$$\mathcal{E}(k) = \frac{\hbar^2 k_B^2}{2m_B^*} \quad (5)$$

where, m_B^* is the electron effective mass and $k_B = \sqrt{\frac{(V_0-E)}{\beta_B}}$ is the acceptable electron wave vector with $\beta_B = \frac{\hbar^2}{2m_B^*}$.

Accordingly, in the barrier region (1) is modified to the form

$$-\beta_B \frac{d^2\psi}{dx^2} + V_0\psi = E\psi, \quad (6)$$

Now, we consider an electric field F applied along the width of the well and intend to estimate the resulting energy levels and their shifts, both in absence and presence of the effect of band non-parabolicity.

Under the influence of an electric field, the confining potential well can still be treated as a square one, only with some perturbation, as long as the field is quite small [11]. The perturbation method can then be employed to determine the energy levels.

Solutions of (4) and (6), under proper boundary conditions, provide the energy eigen value and corresponding wave function for each quantum state of the finite well. Energy of odd and even modes can be found out respectively from solutions of the following equations [2]

$$\tan\left(\frac{k_W a}{2}\right) = \frac{k_B}{k_W} \frac{m_W^*}{m_B^*}$$

and

$$\cot\left(\frac{k_W a}{2}\right) = -\frac{k_B}{k_W} \frac{m_W^*}{m_B^*} \quad (7)$$

For electron in states with odd quantum numbers, wavefunctions are even in x and is given by

$$\begin{aligned} \psi_W(x) &= A_{\text{even}} \cos(k_W x) \text{ for } -\frac{a}{2} \leq x \leq \frac{a}{2}, \\ \psi_B(x) &= B_{\text{even}} \exp(k_B x) \text{ for } x < -\frac{a}{2}, \\ \psi_B(x) &= B_{\text{even}} \exp(-k_B x) \text{ for } x > \frac{a}{2}, \end{aligned} \quad (8)$$

where, the amplitudes A_{even} and B_{even} are determined from appropriate normalization conditions to obtain

$$|A_{\text{even}}| = \frac{1}{\sqrt{C_{2,\text{even}}}} \text{ and } |B_{\text{even}}| = \frac{C_{1,\text{even}}}{\sqrt{C_{2,\text{even}}}}, \text{ with } C_{2,\text{even}} = \frac{1+\cos(k_W a)}{2k_B} + \frac{ak_W + \sin(k_W a)}{2k_W} \text{ and } C_{1,\text{even}} = \cos\left(\frac{k_W a}{2}\right) \exp\left(\frac{k_B a}{2}\right).$$

Similarly, wave functions for the states with even quantum number are odd in x and take the form

$$\psi_W(x) = |A_{\text{odd}}| \sin(k_W x) \text{ for } -\frac{a}{2} \leq x \leq \frac{a}{2}$$

$$\begin{aligned}\psi_B(x) &= -|B_{odd}| \exp(k_B x) \text{ for } x < -\frac{a}{2} \\ \psi_B(x) &= |B_{odd}| \exp(-k_B x) \text{ for } x > \frac{a}{2},\end{aligned}\quad (9)$$

$$\text{with } |A_{odd}| = \frac{1}{\sqrt{C_{2,odd}}}, |B_{odd}| = \frac{C_{1,odd}}{\sqrt{C_{2,odd}}}, C_{2,odd} = \frac{1 - \cos(k_w a)}{2k_B} + \frac{ak_w - \sin(k_w a)}{2k_w} \text{ and } C_{1,odd} = \sin\left(\frac{k_w a}{2}\right) \exp\left(\frac{k_B a}{2}\right)$$

According to the 1st order perturbation theory, shift in the n^{th} energy level due to the electric field F is given by [12]

$$\Delta E_n^{(1)} = eF \langle \psi_n | x | \psi_n \rangle \quad (10)$$

where, $\langle \psi_n | x | \psi_n \rangle = \int_{-a/2}^{a/2} \psi_n^*(x) x \psi_n(x) dx$ and ψ_n is electron wavefunction for the n^{th} quantum state. For the QW considered, the 1st order perturbation term vanishes.

It is, therefore, necessary to calculate the 2nd order perturbation term, given as

$$\Delta E_n^{(2)} = e^2 F^2 \sum_{m \neq n} \frac{\langle \psi_m | x | \psi_n \rangle^2}{E_n^0 - E_m^0} \quad (11)$$

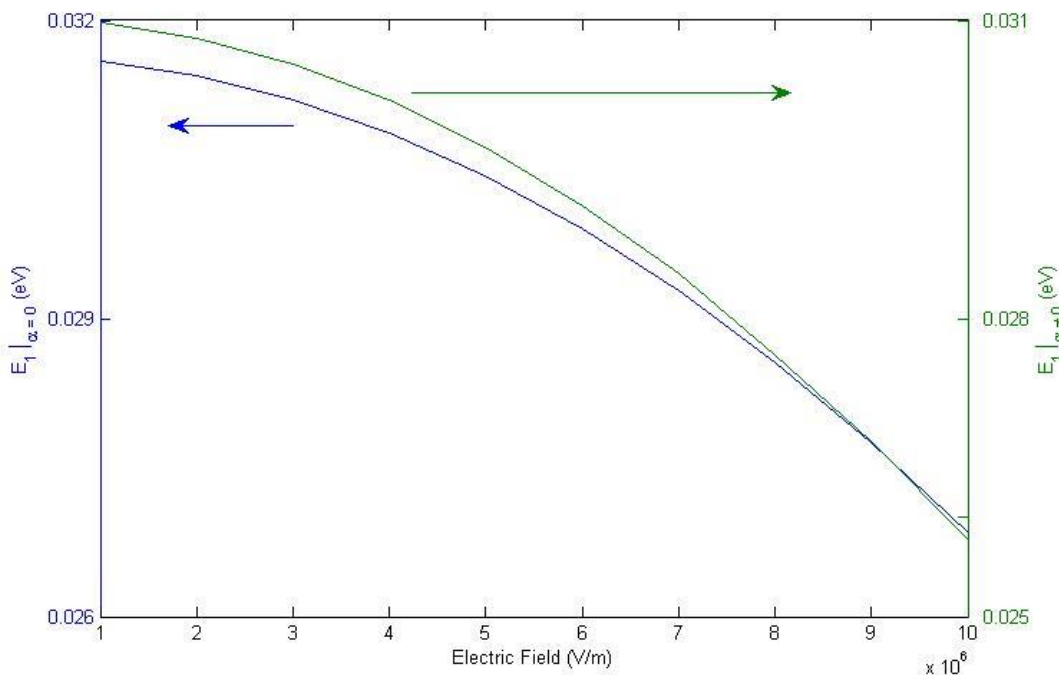
where, $\langle \psi_m | x | \psi_n \rangle = \int_{-a/2}^{a/2} \psi_m^*(x) x \psi_n(x) dx$, ψ_m is electron wavefunction for the m^{th} quantum state, E_n^0 and E_m^0 are unperturbed energies of the n^{th} and m^{th} quantum states. Equation (11) determines the field induced shifts estimated from overlapping of wavefunctions of all the neighbouring states. The energy difference appeared in each contributing term under summation in (11) implies that states lying above the level of interest will produce downward shifts, while those lying below will give rise to upward shifts. The magnitude of such energy shift depends further on the location of the contributing level w.r.t. the original level, the largest shift being induced by the nearest neighbour. Moreover, each of such shifts increases with square of the strength of applied field.

The shift in the bound energy states in a finite SQW under the influence of electric field and band non-parabolicity can be estimated from (11) on use of wavefunctions (8) and (9).

III. Results

To compute the derived results, we consider a GaAs SQW of width 10 nm and depth 0.3093 eV, subjected to an electric field ranging from $(1-10) \times 10^6$ V/m. The barrier material is chosen as $Al_{0.4}Ga_{0.6}As$ and the material parameters required for computation are taken from [13]. The lowest three energy levels are plotted with the applied electric field in Figs. 1 to 3, without and with the consideration of band non-parabolicity.

Fig 1: Ground State energy (E_1) vs. electric field for a 10 nm GaAs/ $Al_{0.4}Ga_{0.6}As$ QW



In order to explain the computed results, we first look into energy levels under the influence of band non-parabolicity alone.

The presence of a negative term in the $\mathcal{E}$ - k relation (3) indicates that band non-parabolicity causes lowering in all the energy states. The 2nd term in (3) involves square of the wave vector, and therefore, the energy states located away from the conduction band edge get strongly influenced by the band non-parabolicity and suffer greater energy lowering.

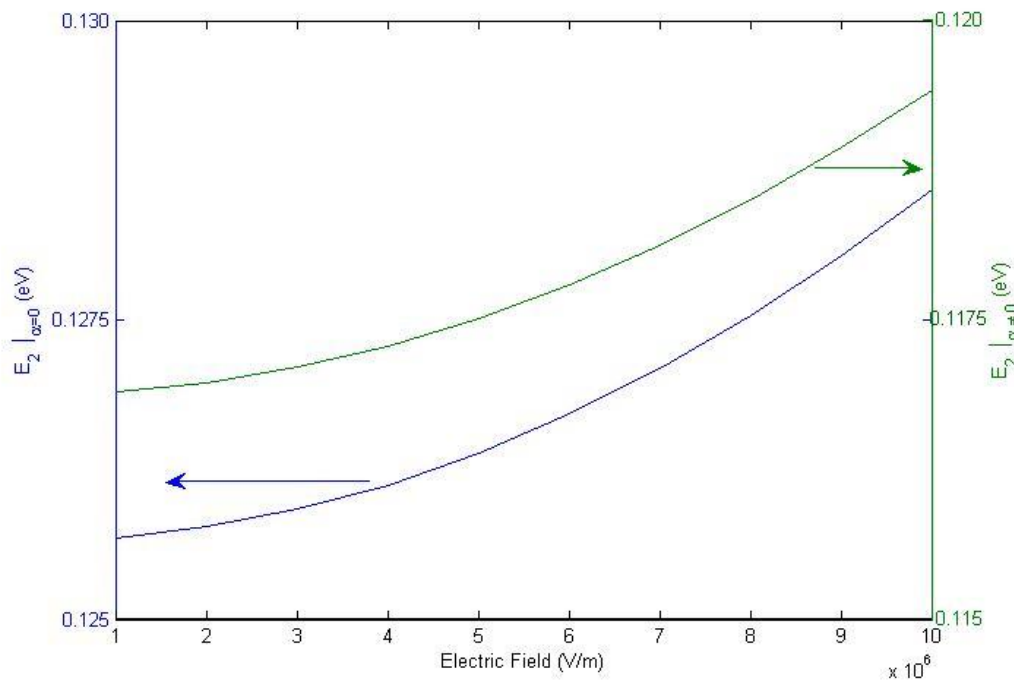
The ground state (E_1) undergoes a downward shift of 0.6 meV due to the effect of band non-parabolicity. When an electric field of 10^7 V/m is applied to the SQW, E_1 suffers a field induced shift of 5.23 meV, as indicated in Fig.1. However, if the band non-parabolicity effect is neglected, the field induced shift is reduced to only 4.78 meV under the influence of the same field strength.

Now, for the QW considered here, only three bound states exist. For excited states, the neighbouring lower state being the closest one, its interaction dominates most and is responsible for an overall upward shift in energy with electric field. Reduction in inter-subband separation due to the effect of band non-parabolicity makes the field dependence of such shift stronger.

But the first excited state E_2 experiences an overall upward shift, which is the result of stronger upward shift due to E_1 and a relatively smaller downward shift due to E_3 . In presence of band non-parabolicity, greater lowering in E_3 w.r.t. E_1 produces a larger downward shift in E_2 and thus makes the overall upward shift less sensitive to applied field strength, as evident from Fig. 2. In case of the 2nd excited state, E_3 . Both E_1 and E_2 lie below it and an overall upward field induced shift is produced as shown in Fig. 3.

However, with varying well width the number of bound states and their location changes, and the picture described above changes. We, therefore, reinvestigate the situation for another similar SQW, having the same barrier height with its width doubled. The QW possesses a greater number of bound states and the corresponding results are presented in Fig.4. In the wider QW, both the energies and separations of the bound states decrease. Compared to the narrower QW, the influence of band non-parabolicity on individual state is here reduced, but the interactions between them and thereby, field dependence of the energy shifts become much more pronounced. Fig. 4 also reveals the fact. Apart from the above general features, the case of energy state E_3 needs a special mention. In the QW of width 20 nm, E_3 is not the top most state and thus, experiences additional downward shifts induced by a number of states lying above it. Thus, the overall upward shift in E_3 is smaller than that in the immediate lower state E_2 , as a contrary to the case observed in a 10 nm QW.

Fig 2: Energy of the first excited state (E_2) vs. electric field for a 10 nm GaAs/Al_{0.4}Ga_{0.6}As QW



To highlight the influence of band non-parabolicity on the bound state energy along-with their shifts due to external electric field, results estimated for field strength 10^7 V/m applied to a 10 nm QW are presented in Table 1 and Table 2 respectively. Table 3 presents the contributions of band non-parabolicity and electric field separately to the total energy shift for each energy level. It indicates that for the electric field strength and QW

considered, the field induced shift in the ground state energy is 8.83 times greater than the shift due to band non-parabolicity. However, the influence of band non-parabolicity dominates over that of electric field for the first excited state, which in this case is 3.44 times. It is most prominent in the highest energy level, where the effect of electric field is negligible compared to the band non-parabolic effect. It supports the fact that the consideration of band non-parabolicity is more relevant for states away from the band edges.

Fig 3: Energy of the 2nd excited state (E_3) vs. electric field for a 10 nm GaAs/Al_{0.4}Ga_{0.6}As QW

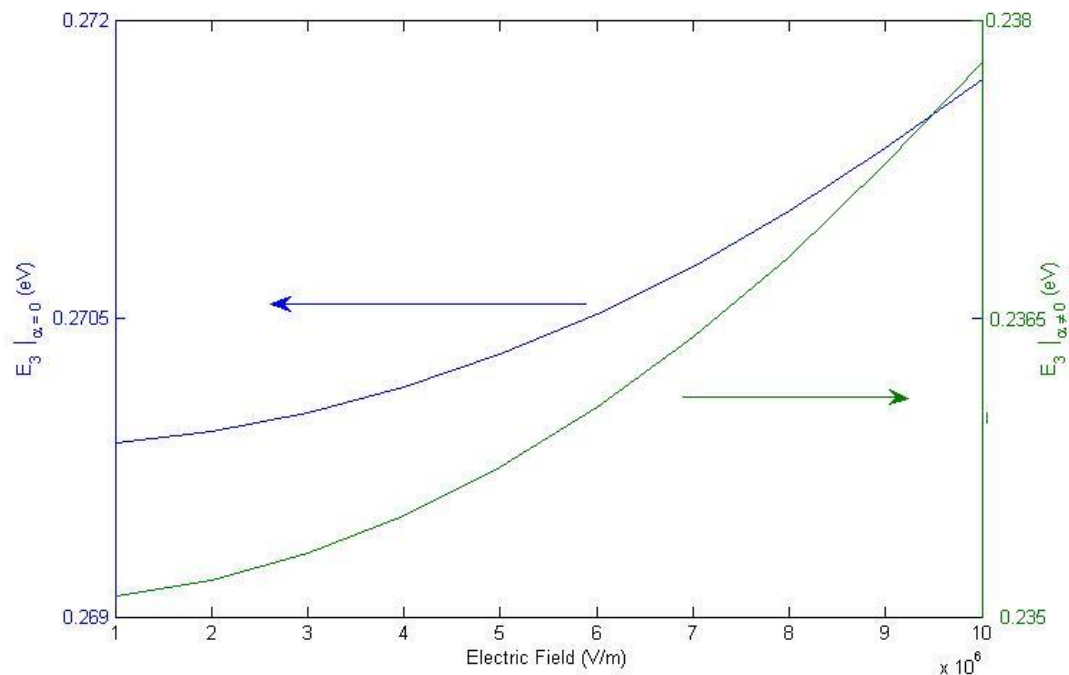


Fig 4 Electric field induced shifts in 10 nm GaAs/Al_{0.4}Ga_{0.6}As square QW for: (a) E_1 , (b) E_2 and (c) E_3 ; (a'), (b'), (c') represent corresponding shifts in a 20 nm QW.

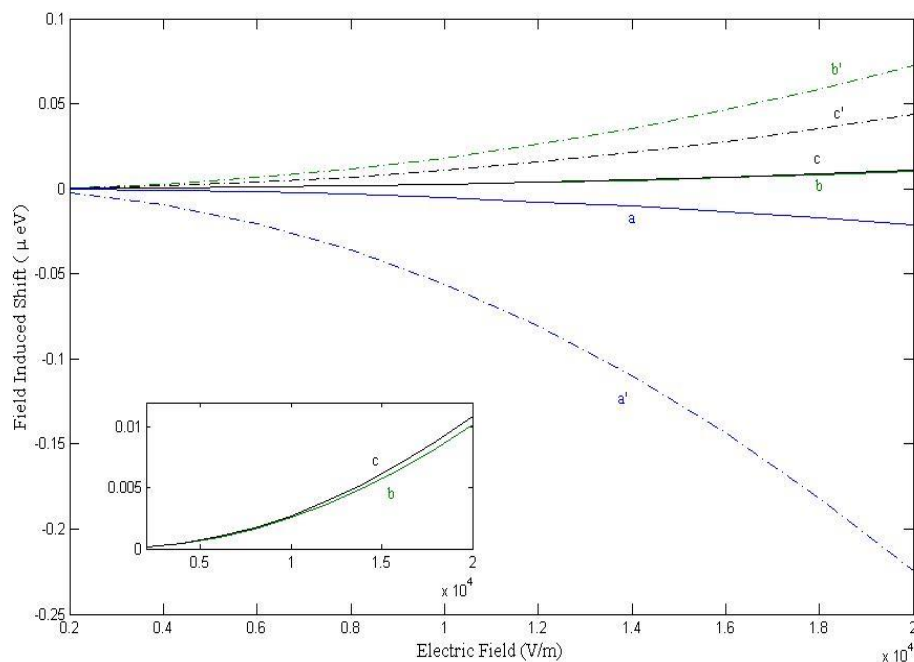


Table 1: Energy levels and their shifts due to band non-parabolicity

Energy level	Energy neglecting band non-parabolicity $E_n _{\alpha=0, F=0}$ (meV)	Energy considering band non-parabolicity $E_n _{\alpha \neq 0, F=0}$ (meV)	Shift due to band non-parabolicity $\Delta E_n _{F=0} = \left(E_n _{\alpha \neq 0, F=0} - E_n _{\alpha=0, F=0} \right)$ (meV)
E_1	31.6319	31.0355	-0.5964
E_2	125.6541	116.8785	-8.7755
E_3	269.8588	235.0739	-34.7839

Table 2: Energy levels and their shifts due on application of electric field

Energy level	$F=10^7 \text{V/m}$ $\alpha=0$			$\alpha \neq 0$		
	Energy application on electric field $E_n _{\alpha=0, F \neq 0}$ (meV)	Field Induced Shift $\Delta E_n _{\alpha=0} = \left(E_n _{\alpha=0, F \neq 0} - E_n _{\alpha=0, F=0} \right)$ (meV)		Energy application on electric field $E_n _{\alpha \neq 0, F \neq 0}$ (meV)	Field Induced Shift $\Delta E_n _{\alpha \neq 0} = \left(E_n _{\alpha \neq 0, F \neq 0} - E_n _{\alpha \neq 0, F=0} \right)$ (meV)	
E_1	26.8401	-4.7918		25.7671	-5.2684	
E_2	128.5931	2.9390		119.4231	2.5446	
E_3	271.7116	1.8528		237.7977	2.7238	

Table 3: Contribution of electric field and band non-parabolicity in total energy shift for the 10 nm QW under application of $F=10^7 \text{V/m}$

Energy level	Shift due to band non-parabolicity $\Delta E_n _{F=0}$ (meV)	Field Induced Shift $\Delta E_n _{\alpha \neq 0}$ (meV)	Total Shift (meV)	Percentage change in energy shift due to band non-parabolicity $\frac{\Delta E_n _{F=0}}{ \Delta E_n _{\alpha \neq 0} + \Delta E_n _{F=0} }$ (%)	Percentage change in energy shift due to electric field $\frac{\Delta E_n _{\alpha \neq 0}}{ \Delta E_n _{\alpha \neq 0} + \Delta E_n _{F=0} }$ (%)
E_1	-0.5964	-5.2684	-5.8648	-10.17	-89.83
E_2	-8.7755	2.5446	-6.2309	-77.52	22.48
E_3	-34.7839	2.7238	-32.0601	-92.74	7.26

IV. Conclusion

Considering the effect of band non-parabolicity, the energy levels of a finite SQW have been estimated in presence of an electric field ($\sim 10^7 \text{V/m}$). In case of the ground state of a 10 nm QW, energy shift due to application of electric field of 10^7V/m is much stronger than that due to band non-parabolicity. However, for the excited states, the influence of band non-parabolicity dominates over electric field and becomes more and more prominent for higher energy levels and in narrower QWs. On the other hand, field induced shifts are found to increase obviously with the applied field strength and also with well width. Thus, along with the shifts resulting from applied electric field, correction due to band non-parabolicity in estimation of energy levels, becomes essential in order to describe the real energy level configuration, and thereby, related properties of a finite QW.

VI. References

- [1] U. Ekenberg, "Quantum Well Enhancement Of Nonparabolicity Effects On The Effective Electron Mass", J. Phys. Colloques, vol.48, 1987, pp. C5-207-C5-210.
- [2] T. Hiroshima and R. Lang, "Effect of conductionbandnonparabolicity on quantized energy levels of a quantum well", Appl. Phys. Lett., vol. 49, 1986, pp. 456-457.
- [3] D. F. Nelson, R. C. Miller and D. A. Kleinman, "Band Nonparabolicity Effects In Semiconductor Quantum Wells", Phys. Rev. B, vol. 35(1), 1987, pp. 7770-7773.
- [4] G. Bastard, E. E. Mendez, L. L. Chang and L. Esaki, "Variational calculations on a quantum well in an electric field", Phys. Rev. B, vol. 28(6), 1983, pp. 3241-3245.
- [5] W. L. Bloss, Electric field dependence of quantum-well eigenstates, J. Appl. Phys., vol. 65, 1989, pp. 4789-4794.
- [6] D. Ahn and S. L. Chuang, "Variational calculations of subbands in a quantum well with uniform electric field: Gram-Schmidt orthogonalization approach", Appl. Phys. Lett., vol. 49, 1986, pp. 1450-1452.
- [7] D. C. Hutchings, "Transfer matrix approach to the analysis of an arbitrary quantum well structure in an electric field", Appl. Phys. Lett., vol. 55, 1989, pp. 1082-1084.
- [8] C. Juang, "Electric Field Effects in Parabolic Quantum Wells", J. Appl. Phys., vol. 30, 1991, pp. 827-831.
- [9] D. Bala, S. Biswas Sett and C. Bose, "Influence of Band non-parabolicity on electric field induced shift in ground state energy of infinite quantum well", Int. J. Appl. Engg. Research, vol. 9(6), 2014, pp. 727-732.
- [10] H. Luttinger and W. Kohn, "Motion of Electrons and Holes in Perturbed Periodic Fields", Phys. Rev., vol. 97, 1955, pp. 869-883.
- [11] J. H. Davies, The Physics of Low-Dimensional Semiconductors An Introduction, 1st ed., Cambridge: Cambridge University Press, 1998.
- [12] P. Harrison, Quantum Wells, Wires and Dots: Theoretical and Computational Physics of Semiconductor Nanostructures, 2nd ed., England: John Wiley & Sons Ltd., 2005.
- [13] S. Adachi, "GaAs, AlAs, and AlxGa1-xAs: Material parameters for use in research and device applications", J. Appl. Phys., vol. 58(3), 1985, pp. R1-R29.