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Study of Defects Effect on Electronic Conductance Through Binomially Tailored Quantum Wire

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Abstract: This study considers the effect of the defects on the electronic conductance properties in Binomially Tailored Quantum Wires (BTQW), in which each Dirac delta function's potential strength have been weight on the binomial distribution law. A single free-electron channel is incident on the structure and the scattering of electrons is solely from the geometric nature of the problem. We found that this novel structure has a good defect tolerance within $\pm 5\%$ or more for the following defects: single strength defect, dislocation defect, or both defects. Finally, we found this structure has somehow good tolerance for flipped order of the delta potential and missing Dirac delta potential from the binomial pattern.

Key words: Mesoscopic systems, quantum waveguide, quantum wire

INTRODUCTION

Electronic conductance behavior in one dimensional periodic structure, like a finite series of Dirac delta function potential, is an important subject in condensed matter after the major advances in nano-technology and micro-fabrications. Quantum wires are one dimensional mesoscopic device, in which the electrons can transport coherently across the whole system with negligible inelastic scattering (Sprung *et al.*, 1993; Singha Deo and Jayannavar, 1994). The recent progress in modern crystal growth techniques such as Molecular Beam Epitaxy (MBE) and the Metal-Organic Chemical Vapor Deposition (MOCVD), has demonstrated that we can grow semiconductor substrate with monolayer precision. These advances make it possible to confine electrons within a lateral extent of 100 nm or less resulting one dimensional quantum wave-guide. In this wave guide, the electron transport can be considered ballistic or quasiballistic and the electron-electron scattering and the electron-phonon interaction can be neglected if the temperature is low enough. So, the phase-coherence length become large enough compared with the device dimension. Therefore, the electron transport properties solely depend on the geometrical structure of the problem in hand. Recently, the electronic conductances in a series of Dirac delta function potential grasp many researches interest (Sprung *et al.*, 2008; Ashour *et al.*, 2006; Martorell *et al.*, 2004; Fayad *et al.*, 2001; Jin *et al.*, 1999; Bolton-Heaton *et al.*, 1999; Ferry and Goodnick, 1999). The researcher used different methods to study the electronic conductance through quantum wires and rings (Midgley and Wanc, 2000; Tachibana and Totsuji, 1996; Macucci *et al.*, 1995; Sprung *et al.*, 1993; Takagaki and Ferry, 1992a, b).

Recently, Ashour *et al.* (2006) has proposed a novel structure which is the Binomially Tailored Waveguide Quantum Wires (BTQW), in which each Dirac's Delta function potential strength has been weighted on the binomial distribution law. In this study, we study the defects effect on the electronic conductance on the novel structure proposed by Ashour *et al.* (2006).

TRANSMISSION THROUGH PERIODIC STRUCTURE

Here, let us consider a finite periodic structure of Dirac delta function potential (Dirac Comb). Also, we have assumed that the structure is narrow enough so that just single channel of electrons can be considered. In this treatment, we assume the temperature is low enough to ignore the electron-electron interaction and electron-phonon interaction. We assumed the scattering of electrons mainly form the geometrical structure of the potential. The potential can be written as:

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

where, U_j and x_j represent the strength and the position of the j th delta function respectively and N is the number of the Dirac delta functions in Dirac Comb. The distance between the adjacent barriers are given by $d_j = x_{j+1} - x_j$. The Schrödinger wave equation in one dimension can be written as:

$$-\frac{\hbar^2}{2m^*} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (2)$$

where, $V(x)$ is the periodic potential given by Eq. 1, m^* is the electron effective mass, which is considered approximately constant over the interaction range. The solution of Schrodinger wave equation for single Delta function potential can be found in literature and also the transfer matrix formulism (Kostyrko, 2000; Sheng and Xia, 1996; Wu and Sprung, 1994; Wu *et al.*, 1991; Merzbacher, 1997). The transfer matrix for periodic structure has been used also to study the transmission of electron through Comb structure (Ashour *et al.*, 2006; Fayad *et al.*, 2001; Kostyrko, 2000; Sheng and Xia, 1996; Wu *et al.*, 1991). In the following, we are going to outline the matrix transfer matrix method and we are closely following the references (Landau and Lifshitz, 1981). To derive the transfer matrix for the j th Delta function potential, we express the electron wave function in the leads, where the potential is zero, as:

$$\psi_L(x) = Ae^{ikx} + Be^{-ikx} \quad (3)$$

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

$$\psi_R(x) = Ce^{ikx} + De^{-ikx} \quad (4)$$

for the right lead ($x_j < x < x_{j+1}$).

Thus $k = \sqrt{2mE}/\hbar$ and the wave amplitudes on either side of the j -th Dirac delta function after imposing the boundary conditions satisfies,

$$\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} = T_j \begin{pmatrix} A_j \\ B_j \end{pmatrix} \quad (5)$$

In this expression T_j is the transfer matrix,

$$T_j = \begin{pmatrix} 1 - i\beta & -i\beta e^{-2ikx_j} \\ i\beta e^{2ikx_j} & 1 + i\beta \end{pmatrix} \quad (6)$$

Thus β_j is $\gamma_j/2k$, where γ_j is $2m^*U_j/\hbar^2$

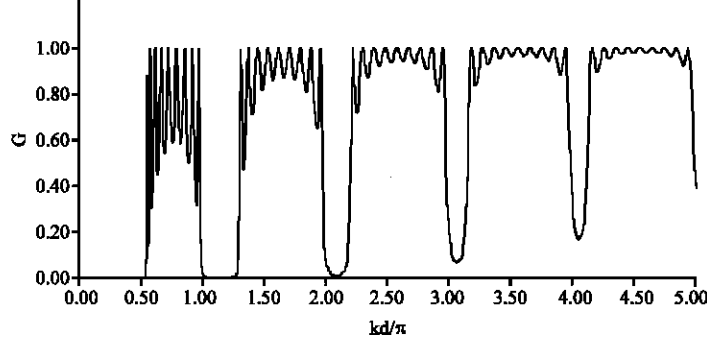


Fig. 1: Conductance spectrum G in the units of $2e^2/h$ as a function of kd/π for a sequence of Dirac delta function potential with $N = 10$. The strength of the potential here is $\Omega = 0.2$. Notice that the number of ripples in the allowed band is $N-1$

The transfer matrix for Dirac comb, which is a series of equally spaced Dirac delta function potentials, has the following form:

$$\tilde{T} = \begin{pmatrix} \tilde{T}_{11} & \tilde{T}_{12} \\ \tilde{T}_{21} & \tilde{T}_{22} \end{pmatrix} \quad (7)$$

and is given by the product of the transfer matrices of each individual Dirac delta function potential

$$\tilde{T} = T_N T_{N-1} \dots T_1 \quad (8)$$

Then the transmission amplitude is given by Sprung *et al.* (1993):

$$T = \frac{1}{\tilde{T}(2,2)} \quad (9)$$

thus $\tilde{T}(2,2)$ is the second element in the second row in a 2×2 matrix. The electron conductance through this structure, according to the Landauer-Buttiker formula, is (Landau and Lifshitz, 1981; Baym, 1974):

$$G = \frac{2e^2}{h} |T|^2 \quad (10)$$

We rescale the strength of the Dirac delta function potential by the following parameter (Takagaki and Ferry, 1992b) $\Omega_j = md_j U_j / \pi^2 \hbar^2$. In Fig. 1, we show the conductance through $N = 10$ Dirac delta function potential with strength $\Omega = 0.2$. A perfect transmission, in this case, is in general impossible as predicted by Ashour *et al.* (2006) and Blundell (1993). According to Blundell (1993) we can not have a resonant transmission, $T = 1$, even if N is very large.

BINOMIALLY TAILORED DIRAC DELTA FUNCTION POTENTIAL

Here, we reintroduce a novel simple structure of the waveguide quantum wires based on the binomial distribution (Ashour *et al.*, 2006), this propose a new structure based upon the similarities between the electromagnetic waves and the electronic plane waves. We have noticed a similarity between the diffraction of plane waves from multiple narrow slits and the electrons diffraction from Dirac comb. Because of this situation, we introduced a novel simple structure of the quantum

waveguide based upon the binomial distribution (Fig. 2) to get tunneling transmission to reach the unity over a significant range of incident electron energy and to get rid of the undesired ripple in the conductance band in the previous structure. The Dirac delta function has been equally spaced but their strength, Ω_j and has been weighted according to the binomial distribution law, which is:

$$\Omega(N_j) = \binom{N}{N_j} / 2^N, \quad N = 0, \dots, N \quad (11)$$

Thus, $\Omega(N_j)$ represents the strength of the Dirac delta potential. $N+1$ represents the total number of Dirac delta function potentials in the quantum wire and N_j represents the order of the Dirac delta potential. This novel structure of quantum wires can be realized by putting metallic gates on top of a one-dimensional electron gas and then by applying voltages, according to the binomial distribution law, to deplete the electron gas underneath. In this case, Eq. 8 is no longer valid for our new structure so that, the total transmission matrix can be written as follows:

$$\tilde{T} = T_3(\Omega_3) T_4(\Omega_4) T_3(\Omega_3) T_2(\Omega_2) T_1(\Omega_1) \quad (12)$$

Notice that the potential strength is weighted according to Eq. 11. In Fig. 3, we show the conductance spectrum through a sequence of binomially tailored Dirac delta function potentials. It is

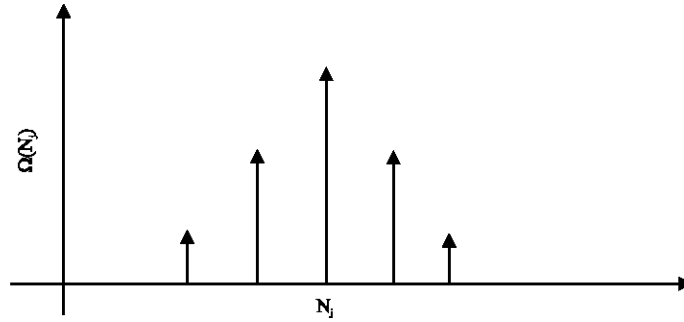


Fig. 2: Binomially tailored Dirac delta function potential. Here, $N = 4$ but the number of Dirac delta functions is 5, and N_j values which can be evaluated by Eq. 11

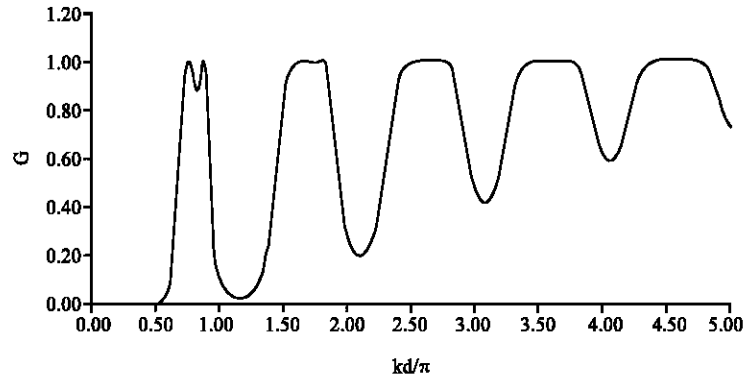


Fig. 3: Conductance spectrum G in the units of $2e^2/h$ as a function kd/π of for a binomially tailored sequence of Dirac delta function potential with $N = 4$. The strength of the potential here is as in Fig. 2

quite interesting to notice that the transmission through this structure approaches unity in the allowed band region without any ripples after some small values of k . We have a resonant tunneling due to coherent interference due to elastic scattering of electrons plane waves, which leads the transmission to reach unity over a considerable range of k values, which is called allowed band or conduction band. Also, we can see that there is a forbidden band, or a conduction gap where the transmission is small.

In Fig. 3, we show the conductance spectrum through a sequence of a binomially tailored Dirac delta function potentials. It is quite interesting to notice that we have reached a transmission through this structure approaches to unity in the allowed band region without any spikes after some k value. Here, we have a resonant tunneling due to coherent interference effects due to elastic scattering of electrons, which leads the transmission to reach unity and also to have constant value over the allowed band or conduction band. Also, we see that there are forbidden bands or conduction gap where the transmission is small.

DEFECT EFFECT ON THE ELECTRONIC CONDUCTANCE

Strength Defect

In this subsection, we study strength defect effect on the central element of the binomial tailored quantum wire and keeping the other elements and the spacing between the Dirac delta function potentials intact. First, in Fig. 4a, we consider defect free binomially tailored quantum wire with $N = 35$, with two scaling factors. We notice that when the scaling factor increase the conduction bands become narrower but the forbidden bands become wider and well defined. In Fig. 4b, we consider the strength defect does not exceed $\pm 5\%$ of the Dirac delta function potential strength. That is, when the central Dirac delta function potential strength is, for odd number of Dirac delta function potential in the binomial distribution. In Fig. 4b, we plot the electronic conductance spectrum for both strengths (with scaling factor of one and three) with N_j is 35 and scaling factor of three. As can noticed there is slight difference between the two curves, and compared to Fig. 4a. In Fig. 4c, we increase the strength defect up to $\pm 20\%$, we have noticed some measurable differences between the two curves and compared to Fig. 4a, we have noticed some measurable differences between the two curves, but still the conduction band and the forbidden bands are well defined, which is a very good feature for the binomially tailored quantum wires.

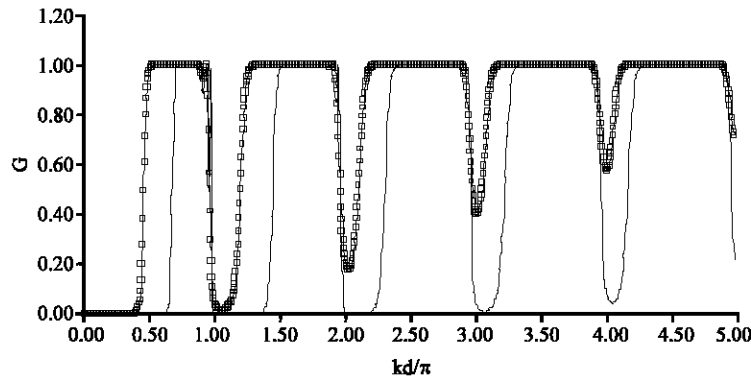


Fig. 4a: The electronic conductance, in the units of $2e^2/h$ as a function of kd/π . The curve with squares is for $N = 35$ without scaling the binomial distribution. The second curve also with $N = 35$ but with a scaling factor of three

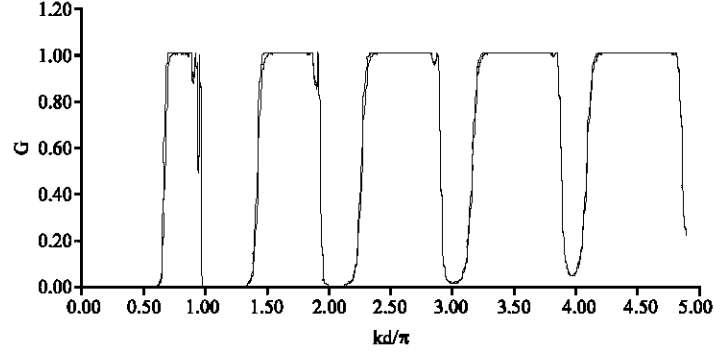


Fig. 4b: The electronic conductance, in the units of $2e^2/h$ as a function of kd/π . Here, $N = 35$ with scaling the binomial distribution by factor of three. In the case where the defect is only $\pm 5\%$, in the strength of the central Dirac delta function, there is slight difference between the two curves and compared to Fig. 4a

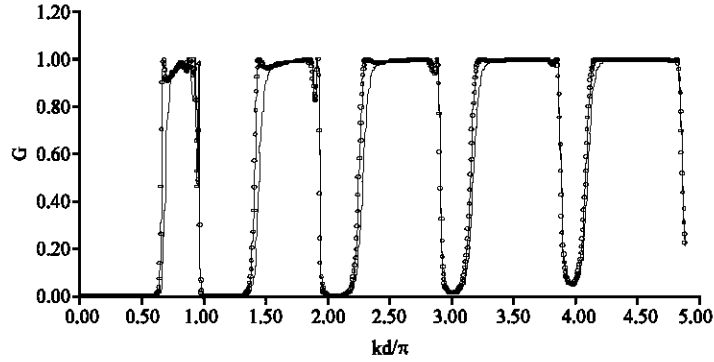


Fig. 4c: The electronic conductance, in the units of $2e^2/h$ as a function of kd/π . Here, $N = 35$ with scaling the binomial distribution by factor of three. In the case where the defect is only $\pm 20\%$, in the strength of the central Dirac delta function, there some measurable differences between the two curves and compared to Fig. 4a. The curve with circles, has potential strength defect $+20\%$ higher

Dislocation Effect

In this research, we study dislocation defect effect on the position of the central element in the binomial tailored quantum wire and keeping all other elements and the spacing between the Dirac delta function potentials unchanged. First, We consider the position defect does not exceed $\pm 5\%$ of the Dirac delta function potential spacing constant. That is, when the central Dirac delta function potentials spacing is $d = \pm 0.05 d$. In Fig. 5a, we plot the electronic conductance spectrum for both dislocations with $N = 35$ and scaling factor of three. Compared to Fig. 4a, as can noticed there is a difference between the two curves. The conduction band starts to lose its flatness and the forbidden band become sharper spacing increase between the central Dirac delta function and the adjacent one. In Fig. 5b, we increase the dislocation defect up to $\pm 20\%$, we have noticed measurable differences between the two curves and the curve in Fig. 4a, but the conduction band is still well defined but the forbidden bands have a split compared to forbidden band in no defect curves (Fig. 5). This splitting is due to resonant state in the forbidden energy band which leads to a bound state in the structure (Singha Deo and Jayannavar, 1994). This is because the particle mode cannot propagate and hence get trapped.

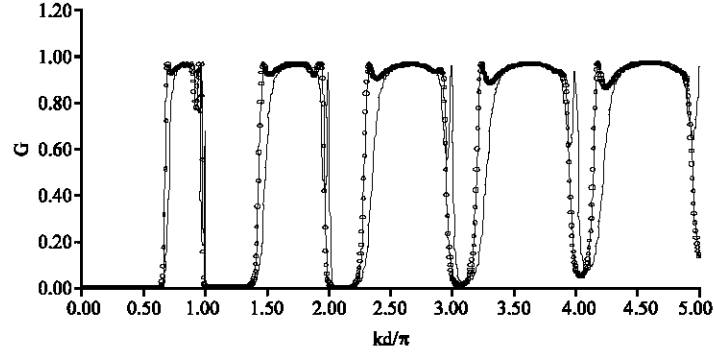


Fig. 5a: The electronic conductance, in the units of $2e^2/h$ as a function of kd/π . Here, $N = 35$ with scaling the binomial distribution by factor of three. In the case where the defect is only $\pm 5\%$, in the position of the central Dirac delta function, there is some difference between the two curves and compared to the curve in figure 4-a. The curve with circles, dislocation in position $+5\%$ wider

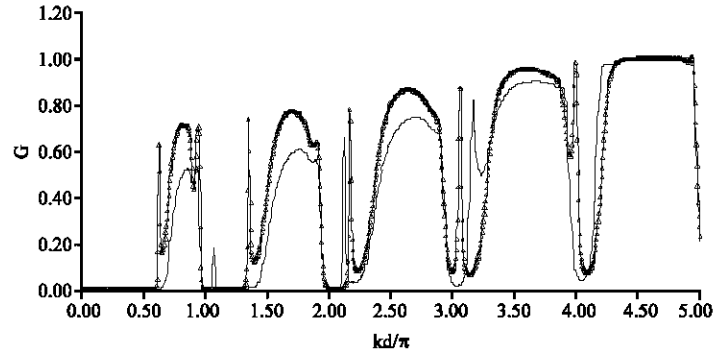


Fig. 5b: The electronic conductance, in the units of $2e^2/h$ as a function of kd/π . Here, $N = 35$ with scaling the binomial distribution by factor of three. In the case where the defect is only $\pm 20\%$, in the position of the central Dirac delta function, there some measurable differences between the two curves. The curve with circles, dislocation in position $+20\%$ wider

Dislocation and Strength

In this research, we study both the dislocation defect and the strength effect on the central element in of the binomially tailored quantum wire and keeping the other elements strength and spacing in between intact. In Fig. 6a, we plot the electronic conductance spectrum considering the position defect is $d \pm 0.05 d$ and the strength defect is $\Omega_j (N/2+1) \pm 0.05 \Omega_j (N/2+1)$. As can be seen from the Fig. 6a there measurable difference between the defect free structure and the structure with both defects, but the conductance spectrum from the defected structure still maintain the main features of the original transmission spectrum. This leads us to conclude that this structure has a significant tolerance for both defects in position and strength which makes this structure more reliable.

In Fig. 6b, we plot the electronic conductance spectrum considering the position defect is $d \pm 0.2d$ and the strength defect is $\Omega_j (N/2+1) \pm 0.2 \Omega_j (N/2+1)$. Here, there is a significant and measurable difference in the conductance spectrum between the defect free case and this case. So, we can say that this structure cannot tolerate this high defect in both the position and strength. As can be noticed from

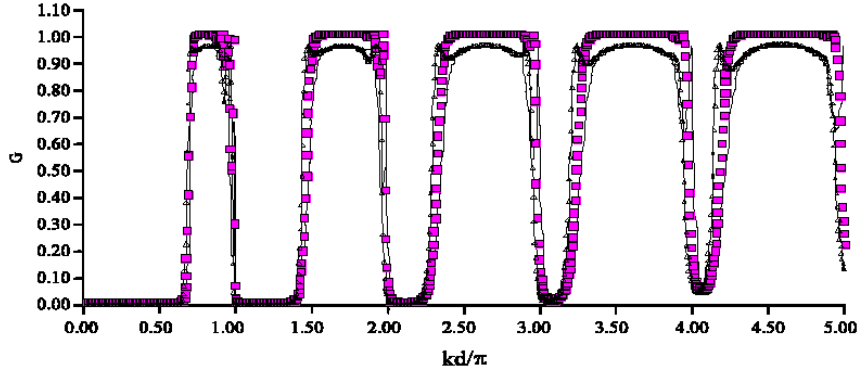


Fig. 6a: The electronic conductance, in the units of $2e^2/h$ as a function of kd/π . Here, $N = 35$ with scaling the binomial distribution by factor of three. In this case, where the defect is only $\pm 5\%$, in the position and the strength of the central Dirac delta function, there is some difference between the two curves and compared to the upper curve. The curve with triangles, dislocation in position $+5\%$ wider and $+5\%$ higher in strength

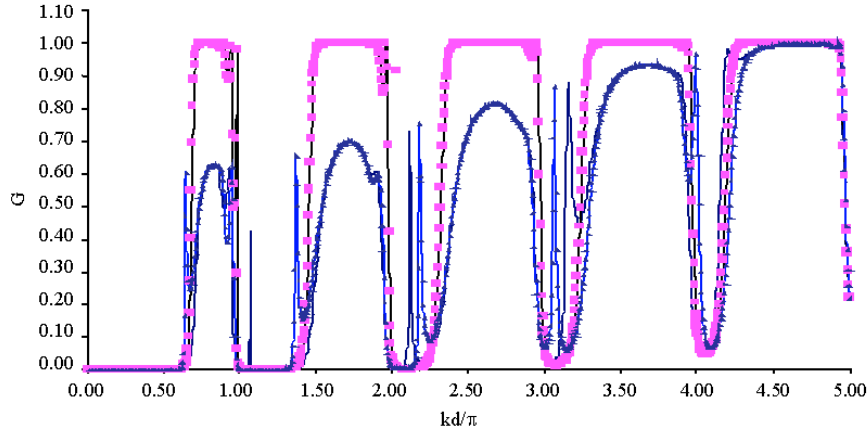


Fig. 6b: The electronic conductance, in the units of $2e^2/h$ as a function of kd/π . Here, $N = 35$ with scaling the binomial distribution by factor of three. In this case, where the defect is only $\pm 20\%$, in the position and the strength of the central Dirac delta function, there is some difference between the two curves and compared to the upper curve. The curve with triangles, dislocation in position $+20\%$ wider and $+20\%$ higher in strength. The peaks in the forbidden bands are due to bound states

the Fig. 6b, the conduction band conductance get lowed by this double defect and the forbidden band has splitting. Also, this splitting is due to resonant state in the forbidden energy band. However, the peaks increase in its height as we increase kd/π . Increasing the defect in both the position and strength increases the chance the particle mode not to propagate through the structure, which increases the chance of the entrapment as the factor kd/π increases (Wu *et al.*, 1991).

In Fig. 6c, We plot the electronic conductance spectrum considering the position defect is $d \pm 0.05d$ and the strength defect is $\Omega_j(N/2+1) \pm 0.2 \Omega_j(N/2+1)$. In this plot, we notice that the structure can tolerate a double defect with $+5\%$ in position and a $+20\%$ in strength without losing the conductance spectrum pattern. From this we can set the maximum limit of the defect tolerance of this structure

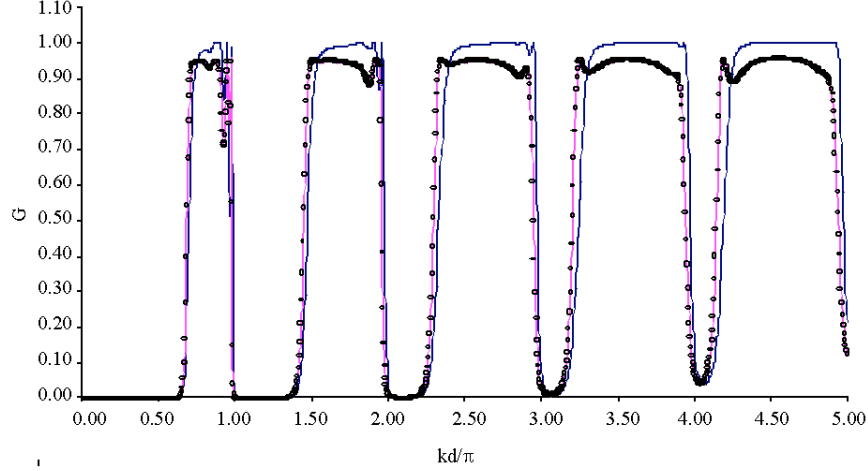


Fig. 6c: The electronic conductance, in the units of $2e^2/h$ as a function of kd/π . Here, N_j with scaling the binomial distribution by factor of three. In this case, where the defect is only +5% in position and +20% in strength of the central Dirac delta function. Notice that there is some difference between upper curve, defect free Fig. 4a and curve with circles

which is $\pm 5\%$ in position and $\pm 20\%$ in strength of the central Dirac delta function potential in the binomially tailored quantum wire.

Missing and Reversed Order Dirac Delta Function Defect

Finally, in this subsection, we are going to study the effect of missing and reversed order, when two adjacent Dirac delta function strength switched, Dirac delta function potential form the binomially tailored quantum wire. In this case, the binomially tailored quantum wire would not function as a good quantum waveguide as it should be, as in Fig. 4a. We assumed the central Dirac delta function potential is missing from the pattern and keeping all other elements strength and spacing intact. Also, we have assumed the central Dirac delta function switched its strength with the adjacent delta function. In Fig. 7a, we illustrate and compare the effect of these defects with defect-free binomially tailored quantum wire. In Fig. 7a, the number of Dirac delta functions in the quantum wire pattern is seven and their strength is weighted according to Eq. 11. As we can see, the electronic conductance through this structure is largely affect when the central Dirac delta function is missing from the pattern at low values of kd/π , but at high values of kd/π the conductance spectrum starts to match that of no-defect spectrum. In the case of the switched order, we see this structure has a good tolerance and conductance spectrum is almost equals that is of no-defect conductance spectrum at moderate values of kd/π . In Fig. 7b, we study the effect of the number Dirac delta functions in the binomially tailored quantum wire on the electronic conductance in the defected quantum wire. We have increase the number of Dirac delta functions to eleven and their strength weight by scaling factor of three. Its worthwhile to notice that when the number of Dirac delta function is increased in the quantum waveguide the difference between the no defect electronic conductance spectrum and the one switched delta function potential case in negligible and in the case of missing Dirac delta function potential the electronic conductance spectrum starts to come close to the no-defect spectrum at lower values of kd/π . As we can notice, these defects destruct of the phase coherence of the electrons wave functions interacting with the binomially tailored quantum wire, which leads to the irregularities in the tunneling and consequently the electronic conductance spectrum.

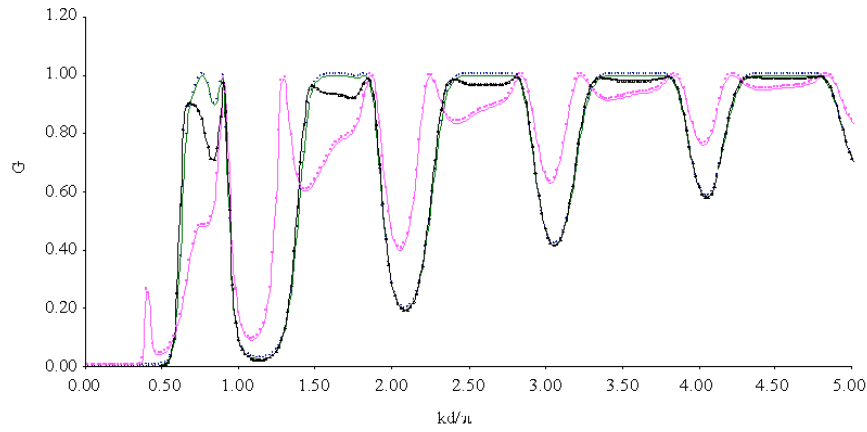


Fig. 7a: The electronic conductance, in the units of $2e^2/h$ as a function of kd/π , the number of Dirac delta function in the quantum wire pattern is seven and the scaling factor is one. The curve with circles is the electronic conductance through the quantum wire without defect, the curve with squares the quantum wire has the central Dirac delta function missing and the curve with triangles the central Dirac delta function switched with the adjacent one

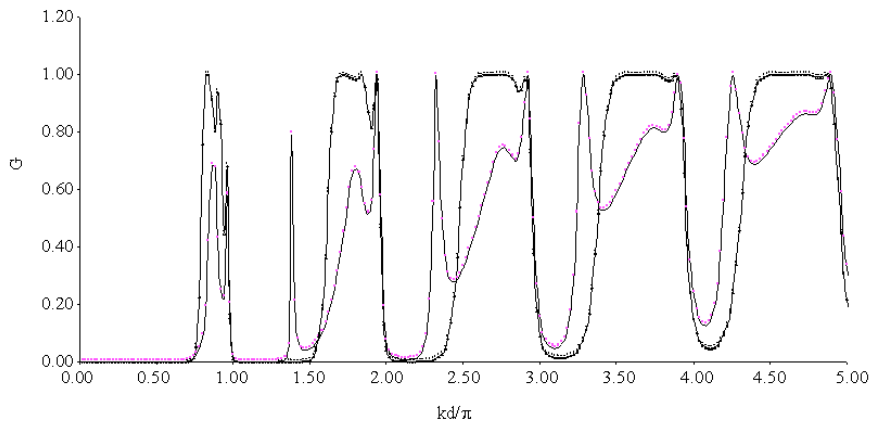


Fig. 7b: The electronic conductance, in the units of $2e^2/h$ as a function of kd/π , the number of Dirac delta function in the quantum wire pattern is eleven and the scaling factor is three. The curve with circles is the electronic conductance through the quantum wire without defect, the curve with triangles the quantum wire has the central Dirac delta function missing and the curve with squares the central Dirac delta function switched with the adjacent one

CONCLUSION

We reintroduced the novel structure of the waveguide quantum wires which is the BTQW. We show that it is possible to have perfect transmission, coherent tunneling, due the interference effects, which gives rise to allowed band and forbidden bands in the transmission spectrum. We found that the

increase of Dirac delta function in the structure and their strength the conduction band become wider and the forbidden bands become sharper and narrower. Besides that, we found the structure tolerate the following defects: up to $\pm 20\%$ in strength defect and $\pm 5\%$ in position defect for the central Dirac delta function in the binomial distribution; can tolerate both defect up to $\pm 20\%$ in strength and $\pm 5\%$ in position dislocation; has a little tolerance when we replace the central Dirac delta function potential with the adjacent one. So, we can conclude that this novel structure offer a good electronic conductance spectrum with considerably high tolerance for defects.

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