Comparison of Electron Transmittance and Tunneling Current through a Trapezoidal Potential Barrier with Spin Polarization Consideration by using Analytical and Numerical Approaches

Ezra Nabila, Fatimah A. Noor* and Khairurrijal

Physics of Electronic Materials Research Division, Faculty of Mathematics and Natural Sciences, Institut Teknologi Bandung, Bandung 40132, Indonesia

*Email: fatimah@fi.itb.ac.id

Abstract. In this study, we report an analytical calculation of electron transmittance and polarized tunneling current in a single barrier heterostructure of a metal-GaSb-metal by considering the Dresselhaus spin orbit effect. Exponential function, WKB method and Airy function were used in calculating the electron transmittance and tunneling current. A Transfer Matrix Method, as a numerical method, was utilized as the benchmark to evaluate the analytical calculation. It was found that the transmittances calculated under exponential function and Airy function is the same as that calculated under TMM method at low electron energy. However, at high electron energy only the transmittance calculated under Airy function approach is the same as that calculated under TMM method. It was also shown that the transmittances both of spin-up and spin-down conditions increase as the electron energy increases for low energies. Furthermore, the tunneling current decreases with increasing the barrier width.

1. Introduction

Modern technology relies hugely on semiconductor transistors, in which data processing and computing take place. For decades, the growth and improvement of microelectronic devices was mainly driven by attempts to miniaturize device dimensions. This miniaturization is reflected in Moore’s Law [1], which predicts that the number of transistors per area doubles every 18 months. However, this progressive trend will come into conflict with fundamental physical limitations because of which the size of transistors cannot be further reduced. Earlier this decade indications of a decline in the growth of miniaturization have emerged. A semiconductor technology only utilizes electron charge and completely ignores the associated spin state of the electron. However, integrating spin polarized currents and using electron spin as a new degree of freedom could not only further enhance and improve this technology but could also unveil a new kind of technology.

This is enabled by the invention of diluted magnetic semiconductors (DMS) [2], in which the spin polarization in semiconductors can be obtained by inducing a ferromagnetic material to become a semiconductor material. Hideo Ohno et al. in 1998 were the first to determine the ferromagnetic properties of semiconductor materials doped with transition metals [2]. Since then, research regarding DMS has become one of the core research areas in the magnetic semiconductor field. Additionally, Voskoboynikov et al. [3] proposed the idea of using Rashba spin orbit coupling in nonmagnetic
semiconductors as a spin filter [4]. Meanwhile, Hall et al. [5,6] suggested the idea of using nonmagnetic semiconductors as a spin transistor, which exploits bulk inversion asymmetry (BIA) in the (110)-oriented semiconductor heterostructure as the spin polarizer. Perel et al. [7] in their report showed that spin polarization affects the process of electron tunnelling through zinc blende material. Wang et. al [8] reported that the Dresselhaus effect caused by BIA occurs in zinc blende material, which causes tunnelling current enhancement in the case of a thin barrier. Here, the study of electron tunnelling through a nanometer-thick trapezoidal barrier with spin polarization consideration is reported.

2. Theoretical model
The potential profile of the heterostructure composed by metal-GaSb-metal grown along the z-axis is shown in Fig. 1, where q is an electron charge, $V_0$ is the GaSb height, $V_b$ is the bias voltage applied to the GaSb, and d is the GaSb width. The mathematical representation of the potential profile is given by:

$$V(z) = \begin{cases} 
0, & z \leq 0 \\
V_0 - \frac{qV_b}{d} z, & 0 < z \leq d \\
-qV_b, & z > d 
\end{cases}$$

(1)

![Figure 1. Potential energy profile by applying bias voltage to the barrier.](image)

The alignment of the electron spin was caused by the inversion asymmetry effect, namely bulk inversion asymmetry (BIA). The asymmetry effect is represented by the Dresselhaus Hamiltonian which is given by [6,9]:

$$H_D = \gamma (\sigma_x k_x - \sigma_y k_y) \frac{\partial^2}{\partial z^2}$$

(2)

here $\gamma$ is the Dresselhaus constant, for the material grown only along the z axis the (k) wave number represented for every axis is $k_x^2 = k_y^2 = 0$ and $k_z = -i \frac{\partial}{\partial z}$. By calculating the eigenvalue and eigenfunction we can calculate the total Hamiltonian system ($H = H_0 + H_D$), which can be represented by [10,11]:

$$H = -\frac{\hbar^2}{2m^*_\pm} \frac{\partial^2}{\partial z^2} + V(z) + \frac{\hbar^2 k_z^2}{2m^*_\pm}$$

(3)

here $m^*_\pm$ is the effective mass of a spin dependant electron, which can be represented as:
\[ m_\pm = m^* \left( 1 \pm 2 \frac{y m^* k^2}{\hbar^2} \right) \] (4)

with \( \phi \) as the smallest angle between \( k_y \) and \( k_x \) vector, \( k_p \) can be written as:

\[
\begin{align*}
\vec{k}_p &= k_x \hat{x} + k_y \hat{y} \quad (5) \\
k_y &= k_p \cos \phi \quad (6) \\
k_x &= k_p \sin \phi \quad (7)
\end{align*}
\]

2.1. Exponential wavefunction-approach

Using the exponential function, the solution for every region is represented by:

\[
\varphi(z) = \begin{cases} 
A \exp(ik_1z) + B \exp(-ik_2z), & z \leq 0 \\
C \exp\left(\int_0^z k_2(z')dz'\right) + D \exp\left(-\int_z^d k_2(z')dz'\right), & 0 < z \leq d \\
F \exp(ik_3z), & z > d
\end{cases} \quad (8)
\]

with the wavenumber as follows:

\[
\begin{align*}
k_1 &= \left(\frac{2m_1 \beta_x}{\hbar^2}\right)^{\frac{1}{2}} \quad (9) \\
k_2 &= \left(\frac{2m_2 \beta_x}{\hbar^2}(V_0 - \frac{qV_b z}{d})\right)^{\frac{1}{2}} \quad (10) \\
k_3 &= \left(\frac{2m_3 \beta_x}{\hbar^2}(E_z + qV_b)\right)^{\frac{1}{2}} \quad (11)
\end{align*}
\]

The transmission coefficient then can be derived as:

\[
\left(\frac{F}{A}\right) = 2k_1 \left(\frac{k_2(d)}{k_2(0)}\right) \exp(-ik_3d) \times \left[ \left(k_3 + \left(\frac{k_2(d)}{k_2(0)}\right)\cosh(a)\right)^2 + \left(\frac{m_2 k_3}{m_1 k_2(0)} - \frac{m_1 k_2(d)}{m_2}\sinh(a)\right) \right] \quad (12)
\]

with

\[
a = \int_0^d k_2z \quad (13) \\
a = \left(\frac{2m_2}{\hbar^2}\right)^{\frac{1}{2}} \frac{2d}{3qV_b} \left( (V_0 - E)^{\frac{3}{2}} - (V_0 - E - qV_b)^{\frac{3}{2}} \right) \quad (14)
\]

2.2. Airy wavefunction-approach

By defining a function \( \eta \) as:

\[
\eta(z) = \left(\frac{2m qV_b}{\hbar^2 d}\right)^{\frac{1}{3}} \left( (V_0 - E_z)^\frac{d}{qV_b} - z \right) \quad (15)
\]

the solution for every region can be represented as:

\[
\varphi(z) = \begin{cases} 
A \exp(ik_1z) + B \exp(-ik_1z), & z \leq 0 \\
C \text{Ai}\left(\eta(z)\right) + D \text{Bi}\left(\eta(z)\right), & 0 < z \leq d \\
F \exp(ik_3z), & z > d
\end{cases} \quad (16)
\]

with the wavenumber as follows:
The transmission-coefficient then can be derived as:

\[
\left(\frac{k}{A}\right) = -2i \frac{k a_1}{m_1} \exp(-ik_3 d) \times \left[ \left( \frac{2}{m_2 \hbar^2} \frac{q V_b}{d} \right)^{\frac{1}{3}} a_2 + i \left( \frac{k a_3 k_2 a_4}{m_2 m_3} - \frac{k_3}{m_1 m_3} \left( \frac{2}{m_2 \hbar^2} \frac{q V_b}{d} \right)^{\frac{1}{3}} a_5 \right) \right]
\]

(19)

with the Airy function as follows:

\[
a_1 = A_1 \exp(i \eta(d)) B_1(\eta(d)) - A_1(\eta(d)) B_1'(\eta(d))
\]

(20)

\[
a_2 = A_2 \exp(i \eta(d)) B_2(\eta(0)) - A_2(\eta(0)) B_2'(\eta(d))
\]

(21)

\[
a_3 = A_3(\eta(0)) B_3(\eta(d)) - A_3'(\eta(0)) B_3(\eta(0))
\]

(22)

\[
a_4 = A_4(\eta(0)) B_4'(\eta(0)) - A_4'(\eta(0)) B_4(\eta(0))
\]

(23)

\[
a_5 = A_5(\eta(0)) B_5(\eta(d)) - A_5(\eta(d)) B_5'(\eta(0))
\]

(24)

2.3. Matrix transfer method

Using the matrix transfer method, the GaSb region is divided into N regions, with \( n = 2, 3, \ldots, N-1 \). The solution can be represented as:

\[
\phi_n = A_n \exp(ik_n z_n) + B_n \exp(-ik_n z_n), \quad 0 \leq z < z_n
\]

(26)

\[
\phi_n = A_{n+1} \exp(ik_{n+1} z_n) + B_{n+1} \exp(-ik_{n+1} z_n), \quad 0 < z \leq z_n
\]

(27)

\[
\phi_N = A_N \exp(ik_{N-1} z_n), \quad z \leq z_N
\]

(28)

By applying the boundary conditions, the solution can then be written into matrix

\[
\begin{pmatrix}
1 \\
B_1
\end{pmatrix} =
\begin{pmatrix}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{pmatrix}
\begin{pmatrix}
A_N \\
0
\end{pmatrix}.
\]

(29)

and the transmission coefficient then can be defined as:

\[
t = A_N = \frac{1}{a_{11}}
\]

(30)

2.4. WKB approximation

The solution of the Schrödinger equation is written as:

\[
\phi(z) = R(z) \exp \left( \frac{i \tilde{z}(z)}{\hbar} \right)
\]

(31)

and the transmission coefficient can then be written as:

\[
T = \left| \frac{\varphi_{\text{trans}}}{\varphi_{\text{inc}}} \right|^2 = \exp \left( \int_{z_1}^{z_2} (2m(V(z) - E)^{\frac{1}{2}}(dz)^{-1} \right)
\]

(32)

2.5. Spin dependent transmittance

The effective Schrödinger equation for each region can be written as:
\[
\frac{d^2 \varphi_\pm}{dz^2} + \frac{2m_1}{\hbar^2} \left( 1 \pm \frac{2ym_1 k_p}{\hbar^2} \right)^{-1} E_{x\pm} \varphi_\pm = 0, \quad z \leq 0 \\
\frac{d^2 \varphi_\pm}{dz^2} + \frac{2m_2}{\hbar^2} \left( 1 \pm \frac{2ym_2 k_p}{\hbar^2} \right)^{-1} \left[ (V_0 - E_{x\pm}) \frac{d}{qV_b} - z \right] \varphi_\pm = 0, \quad 0 < z \leq d \\
\frac{d^2 \varphi_\pm}{dz^2} + \frac{2m_1}{\hbar^2} \left( 1 \pm \frac{2ym_1 k_p}{\hbar^2} \right)^{-1} (E_{x\pm} + qV_b) \varphi_\pm = 0, \quad z > d
\]

Using the Airy function, the solution then can be written as:

\[
\varphi_\pm(z) = \begin{cases} 
A_\pm \exp(ik_{z1\pm}z) + B_\pm \exp(-ik_{z1\pm}z), & z \leq 0 \\
C_\pm Ai\left( \eta_\pm(z) \right) + D_\pm Bi\left( \eta_\pm(z) \right), & 0 < z \leq d \\
F_\pm \exp(ik_{z3\pm}z), & z > d
\end{cases}
\]

with

\[
k_{z1\pm} = \left( \frac{2m_1 E_{x\pm}}{\hbar^2} \right)^\frac{1}{2} \left( 1 \pm \frac{2ym_1 k_p}{\hbar^2} \right)^{-\frac{1}{2}}
\]

\[
k_{z3\pm} = \left( \frac{2m_1}{\hbar^2} (E_z + qV_b) \right)^\frac{1}{2}
\]

\[
\eta_\pm(z) = \left( \frac{2m_2}{\hbar^2} qV_b^2 \right)^\frac{1}{2} \left[ (V_0 - E_z) \frac{d}{qV_b} - z \right]
\]

the transmission coefficient can then be derived as:

\[
\left( \frac{F_\pm}{A_\pm} \right) = -2i \frac{k_{z1\pm} a_1}{m_{1\pm}} \exp(-ik_{z3\pm}d) \times \left[ \frac{2}{m_{z\pm}^2 \hbar^2} \frac{qV_b}{d} \right]^{\frac{1}{3}} a_2 + i \left( \frac{k_{z1\pm} a_3 k_{z3\pm} a_4}{m_{1\pm} m_{3\pm}} - \frac{k_{z1\pm} k_{z3\pm}}{m_{1\pm} m_{3\pm}} \left( \frac{2}{m_{z\pm}^2 \hbar^2} \frac{qV_b}{d} \right)^{-\frac{1}{3}} a_5 \right)
\]

2.6. Spin dependent tunneling current

The tunneling current can be calculated by deriving the following equation [12,13]:

\[
J = \int_0^\infty \frac{q m_1 k_p T}{2\pi^2 \hbar^3} T(z) \ln \left( \frac{1 + \exp(E_f - E_z)}{1 + \exp(E_f - E_z - qV_b)} \right) dE_z.
\]

with

\[
T(z) = T_+(z) + T_-(z)
\]

In which \(T(z)\) is the total of the transmittance in spin up and spin down state, \(m_1\) is the electron mass in the metal, \(k_p\) is the Boltzmann constant, \(T\) is the temperature in Kelvin, \(E_f\) is the Fermi energy, \(E_z\) is the electron energy.
3. Results and Discussion

Figure 2. Comparison of methods with electron energy lower than potential barrier.

Figures 2 (a) and (b) show the transmittance versus electron energy at low and high energy regimes, respectively. The transmittances are calculated by using Airy- and Exponential-wavefunction approaches, matrix transfer method, and WKB approximation. It is shown that only the transmittances computed by Airy wavefunction-approach fit those calculated by TMM. In addition, the transmittances computed under Exponential wavefunction-approaches and WKB approximation show the deviation results from TMM. They indicate that the Airy wavefunction-approach is the best analytical method in calculating the transmittance in the spintronic devices. These results are the same as those obtained for MOSFETs device without spin polarization consideration [14].

Figure 3. Transmittance versus energy with variation of the barrier width.

Fig. 4 shows transmittance as a function of energy for the barrier width of 5 and 10 nm. It is seen that the transmittances increase as energy increases for the energy lower than barrier height. It is also seen that the transmittances show the oscillatory behaviour for energy higher than barrier height. The transmittance of the spin up state is greater than the spin down state. Moreover, the transmittance increase with decreasing the barrier width.
Figure 4. Tunneling current density as a function of bias voltage with variation of the barrier width.

Fig. 4 illustrates the tunnelling current density versus bias voltage plotted against external voltage with variation of the barrier width. It is seen that the width of the barrier is very influential on the tunnelling current density obtained: the smaller the width of the barrier, the greater the value of the tunnelling current density obtained. This is due to the narrower width of the barrier making it easier for the electrons to tunnel through the potential barrier, resulting in a higher electron transmittance and tunnelling current density.

4. Conclusion
We have derived the analytical expression of transmittance and tunnelling current through a trapezoidal potential barrier by including the spin polarization effect. It is shown that the transmittances calculated under the Airy wavefunction-approach match those computed under the matrix transfer method. It is also shown that the transmittances in the spin up state are higher than those in the spin down state. In addition, the tunnelling currents increase as the bias voltage increases and the barrier width decreases.

5. References
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