مجلة المثنى للعلوم الصرفة
AL-Muthanna Journal of Pure Sciences (MJPS)
VOL.(3), NO.(2), 2016

Study The Electron Transport Properties of Nanowire and its applications in a Nano Electronic Device

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Received 23-3-2016, Accepted 27-2-2016, Published 27-12-2016
DOI: 10.18081/2226-3284/016-12/295-302

Abstract

In this paper, the electronic transport properties were studied for nanowire, by using non-equilibrium Green function (NEGF) theory. The results that we have obtained in this study were not noticed by other researchers previously and the electronic transport properties were calculated for a number of an even molecules ranging from (2-16) then the conductivity was calculated. This method enables us to get a good and accurate calculations and appearance of shapes agreed with the shape of (Breit Wigner) perfectly symmetrical on both left and right sides, then emergence of a magic number were conductive accumulate significantly.

Introduction

Recently, nanowires and nanorods of metallic and semiconducting materials have a lot of research interest because of their unique physical properties [1]. In 2015 S. M Al-Mutoki was studied the ZnO Nanowire/ N719 dye/ Polythiophene-SWNTnanocomposite solid state dye sensitized solar cell which designed and fabricated at high efficiency solid state dye sensitized solar cells, based on vertical ZnO nanowire[2]. As well as in 2013 S. M Al-Mutoki studied a new novel approach for synthesizing ZnO nano plate (ZNONPLs), ZnO nanowire, ZnO doped by Al, ZnO thin film by ALD on Indium Titanium Oxide(ITO) coated glass substrates for photo-voltaic applications [3].

As in 2012 studied a facile method to fabricate an AZO/PANI hetero-structure by a sandwiching technique. Aluminum-doped ZnO (AZO) films were deposited onto indium tin oxide (ITO) glass using the sputtering technique while PANI films were deposited on to ITO glass using electro-polymerization [4].

NWs are considered an essential component for these interconnects and have been used extensively to build nano electronic devices for applications in: sensors, waveguides, photonics, and piezo-electronics. Gold (Au) nano-wire is chemically inert and has very low resistivity. These properties make Au-NWs an ideal candidate as interconnects for linking molecular devices [5]. Its, unlike other two-dimensional systems, have two quantum-confined directions but one unconfined direction available for electrical conduction. This allows nano wires to be used in an applications where electrical conduction, rather than tunneling transport, is required. Because of their unique density of electronic states, in the limit of small diameters nano wires are expected to exhibit significantly different optical, electrical and magnetic properties to their bulk 3-D crystalline counterparts. Structural and geometric factors play an important role in determining the various attributes of nano wires, such as their electrical, optical and magnetic properties. Therefore, various novel tools have been developed and employed to obtain this important structural information at the nano scale. At the micrometer scale, optical techniques are extensively used for imaging structural features. Since the sizes of nano wires are usually comparable to or, in most cases, much smaller than the wavelength of visible light, traditional optical microscopy techniques are usually limited when characterizing the morphology and surface features of nano wires [6]. Strength of it is considerably higher than bulk materials, depends on wire size and cannot be predicted by ideal bulk strength theories. Atomistic simulations reveal that size-dependent nano wire strengths for wires under 10 nm in diameter are influenced by wire structure, surface stress, and defect formation mechanism [7]. The nano wires can be grown by the (VLS) method possess, Already in 1960s the growth of whisker or wire-like semiconductor crystals the growth mechanism called vapor- liquid-solid (VLS) growth, is still the governing principle in most present-day nano wire growths. The starting point of the NWs growth is a substrate prepared with metal (usually gold) nano particles either by deposition from commercially available colloidal suspensions, by direct deposition using aerosol techniques or made by metal evaporation and subsequent thermal annealing, physical properties of it are influenced by the morphology of the nano wires, diameter dependent band gap, carrier density of states etc [8]. Nano wires hold lot of promises for different applications. Basic electronic devices like junction diodes, transistors, FETs and logic gates can be fabricated by using semiconductor and super lattice nano wires. Thermoelectric cooling system can be fabricated by using metallic nano wires. Semiconductor nano wire junctions can be used for different opto-electronic applications. Moreover, periodic arrays of magnetic nano wires hold high potential for recording media application, Also it is used as potential candidates for sensor and bio-medical applications. Electron transport properties of nano-wires are very important for electrical and electronic applications as well as for understanding the unique one dimensional carrier transport mechanism. It has been noticed that the wire diameter, wire surface condition, crystal structure and its quality, chemical composition, crystallographic orientation along the wire axis are important parameters, which influence the electron transport mechanism of nano wires [1].

In view of the interest and immense importance that has been attached to the different properties and applications of nano wires, a review on the electron transport of nano wire research contain from (2-16) an even molecules were presented below.

The review aims at highlighting on the electronic transport properties of nano wires and their applications in electronic device. In this paper, calculations was made as follows; In section 1.1 the theoretical model, in section 1.2 the calculations and results of own work and in section 1.3 the discussion of the results and conclusions.

1.1: Theoretical Model

In this research, we studied a nano wire consisting from number of molecules which represented by N, where N = 2-16 an even molecules, assuming that the nano wire linked with leads from the right and left sides, as shown in figure (1-1):

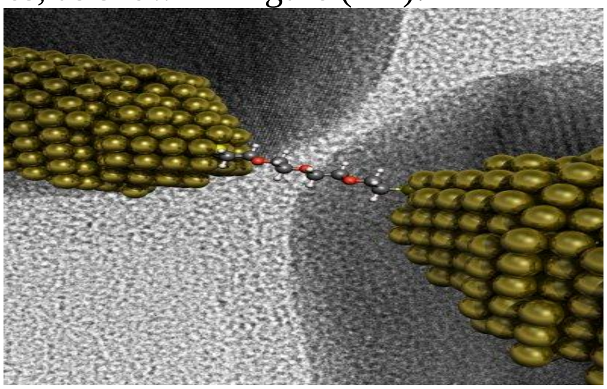

Figure 1: Illustrated the structure of the designed system.

By using theories of the strong bonding, and show if it was possible to put this model and explain the results and if they are in good matching to other researchers in practical applications. Where was the representation of the overlap between molecules in left and right leads as γ_R and γ_L, as well as symbolizes to the energy levels for two leads as $\overset{\circ}{\varepsilon}_R$ and $\overset{\circ}{\varepsilon}_L$, also the coefficient of overlap in nano wire molecules, it's the molecules close to the central region has been represent it by a factor of overlap $\propto_R$, $\propto_L$ and by using Schrodinger equation as:

$$\mathrm{H}\psi = \mathrm{E}\psi \qquad (1)$$

From this equation at the left

$$\psi = A\, e^{ik_R j} + B\, e^{-ik_l j} \qquad (2)$$

And at the right

$$\psi = C\, e^{ik_R j} \qquad (3)$$

As well known that the speed of the group in solid-state physics as:

$$v = 2\, \gamma_{L,R} \sin k_{L,R} \qquad (4)$$

$$G = G\, \Sigma\, T(E) \qquad (5)$$

Where T it's the probability of transition, then can be calculate the conductivity of nano wire, which consists of a number of molecules also by following number of mathematical steps with using equation (1), (2) and (3).

$$G = G_O\ v_L \left(\frac{q_L}{\gamma_L}\right)^2 |\Delta_{RL}|^2 \left(\frac{B_R}{\gamma_R}\right) v_R \qquad (6)$$

Where Δ_{RL} it's a function represented to number of variables obtained after dependence on a number of mathematical steps.

$$\Delta_{RL} = y^2 - (\mathcal{E}_L^0 - \mathrm{E} - (\frac{\alpha_L^2}{\gamma_L}) \cos k_L - X_L)\, (\mathcal{E}_R^0 - \mathrm{E} - (\frac{\alpha_R}{\gamma_R}) \cos k_R - X_R) \qquad (7)$$

$$X_L = \alpha_L^2 \sin K_L\ N/\gamma_L \sin k_L\ (\mathrm{N}+1) \qquad (8)$$

$$X_R = B^2 \sin K_L\ N/\gamma_L \sin k_R\ (\mathrm{N}+1) \qquad (9)$$

$$y = \alpha_L\, \mathrm{B_L} \sin k_L/\gamma_L \sin k_L\ (\mathrm{N}+1) \qquad (10)$$

Where E it represented to the overall energy system, then by implementation equation (6) and utilizing the D.P.S program where it used first time in such calculations, the results achieve high precision in conductivity calculations and its perfectly matched to the practical results, all interactions in transition which is difficult for the experimental work employers incorporated it in calculation, results shown in figures (1, 2 and 3). The electronic transport process in nano wire, is one of the challenges in standards nano scale, our calculations done with less than 10 nm, therefore we could study and understand the behavior of molecules formed nano wire between two electrodes, and compare the results with calculations in real and practical system.

1.2: Calculations and Results:

The Calculations are done by drawing a relationship between conductivity and power system for the Fermi energy when the nano wire composed of an even number of molecules. Illustrated below the results when the nanowire composed of (2-16) molecules:

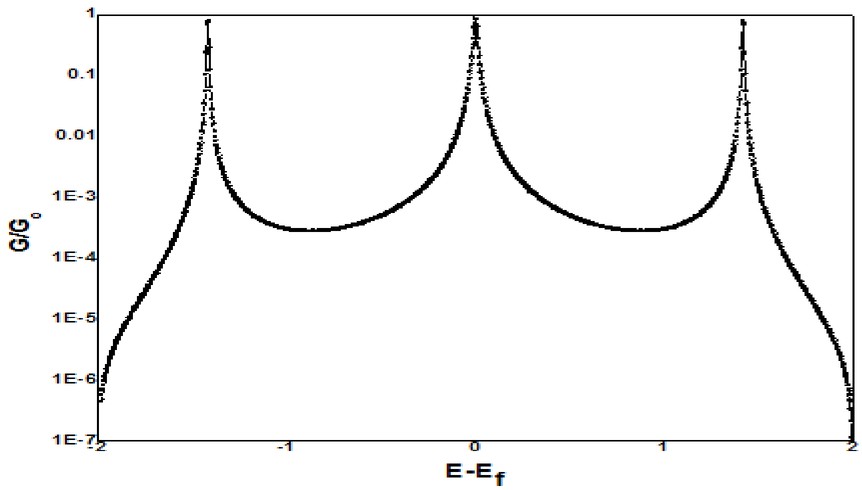

Figure 2: Nanowire compose of 2 molecules.

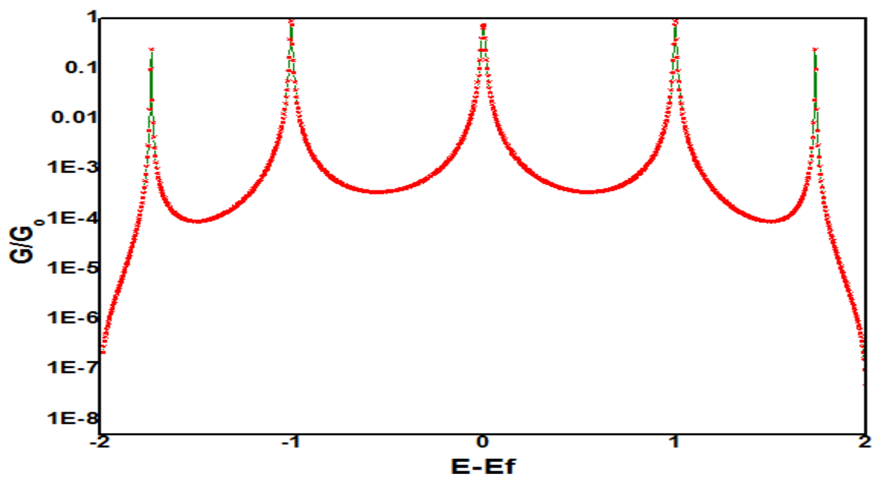

Figure 3: Nano-wire compose of 4 molecules.

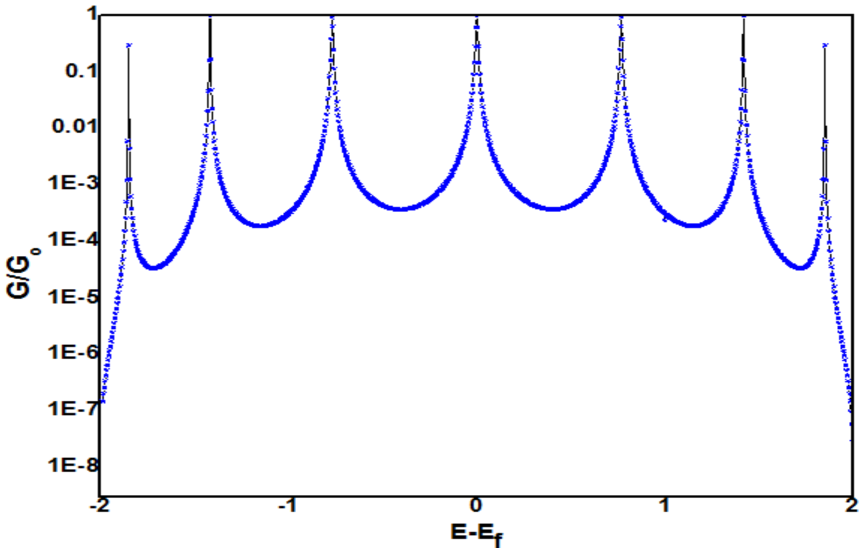

Figure 4: Nanowire compose of 6 molecules.

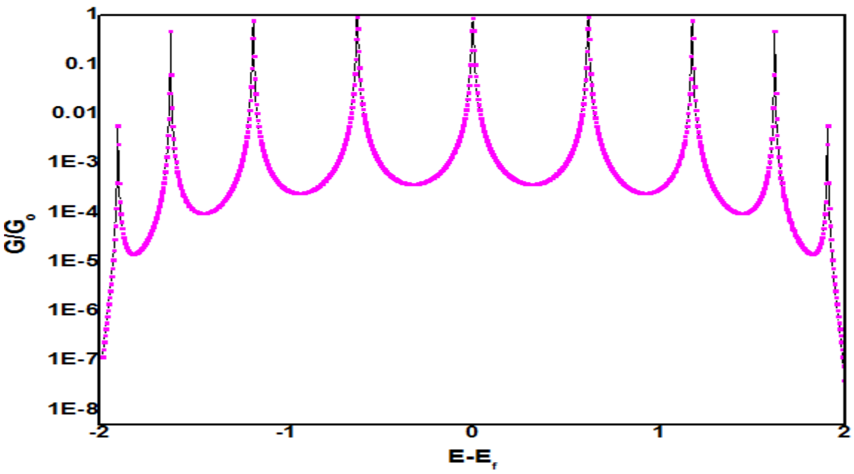

Figure 5: Nanowire compose of 8 molecules.

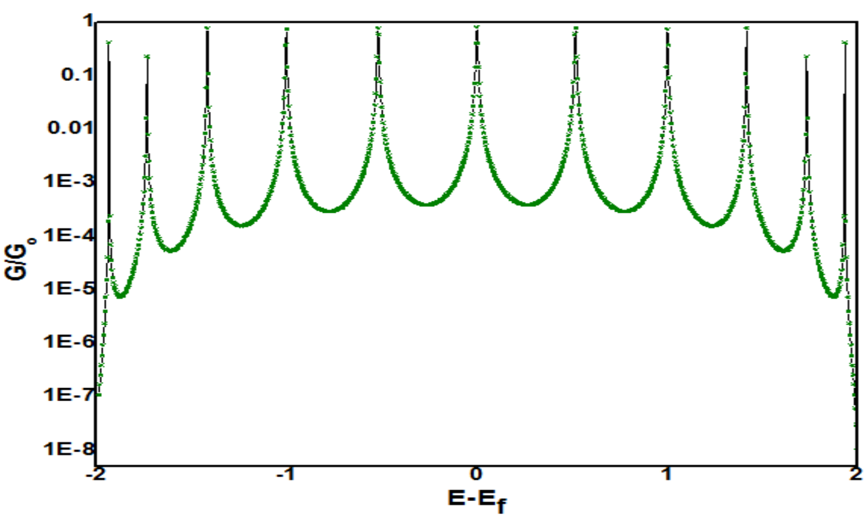

Figure 6: Nanowire compose of 10 molecules.

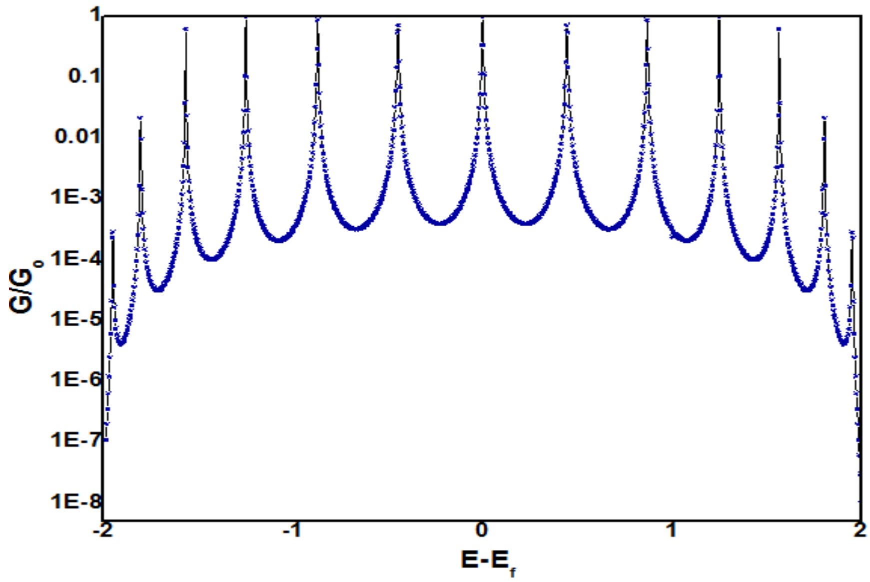

Figure 7: Nanowire compose of 12 molecules.

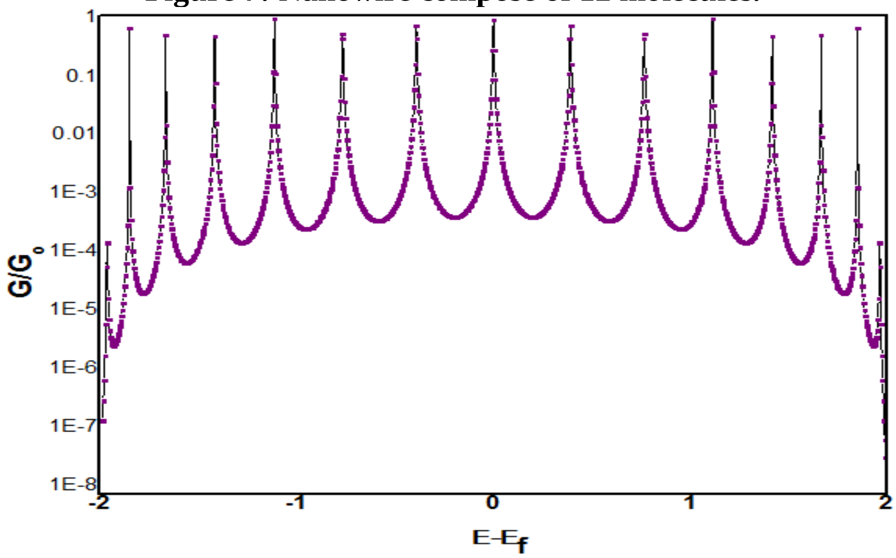

Figure 8: Nanowire compose of 14 molecules.

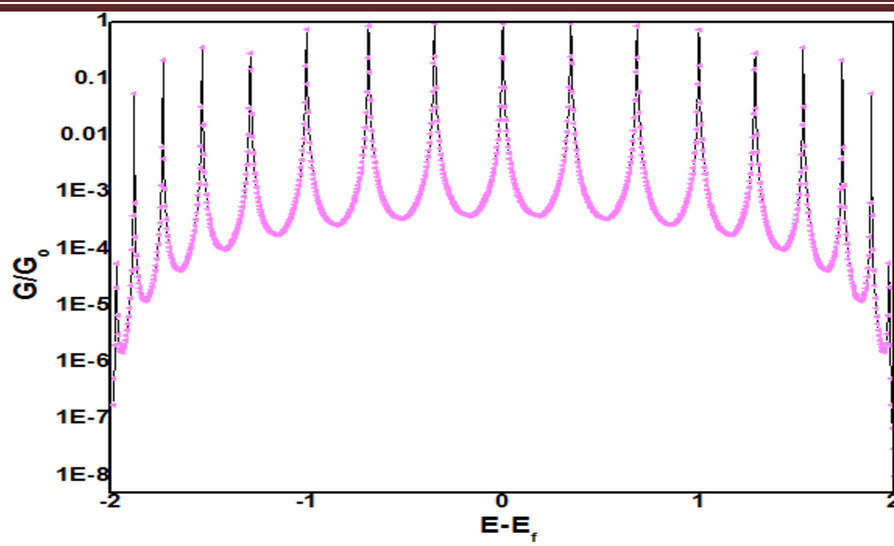

Figure 9: Nanowire compose of 14 molecules.

After calculated the conductivity and power of system for (2-16) even molecules, then compared all results in one curve, as shown in the following figure:

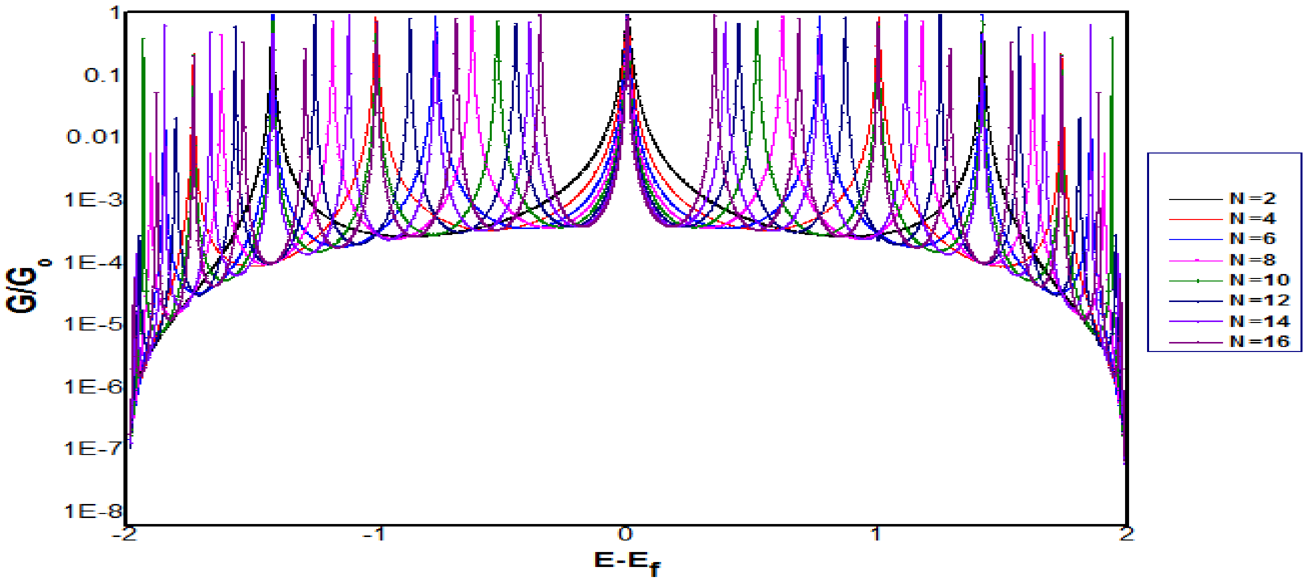

Figure 10 : Illustrated the comparison results of (2-16) molecules.

1.3: Conclusions:

In brief, we have studied the electronic transport properties in nanowire by using NEGF theory. After comparing the marital molecules (2-16) impressive results, it has an exact match on both sides of the left and right as well as the emergence of two nodes before 1.5 in the right side and also appeared before -1.5 in the left side of the chart. The magic number, which collects the conductivity dramatically and also, appeared in the zero point. Therefore, the electrical conductivity increase with adding more amount of nanowires due to rise the electron transport which make it widely applied in several applications such as a nano electronic devices.

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الخلاصة:

في هذا البحث تدرس خصائص الانتقال الالكتروني للسلك النانوي بواسطة استخدام نظرية (NEGF). النتائج التي حصلنا عليها من هذه الدراسة لم تعهد سابقا من قبل الباحثين حيث تم حساب خصائص الانتقال الالكتروني لنظام يتكون من عدد من الجزيئات يتراوح عددها بين (2-16) جزيئة كما تم قياس التوصيلية الكهربائية لهذا النظام. هذه النظرية تمكننا من الحصول على نتائج دقيقة وموثوقة حيث اظهرت النتائج اشكال تتوافق مع نظام (Breit Wigner) بشكل تام والتي تتناظر في الجانبين الايمن والايسر اضافة الى ظهور نقطة حقيقية تتجمع فيها التوصيلية بشكل كبير.