



جامعة  
بنغازي الحديثة



**مجلة جامعة بنغازي الحديثة للعلوم  
والدراسات الإنسانية  
مجلة علمية إلكترونية محكمة**

**العدد الثامن**

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حقوق الطبع محفوظة

## شروط كتابة البحث العلمي في مجلة جامعة بنغازي الحديثة للعلوم والدراسات الإنسانية

- 1- الملخص باللغة العربية وباللغة الانجليزية (150 كلمة).
- 2- المقدمة، وتشمل التالي:
  - ❖ نبذة عن موضوع الدراسة (مدخل).
  - ❖ مشكلة الدراسة.
  - ❖ أهمية الدراسة.
  - ❖ أهداف الدراسة.
  - ❖ المنهج العلمي المتبع في الدراسة.
- 3- الخاتمة. (أهم نتائج البحث - التوصيات).
- 4- قائمة المصادر والمراجع.
- 5- عدد صفحات البحث لا تزيد عن (25) صفحة متضمنة الملاحق وقائمة المصادر والمراجع.

### القواعد العامة لقبول النشر

1. تقبل المجلة نشر البحوث باللغتين العربية والانجليزية؛ والتي تتوفر فيها الشروط الآتية:
  - أن يكون البحث أصيلاً، وتتوافر فيه شروط البحث العلمي المعتمد على الأصول العلمية والمنهجية المتعارف عليها من حيث الإحاطة والاستقصاء والإضافة المعرفية (النتائج) والمنهجية والتوثيق وسلامة اللغة ودقة التعبير.
  - ألا يكون البحث قد سبق نشره أو قُدم للنشر في أي جهة أخرى أو مستل من رسالة أو اطروحة علمية.
  - أن يكون البحث مراعيًا لقواعد الضبط ودقة الرسوم والأشكال - إن وجدت - ومطبوعاً على ملف وورد، حجم الخط (14) وبخط (Arial 'Body') للغة العربية. وحجم الخط (12) بخط (Times New Roman) للغة الإنجليزية.
  - أن تكون الجداول والأشكال مدرجة في أماكنها الصحيحة، وأن تشمل العناوين والبيانات الإيضاحية.
  - أن يكون البحث ملتزماً بدقة التوثيق حسب دليل جمعية علم النفس الأمريكية (APA) وتثبيت هوامش البحث في نفس الصفحة والمصادر والمراجع في نهاية البحث على النحو الآتي:
  - أن تُثبت المراجع بذكر اسم المؤلف، ثم يوضع تاريخ نشره بين حاصرتين، يلي ذلك عنوان المصدر، متبوعاً باسم المحقق أو المترجم، ودار النشر، ومكان النشر، ورقم الجزء، ورقم الصفحة.
  - عند استخدام الدوريات (المجلات، المؤتمرات العلمية، الندوات) بوصفها مراجع للبحث: يُذكر اسم صاحب المقالة كاملاً، ثم تاريخ النشر بين حاصرتين، ثم عنوان المقالة، ثم ذكر اسم المجلة، ثم رقم المجلد، ثم رقم العدد، ودار النشر، ومكان النشر، ورقم الصفحة.
2. يقدم الباحث ملخص باللغتين العربية والانجليزية في حدود (150 كلمة) بحيث يتضمن مشكلة الدراسة، والهدف الرئيسي للدراسة، ومنهجية الدراسة، ونتائج الدراسة. ووضع الكلمات الرئيسية في نهاية الملخص (خمس كلمات).

3. تحتفظ مجلة جامعة بنغازي الحديثة بحقها في أسلوب إخراج البحث النهائي عند النشر.

## إجراءات النشر

ترسل جميع المواد عبر البريد الإلكتروني الخاص بالمجلة جامعة بنغازي الحديثة وهو كالتالي:

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- ✓ لا يقبل استلام الورقة العلمية الا بشروط وفورمات مجلة جامعة بنغازي الحديثة.
- ✓ في حالة قبول البحث مبدئياً يتم عرضة على مُحكمين من ذوي الاختصاص في مجال البحث، ويتم اختيارهم بسرية تامة، ولا يُعرض عليهم اسم الباحث أو بياناته، وذلك لإبداء آرائهم حول مدى أصالة البحث، وقيمتها العلمية، ومدى التزام الباحث بالمنهجية المتعارف عليها، ويطلب من المحكم تحديد مدى صلاحية البحث للنشر في المجلة من عدمها.
- ✓ يُخطر الباحث بقرار صلاحية بحثه للنشر من عدمها خلال شهرين من تاريخ الاستلام للبحث، وبموعد النشر، ورقم العدد الذي سينشر فيه البحث.
- ✓ في حالة ورود ملاحظات من المحكمين، تُرسل تلك الملاحظات إلى الباحث لإجراء التعديلات اللازمة بموجبها، على أن تعاد للمجلة خلال مدة أقصاها عشرة أيام.
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# Transmission and Reflection Coefficients of the Random Electron Energy Profile With Respect to a Step Potential Barrier

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## Abstract.

An electron beam one-dimensional scattering problem has been treated in terms of quantum mechanics perspective by the agency of FORTRAN code to simulate the electron generator. One thousand different incident energies were examined within the range of (0.5 – 1.0 keV) to cross a step potential energy barrier of 0.5 keV. The percentage of the electrons that more likely to transmit or reflect due to the existence of the step-potential were investigated by the route of transmission and reflection coefficients. Unblemished curves obtained to represent the relation between the coefficients and the electron incident energies. The two coefficients are found, as it is intuitively expected to complement each other; their sum is unity everywhere.

**Key words:** Scattering problem, Transmission coefficient, Reflection coefficient.

## المخلص:

تمت معالجة مشكلة التشتت لحزمة من الالكترونات على ضوء مبادئ ومسلّمات ميكانيكا الكم كما تمت محاكات مولد الالكترونات وبطاقات مختلفة بواسطة برنامج تمت كتابته خصيصا لهذا الغرض بلغة الفورتران. طاقات الالكترونات الساقطة التي تم اختبارها كانت 1000 قيمة مختلفة لتغطي نطاق طاقي يتراوح من 0.5 keV الي 1 keV لتجتاز عتبة جهد قدرها 0.5 keV. استخدم معاملي المرور والانعكاس لتحديد نسبة الالكترونات المارة والمنعكسة. اظهرت النتائج منحنيين خاليين من العيوب عند رسم المعاملات مع الطاقة. كما كان متوقعا فان المعاملين مكملين لبعضهما البعض وحاصل الجمع عند أي قيمة من قيم الطاقة يساوي الواحد الصحيح.

## Introduction.

In quantum mechanics realm, a particle (say an electron) penetrates a potential barrier and end up in the other region, whereas, it is completely forbidden according to classical mechanics point of view. The analogy of this statement in macroscopic level is having a hill of height  $h$  and a ball of mass  $m$  ascends up the hill with a kinetic energy  $KE$ . At the top all the kinetic energy will be transferred to a potential energy. We do know, classically, if the kinetic energy is happened to be less than the gravitational potential energy, it is absolutely impossible for the object to be at the other side of the hill (Halliday, 2013). On the other hand, in quantum mechanics the scenario is absolutely deferent; always there is some probability that the particle will appear at the other side where the potential barrier exist. In other words, even though the potential barrier that the moving particle encounters is greater than the incident kinetic energy, the particle might be detected at the other side. In the last twenty years a numerous number of researches have been conducted as well as many applications of the electron quantum transport in mesoscopic and nanoscopic systems emerged (Dyndyk, 2013). The electron hopping mechanism while transporting from the left to the right lead through the central part has attracted a number of authors (Ryndyk, 2009), (Nazarov, 2009), (Ventra, 2008). This problem is well known in the research area as quantum junction. As we shall see in the following, the main formal situation to be discussed is the one dimensional electron transport problem with respect to the quantum mechanics postulates. Precisely, a confined particle to move only in one-dimension (in  $x$ -axis) with mass of  $m$  under the influence of variable potential field  $V(x)$ . The ultimate objective of this work is to figure out the one-dimensional electron scattering problem with the aid of the exquisite one-dimensional Schrödinger equation for booth bound and unbound states. This work will precede to identify the transmission and reflection coefficients ( $T$  and  $R$  respectively) of the incident electron facing a potential barrier. Taking into account the particle total energy is  $E = KE + V$  we can express the time independent Schrödinger equation as

$$\frac{\partial^2 \varphi}{\partial x^2} = -\frac{2m}{\hbar^2} (E - V)\varphi \quad (1)$$

Here we must treat two cases individually. When the particle in the allowed region where the total energy is greater than the potential energy ( $E > V$ ); in this context it is obvious that the kinetic energy is positive and identified to be

$$KE = E - V = \frac{\hbar^2 k^2}{2m} \quad (2)$$

In the above,  $k$  is the electron wave number. With this assumption one may recast the differential Equation (1) and its general basic solution as<sup>1</sup>

$$\frac{\partial^2 \varphi}{\partial x^2} = -k^2(x)\varphi \quad (3)$$

$$\varphi(x) \sim e^{\pm ikx} \quad (4)$$

On the other hand, if the potential energy barrier is greater than the total electron incident energy ( $E < V$ ), the electron is said to be in the classical forbidden region<sup>2</sup>. Under this condition, the differential Equation (1) and its basic solution are

$$\frac{\partial^2 \varphi}{\partial x^2} = k^2(x)\varphi \quad (5)$$

$$\varphi(x) \sim e^{\pm kx} \quad (6)$$

The insight eye can readily recognize that if the particle is in the allowed region, the solution is an oscillatory wave function ( $\sim e^{\pm ikx}$ ). In contrast, the solution is represented by a decaying wave ( $\sim e^{-kx}$ ) or a growing wave ( $\sim e^{+kx}$ ) if the particle happened to be in the classically forbidden region. The classical turning point is distinctly detected at  $E = V$  that corresponding to  $\partial^2 \varphi / \partial x^2 = \partial \varphi / \partial x = 0$ ; which means, the solution of our Schrödinger equation at the classical turning point is a wave function  $\varphi(x)$  with a constant slop.

### Bound and unbound states of the electron.

In one-dimensional system, a normalizable wave function can exquisitely represent the electron bound state (Veszprémi, 2012). Mathematically, it is always true that a bound state  $\psi$  complies the condition

$$|\psi|^2 \rightarrow 0 \text{ for } |x| \rightarrow \infty \text{ (for all values of } t) \quad (7)$$

The norm integral of the electron bound state over a broad interval gives a specific finite value

$$\int_{-\infty}^{+\infty} |\psi|^2 dx < \infty \quad (8)$$

On the contrary, the norm integral of unbound state results a finite number only over a narrow finite interval

<sup>1</sup> The incident electron kinetic energy  $\frac{\hbar^2 k^2}{2m} = E - V > 0$

<sup>2</sup> The electron possess a negative kinetic energy:  $KE = E - V = -\frac{\hbar^2 k^2}{2m}$  and  $\frac{\hbar^2 k^2}{2m} = V - E > 0$

$$\int_a^b |\psi|^2 dx < \infty \text{ for } |a - b| < \infty \quad (9)$$

It is time to reminiscence some basic information pertain to the one-dimensional linear momentum operator (in x-axis)

$$\hat{P}_x = -i\hbar \frac{\partial}{\partial x} \quad (10)$$

If the momentum operator operates the electron wave function, the general eigenvalue equation ( $\hat{A}\varphi = a\varphi$ ) will expressed as

$$-i\hbar \frac{\partial \varphi}{\partial x} = P_x \varphi \quad (11)$$

Within this framework if we measure the  $x$ -component of the linear momentum the most likely values that we might obtain are  $P_x$ . In the event that the electron is free and has no boundary condition, the solution of the previous equation is seen to be

$$\varphi(x) = A e^{\frac{iP_x x}{\hbar}} \quad (12)$$

In quantum mechanics it is customary to work with wavenumber in the lieu of linear momentum and thus, the eigenfunction and the eigenvalues of one-dimensional linear momentum operator are

$$\varphi_k(x) = A e^{ikx} \quad (13)$$

Consequently, the eigenstates of the one dimensional momentum operator are

$$\varphi_k(x) = A e^{ikx} = \frac{1}{\sqrt{2\pi}} e^{ikx}, \quad (14)$$

These eigenstates are relevant to that of the unbound or free electron state<sup>3</sup>. In actuality, a proper treatment of the electron scattering problem, demands entire description of bound and unbound states. Predominantly, this sort of problems customarily contain a bunch (or, beam) of particles, can be, electrons or neutrons of equal energies or momenta, which is incident on a step potential barrier. It is evident that the norm integral of the wave function over an infinite domain ( $\int_{-\infty}^{+\infty} |\psi|^2 dx$ ) does not converge for the free electron state, dealing with a normalized wave function with respect to the particle density is preferred. In one-dimensional problem, the incident particle density  $\rho$  can be defined as  $\rho = dN/dx$ ; it is simply the differential number of particles divided by the differential length. It is essential that the wave function norm at any point  $x$  is

<sup>3</sup> The coefficient in equation (14) appears from the orthonormality condition of the electron eigenstates.

directly proportional to the existence of the electron there<sup>4</sup> (Feynman, 1965), we might write

$$|\psi|^2 dx = \rho dx = dN, \quad (15)$$

Or simply the total number of electrons that exist in a finite interval is (Liboff, 2003)

$$\int_a^b |\psi|^2 dx = N \quad (16)$$

### Current density and continuity equation.

In three-dimensional systems, the relationship between the incident electron density  $\rho$  and its relevant current density  $\mathbf{J}$  can perfectly described by continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0 \quad (17)$$

The integration of the left-hand side over a closed volume gives

$$\oint_V \frac{\partial \rho}{\partial t} d\mathbf{r} + \oint_V \nabla \cdot \mathbf{J} d\mathbf{r} = 0 \quad (18)$$

Taking into account the definition of the total number of electrons ( $N = \oint_V \rho d\mathbf{r}$ ), we obtain<sup>5</sup>

$$\frac{\partial N}{\partial t} + \oint_S \mathbf{J} \cdot d\mathbf{S} = 0 \quad (19)$$

A quick insight to equations (17) and (19), tells the verification concept of conservation of matter. For a bunch of electrons restricted to move in one-dimension ( $x$ -direction), the reduced form of the current density vector is written as  $\mathbf{J} = J_x \hat{\mathbf{x}}$ , whereas the continuity equation is

$$\frac{\partial \rho}{\partial t} + \frac{\partial J_x}{\partial x} = 0 \quad (20)$$

We have shortly in equation (15) associated the square norm of the electron wave-function with the electron density. In order to establish a mathematical expression that represents the current density in terms of the

<sup>4</sup> At any point  $x$ , we are specific that  $|\psi|^2 dx \propto \rho dx$ . In this study, the proportionality constant arbitrary has been taken to be unity.

<sup>5</sup> Here, the Gauss's theorem ( $\oint_V \nabla \cdot d\mathbf{r} = \oint_S \mathbf{J} \cdot d\mathbf{S}$ ) has been utilized to simplify the integral.



electron wave-function, we have to follow the same concept for the wave norm and the electron density (Feynman, 1965), (Liboff, 2003). To do so, the perfect way is to invest the one-dimensional-time-dependent Schrödinger equations in the form of

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} \hat{H} \psi \quad \text{and} \quad \frac{\partial \psi^*}{\partial t} = +\frac{i}{\hbar} \hat{H} \psi^* \quad (21)$$

The one-dimensional Hamiltonian operator is defined as

$$\hat{H} = \frac{\hat{P}_x^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (22)$$

Taking into consideration that  $|\psi|^2 = \psi^* \psi$ , concurrently, it is the electron density  $\rho$ , we may readily write

$$\frac{\partial \psi^* \psi}{\partial t} = \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} = \psi^* \left( \frac{-i\hat{H}}{\hbar} \psi \right) + \psi \left( \frac{+i\hat{H}}{\hbar} \psi^* \right) \quad (23)$$

Substitution of the Hamiltonian from equation (22) yields

$$\frac{\partial \psi^* \psi}{\partial t} = \frac{i\hbar}{2m} \left( \psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x^2} \right) \quad (24)$$

Or simply

$$\frac{\partial \psi^* \psi}{\partial t} + \frac{\partial}{\partial x} \left[ \frac{i\hbar}{2m} \left( \psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \right] = 0 \quad (25)$$

If we correlate equation (20) with equation (25) with respect to the above mentioned definitions, one may conclude that the one-dimensional current density can be identified as

$$J_x = \frac{\hbar}{2mi} \left( \psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \quad (26)$$

One more thing we should emphasize here is the dimension of  $x$ -component of the current density, which is obviously seen from equation (20) to be particle/time.

## Material and methods.

The electron one-dimensional scattering problem can be utterly treated on the light of transmission and reflection concept. The particles (or electrons) that have definite momenta are said to be in plane-wave states. The wave-functions relevant to incident, reflected, and transmitted particles are assumed to be known. As a consequence, the current densities of those beams are identified in agreement with equation (2). Intuitively, the definition of the transmission ( $T$ ) and reflection coefficient ( $R$ ) will satisfy the following

$$T \equiv \left| \frac{J_{tran}}{J_{inc}} \right| \text{ and } R \equiv \left| \frac{J_{ref}}{J_{inc}} \right| \quad (27)$$

The reader should be aware that, if we presuppose that the incident electrons all have the same definite linear momentum ( $P_{inc} = \hbar k_1$ ) then, the reflected electrons will have precisely the opposite value ( $P_{ref} = -\hbar k_1$ ). Apart from the incident and reflected momenta, the transmitted momentum because of the potential barrier ( $V(x)$ ), will have a distinguishable momentum ( $P_{tran} = \hbar k_2$ ). In this study, we assume that the potential energies of the electrons out of the central region are constants to some definite values. In other words, a one dimensional wire-like structure centered horizontally on  $x$ -axis and extended from -1 to 1 mm has been chosen as a path of electron beam. The potential energy is zero for all values of  $x$  being within the range of  $-1 \leq x < 0$ , in contrast, it is 0.5 keV for  $0 \leq x \leq 1$ . A FORTRAN code has been written to produce 1000 energies that varies from 0.5 to 1.0 keV with nine digits accuracy after the decimal point. Each energy value commensurate with the condition that; for  $-1 \leq x < 0$ , the incident electron energy is greater than the potential energy. The written code has an ability to calculate the corresponding electron incident and transmitted velocities ( $v_{inc}$  &  $v_{tran}$ ), wavelengths ( $\lambda_{inc}$  &  $\lambda_{tran}$ ), momenta ( $P_{inc}$  &  $P_{tran}$ ), wavenumbers ( $k_1$  &  $k_2$ ), and coefficients ( $T$  &  $R$ ). The wave-functions of the incoming and outgoing electron beam might be represented as

$$\psi_{inc} = A e^{i(k_1 x - \omega_1 t)}, \quad \hbar \omega_1 = E_{inc} = \frac{\hbar^2 k_1^2}{2m} \quad (28)$$

$$\psi_{ref} = B e^{-i(k_1 x - \omega_1 t)}, \quad \hbar \omega_1 = E_{ref} = E_{inc} = \frac{\hbar^2 k_1^2}{2m} \quad (29)$$

$$\psi_{tran} = C e^{i(k_2 x - \omega_2 t)}, \quad \hbar \omega_2 = E_{tran} = \frac{\hbar^2 k_2^2}{2m} + V = E_{inc} = \hbar \omega_1 \quad (10)$$

In equation (29), we have robustly stated the fact that the electron beam total energy is conserved and the angular frequency of the incident and reflected electron must be equal. Employing the current density definition (equation 26) with the above three general solutions of the Schrödinger equations we end up with

$$J_{inc} = \frac{\hbar}{m} k_1 |A|^2 \quad (11)$$

$$J_{tran} = \frac{\hbar}{m} k_2 |C|^2 \quad (12)$$

$$J_{ref} = \frac{\hbar}{m} k_1 |B|^2 \quad (13)$$

It is precious to mention here that the last three equations are the particle currents conforming to the quantum mechanics point of view<sup>6</sup>. Inserting the recently obtained values of the particles currents into equation (27), we obtain the coefficients that we are after as

$$T = \left| \frac{C}{A} \right|^2 \frac{k_2}{k_1} \quad (14)$$

$$R = \left| \frac{B}{A} \right|^2 \quad (35)$$

It is recognized that in the event that the incident wavenumber and the transmitted one are equal ( $k_1 = k_2$ ) the simplest form of the transmission coefficient will be obtained. In this work we put into form the way that quantum mechanics work of treating the simple step problem. The total energy of the incident electrons has been altered automatically 1000 times. Our aim is to elucidate which energies are more likely to transmit to the other region of the entire energy profile. As it is depicted in Figure 1; all the incident energy values are greater than the step potential energy. Further, it is clear from the figure that there are two distinct regions, to demonstrate; in the first region  $V(x) = 0$  for  $x < 0$ , while the second region is characterized by constant potential for  $x \geq 0$ .

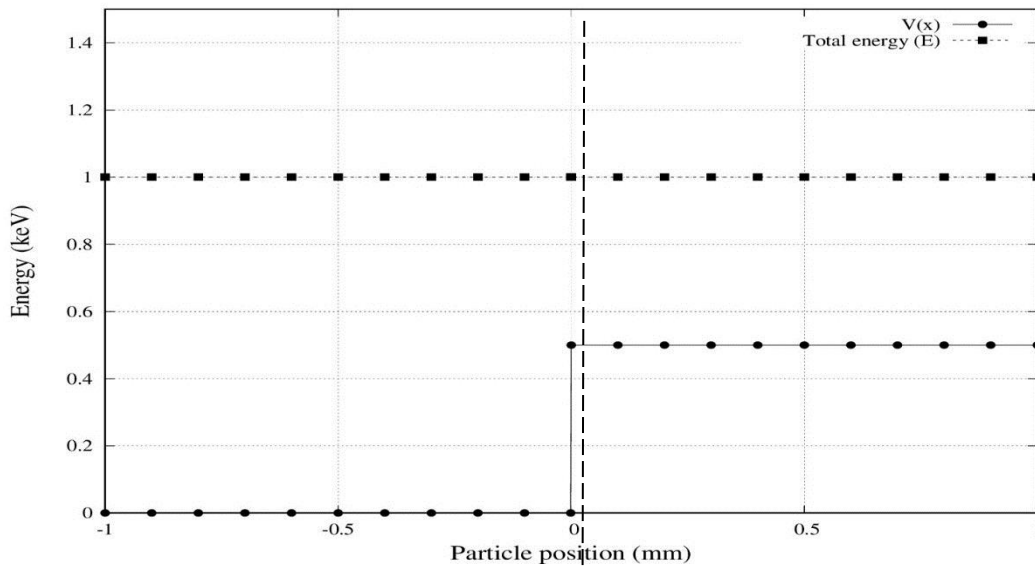


Figure 1 The step potential barrier with the maximum incident electron energy.

In the first region (region  $a$ ), the total energy is purely kinetic due to the omission of the potential energy, to obtain the wave-function ( $\varphi_a$ ) we have to solve the time-independent Schrödinger equation of this region

<sup>6</sup> The interrelationship between classical and quantum mechanics is built by means of  $\rho = |\psi|^2$ ,  $J = \rho v$ , and  $v = \frac{\hbar k}{2m}$  with  $v$  being the electron speed.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \varphi}{\partial x^2} = E\varphi \quad (36)$$

By taking  $E = \hbar^2 k_1^2 / 2m$  we end up with

$$\frac{\partial^2 \varphi}{\partial x^2} = -k_1^2 \varphi \quad (37)$$

In region  $b$ , the scenario is quite different where the kinetic energy is observed to be reduced by the amount of potential energy there, and time-independent Schrödinger equation of this region is formulated as

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \varphi}{\partial x^2} = (E - V)\varphi \quad (38)$$

If we express the kinetic energy as;  $E - V = KE = \hbar^2 k_2^2 / 2m$  then, we may write equation (38) in the form of

$$\frac{\partial^2 \varphi}{\partial x^2} = -k_2^2 \varphi \quad (39)$$

The abecedarian or elementary solutions of the differential equations (37 and 39) of the electrons in regions  $a$  and  $b$  in their most generic forms respectively are

$$\psi_a = Ae^{ik_1x} + Be^{-ik_1x} \quad (40)$$

$$\psi_b = Ce^{ik_2x} + De^{-ik_2x} \quad (41)$$

It is conspicuous that the solutions have no time-dependent factors, to put into work, we have to include these factors which is visibly seen in Table 1. The solutions that comprise the time factors can readily interpreted as we mentioned in the last column of Table 1.

Table 1 The terms of the wave-functions in regions before and after the potential barrier with their interpretation.

Region	Wave-function term	Interpretation
$a$	$Ae^{ik_1x}e^{-i\omega_1t} = Ae^{i(k_1x - \omega_1t)}$	Incident wave traveling to the right
$b$	$Ce^{ik_2x}e^{-i\omega_2t} = Ce^{i(k_2x - \omega_2t)}$	Transmitted wave traveling to the right
$a$	$Be^{-ik_1x}e^{-i\omega_1t} = Be^{-i(k_1x + \omega_1t)}$	Reflected wave traveling to the left
$b$	$De^{-ik_2x}e^{-i\omega_2t} = De^{-i(k_2x + \omega_2t)}$	Wave traveling to the left (originate from positive infinity)

Our authentic problem demands no electrons traveling from positive infinity to the left, as a consequence, the factor  $D$  is simply zero and one may recast the solutions as

$$\psi_a = Ae^{ik_1x} + Be^{-ik_1x} \quad (42)$$

$$\psi_b = Ce^{ik_2x} \quad (43)$$

Because the solutions and their first spatial derivatives being continuous at  $x = 0$ ; in fact, this condition must be always true to guarantee that the Schrödinger equation has a single solution. Mathematically, this condition is wording as

$$\psi_a(0) = \psi_b(0) \quad (44)$$

$$\frac{\partial}{\partial x}\psi_a(0) = \frac{\partial}{\partial x}\psi_b(0) \quad (45)$$

It turns out that

$$A + B = C \ \& \ A - B = \frac{k_2}{k_1}C \quad (46)$$

Solving the above for the sake of the aimed unknown factors, we attain the following

$$\frac{C}{A} = \frac{2}{1 + k_2/k_1} \ \& \ \frac{B}{A} = \frac{1 - k_2/k_1}{1 + k_2/k_1} \quad (47)$$

Lastly, feeding the recently obtained equation into equations (34) and (35) we reach the transmission and reflection coefficients that we have eyes for, to be as

$$T = \frac{4 k_2/k_1}{[1 + (k_2/k_1)]^2} \ \& \ R = \left| \frac{1 - k_2/k_1}{1 + k_2/k_1} \right|^2 \quad (48)$$

## Results and discussion.

The incident electron energy values and their associated transmitted energies that generated from the written code were plotted in Figure 2. The incident energy profile is perfectly cover a rectangular area in region  $a$  above the step potential value within the limited borders. As it is mentioned above, those energies are mainly kinetic. By virtue of the constant value of potential in region  $b$ , all the values are seen to be logically reduced by  $V(x)$ . It is remarkable to notice here that the elementary condition ( $E_{inc} > V(x)$ ) in region  $a$  is attained. In the above, we have met that the transmission and reflection coefficients are just functions of the angular wavenumbers only. All the needful physical quantities that lead to the angular wavenumber of the incident and transmitted electron wave-functions have been calculated automatically with aid of the written code. Of course, the performance and reliability of the code has been checked in every step by handwriting calculations. From the contour depiction (Figure 3), it is

manifested that the step potential has strictly divided the graph into two distinguished regions. The first region represents the wave-functions of fairly high wavenumbers (the area between  $0.11 \times 10^{11} (1/m) \leq k \leq 0.14 \times 10^{11} (1/m)$ ). On the other hand, wave-functions of low wave-numbers appear in the area of  $0.06 \times 10^{11} (1/m) \leq k \leq 0.09 \times 10^{11} (1/m)$  in region *b* after the potential barrier. Broadly speaking, in Figure 3, the bright areas are the places where the coming electrons have higher energies and higher wavenumbers. In contrast the dark regions representing low energies and low wave numbers.

After having the angular wave-numbers being calculated via the written code, it is time to demonstrate the relationship between the incident electron energy and its transmission and reflection coefficients by means of Figure 5. Two flawless curves were appeared exhibiting the tendency of *T* and *R* with no abrupt drop or raise. Furthermore, as the incident energy increase, the value of the transmission coefficient also increase, whereas its counterpart behaves adversely. It is recognized also that in small domain ( $0.5 \text{ keV} \leq E_{inc} \leq 0.5125 \text{ keV}$ ) the transmission coefficient drastically ascend. In contrast, within the same energy range the reflection coefficient abruptly drop. At nearly  $E_{inc} = 0.5125 \text{ keV}$ , the transmission and reflection coefficients are nearly equal, which means that; a beam of electrons, all of energy amount to  $0.5125 \text{ keV}$ , 50 percent of them will transmit passing the potential barrier and the rest of them will reflect back. With incident electron energy being increased, the transmission (reflection) coefficient will gradually increase (decrease) to be near from one (zero) but not one (zero).

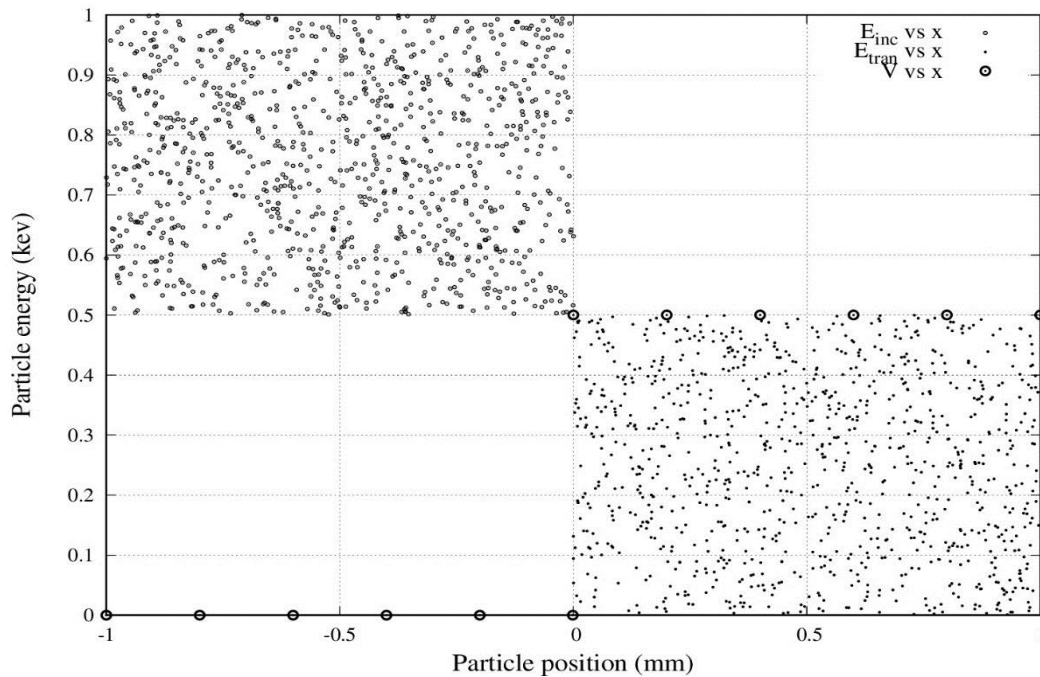


Figure 2: The examined energy profile of 1000 random values with its corresponding transmission profile as a function of *x*.

## Conclusion.

The programming language is considered a powerful tool in simulating this sort of problems exquisitely. Apart from any other perspectives, the energy profile domain in this study has been chosen only for curiosity; in subsequent works we may study a broad range of electron energies or different values of step potential. Realistically, this article just paved the way to go deeply in one-dimensional electron hopping mechanism. Each pair of electron incident energy and its associated angular wavenumber ( $E_{inc}, k_1$ ) is perfectly reflected under the influence of the step potential by reducing its values with specific amount to be ( $E_{tran}, k_2$ ). To recast, it is always true that ( $\{E_{inc}, k_1\} > \{E_{tran}, k_2\}$ ).

We have seen that modeling and solving the Schrödinger equations in their most general forms for incident, reflected, and transmitted beams with the aid of quantum mechanics postulates, leads to a fabulous plain applicable formulas. For instance, both transmission and reflection coefficients are functions of incident and transmitted angular wavenumbers only. It is worthy to mention here that there is a robust proportionality between that coefficients (transmission and reflection) and the incident electron energy. To repeat, the electron beam energy plays a substantial role to overcome the step potential barrier. In the event that the incident beam of high kinetic energy ( $E_{inc} \cong 1 \text{ keV}$ ) happens to cross the barrier, one may fairly say that more than 95% of the electrons will manage to transmit. On the other hand, only less than 5% will reflect.

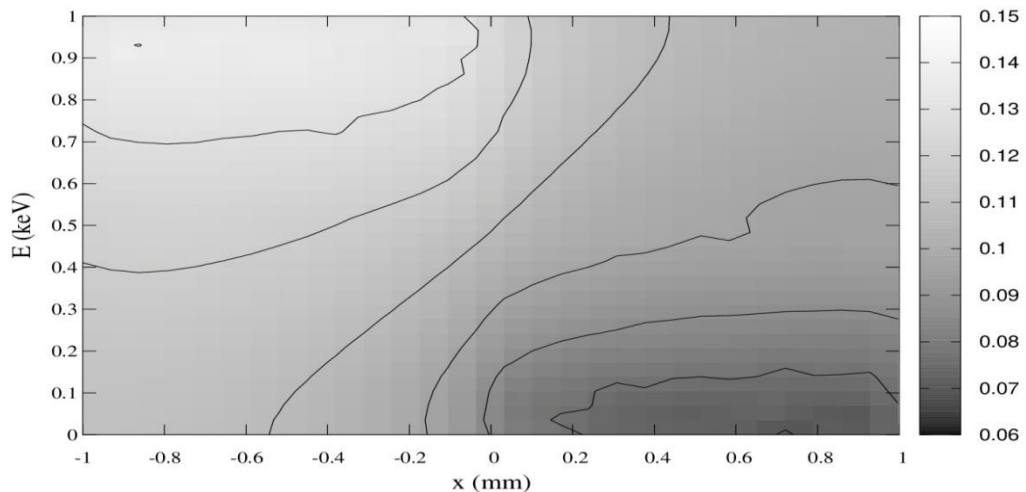


Figure 3 The studied energy profile against the particle position with their correlated wave-numbers been the contour lines<sup>7</sup>.

<sup>7</sup> The contour lines are simply the angular wave numbers of dimension of  $m^{-1}$  multiplying by  $10^{11}$ .

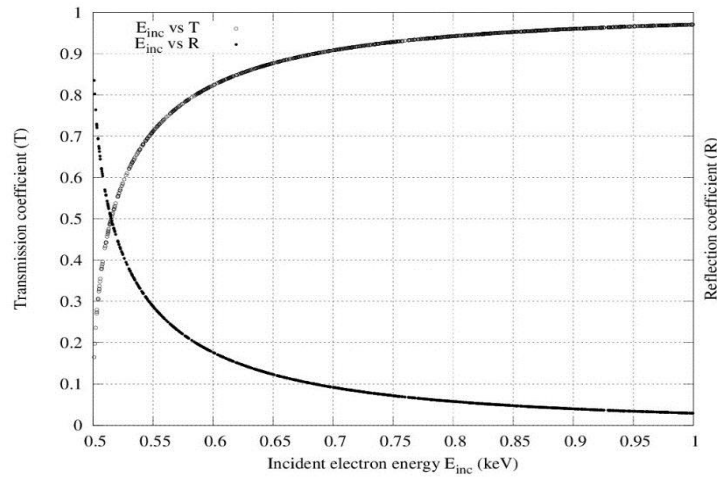


Figure 4 Transmission ( $T$ ) and reflection ( $R$ ) coefficients against the incident electron energy ( $E_{inc}$ ).

## References.

- Di Ventra, M. (2008). Electrical transport in nanoscale systems. etns.
- Feynman, R. P. (1965). Feynman lectures on physics. Volume 3: Quantum mechanics. flp.
- Halliday, D., Resnick, R., & Walker, J. (2013). Fundamentals of physics. John Wiley & Sons.
- Liboff, R. L. (2003). Introductory quantum mechanics. Pearson Education India.
- Nazarov, Y. V., Nazarov, Y., & Blanter, Y. M. (2009). Quantum transport: introduction to nanoscience. Cambridge university press.
- Ryndyk, D. A., Gutiérrez, R., Song, B., & Cuniberti, G. (2009). Green function techniques in the treatment of quantum transport at the molecular scale. In Energy Transfer Dynamics in Biomaterial Systems (pp. 213-335). Springer, Berlin, Heidelberg.
- Ryndyk, D. A., D'Amico, P., & Richter, K. (2010). Single-spin polaron memory effect in quantum dots and single molecules. Physical Review B, 81(11), 115333.
- Ryndyk, D. A., Donarini, A., Grifoni, M., & Richter, K. (2013). Many-body localized molecular orbital approach to molecular transport. Physical Review B, 88(8), 085404.
- Ryndyk, D. A. (2018). Theory of Quantum Transport at Nanoscale (introduction and contents). arXiv preprint arXiv:1812.10531.
- Veszprémi, T., & Fehér, M. (2012). Quantum chemistry: fundamentals to applications. Springer Science & Business Media.