the
abdus salam
international
centre
for theoretical
physics

united nations
educational, scientific
and cultural
organization

international atomic
energy agency

ELECTRONIC CONDUCTANCE OF QUANTUM WIRE WITH SERIAL PERIODIC POTENTIAL STRUCTURES

Hisham M. Fayad

Mohammed M. Shabat

and

Hala - M. Khalil

31/46

preprint

Please be aware that all of the Missing Pages in this document were originally blank pages

IC/2000/92

United Nations Educational Scientific and Cultural Organization
and
International Atomic Energy Agency

THE ABDUS SALAM INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

ELECTRONIC CONDUCTANCE OF QUANTUM WIRE WITH SERIAL PERIODIC POTENTIAL STRUCTURES

Hisham M. Fayad
Department of Physics, College of Education,
Gaza, Gaza Strip, Palestinian Autonomous Territories,

Mohammed M. Shabat *
Department of Physics, The Islamic University,
Gaza, P. O. Box 108, Gaza Strip, Palestinian Autonomous Territories
and
The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy

and

Hala - M. Khalil
Department of Physics, College of Women's, Ain Shams University,
Heliopolise, Cairo, Egypt.

Abstract

A theory based on the total transfer matrix is presented to investigate the electronic conductance in a quantum wire with serial periodic potentials. We apply the formalism in computation of the electronic conductance in a wire with different physical parameters of the wire structure. The numerical results could be used in designing some future quantum electronic devices.

MIRAMARE – TRIESTE

August 2000

* Regular Associate of the Abdus Salam ICTP.

Introduction:

In recent years, there has been a significant advancement in the fabrication technology of ultra-small structures[1], using the molecular beam epitaxy together with electron-beam lithography, which can provide us with many mesoscopic metal or semi conductor structures. Furthermore, the scanning tunneling microscope has made it possible to visualize atomic-scale structures. Using these techniques, one can make extremely high mobility quantum wires with narrow widths, in which the lowest subbands are occupied and the transport is approximately ballistic. The allowed modes in the quantum wires are then considered to be the waveguide modes.

Electronic behavior in one-dimensional periodic, disordered and quasi-periodic structures is a very important subject in mesoscopic physics[2, 3], where in the nano-meter sizes, the mean free path of electrons at low temperature can be larger than the sample dimension. Therefore, the electron motion is dominated by the wave nature and is mainly governed by quantum mechanics. One of the most important problems in mesoscopic physics is to obtain an understanding of the electron transport in a quasi-one dimensional system where the electrons are confined in a narrow channel. For a structure with transverse dimensions comparable to the electron wavelength, the essence is that an electron can transport coherently across the whole system with negligible inelastic scattering. As a result, a variety of interesting interference phenomena can be exhibited, such as the quantized conductance in the point contacts, persistent currents in metallic loops, universal conductance fluctuations. These may provide potential applications to the fabrication of new quantum interference devices[4].

Over the past few years, several analytical and numerical approaches to ballistic transport have been established. In the theoretical studies, the single-electron and effective-mass approximations are usually applied, and it is often supposed that the waveguide structures have hard potential walls and they do not allow any penetration of the electron wave function into the lateral barriers. Several theoretical and numerical methods, such as the recursive Green's-function method[5], the mode-matching method[6], the finite element method[7], and the finite difference method[8], have been extensively used for the investigation of electron conduction in quantum waveguides. The transfer matrix approach[9, 10] is another important tool in the investigation of electron transport in low-dimensional systems, particularly useful for a wire consisting of several distinct

units. In addition, the transfer matrix method also proves to be very efficient in studies of disordered systems[2].

Recently, J. B. Xia[11] have considered the transmission across a T-shaped device consisting of a main wire of constant width attached to a stub perpendicular to the wire. Many interesting conductance characteristics in this structure were revealed, such as a sharp drop to zero transmission at certain values of the stub length, repeated periodically.

Now if a multiple stub configuration is taken, the sharp drops to zero in transmission become extended to forbidden bands and the round tops become squared, along with resonances to form allowed bands. The theoretical calculation showed that relatively small changes in the stub length could induce significant variation in the electron transmission across the structure[12].

In a different manner, Griffith and Taussig have considered a one-dimensional scattering from a series of delta-function barriers[3]. In their structure, the band formation characteristic of periodic potentials had emerged even when the number of barriers was quite small. In contrast to the multiple-stub structure, the zero transmission has not been shown in delta-function potential with finite scatters.

In this paper, we study the electronic conductance in a one-dimensional wire with a series of delta-function potentials by using the transfer matrix approach. We demonstrate the evolution of a conductance for delta-function potentials with, different strength, double periodicity and single defect at the center of a periodic arrangement of delta-function potentials. Disordered effects are also illustrated.

The One Dimensional Periodic Potential

In this section, we study the electronic transport in quasi-one dimensional waveguide systems. The structure under investigation consists of one main quantum wire with uniform section containing a row of periodic potential, as the periodic potential has a value on a finite interval and zero value elsewhere. Two semi-infinite leads are also attached on either side of the wire at each end, which serve as reservoirs.

The proposed periodic potential is characterized by a delta-function potential, where the potential is given by

$$V(x) = \sum_{j=1}^{N} U_j \delta(x - x_j) \qquad (1)$$

where U_j and x_j represent the "strength" and the position of the jth barrier respectively. Therefore N barriers are formed in the main wire. The distance between the adjacent barriers are given by $d_j = x_{j+1}-x_j$ (j = 1,2,3,..., N – 1). Noting that the centers of the peaks have the coordinates $x = x_j$. In general, the "strengths" and positions of barriers vary along the wire.

The wire structure may be considered as modified models of the previous work[3, 13] as we assume both variation of the strengths and positions of the potential barriers, where they[3, 13] considered these parameters as constants over the entire device.

As a model system, we consider a sufficiently narrow wire that only electron motion is in the direction of the wire. This single-channel case provides a good approximation to a real wire with narrow width at low temperatures at which only the lower subband is filled[12].

The single-electron and the effective-mass approximations are applied as is usual in the literature. We also assume that the structure has hard-wall boundaries.

We start from the one-dimensional Schrödinger equation in order to get the electron wave function in the wire as

$$\frac{-\hbar^2}{2m}\frac{d^2\Psi}{dx^2}+V(x)\Psi = E\Psi \tag{2}$$

where m is the electron effective mass.

The solutions of the Schrödinger equation in quantum wires are well known as given in Ref.14. We first derive the transfer matrix for the jth barrier. This matrix relates the coefficients of the wave function at one end to those at the other end.

The potential in the two leads connected to the jth barrier is zero. We express the wave function in these two leads as

$$\Psi^L(x) = Ae^{ikx} + Be^{-ikx} \tag{3}$$

for the left lead ($x_{j-1} < x < x_j$),and

$$\Psi^R(x) = Ce^{ikx} + De^{-ikx} \tag{4}$$

for the right lead ($x_j < x < x_{j+1}$), where the wave number is $k = \left(2mE/\hbar^2\right)^{1/2}$.

The normal derivative of the wave function is no longer continuous whenever $V(x) \neq 0$. We need to derive the generalized boundary conditions applicable when the delta-function potential is present.

Integrating the Schrödinger equation at x_j from ($x_j - \varepsilon$) to ($x_j + \varepsilon$), and taking the limit $\varepsilon \rightarrow 0$, we have

$$\left.\frac{d\Psi^R}{dx}\right|_{x^R=x_j} - \left.\frac{d\Psi^L}{dx}\right|_{x^L=x_j} = \gamma_j \Psi(x_j) \tag{5}$$

where " x^R " and " x^L " refer to the limits from the right to left respectively, and $\gamma_j = 2mU_j/\hbar^2$.

We also see that the continuity of the wave function at $x = x_j$ is preserved, that is:

$$\Psi^R(x)\big|_{x=x_j} = \Psi^L(x)\big|_{x=x_j}. \tag{6}$$

Imposing the above mentioned boundary conditions at $x = x_j$, we obtain the coefficients C and D in terms of A and B, thus we obtain

$$C = (1 - i\beta_j)A - i\beta_j B e^{-2ikx_j} \tag{7}$$

$$D = i\beta_j A e^{2ikx_j} + (1 + i\beta_j)B \tag{8}$$

where $\beta_j = (\gamma_j/2k)$.

The above two equations can be rewritten in a matrix form as:

$$\begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} e^{ikx_j} & 0 \\ 0 & e^{-ikx_j} \end{pmatrix}^{-1} \begin{pmatrix} 1 - i\beta_j & -i\beta_j \\ i\beta_j & 1 + i\beta_j \end{pmatrix} \begin{pmatrix} e^{ikx_j} & 0 \\ 0 & e^{-ikx_j} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}. \tag{9}$$

Accordingly, we define the transfer matrix at a given barrier. For instance, at barrier j, we have

$$M_j = S^{-1}(ikx_j).\Gamma(\beta_j).S(ikx_j). \tag{10}$$

where S represents the first and the third matrices in Eq. 9, while Γ represents the middle one.

The total transfer matrix that represents the electron wave propagation through the entire device is just the product of the transfer matrices of the barriers in order. Thus we obtain

$$M_{tot} = S^{-1}(ikd_{N-1}).\Gamma(k\beta_N).\left[\prod_{j=1}^{N-1} S(ikd_j).\Gamma(\beta_j)\right].S(0) \tag{11}$$

The transmission amplitude of the electrons is related to the element of M_{tot} as

$$T(k) = \frac{1}{M_{tot}(2,2)}. \tag{12}$$

The two terminal conductance G, which is the ratio of the transmitted current to the potential difference between two reservoirs is evaluated using the two Probe Landauer-Büttiker formula[15, 16]

$$G = \frac{2e^2}{h}|T|^2. \qquad (13)$$

Numerical Results for the delta-function potentials

The discussion in the previous section makes the calculations very straightforward and allows an easy using of the different parameters defining the device. In the following, we assume a dimensionless strength for the delta- function potentials[17], $\Omega_j = md_jU_j/\pi^2\hbar^2$, with $\beta_j = mU_j/k\hbar^2$, we find, $\beta_j = \pi^2\Omega_j/kd_j$. In Fig.1 we plot the one dimensional conductance as a function of the wave number of electrons for two values of the barrier strengths. The distance between adjacent barriers is fixed at $d_j = d$. The standard strength of the barriers is Ω, and the number of the barriers is $N = 5$. The strength of the potentials considered in Fig.1 is (a) $\Omega = 0.2$, and (b) $\Omega = 0.5$. It is seen from the graphs that, the allowed and forbidden regions are appearing although the number of barriers is quite small, and each allowed band contains N-1 maxima "spikes". Such spikes are a feature for delta- function potential[18]. Also, we note that the allowed bands become slowly wider as k increases, and this is because $\beta = \pi^2\Omega/kd$ has a slow decline. The standard analysis of the transmission through a row of delta- function potentials is given in Refs. 3,13, and 18. The conclusion is quite simple that is the transmission is not simply unity when k is in an allowed region, even in the limit of $N \to \infty$, but is almost always less than unity. Graphs a and b in Fig.1 display the variation of the calculated conductance G (in units of $2e^2/h$) versus λ ($\lambda = kd/\pi$) through a row of delta function potentials. The dimensionless strength values of the potentials in the Fig. 1.a equal 0.2 and in the Fig. 1.b equal 0.5. If one wants to compare the two pictures, he can easily notice that the increasing of the potential strength leads to form the allowed region rapidly. The increasing of the potential strength from 0.2 to 0.5 forms two complete allowed regions in Fig.1b while it does not form any complete region in Fig.1a for the small value of Ω. We also notice that the increasing of the potential strength makes the allowed regions to be narrower, and then the spikes become very sharp and very deep. So it is easy to state that the number of potential barriers and the potential strength can control the conductance spectra in these kinds of potentials.

Fig.2. illustrates the one dimensional conductance as a function of the Fermi wave

number k, as in Fig.1.The distance between adjacent barriers is fixed at $d_j=d$. The strength of the potential barriers is taken double periodic with values {Ω=0.2, Ω=0.3}in Fig.1a, and {Ω=0.2,Ω=0.5}in Fig.1b. The number of potential barriers N is taken to be 6. Fig.2 shows that the double periodic arrangement leads to split the allowed regions and the splitting of the allowed region in Fig.2a become a valuable due to the reduction of the medium spike in every allowed region due to the small value of the difference of the potential strength ($\Delta\Omega$= 0.1). The increasing of the difference of the potential strength ($\Delta\Omega$= 0.3) is leading to the reflection process of the medium spike in every allowed region as this reflection appears in the form of a deep valley where this valley is well fitted with the size of its region. It means that the increasing of the difference of the strength potential leads to a complete split of the allowed region forming a forbidden region inside the allowed region at small values of k. These phenomena can be explained due to the destruction interference between the incident and reflected waves at the potential barriers.

In Fig.3. we present the calculated conductance as a function of the Fermi wave number k for the row of delta- function potentials. Here we shall show how a single defect at the center of the row can alter the band formation, which changes with the strength of the defect. The strengths of all the barriers are assumed to be identical, except the central one. The distance between adjacent barriers is fixed at $d_j = d$. We have taken three barriers on either side of the defect barrier. We clearly observe two cases. The first one can be observed where the defect strength Ω_d is less than values of the potential as in Fig.3a where $\Omega = 0.5$ and $\Omega_d = 0.2$. We notice that some changes have occurred in the internal structure of the allowed regions and at the same time keeping the general form of that region. The changes take the form of multiple splitting inside the allowed region. This splitting varies in the strength inside the one region and it varies according to the size of the region where they exist. We also notice that the number of spikes in the structure has kept its distinguished feature for delta function potential which equals (N-1) in every allowed region. So we have six spikes in this case. If we look at the spikes at both sides of the graph in every allowed region, we notice that the spikes become deeper and sharper. But at the lower value of the wavelength k, the spikes tend to form, which is called quasi-bound state. The second case as the defect strength is bigger than the potential value ($\Omega = 0.2$ and $\Omega_d = 1$) as in Fig.3b. We found that the spectra of the conductance have changed totally from which has been shown previously in Fig.3a, as

the number of the spikes has changed in every allowed region and becomes as [(N-1)/2]. This value is equal to the number of the potential barriers at each side of the defect strength. We also notice that the difference of the height of the spikes is bigger at the lower values of k than at the higher values. This difference will also be reduced by increasing the values of k. It is easy to state in general that the above mentioned cases can be the distinguished feature for these kinds of the potentials as the conductance spectra will have similar features for the two cases taking into account the effects of the number of the potential barriers and their strengths.

Fig.4. Presents the calculated conductance for the disordered lead connections between adjacent barriers (barrier distances). We assume that the average barrier distance is d and the number of the barriers is $N = 5$. To produce disorder configurations, the barrier distances are given by $d_j = (1+LR)\ d$, where R represents the random values with a uniform distribution in the range [-0.5,0.5] as L describes the extent of the disorder. In Fig.4 graphs a, b, and c correspond to different barrier distance disorders of L: 0.1, 0.15, and 0.2 respectively. The process of disorder in the distance between the potential barriers leads to a clear change in the conductance spectra as shown in Figs.4. as the spikes at each side in each allowed region have been changed rapidly. The reduction of the spikes is increasing due to the increasing of the parameter L at the lower value of the wave number k. The conductance spectra also takes the form of the oscillations at the bigger value of k, which has been caused due to the reflection of the separated valleys between the allowed regions. We also notice that the values of the disorder L do not lead to the bigger differences between the conductance spectra for the three figures.

Conclusions

In conclusion, we have presented the transfer matrix method to model a quantum wire containing a row of delta-function barriers. We hope that this article will act as a stimulus for further work in this promising area. The results could be useful in introducing quantum wires for designing some future nano-electronic devices.

Acknowledgments:

This work was done within the framework of the Associateship Scheme of the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy. M.M.S. gratefully acknowledges the director of the Abdus Salam ICTP, Prof. Virasoro and Prof. Denardo for their kind hospitality and helpful support.

References:

[1]T. J. Thornton. Rep. Prog. Phys. 58. 311 (1995).

[2]Ben-Yuan Gu, Phys. Rev. B51, 16840 (1995).

[3]J. Griffiths and N. F. Taussig, Am. J. Phys. 60, 883 (1992).

[4]F. Capasso and S. Datta, Phys. Today LB (2), 74 (1992).

[5]F. Sols, M. Macucci, U. Ravaioli, and K. Hess, J. Appl. Phys. 66, 3892 (1989).

[6]Y. Takagaki and D. K. Ferry, Phys. Rev. B 45, 6715 (1992).

[7]H. Tachibana and H. Totsuji, J. Appl. Phys. 79, 7021 (1996).

[8]C. Berthod, F. Gagel, and K. Maschke, Phys. Rev. B 50, 18299 (1994).

[9]Hua Wu, D. W. L. Sprung, J. Martorell, and S. Klarsfeld, Phys. Rev. B 44, 6351 (1991).

[10]W. D. Sheng and J. B. Xia, J. Phys.: Condens. Matter 8, 3635 (1996).

[11]J. B. Xia, Phys. Rev. B 45, 3593 (1992).

[12]P. S. Deo and A. M. Jayannavar,Phys. Rev. B 50, 11629 (1994).

[13]D. W. L. Sprung, Hua Wu, and J. Martorell. Am. J. Phys. 61, 1118 (1993).

[14]J. E. Avron, A. Raveh, and B. Zur, Rev. Mod. Phys. 60, 873 (1988).

[15]R. Landauer, Z. Phys. B 68, 217 (1987); J. Phys. Condens. Matter 1, 8099 (1989).

[16]M. Buuttiker, Y. Imry, R. Landauer, and S. Pinhas, Phys. Rev. B 31, 6207 (1985).

[17]Y. Takagaki and D. K. Ferry, Phys. Rev. B 45, 8506 (1992).

[18]S. J. Blundell, Am. J. Phys. 61, 1147(1993).

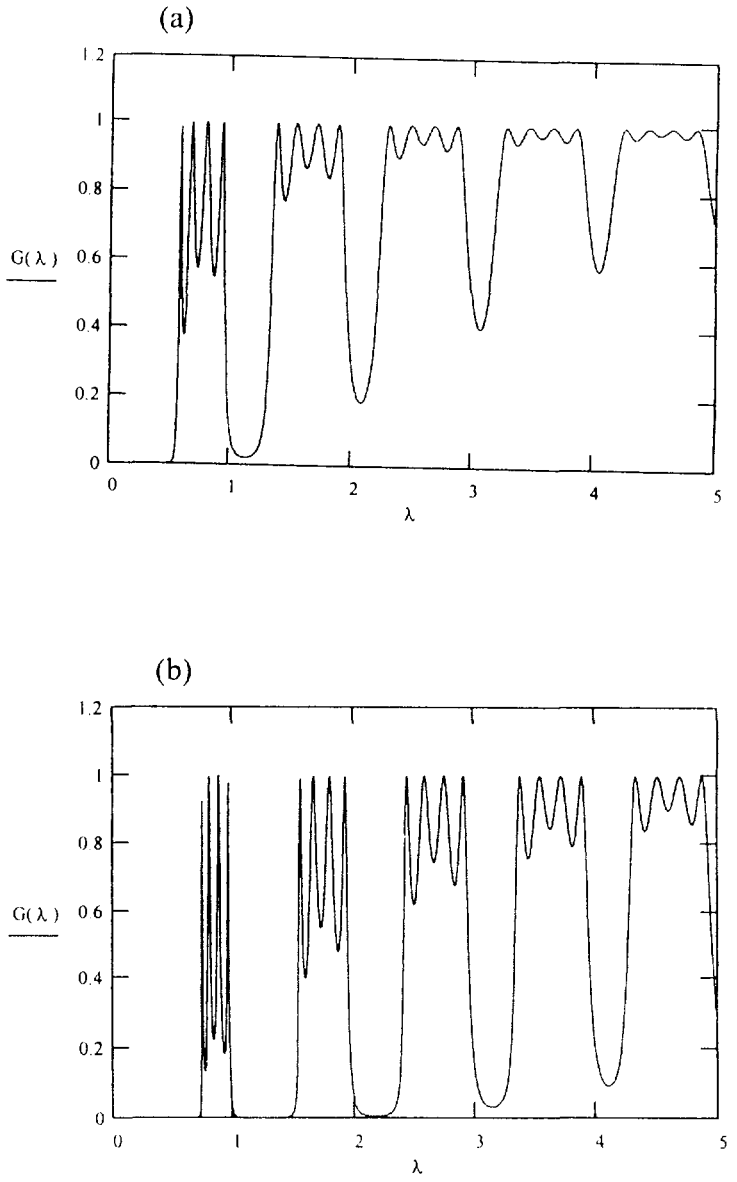

Fig.1. Calculated conductance G (in units of $2e^2/h$) through a row of N=5 delta function potentials, plotted against ($\lambda = kd/\pi$). The dimensionless strength of the potential is (a) $\Omega = 0.2$, and (b) $\Omega = .5$.

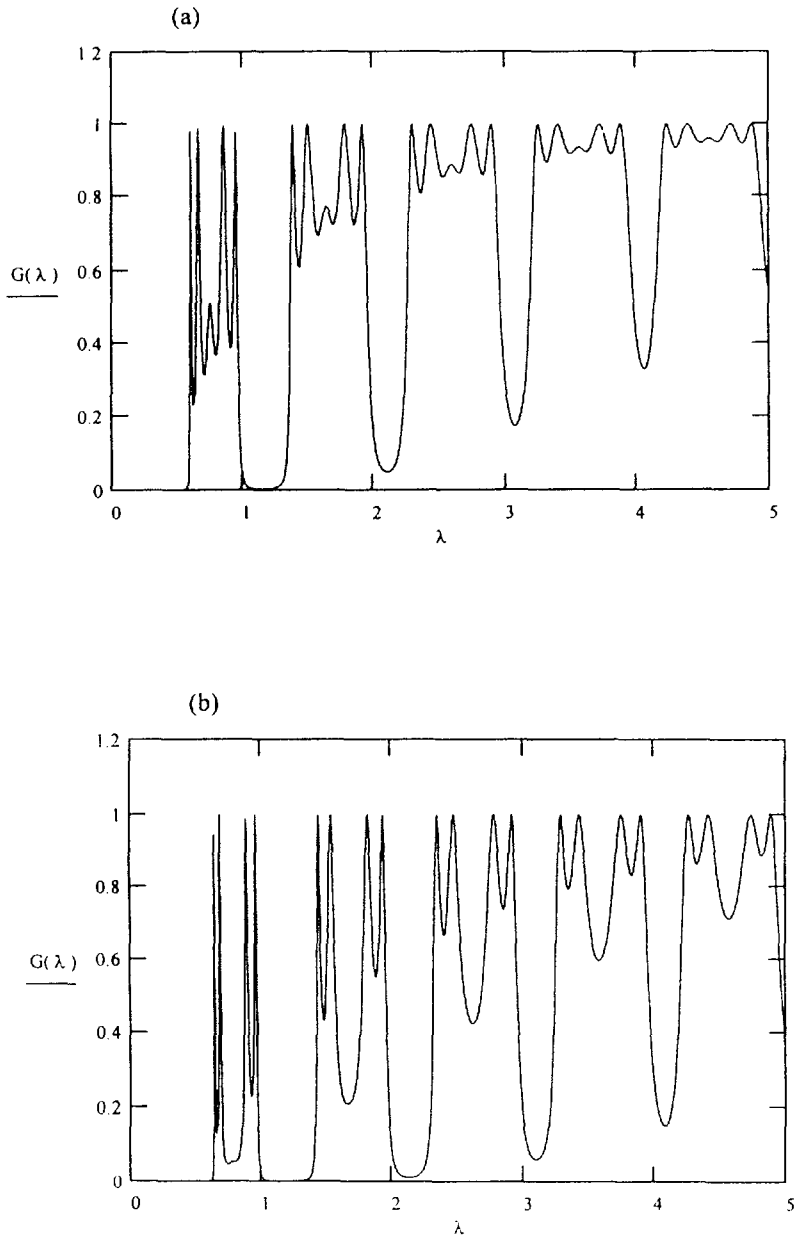

FIG. 2 . Calculated conductance G (in units of $2e^2/h$) through an row of $N = 6$ delta function potentials, plotted against ($\lambda = kd/\pi$). The strength of the potential is double periodic taking values of: (a){Ω =0.2, 0.3}, and (b){Ω =0.2, 0.5}.

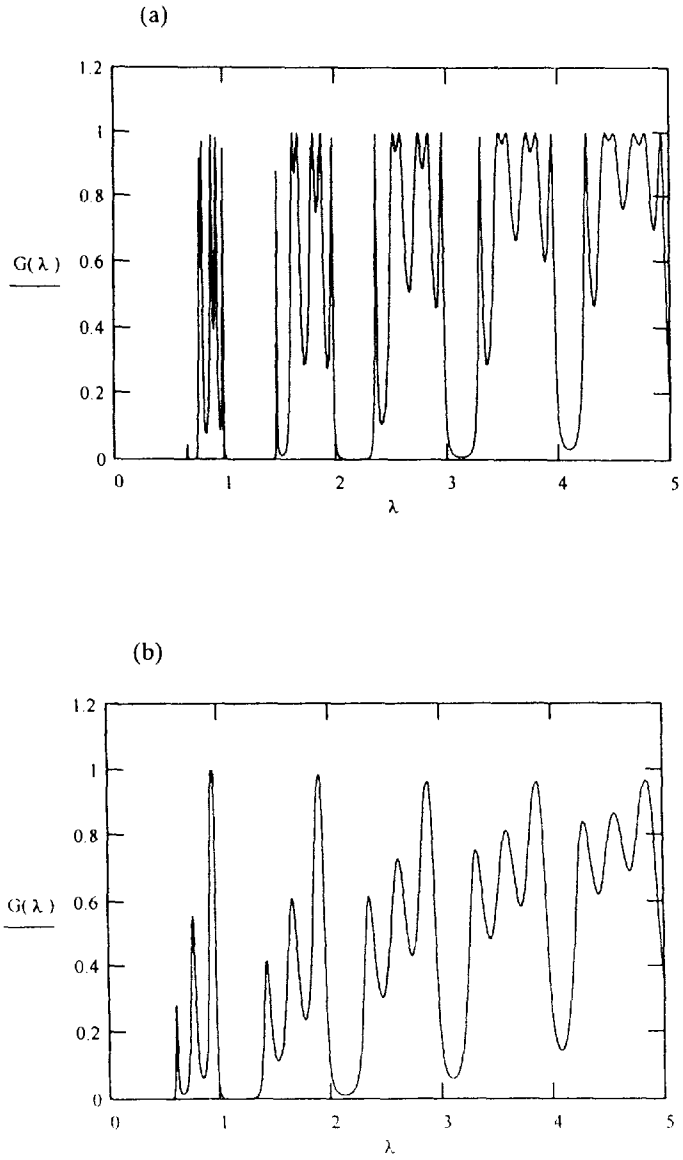

FIG.3. Calculated conductance, G (in units of $2e^2/h$) through an row of delta function potentials, plotted against ($\lambda = kd/\pi$). A single defect strength Ω_d at the centre of an otherwise periodic arrangement of 3 delta function potentials on either side of the defect strength. Where the strengths potentials as follow: In (a) $\{\Omega = 0.5, \Omega_d = 0.2\}$, and (b) $\{\Omega = 0.2, \Omega_d = 1\}$.

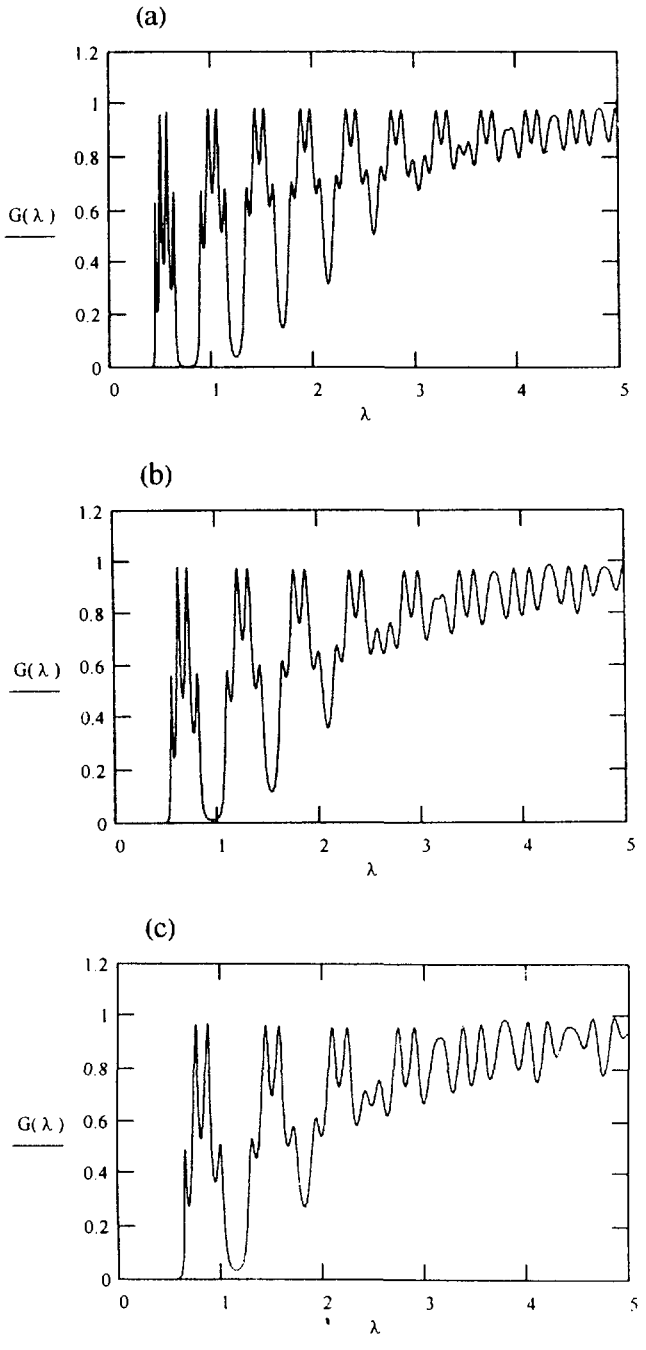

FIG 4 The same parameters as Fig.1(a). Figs. (a)-(c) correspond to different values of L, 0.1, 0.15, and 0.2.