Theoretical analysis quantum tunnelling three potential barriers to the Schrodinger equation in graphene

S H B Prastowo, B Supriadi, Z R Ridlo, M K Huda, W Baririoh and U Sholihah
1Departemen of Physic Education, University of Jember, Indonesia

Email: physicshuda@gmail.com

Abstract. Quantum mechanics is a branch of physics that can answer problems involving atomic nuclei, atoms, molecules, and matter in solids rather than classical mechanics. The phenomenon of three barrier tunnelling effects is the development of a double barrier tunnelling effect. This study aims to determine the transmission coefficient on three barriers. This study uses a barrier with the semiconductor material, graphene. Graphene material has a band gap energy close to 0 eV with a lattice distance of 0.246 nm. Analysis of tunnelling effects using the Schrodinger equation does not depend on time with the matrix propagation method. The results shown get the largest transmission coefficient is 1.00 of energy electron 0.9225 eV, meaning the chance of electrons in breaking through the barrier to 100%. However, after reaching the largest coefficient point on the three electron barriers the transmission coefficient decreases even though the energy is getting higher. But on one and two electron energy barriers and the transmission coefficient increases and does not decrease. The properties of this very special graphene can create a new opportunity in the utilization to produce better electronic field products such as supercapacitors and transistors.

1. Introduction

Quantum mechanics is a branch of physics that can answer problems involving atomic nuclei, atoms, molecules, and matter in solids rather than classical mechanics. This science provides a mathematical framework for various branches of physics and chemistry. Quantum mechanics was developed through approaches developed by Erwin Schrödinger, Warner Heisenberg, and others. Quantum mechanics produces observable quantities such as opportunities (possibilities) in observing and ascertaining in atomic problems, for example in experiments using the radius of the orbit of electrons in the ground state of a hydrogen atom it will produce almost the same price, but most provide the greatest chance ± 5 3 x 10−11 m [2]. The development of quantum mechanics has begun to be felt in the present century, much research on quantum mechanics such as research on the effects of stark. The Stark effect is the effect of shifting or polarizing the atomic spectrum caused by an external electrostatic field [9].

Another development in quantum mechanics in the present century is the tunnelling phenomenon. The principle of breakthrough or tunnelling effects in the theory of quantum physics is a very interesting phenomenon studied at the same time that distinguishes it from classical physics. The development of science in quantum physics needs to be done including developing the concept of tunnelling by analyzing it more deeply. In the breakthrough effect phenomenon, there is a principle of resonance wherein, with energy that is small enough to produce coefficients that are equal to one. The application of theoretical analysis of the effects of resonance on potential double barriers is used to design and develop new structures of materials for semiconductor devices (diodes, transistors, and integrated circuits) [7].

Graphene is the thinnest, strongest and most superior new material in the world today that is formed from a single layer of carbon atoms that have a hexagonal structure resembling a honeycomb. Stacked graphene sheets will form carbon-based materials such as graphite. The sheets are bound by van der Waals bonds with a gap between 0.335 nm. Graphene has a distance between atoms of 0.142
nm and is bound by covalent bonds. The advantages of graphene in terms of conductivity are single-layer layers which have a conductivity of $0.96 \times 10^6 \Omega^{-1} \text{cm}^{-1}$ [3]. The conductivity of graphene material can also be determined by the influence of zinc content and hydrothermal temperature. The biggest electrical conductivity value is produced from variations of zinc powder addition of 0.8 gram and hydrothermal temperature of 200°C with a value of $0.10281 \text{S/cm}$ and iodine number 11384.64 [1]. In addition, graphene electronic tape structure can be described analytically using strong, and numerical bonding models such as Density Functional Theory, GW approximation, and Tight Binding with TDSE completion [8], besides graphene crystals can be chipped into [(CH) N or (C6H6) N] with a two-hour exposure to cold disposal of hydrogen atoms, after annealing in Ar for four hours at 300°C [10].

The development of the theory of breakthrough effects on a barrier can be solved by several approaches, namely the approach with the Schrodinger equation, WKB, and also Matrix Propagation. Wentzel-Kramers-Brillouin (WKB) is an approach to calculating the probability of quantum tunnelling a potential barrier function [6]. The WKB approach includes a technique for obtaining an estimate of the time-dependent Schrodinger equation solution in one dimension [4]. But this approach is quite complex and many must be understood, so that researchers use the matrix propagation approach because it is easier to understand and simpler to operate. Propagation matrix is very easy to use and easy to understand, only requires mathematical capabilities in the matrix.

2. Methods
The method used in the research is the method of matrix propagation. The steps in the matrix propagation method are as follows.

![Figure 1. scheme tunnelling effect on triple barrier](image)

Step 1: write down the wave function in each area

\[
\psi_1(x) = O e^{i k_1 x} + P e^{-i k_1 x}, \\
\psi_2(x) = Q e^{k_2 x} + R e^{-k_2 x}, \\
\psi_3(x) = S e^{i k_1 x} + T e^{-i k_1 x}, \\
\psi_4(x) = U e^{k_2 x} + V e^{-k_2 x}, \\
\psi_5(x) = W e^{i k_1 x} + X e^{-i k_1 x}, \\
\psi_6(x) = Y e^{k_2 x} + Z e^{-k_2 x}, \\
\psi_7(x) = A A e^{i k_1 x}
\]

Electron or a particle has a wave vector in each region,

\[
k_1 = \frac{(2m(E))^{1/2}}{\hbar} \text{and} k_2 = \frac{(2m(E-eV))^{1/2}}{\hbar}
\]

Step 2: Determine Step Up Propagation
Using continuity requirements on step up1,

\[
\begin{align*}
\psi_1(0) &= \psi_2(0) \\
O + P &= Q + R \quad (8) \\
d\psi_1(0) &= d\psi_2(0) \\
dx &= dx \\
\frac{dx}{ik_1} O - \frac{dx}{ik_1} P &= \frac{dx}{k_2} Q - \frac{dx}{k_2} R \\
\end{align*}
\]

So that from equation (9) divided by $ik_1$ the following equation will be obtained.

\[
O - P = \frac{k_2}{ik_1} Q - \frac{k_2}{ik_1} R
\]

For example $\hat{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$
Then the inverse matrix above is
\[
\hat{A}^{-1} = \frac{1}{\det} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}
\] (11)

Where the determinant of the matrix \( \hat{A} \) is
\[
\det = a_{11}a_{22} - a_{12}a_{21}
\]

Then equations (8) and (9) are changed in the form of a matrix and the matrix is obtained as follows.
\[
\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} p \end{bmatrix} = \frac{1}{2} \begin{bmatrix} k_2 & -k_2 \\ ik_1 & -ik_1 \end{bmatrix} \begin{bmatrix} Q \\ R \end{bmatrix}
\] (12)

So equation (10) can be simplified into the following equation.
\[
\begin{bmatrix} p \end{bmatrix} = \hat{p}_{\text{step}} \begin{bmatrix} Q \\ R \end{bmatrix}
\]

where \( \hat{p}_{\text{step}} \) is a matrix \( 2 \times 2 \) that describes the propagation wave at a step potential, to get this equation, we need to remove the matrix \( 2 \times 2 \) on the left side of equation (12) [5].

Then the inverse of the matrix \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} is the same with \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{-1} & \frac{1}{-1} \end{bmatrix}, so that the equation can be written as follows.
\[
\begin{bmatrix} Q \\ P \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ \frac{k_2}{ik_1} \\ -\frac{k_2}{-ik_1} \end{bmatrix} \begin{bmatrix} Q \\ R \end{bmatrix} = \hat{p}_{\text{step}} \begin{bmatrix} Q \\ R \end{bmatrix}
\] (13)

So the matrix step up is
\[
\hat{p}_{\text{step up} \ 1} = \frac{1}{2} \begin{bmatrix} 1 + \frac{k_2}{ik_1} & 1 - \frac{k_2}{ik_1} \\ 1 - \frac{k_2}{ik_1} & 1 + \frac{k_2}{ik_1} \end{bmatrix}
\] (14)

Then, in the same way, the next step matrix can be determined.
\[
\hat{p}_{\text{step up} \ 2} = \frac{1}{2} \begin{bmatrix} 1 + \frac{k_2}{ik_1} & 1 - \frac{k_2}{ik_1} \\ 1 - \frac{k_2}{ik_1} & 1 + \frac{k_2}{ik_1} \end{bmatrix}
\]
\[
\hat{p}_{\text{step up} \ 3} = \frac{1}{2} \begin{bmatrix} 1 + \frac{k_2}{ik_1} & 1 - \frac{k_2}{ik_1} \\ 1 - \frac{k_2}{ik_1} & 1 + \frac{k_2}{ik_1} \end{bmatrix}
\]

Step 3: determine the propagation matrix step down
\[
\begin{align*}
\psi_2(0) &= \psi_3(0) \\
Q + R &= S + T \\
\frac{d\psi_2(0)}{dx} &= \frac{d\psi_3(0)}{dx} \\
k_2Q - k_2R &= ik_1S - ik_1T
\end{align*}
\] (15)

So that from equation (16) divided by \( ik_1 \) the following equation will be obtained.
\[
Q - R = \frac{ik_1}{k_2}S - \frac{ik_1}{k_2}T
\] (17)

For example \( \hat{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \)

Then the inverse matrix above is
\[
\hat{A}^{-1} = \frac{1}{\det} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}
\] (18)

Where the determinant of the matrix \( \hat{A} \) is
\[
\det = a_{11}a_{22} - a_{12}a_{21}
\]

Then equations (15) and (16) are changed in the form of a matrix and the matrix is obtained as follows.
\[
\begin{bmatrix}
1 & 1 \\
-1 & 1
\end{bmatrix}
\begin{bmatrix}
Q \\
R
\end{bmatrix}
= 
\begin{bmatrix}
1 & 1 \\
\frac{k_2}{ik_1} & -\frac{k_2}{ik_1}
\end{bmatrix}
\begin{bmatrix}
S \\
T
\end{bmatrix}
\]

So equation (17) can be simplified into the following equation.

\[
\begin{bmatrix}
Q \\
R
\end{bmatrix}
= \hat{p}_{\text{step}}
\begin{bmatrix}
S \\
T
\end{bmatrix}
\]

where \(\hat{p}_{\text{step}}\) is a matrix \(2 \times 2\) that describes the propagation wave at a step potential, to get this equation, we need to remove the matrix \(2 \times 2\) on the left side of equation (19).

Then the inverse of the matrix \(\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\) is the same with \(\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\), so that the equation can be written as follows.

\[
\begin{bmatrix}
Q \\
R
\end{bmatrix}
= \frac{1}{2}
\begin{bmatrix}
1 & 1 \\
1 & -1
\end{bmatrix}
\begin{bmatrix}
1 & 1 \\ \frac{ik_1}{k_2} & \frac{ik_1}{k_2}
\end{bmatrix}
\begin{bmatrix}
S \\
T
\end{bmatrix}
\]

So the step-down matrix is

\[
\hat{p}_{\text{step down 1}} = \frac{1}{2}
\begin{bmatrix}
1 + \frac{ik_1}{k_2} & 1 - \frac{ik_1}{k_2} \\
1 - \frac{ik_1}{k_2} & 1 + \frac{ik_1}{k_2}
\end{bmatrix}
\]

Then, in the same way, the next step matrix can be determined.

\[
\hat{p}_{\text{step down 2}} = \frac{1}{2}
\begin{bmatrix}
1 + \frac{ik_1}{k_3} & 1 - \frac{ik_1}{k_3} \\
1 - \frac{ik_1}{k_3} & 1 + \frac{ik_1}{k_3}
\end{bmatrix}
\]

\[
\hat{p}_{\text{step down 3}} = \frac{1}{2}
\begin{bmatrix}
1 + \frac{ik_1}{k_4} & 1 - \frac{ik_1}{k_4} \\
1 - \frac{ik_1}{k_4} & 1 + \frac{ik_1}{k_4}
\end{bmatrix}
\]

Step 4: determine propagation in area E < V

\[
\psi Q e^{k_2 L_1} = \psi S
\]

\[
\psi R e^{-k_2 L_1} = \psi T
\]

Equations (15) and (16) can be changed to the matrix as follows.

\[
\begin{bmatrix}
e^{k_2 L_1} & 0 \\
0 & e^{-k_2 L_1}
\end{bmatrix}
\begin{bmatrix}
Q \\
R
\end{bmatrix}
= 
\begin{bmatrix}
S \\
T
\end{bmatrix}
\]

So that is obtained

\[
\begin{bmatrix}
Q \\
R
\end{bmatrix}
= 
\begin{bmatrix}
e^{-k_2 L_1} & 0 \\
0 & e^{k_2 L_1}
\end{bmatrix}
\begin{bmatrix}
S \\
T
\end{bmatrix}
\]

Then,

\[
\hat{p}_{\text{free 1}} = 
\begin{bmatrix}
e^{-k_2 L_1} & 0 \\
0 & e^{k_2 L_1}
\end{bmatrix}
\]

In the same way, it will be obtained,

\[
\hat{p}_{\text{free 3}} = 
\begin{bmatrix}
e^{-k_3 L_3} & 0 \\
0 & e^{k_3 L_3}
\end{bmatrix}
\]

\[
\hat{p}_{\text{free 5}} = 
\begin{bmatrix}
e^{-k_4 L_5} & 0 \\
0 & e^{k_4 L_5}
\end{bmatrix}
\]

Step 5: determine propagation in area E> V

\[
\psi S e^{k_2 L_1} = \psi U
\]

\[
\psi T e^{-k_2 L_1} = \psi V
\]
Equations (24) and (25) can be changed to the matrix as follows.

\[
\begin{bmatrix}
e^{ik_1L_2} & 0 \\
0 & e^{-ik_1L_2}
\end{bmatrix}
\begin{bmatrix}
|S| \\
|T|
\end{bmatrix}
= \begin{bmatrix}
|U| \\
|V|
\end{bmatrix}
\]

So that is obtained

\[
\begin{bmatrix}
|Q| \\
|R|
\end{bmatrix}
= \begin{bmatrix}
e^{ik_1L_2} & 0 \\
0 & e^{-ik_1L_2}
\end{bmatrix}
\begin{bmatrix}
|S| \\
|T|
\end{bmatrix}
\]

Then,

\[
\hat{p}_{\text{free}} 2 = \begin{bmatrix}
e^{-ik_1L_2} & 0 \\
0 & e^{ik_1L_2}
\end{bmatrix}
\]

In the same way it will be obtained,

\[
\hat{p}_{\text{free}} 4 = \begin{bmatrix}
e^{-ik_1L_4} & 0 \\
0 & e^{ik_1L_4}
\end{bmatrix}
\]

Step 6: determine the transmission coefficient of the propagation matrix of a total of 3 barriers

\[
P = \hat{p}_{\text{up}} 1 \cdot \hat{p}_{\text{free}} 1 \cdot \hat{p}_{\text{down}} 1 \cdot \hat{p}_{\text{free}} 2 \cdot \hat{p}_{\text{up}} 2 \cdot \hat{p}_{\text{free}} 3 \cdot \hat{p}_{\text{down}} 2 \cdot \hat{p}_{\text{free}} 4 \cdot \hat{p}_{\text{up}} 3 \cdot \hat{p}_{\text{down}} 3
\]

3. Result and Discussion

Based on the simulation results of the transmission coefficient data collection with a computer program, that electrons have little energy but can break through a potential barrier of one barrier with the same semiconductor material. Data retrieval from 0 to 1 eV. From the retrieval of the data, the results are obtained as follows

![Graph 2](image)

**Figure 2.** Graph the relationship between electron energy and the transmission coefficient on one barrier

Graphs above breakthrough phenomena in one barrier with graphene material produces graphs that continue to increase followed by energy which also continues to increase. This suggests that the breakthrough effect on graphene is still said that electrons are well able to break through the barrier well.
Figure 3. Graph the relationship between electron energy and the transmission coefficient on two barriers

Likewise in the graph above the breakthrough phenomenon in two barriers with graphene material produces a graph that continues to increase followed by energy which also continues to increase as a graph on a one barrier graph. This suggests that the breakthrough effect on graphene is still said that electrons are well able to break through the barrier well.

Based on the simulation results of the transmission coefficient data collection with a computer program, that electrons have little energy but can break through a potential barrier of three barriers with the same semiconductor material. Data retrieval from 0 to 1 eV. From the retrieval of the data, the results are obtained as follows.

Figure 4. Graph the relationship between electron energy and the transmission coefficient on three barriers

Based on the graph data it can be explained that the results obtained from data retrieval with the help of a computer program are the energy electrons which are at least 0.0025 eV resulting in a transmission coefficient of 0.0001 and at 1 eV energy producing a transmission coefficient of 0.9702. From the graph above electrons are able to get a transmission coefficient of 100% in the energy range 0.9200-0.9225 eV, then begin to experience a decline in energy electron 0.9975 eV. This result shows
that in graphene semiconductor material which has a lattice distance of 0.246 nm with potential energy of 3 eV electrons it perfectly breaks through the semiconductor material.

### Table 1. Result energy and transmission coefficient on three barrier

| Data | Electron Energy (eV) | Transmission Coefficient |
|------|----------------------|--------------------------|
| 1    | 0.0025               | $5.1256 \times 10^{-5}$  |
| 2    | 0.2000               | 0.0101                   |
| 3    | 0.4000               | 0.0590                   |
| 4    | 0.5000               | 0.1297                   |
| 5    | 0.6000               | 0.2826                   |
| 6    | 0.7500               | 0.7199                   |
| 7    | 0.8500               | 0.9573                   |
| 8    | 0.9200               | 1.0000                   |
| 9    | 0.9225               | 1.0000                   |
| 10   | 0.9975               | 0.9717                   |
| 11   | 1.0000               | 0.9702                   |

The table above draws the results of data transmission coefficient from the energy interval 0 to 1 eV. From these results, the observed transmission coefficients continue to increase from 0.0025 to 0.9225 which means that the electrons very well break through the three barriers of the graphene material, but at 0.9975 eV electron energy the transmission coefficient decreases from 100% to 97.17% to 1 eV energy, the transmission coefficient is only around 97.02%. These results indicate that with graphene material as an electron barrier in breaking through the barrier potential it is very good and shows that the material is also very good. The better the electron breaks through the material, the better the material will be used as an electronic device.

Based on some of the graphs above stated that the breakthrough effect can be seen that the smaller the potential width, the better the electron in breaking through the barrier in the semiconductor material because based on previous research on a wider material states that the electron graph is able to return to its original state. We can say that potential and large widths can potentially affect the good and bad of semiconductor materials as electron devices that will be used in everyday life.

### Table 2. Result energy and transmission coefficient on two barriers by Prastowo et.al

| Data | Electron Energy (eV) | Transmission Coefficient |
|------|----------------------|--------------------------|
| 1    | 0.0025               | $3.14 \times 10^{-17}$   |
| 2    | 0.3975               | 0.0035                   |
| 3    | 0.4259               | 0.5229                   |
| 4    | 0.4453               | 0.8249                   |
| 5    | 0.5123               | 0.9982                   |
| 6    | 0.5886               | 0.9616                   |
| 7    | 0.6975               | 0.8993                   |
| 8    | 0.8425               | 0.8524                   |
| 9    | 1.0                  | 0.8291                   |

Try to compare table 1 with table 2, the results of table 2 from the Prastowo et.al study show that the results of the transmission coefficient obtained continue to increase from energy 0.0025 eV to energy 0.8425 eV with the maximum coefficient obtained is 85.24% and decrease back to energy 1 eV until the limit of the coefficient being reached is 82.91%. While in Table 1 of the development research Prastowo et.al showed significantly different results and better than the previous research because the resulting transmission coefficient reaches 100% of the energy range 0.9200-0.9225 eV and at 1 eV energy the coefficient achieved is 97.02%. This result is different because there are several factors that influence the semiconductor material used is different so that the width and height
of the barrier are also different. In table 2 using GaAs and Pb semiconductor materials while in table 1 all barriers use graphene. From these results, it also proves that graphene material is material that can be used as future material for the development of electronic devices in the world. Besides the opportunity to break through three potential barriers can be shown in figure 5. Generally, the graph states that the electron can burst well until the third barrier and continues to increase until the energy is 0.9225 eV.

![Figure 5](image)

**Figure 5.** Graph the relations between electron energy and the transmission coefficient

4. Conclusion
Based on the results obtained, it shows that the transmission coefficient achieved by an electron can break through a barrier with graphene semiconductor material at a maximum transmission coefficient barrier reached 0.7937 or 79.37% of the energy of 1.00 eV. In the two barriers, the maximum transmission coefficient is reached 0.8555 or 85.55% of the energy of 1.00 eV. The results of one and two barrier transmission coefficients continue to increase with energy which also increases. Whereas in the three maximum transmission coefficient barriers reached 1.00 or 100% of energy 0.9200-0.9225 eV and at 0.9975 eV electron energy begins to decrease the transmission coefficient from 100% to 97.17% to energy 1 eV transmission coefficient is only in the range of 97.02%. This shows that resonant graphene tunnelling occurs on three barriers. In general, the transmission coefficients obtained at the three barriers continue to increase to the energy range of 0.9200-0.9225 eV. The results also show that the electron's ability to break through the semiconductor material is so good that graphene is one of the excellent semiconductor materials to produce the best semiconductor from the previous material. The hope is that this very special graphene can create a new opportunity in the utilization to produce a better electronic products such as supercapacitors and transistors. This research still needs further research that is better with other materials and with different barrier widths.

Acknowledgement
We gratefully acknowledge the support of 3rd Research Group Physics Education from FKIP-Jember University of the year 2018.

References
[1] Azizah L N and Susanti D 2014 Pengaruh Variasi Kadar Zn Dan Temperatur Hydrothermal Terhadap Struktur Dan Nilai Konduktivitas Elektrik Material Graphene. JURNAL TEKNIK POMITS. 3 (2) : 209-214.
[2] BeiserA 2003 Concepts of Modern Physics Sixth Edition (New York: The McGraw-Hill Companies, Inc)
[3] Fikri A A and Dwandaru WS B2016 Pengaruh Variasi Konsentrasi Surfactan Dan Waktu Ultrasonikasi Terhadap Sintesis Material Graphene Dengan Metode LiquidSonification
Exfoliation Menggunakan Tweeter Ultrasonication Graphite Oxide Generator. *Jurnal Fisika*. 5 (3) 188-197

[4] Griffith D J 2005 *Introduction To Quantum Mechanics Second edition* (USA:Pearson Education inc)

[5] Levi A F J 2003 *Applied Quantum Mechanics* (Cambridge: Cambridge University Press)

[6] Nufida D A, Rizka N F, Hermawan K D, and FebdianR2017 A Theoretical Study of Monodeuteriation Effect on the Rearrangement of trans-HCOH to H2CO via Quantum Tunneling with DFT and WKB Approximation. *Procedia Engineering*. 170 (119 – 12)

[7] Prastowo S H B, Supriadi B, Ridlo Z R, and Prihandono, T 2018 Tunneling effect on double potential barriers GaAs and PbS. *Journal Of Physics*. Series 1008 (102012) : 1-7.

[8] Qosim M and Santoso I 2015 Kajian Struktur Pita Elektronik Graphene Dan Graphane Menggunakan Model Ikatan Kuat Realistidengan Ketakteraturan. *JurnalFisika Indonesia*. 55 (19) 28-33

[9] Supriadi B, S H B Prastowo, S Bahri, Z R Ridlo, and T Prihandono2018The Stark Effect on the Wave Function of Tritium in Relativistic Condition. *Journal Of Physics*. Series 997 (012045) : 1-7.

[10] Wolf E L 2014 *Graphene* (UK: Oxford University Press)