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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.

Keywords: Bloch NMR; Rashba Energy; Rashba Parameter; Quantum Well; Spin-Split; Hole Spin Velocity

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 ($\alpha_R$) 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 4.8eV. 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 gaint 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 ($\omega_3 = \omega_1$).
3) The macroscopic magnetization of the localized was
equated with the equilibrium magnetization of the Bloch
model.

4) Semiconductors have various electron-hole recom-
bination rates [25,26]. The speed of the holes and elec-
trons is assumed \( v_h v_e = 1 \).

5) Both the g tends to 1, likewise the frequency dif-
fERENCE between Larmor frequencies.

2.1. Spin Splitting Derivations

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

\[
E_R = \frac{\hbar^2 k^2}{2m^*} \tag{1}
\]

\[
k_o = \frac{m^* a_B}{\hbar} \tag{2}
\]

\[\alpha_B = \frac{2E_R}{k_o} \tag{3}\]

The magnetic potential introduced by Zeeman term

\[U = \frac{g^* \mu_B}{2} \sigma \cdot \mathbf{B} \tag{4}\]

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

\[\hbar \omega_k = g^* \mu_B B + \alpha \frac{M_o}{g \mu_B} \tag{5}\]

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

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

where \( E_R \) = Rashba energy, \( \alpha_B \) = Rashba parameter, \( m^* \) = effective mass, \( u \) = magnetic potential, \( \sigma \) = spin index, Pauli spin matrices, for electric spin, it is given as

\[\sigma = \begin{pmatrix} 2a \sqrt{1 - a^2} \cos \phi, & 2a \sqrt{1 - a^2} \sin \phi, & -1 + 2a^2 \end{pmatrix}\]

where \( a = \) lattice constant, \( g = \) g-factor. \( \mu_B = \) 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 crys-
tal structure is analyzed by the \( x, y, z \) component (in the
rotating frame) of magnetization given by the Bloch equa-
tions which may be written as follows

\[\frac{dM_i}{dt} = \Delta \omega M_i - \frac{M_i}{T_i} \tag{7}\]

\[\frac{dM_y}{dt} = -\omega_0 M_y - \frac{M_y}{T_y} \tag{8}\]

\[\frac{dM_z}{dt} = -\omega_0 M_z - \frac{M_z}{T_z} \tag{9}\]

where \( \Delta \omega = \omega_0 - \omega_e \) the frequency difference between
Larmor frequency and frame of reference, \( \omega_0 = -\gamma B_0 \)
the Rabi frequency, \( \omega_e = -\gamma B_e \) is the Larmor fre-
quency, \( M_o, M_e \) are the transverse magnetization, \( M_z \)
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 \( V_h \) at distances
\( L_h \& L_e \) from the conduction and valence bands.

\[\frac{dL_{x}}{dt} = v_e \text{ and } \frac{dL_{y}}{dt} = v_h \]

\[\frac{dM_y}{dL_y} = \frac{\Delta \omega M_y}{v_e} - \frac{M_y}{v_e T_y} \tag{13}\]

\[\frac{dM_y}{dL_y} = -\omega_0 M_y + \frac{\alpha M_z}{v_h} - \frac{M_y}{v_h T_e} \tag{14}\]

\[\frac{dM_y}{dL_y} = -\omega_0 M_y - \frac{M_z - M_y}{v_e T_1} \tag{15}\]

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

\[
\begin{pmatrix}
-v_e & \Delta \omega T_y v_y & 0 \\
-\Delta \omega v_e T_2 & v_y & T_2 \alpha v_h \\
0 & -v_e T_1 \alpha & -v_e
\end{pmatrix}
\begin{pmatrix}
M_x \\
M_y \\
M_z
\end{pmatrix} =
\begin{pmatrix}
0 \\
0 \\
v_e M_o
\end{pmatrix}
\tag{16}
\]

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

\[M_x = \frac{\alpha \Delta \omega v_e T_1^2 M_o}{-v_e^3 - \alpha v_h \gamma v_e T_2^2 + \Delta \omega^2 v_e v_h^2 T_2^2} \tag{17}\]

\[M_y = \frac{v_e T_2 \alpha v_h M_o}{-v_e^3 - \alpha^2 v_h T_2^2 - \Delta \omega^2 v_e v_h^2 T_2^2} \tag{18}\]

\[M_z = \frac{-v_e^3 + \Delta \omega^2 v_e^2 T_2^2 M_o}{-v_e^3 - \alpha^2 v_h T_2^2 - \Delta \omega^2 v_e v_h^2 T_2^2} \tag{19}\]

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 $\alpha^2 v_y T_2 T_z$ is proportional to the radio frequency power $P$. At the state of no saturation i.e. for low power $P$, this term is small $\alpha^2 v_y T_2 T_z \ll 1$.

$$M_x = \frac{\alpha_1^2 v_y v_z T_1^2 M_y}{-v_y^3 - \Delta \alpha^2 v_y^2 T_2^2}$$

$$M_y = \frac{T_2 \alpha_2 v_x M_z}{-v_x^3 - \Delta \alpha^2 v_x^2 T_2^2}$$

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

$$E_R = \frac{k \alpha^2}{2} \left( \frac{2u}{\sigma + M_\mu} \right)^2$$

where $\chi_1 = 2 \left( \frac{u}{\alpha \sqrt{1 - a^2 \cos \Theta}} + \frac{\alpha_1^2 T_2^2 M_\mu}{-u_x^3 - u_y T_2^2} \right)^2$

$$E_{Ry} = \frac{k \alpha^2}{\chi_2}$$

where $\chi_2 = 2 \left( \frac{u}{\alpha \sqrt{1 - a^2 \sin \Theta}} + \frac{T_2 \alpha_1 M_\mu}{-u_x^3 - u_y T_2^2} \right)^2$

Equations (17)-(19) yields when $v_x T_2^2 \ll 1$

$$\alpha_1 v_x T_2 = -v_y \sin \Theta$$

$$\alpha_1 T_2 = -v_y \cos \Theta$$

$$v_x T_2 = \tan \Theta$$

Applying Equations (23)-(27)

$$\chi_1 = 2 \left( \frac{u}{\alpha \sqrt{1 - a^2 \cos \Theta}} + \frac{M_\mu}{u_x^3 \sin (\Theta)} \right)^2$$

$$\chi_2 = 2 \left( \frac{u}{\alpha \sqrt{1 - a^2 \sin \Theta}} + \frac{M_\mu}{u_x^3 \cos (\Theta)} \right)^2$$

Plotting 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

$$E_R^2 = E_{Rx}^2 + E_{Ry}^2$$

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 $9 \times 10^{-9}$ 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 shows the Rashba energies at ground state (in which was calculated at about $\geq 43$ meV) which have two branches synonymous to the spin up state and the spin down state.

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Unlike the findings of Eerdunchaolu et al. [30] an increase in the Rashba energy makes no significant change in $\chi_1$ & $\chi_2$ (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
Figure 4. First term solutions of Equations (28) and (29).

Figure 5. Second term solution of Equation (23).

Figure 6. Solutions of the second term of Equation (24).

Figure 7. Graphical solution of $\chi_1$ in Equation (23).

Figure 8. Graphical solution of $\chi_2$ in Equation (24).

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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-
significant changes in $\chi_1$ & $\chi_2$ (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.

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