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Mathematical Modelling of Bloch NMR to Explain the Rashba Energy Features

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ABSTRACT

The Bloch NMR as an analytical tool was able to address the fundamental features in the learning of spintronics. Beside confirming past assertions on the Rashba spin-orbit interaction, thermal motion of hole and electron spin and features of the quantum well, it was also able to explain the condition necessary for Rashba splitting within the quantum well. When the Rashba energy is 43 meV, it modified the Ehrenfest's theorem to hold for an external magnetic field. The confinement potential which is the strength of the Rashba spin-orbit interaction was shown to be controlled magnetically.

1. Introduction

The Bloch NMR model has over the years proven to be a good diagnostic tool for investigating properties of known quantities. For example, the Bloch NMR equations has shown good success in the study biological and physiological properties of living tissue [1,2]. Besides medical applications, the Bloch NMR equations were used to investigate the thermodynamic properties of system e.g. the Wegner distribution function [3]. Recently, the Bloch NMR was used to analyse the magnetic penetration depth of superconducting material and was also applied to explain the muon-spin [4].

The technological and computational prospects of semiconductor spintronics have been explored in various researches [5-10]. One of the notable works in the semiconductor spintronics is the Rashba term [11-13]. One of the major successes of the Rashba term is the measurement of the strength of spin splitting using the Rashba energy of split state and coupling parameter. The Rashba energies can be tuned by changing the composition parameters of the surface alloy [14,15] while the Rashba coupling parameter (α_R) was calculated as 10^{-1} eVÅ for conventional narrow-gap semiconductor structures. Unfortunately, low Rashba coupling parameter do not supports the 2 d spintronics device. Early this year, a layered semiconductor (bismuth tellurohalides) was found to exhibit a large spin splitting [16] which was about 4.8 eV. The improvements on the spin-split extended to nonmagnetic material where the Rashba-Bychkov effect shows the possibility of producing spin-split energy bands in

nonmagnetic materials without the application of any external magnetic field [17]. The Rashba splitting was believed to have been absent in quantum wells because quantum well states are standing waves [18], but was opposed by Stanley *et al.* [19]. The later proved that Rashba splitting occurs in the quantum well states II-V semiconductors. The giant spin splitting in semiconductor is dependent on the spin-orbit interaction [17,20] which is now referred to as the Rashba spin-orbit interaction [12]. The giant spin splitting was first demonstrated on a noble metal [21,22] and further improved on in thin-film [23,24].

In this paper, the Bloch NMR equations were used as a diagnostic tool to analyze the Rashba energies state in a rotating magnetic frame. Derivations of operational equations were used to solve the Rashba energy with the mind set of investigating the conditions necessary for the presence of Rashba splitting in quantum wells and the possibility of controlling the confinement potential magnetically.

2. Theoretical Derivations

The following theoretical assumptions were made in order to incorporate the Bloch NMR into the spintronics device

1) The Rashba parameter was substituted for the spin coupling in the Bloch NMR because they both are synonymous in operation.

2) Let the excitation frequencies in each concept be the same $(\omega_S = \omega_1)$.

3) The macroscopic magnetization of the localized was equated with the equilibrium magnetization of the Bloch model.

4) Semiconductors have various electron-hole recombination rates [25,26]. The speed of the holes and electrons is assumed $v_h v_e = 1$.

5) Both the g tends to 1, likewise the frequency difference between Larmor frequencies.

2.1. Spin Splitting Derivations

The Rashba energy and Rashba parameter are related in the equations shown below

$$E_R = \frac{\hbar^2 k_o^2}{2m^*} \tag{1}$$

$$k_o = \frac{m^* \alpha_B}{\hbar^2} \tag{2}$$

$$\alpha_B = \frac{2E_R}{k_o} \tag{3}$$

The magnetic potential introduced by Zeeman term

$$U = \frac{g^* \mu_B}{2} \boldsymbol{\sigma} \cdot \boldsymbol{B} \tag{4}$$

The resulting spin-splitting of s-type electron states is given by

$$\hbar \omega_S = g^* \mu_B B + \alpha \frac{M_o}{g \mu_B} \tag{5}$$

From Equations (1)-(5), Equation (6) was derived

$$E_R = \frac{m^* \omega_s^2 \alpha_B^2}{2 \left(\frac{2u}{\sigma} + \frac{\alpha M_o}{g \mu_B} \right)^2} \tag{6}$$

where E_R = Rashba energy, α_B = Rashba parameter, m^* = effective mass, u = magnetic potential, σ = spin index, Pauli spin matrices, for electric spin, it is given as

$$\sigma = \left(2a\sqrt{1-a^2} \cos\varnothing, 2a\sqrt{1-a^2} \sin\varnothing, -1+2a^2 \right)$$

where a = lattice constant, g = g-factor. μ_B = mobility.

2.2. Bloch NMR Derivation Model

In this section, a mathematical algorithm to describe in detail the translational mechanical properties of the Bloch NMR equation was developed. A sample of atomic crystal structure is analyzed by the x, y, z component (in the rotating frame) of magnetization given by the Bloch equations which may be written as follows

$$\frac{dM_x}{dt} = \Delta \omega M_y - \frac{M_x}{T_2} \tag{7}$$

$$\frac{dM_y}{dt} = -\Delta \omega M_x - \omega_1 M_z - \frac{M_y}{T_2} \tag{8}$$

$$\frac{dM_y}{dt} = -\omega_1 M_y - \frac{(M_z - M_o)}{T_1} \tag{9}$$

where $\Delta \omega = \omega_1 - \omega_o$ the frequency difference between Larmor frequency and frame of reference, $\omega_1 = -\gamma B_1$ is the Rabi frequency, $\omega_o = -\gamma B_O$ is the Larmor frequency, M_x, M_y are the transverse magnetization, M_z is the longitudinal magnetization, M_o is the equilibrium magnetization. The movement of the holes and electrons is assumed to move at a velocity V_e and V_h and at distances L_h & L_e from the conduction and valence bands.

$$\frac{dM_x}{dL_h} \frac{dL_h}{dt} = \frac{dM_x}{dt} \tag{10}$$

$$\frac{dM_y}{dL_e} \frac{dL_e}{dt} = \frac{dM_y}{dt} \tag{11}$$

$$\frac{dM_z}{dL_h} \frac{dL_h}{dt} = \frac{dM_z}{dt} \tag{12}$$

where $\frac{dL_h}{dt} = v_h$ and $\frac{dL_e}{dt} = v_e$

$$\frac{dM_x}{dL_h} = \frac{\Delta \omega}{v_e} M_y - \frac{M_x}{v_h T_2} \tag{13}$$

$$\frac{dM_y}{dL_e} = \frac{-\Delta \omega M_x}{v_h} + \frac{\omega_1 M_z}{v_h} - \frac{M_y}{v_e T_2} \tag{14}$$

$$\frac{dM_z}{dL_h} = \frac{-\omega_1 M_y}{v_e} - \frac{(M_z - M_o)}{v_e T_1} \tag{15}$$

The solution of the above equations can be arranged in matrix form as shown below

$$\begin{bmatrix} -v_e & \Delta \omega T_2 v_h & 0 \\ -\Delta \omega v_e T_2 & v_h & T_2 \omega_1 v_h \\ 0 & -v_h T_1 \omega_1 & -v_e \end{bmatrix} \begin{bmatrix} M_x \\ M_y \\ M_z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ v_e M_o \end{bmatrix} \tag{16}$$

The matrix multiplication as shown below leads to the steady solutions of the Bloch equations in the rotating frame of reference are shown below

$$M_x = \frac{\omega_1 \Delta \omega v_h^2 T_2^2 M_0}{-v_e^3 - \omega_1^2 v_h v_e T_1 T_2 - \Delta \omega^2 v_h v_e^2 T_2^2} \tag{17}$$

$$M_y = \frac{T_2 \omega_1 v_h v_e M_o}{-v_e^3 - \omega_1^2 v_h v_e T_1 T_2 - \Delta \omega^2 v_h v_e^2 T_2^2} \tag{18}$$

$$M_z = \frac{-v_e^3 + \Delta \omega^2 v_h v_e^2 T_2^2 M_o}{-v_e^3 - \omega_1^2 v_h v_e T_1 T_2 - \Delta \omega^2 v_h v_e^2 T_2^2} \tag{19}$$

These solutions directly give the frequency response of the magnetization. This idea gives the possibilities of

quantitatively calculating the measured signal if a spin system is characterized by relaxation times T_1 and T_2. The term $\omega_1^2 v_h v_e T_1 T_2$ is proportional to the radio frequency power P. At the state of no saturation *i.e.* for low power P, this term $\left(\omega_1^2 v_h v_e T_1 T_2\right)$ is small $\omega_1^2 v_h v_e T_1 T_2 \square\ 1$.

$$M_x = \frac{\omega_1 \Delta\omega v_e v_h^2 T_2^2 M_0}{-v_e^3 - \Delta\omega^2 v_h v_e^2 T_2^2} \qquad (20)$$

$$M_y = \frac{T_2 \omega_1 v_h v_e M_o}{-v_e^3 - \Delta\omega^2 v_h v_e^2 T_2^2} \qquad (21)$$

2.3. Operational Equations

The operational equations used for the simulations were worked out and systems of equations were generated. Equations (6), (20) and (21) yield

$$E_R = \frac{k\alpha_B^2}{2\left(\dfrac{2u}{\sigma} + \dfrac{M_o}{\mu_B}\right)^2} \qquad (22)$$

$$E_{Rx} = \frac{k\alpha_B^2}{\chi_1} \qquad (23)$$

where $\chi_1 = 2\left(\dfrac{u}{a\sqrt{1-a^2}\cos\varnothing} + \dfrac{\omega_1 T_2^2 \upsilon_h}{-\upsilon_e^3 - \upsilon_e T_2^2}\dfrac{M_o}{\mu_B}\right)^2$

$$E_{Ry} = \frac{k\alpha_B^2}{\chi_2} \qquad (24)$$

where $\chi_2 = 2\left(\dfrac{u}{a\sqrt{1-a^2}\sin\varnothing} + \dfrac{T_2\omega_1}{-\upsilon_e^3 - \upsilon_e T_2^2}\dfrac{M_o}{\mu_B}\right)^2$

Equations (17)-(19) yield when $v_e T_2^2 \square\ 1$

$$\omega_1 v_h T_2^2 = -v_e^3 \sin\theta \qquad (25)$$

$$\omega_1 T_2 = -v_e^3 \cos\theta \qquad (26)$$

$$v_h T_2 = \tan\theta \qquad (27)$$

Applying Equations (23)-(27)

$$\chi_1 = 2\left(\frac{u}{a\sqrt{1-a^2}\cos\varnothing} + \frac{M_o}{\mu_B}\sin(\varnothing)\right)^2 \qquad (28)$$

$$\chi_2 = 2\left(\frac{u}{a\sqrt{1-a^2}\sin\varnothing} + \frac{M_o}{\mu_B}\cos(\varnothing)\right)^2 \qquad (29)$$

Ploting the first and second term of Equations (28) and (29) where $a < 1$.

The Rashba energy along the vertical and horizontal axes are represented diagrammatically (shown in **Figure 1**) which satisfies the mathematical expression $E_R^2 = E_{Rx}^2 + E_{Ry}^2$.
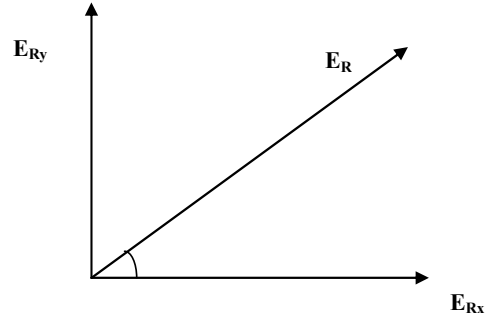
Figure 1. Rashba energy representation.

3. Simulations of Derivations

In this section, the simulations of Equations (22)-(24) under various conditions e.g. the time relaxations and magnetic moments. Time relaxations of 9 ns was applied (Laura Fanea *et al.*, 2011) to investigate the behavior of the Rashba energy with respect to its longitudinal and transverse component.

4. Results and Discussion

Thermal motion of the hole was investigated in **Figure 2** where the hole velocity was plotted against the angle of propagation at a relaxation time 9×10^{-9} s. Its results was in accordance with past papers [27,28] which was interpreted that the stochastic modulation of the interaction between the heavy and light hole sub-bands may induce a nonadiabatic transitions between them, which may eventually lead to J-relaxation and dephasing. In **Figure 3**, the focus was to which type of character is dominant among the subbands. In accordance to the graphical expression given by Winkler [29] it was discovered that the features of **Figure 3** is a heavy hole character. **Figure 4** investigated the relationship between the potential and the spin mobility within the system. The direction of the wavelike structure gives an asymmetric double peak structure which shows that energy exist between the peaks which was as a result of the perpendicular magnetic field. An in-plane inversion asymmetry can induce a contribution from an in-plane potential gradient, which can strongly enhance the spin splitting [22]. **Figures 5** and **6** explain more on effect of the external magnetic fields on the holes or electron in the quantum well. Actually, **Figure 5** supports the idea that quantum well states are standing waves and should therefore show no Rashba splitting while **Figure 6** supports that the Rashba splitting occurs in the quantum well state (two strange events). One of the objectives of this paper was to investigate the conditions necessary for the Rashba splitting within the quantum well. **Figures 7** and **8** are similar in shape *i.e.* showing the strength of the splitting. **Figures 9** and **10** show the Rashba energies at ground state (in which was calculated at about ≥43 meV) which have two branches synonymous to the spin up state and the spin down state.
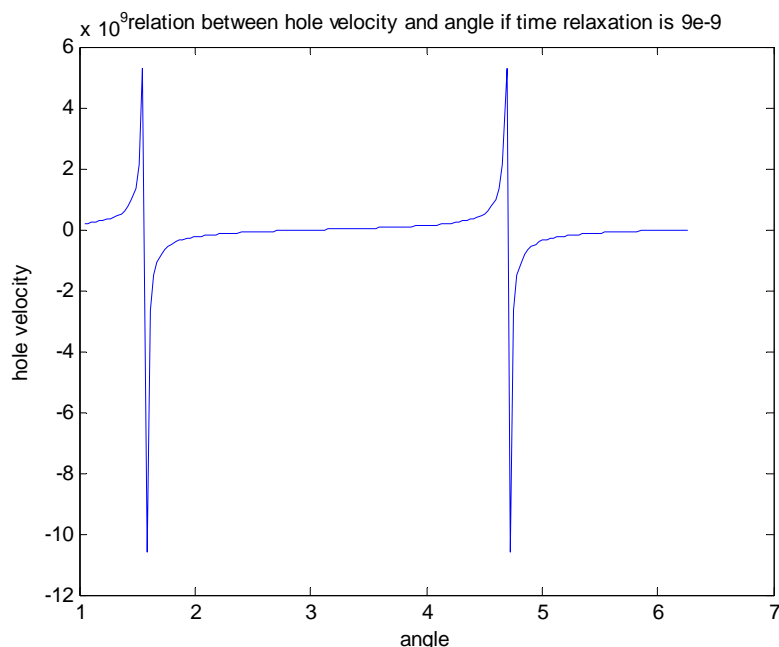
Figure 2. Hole velocity-angle relationship when the time relaxation is 9×10^{-9} s.
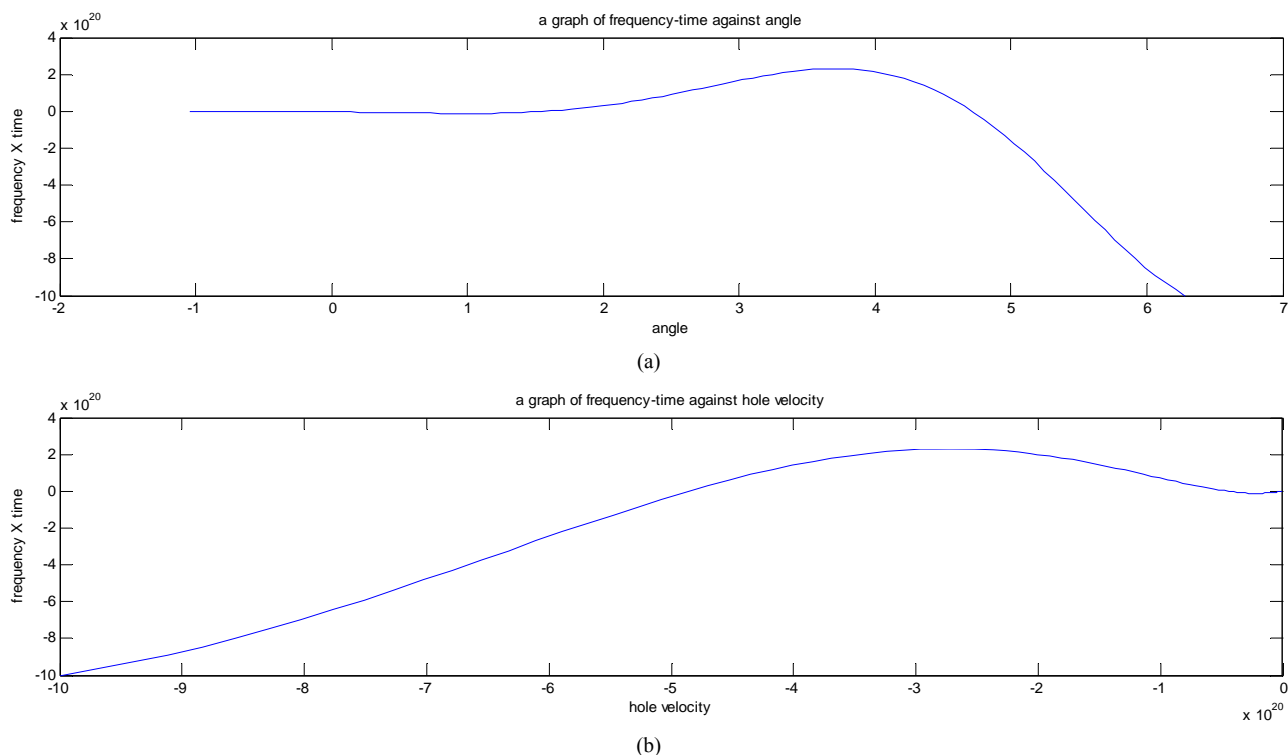

(a)

(b)

Figure 3. (a) Frequency-time versus angular change; (b) Frequency-time versus hole velocity.

Unlike the findings of Eerdunchaolu *et al.* [30] an increase in the Rashba energy makes no significant change in χ_1 & χ_2 (which is described as the height). More importantly, it reveals that Rashba split of orbit interaction effect is not dependent on the height in the y direction. This is because the effective magnetic field which is produced by spin-orbit coupling (due to the lack of structure inversion symmetry) is approximately perpendicular to the electron momentum in the quantum ring. **Figure 11** shows that electron wave function bound in a quantum well in the presence of an external (or built-in) field e.g. M_x, M_y or M_z. Very much like the reaction of the electric
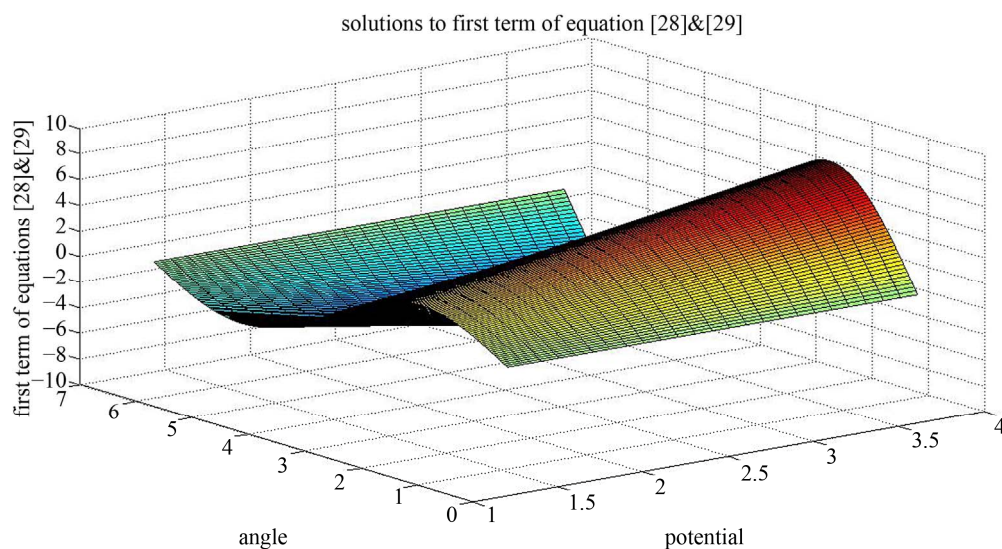
solutions to first term of equation [28]&[29]

Figure 4. First term solutions of Equations (28) and (29).

solution of second term of equation[28]
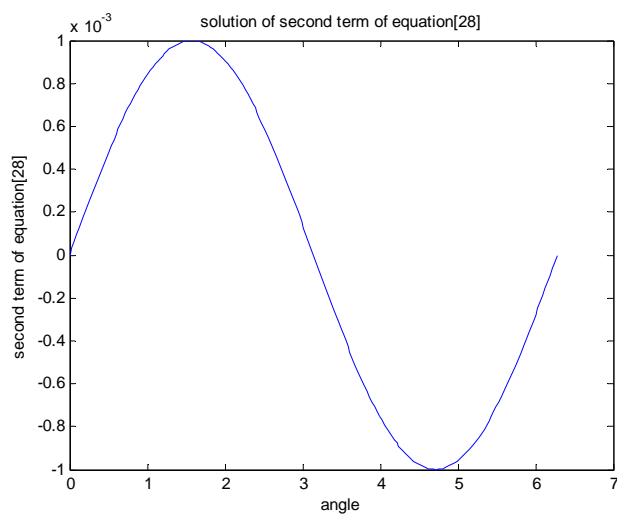
Figure 5. Second term solution of Equation (23).

solution of second term of equation[29]
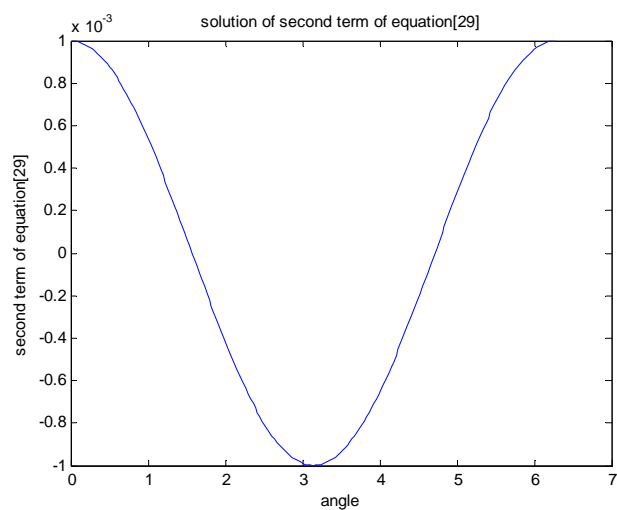
Figure 6. Solutions of the second term of Equation (24).

solution of x in equation[23]
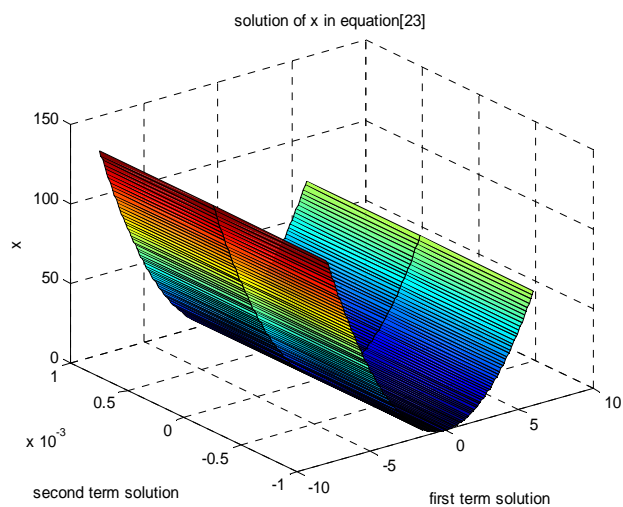
Figure 7. Graphical solution of χ_1 in Equation (23).

solution of x in equation[24]
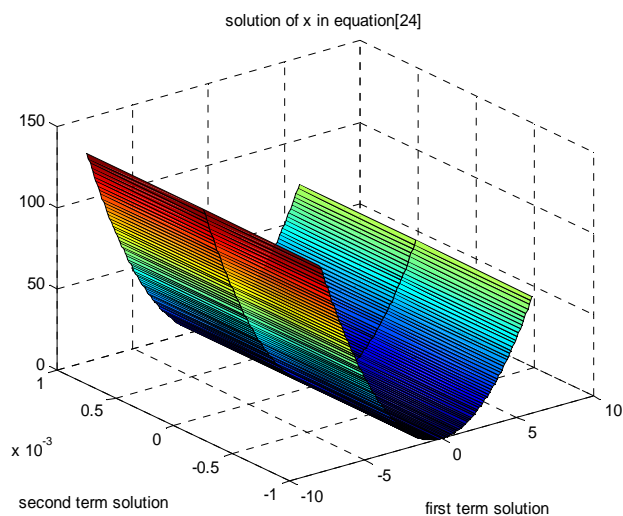
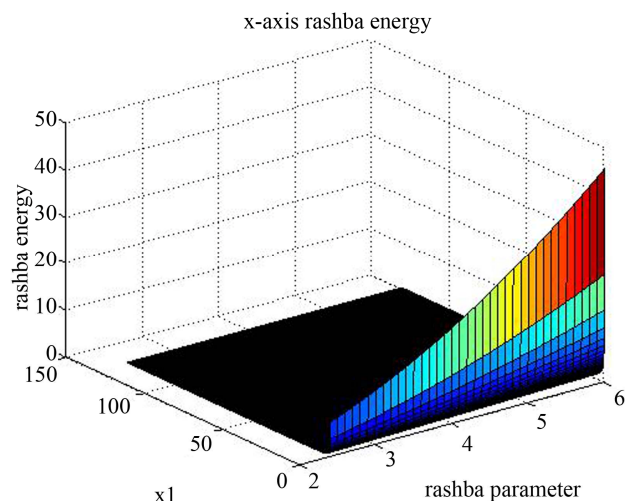**Figure 8. Graphical solution of χ_2 in Equation (24).**

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Figure 9. Solution of the Rashba energy of the horizontal axis.

fields in the quantum well, the behavioral features of the effective magnetic field in the conduction band (upper part of **Figure 11**) and valence band (lower part of **Figure 11**)) is the sum of the magnetic field and the contributions due to the position dependence of the conduction band. In other words, the modification of Ehrenfest's theorem becomes necessary because it is the magnetic field in the valence band that controls the Rashba spin splitting of electron states. **Figure 12** gives a joint feature of **Figures 5** and **6** which may suggest the possibility of the ideas of Petersen *et al*. [18] and Stanley *et al*. [19] occurring simultaneously within the quantum well.

5. Conclusion

The Bloch NMR model has been proven to be efficient in analyzing the fundamentals of spintronics. It was discovered that an increase in the Rashba energy makes no sig-
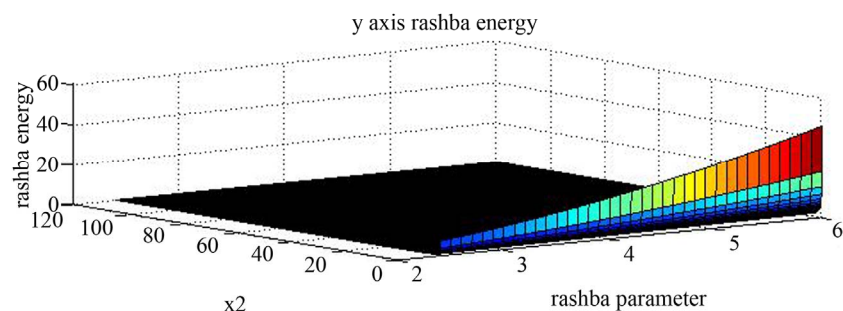

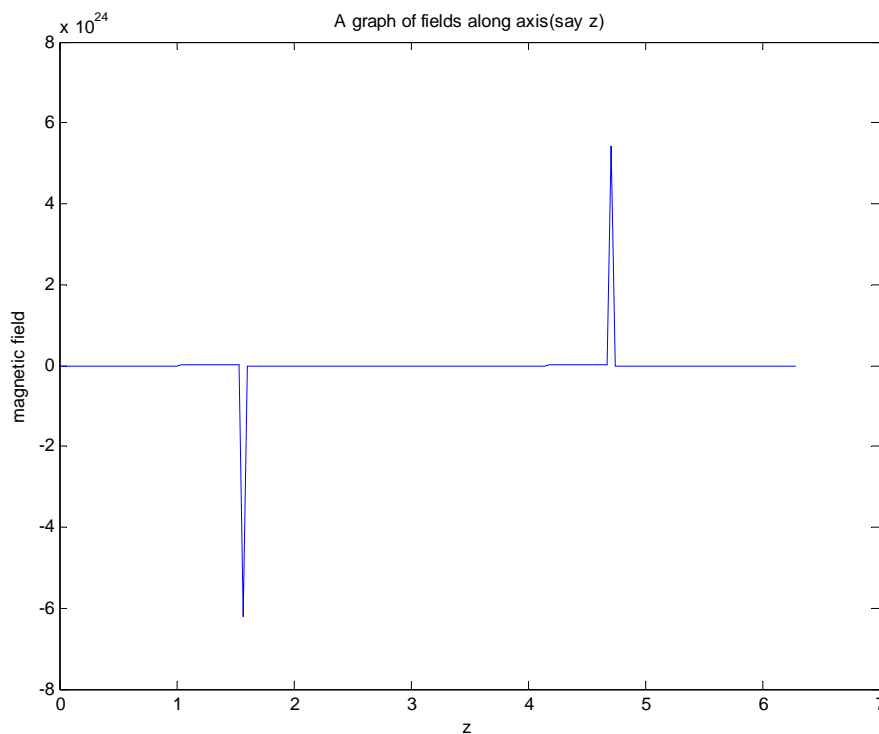**Figure 10. Solution of the Rashba energy of the vertical axis.**
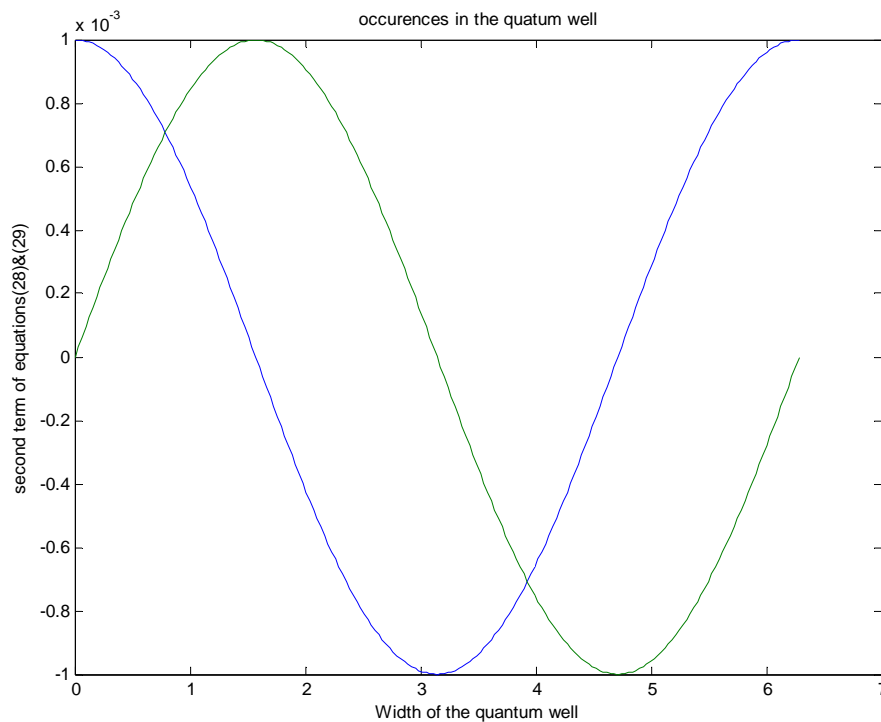

Figure 11. The nature of fields along the axes.

Figure 12. Occurrences in the quantum well state.

nificant changes in χ_1 & χ_2 (which was described as height). This result, makes the Rashba split of orbit interaction effect independent on the height along the y direction as shown in **Figures 9** and **10**. Furthermore, this led to the alteration of Ehrenfest's theorem (which originally applies to the external electric fields), but now applies to the external magnetic field. Therefore, the confinement potential which is the strength of the Rashba spin-orbit interaction can also be controlled magnetically. This idea may be expatiated upon based on further research. Also the Bloch NMR was also effective to analyze the quantum well *i.e.* even though it is a standing wave, it could still experience Rashba splitting when the quantized electron energy $E_e \geq 1$ meV and the length of the quantum well is 6 nm.

6. Appreciation

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