QUANTUM WAVEGUIDE TRANSPORT IN SERIAL STUB AND LOOP STRUCTURES

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Abstract

We have studied the quantum transmission properties of serial stub and loop structures. Throughout we have considered free electron networks and the scattering arises solely due to the geometric nature of the problem. The band formation in these geometric structures is analyzed and compared with the conventional periodic potential scatterers. Some essential differences are pointed out. We show that a single defect in an otherwise periodic structure modifies band properties non trivially. By a proper choice of a single defect one can produce positive energy bound states in continuum in the sense of von Neumann and Wigner. We also discuss some magnetic properties of loop structures in the presence of Aharonov-Bohm

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In the past decade remarkable advances have taken place in micro fabrication, and now it is possible to confine electrons in a conductor with a lateral extent of 100 nm or less, resulting in narrow quantum wires, constrictions and quantum dots[1-4]. This expansion is due to combination of new developments in lithography, patterning and layer growth techniques. Specifically it is now possible to engineer device potentials which vary over the length scale such that the electron motion is ballistic or quasiballistic at low temperatures. The small size of these structures largely eliminate the defect scattering and one can get extremely high mobility conductive channels, thus motivating interest in the ballistic regime. In these mesoscopic systems electron transport is governed by quantum mechanics rather than classical mechanics. At very low temperatures, the scattering of phonons (dephasing scattering) is significantly suppressed and the phase coherence length of the electrons L_ϕ (the length over which the electron can be considered to be in a pure state), becomes large compared to the system dimensions. Mesoscopic system can thus be modelled as a phase coherent elastic scatterer. The idealized sample becomes an electron waveguide where the transport properties are solely determined by the impurity configuration, the geometry of the conductor and by the principles of quantum mechanics. As the phase coherence is maintained over the entire sample, several intrinsic quantum mechanical phenomenon have been observed[1-4]. This has opened a completely new branch of device physics and mesoscopic physics. Convincing demonstration of new quantum transport regime have come from experiments on thin metal or semiconductor films and multiply connected structures. Some of the observed quantum phenomenon include Aharonov-Bohm oscillations in the magneto resistance in doubly connected ring structures[5], universal conductance

fluctuations, reproducible sample specific non-self-averaging fluctuations in conductance as the magnetic field or the chemical potential is varied, quantized conductance in the point contact, quenching of Hall resistances in narrow cross etc[2,3]. Given the coherence of the electrons throughout the sample, several exciting ideas for active quantum devices(transistors, switches etc) have been proposed based on interferometric principles[6]. These are quantum analog of well known optical or microwave devices. In these structures, the electron transport is identical to the microwave propagation through a wave guide.

In recent years, several studies have been reported on the transmission across a T shaped device consisting of a main wire of constant width attached to a stub perpendicular to the wire (fig. 1)[7-11]. In this structure the transmission oscillates between zero(antiresonance) and one(resonance) with kL. Here k is the incident wave vector and L is the length of the stub. Especially for the case of one channel T shaped structures one obtains results similar to the wave guides resonantly coupled to a cavity[9,10]. Here the cavity has a set of resonant states given by kL=nπ. Along the main wire across the stub, transmission zeros (total absence of forward scattering or total backscattering) and resonances occur at $kL = n\pi$ and $kL = (n + 1/2)\pi$ respectively. The existence of transmission zeros are very specific to the geometric nature of the scattering and do not occur in conventional one dimensional potential scattering problems. The resonantly coupled quantum waveguides also exhibits the zero-pole pairs in the structure of transmission amplitude in the complex energy plane[9,10]. The proximity of the zero and the poles lead to sharp variations of transmission coefficients as a function of energy and in certain circumstances lead to asymmetrical Fano resonances[12]. If now a

multiple stub configuration is taken, the sharp drops to zero in transmission become extended to forbidden bands and the round tops get squared, along with resonances to form allowed bands. In ref [7,8] the potential usefulness of such systems as transistor device (quantum modulated transistor) has been discussed. In this the drain current can be modified by remote control where the non-locality of electron waves is exploited, i.e., the transistor action can be achieved by varying the effective length of the vertical terminated lead. Relatively small changes in the stub length can introduce strong variations in the electron transmission across the structure. However, quantum channels have a very high resistance($h/e^2 = 25$ kΩ) and the current through a quantum channel is very small. This practical problem can be resolved by stacking superlattice of many such channels[8]. Other potential switching devices are based on controlling the relative phase between different interfering paths (say in semiconducting loop structures) by applying electrostatic or magnetic fields[6,13]. These ballistic devices promise to be much faster and will consume less power than the conventional devices. The conventional transistors operate in a classical diffusive regime and are not sensitive to variations in material parameters such as dimensions or presence of small impurities. These devices operate by controlling the carrier density of quasiparticles. However, proposed quantum devices are not very robust in the sense that the operational characteristics depend very sensitively on material parameters. For example, incorporation of a single impurity or slight structural variations in the mesoscopic device can change non-trivially the influence of partial waves propagating through the sample and hence electron transmission across the sample. In other words the electron transmission across these devices is very specific to the arrangement of the elastic scatterers and on the Fermi energy. These

devices can be exploited, if we can achieve the technology that can reduce or control the phase fluctuations to a small fraction of 2π. On the positive side it should be noted that quantum devices can exhibit multifunctional property (e.g, single stage frequency multiplier), wherein it can perform the functions of an entire circuit within a single element[14].

In this paper we discuss in detail many features of band structure in multiple stub and ring (in the presence of magnetic field) configurations. Throughout our analysis we have restricted ourselves to one channel case, in that the main wire as well as the stub is taken to be one dimensional. This single channel case provides a good approximation to a real wire with finite width at low temperatures at which only the lower subband is filled. Moreover, energy level spacings produced by transverse confinement must be larger than the energy range of the longitudinal transport and thermal broadening k_BT. In this regime quantum wire behaves as a single moded electron waveguide. It is also well known that to have a optimum performance, the quantum device has to be operated in a fundamental mode, i.e., the Fermi energy should be between the ground and the first excited transverse mode. In this regime one can achieve a sharp and controllable modulation of the electron transmission probability. With higher energies (larger than the first excited transverse modes), the propagation of various modes become possible and due to mode mixing the total transmission becomes very sensitive to the defect structures and oscillations in the total transmission coefficient are averaged out. Thus the energy dependence of the total transmission becomes aperiodic. In the case of single channel one can apply quantum waveguide theory on networks[15-17] and one can easily obtain the transmission and reflection probabilities analytically. In our analysis we have

considered free electron networks, i.e., when quantum potential V throughout the network is assumed to be identically zero. The scattering arises solely due to junctions (or geometric scattering) in free electron networks. The scattering properties of the network can be calculated by using the Griffith's boundary conditions at the junction points[18]. These boundary conditions are due to the single valuedness of the wave functions and the conservation of the current(Kirchoff's law) at the junction. The electron wave function has to be single valued throughout the network. If i segments intersect to form a junction and ϕ_1, ϕ_2...ϕ_i are the wavefunctions on the segments, the boundary condition at the junction point are $\phi_1 = \phi_2 = ... = \phi_i$ (continuity) and $\Sigma_i \frac{\partial \phi_i}{\partial x}$=0 (current conservation). Here all the derivatives are either outward or inward from the junction. We have considered both serial stub structure (figs. (1) and (2)) and loop structures (figs. (3) and (4)). For a single stub of length L as shown in fig. (1) and for a loop structure as shown in fig. (3) with equal arms of length L each and in the presence of magnetic flux ϕ, Xia has obtained an analytical expression for the transmission coefficient τ_s and τ_l, respectively and are given by[15]

$$\tau_s = \frac{4sin^2(kL)}{4sin^2(kL) + cos^2(kL)} \tag{1}$$

$$\tau_l = \frac{16(1 - cos(2kL))(1 + cos(\alpha))}{(1 + 4cos(\alpha) - 5cos(2kL))^2 + (4sin(2kL))^2} \tag{2}$$

where $\alpha = 2\pi\phi/\phi_0$. The eqn. (1) is for a single stub structure, where k is the incident wave vector of an electron and L is the length of the stub. In eqn. (2), L is the length of the single arm of the loop. The two arm lengths are assumed to be equal, ϕ is the magnetic flux and ϕ_0=hc/e is the flux quantum. As expected the transmission coefficient

is flux periodic for all energies with a period ϕ_0. For the expressions of complex reflection and transmission amplitudes we refer to [15]. With the help of these amplitudes one can easily compute the transmission coefficient of regularly placed stub structure (fig. (2)) or ring structure (fig. (4)) with the help of transfer matrix method. We have obtained an analytical result for these cases. The stubs (or rings) are assumed identical and are placed at regular intervals of length l. Coherent interference effects, due to elastic scattering by serial structures can produce broad regions where transmission is vanishingly small and these regions are called conduction gaps (or forbidden gaps) and broad regions with finite transmission along with resonances and these regions are called conduction bands. We compare the evolution of band features to that of band structure in a one dimensional periodic potential scatterers, as a function of the number of scatterers, and point out some notable differences. We next consider the effect of a single defect in an otherwise periodic structure. In particular we show that a single defect stub can change non-trivially the band structure. A single defect stub in such a multiple stub configuration can produce one or more zero transmission in the conduction bands. The length of the defect stub determines precisely where the transmission zero will be formed and adjusting the length we can adjust the zeros (band tailoring). These dramatic changes in the band structure are associated with the existence of transmission zeros in geometric structures, which are absent in the conventional potential scattering problems. With an appropriate choice of the length of a single defect stub, one can produce bound states in continuum in the sense of von Neumann and Wigner[19]. Finally we have studied the band formation due to a periodic structure of mesoscopic loops with a Aharonov-Bohm flux passing through the center of each loop and the effect of magnetic field on the band

evolution is studied. We briefly remark on the paramagnetic and diamagnetic (orbital currents) properties of the bands.

TRANSMISSION IN PERIODIC STRUCTURES

Consider a serial structure shown in fig. (2). We can disassemble the system into basic pieces connected in series. The basic piece is the structure as shown in fig. (1). We consider the system to be one dimensional only to simplify the problem without any loss of generality. If we consider the system to be of higher dimensions (i.e., wires with finite transverse widths) then for small values of incident electron energy (such that there is only one propagating channel), the conductance versus energy plot is similar to that of a 1-d system only the origin being shifted due to the zero point energy of the lowest transverse mode. To get the electron wave function in the wire we have to solve the Schrödinger eqn.

$$\nabla^2\phi + (E - V(x))\phi = 0, \tag{3}$$

we have set throughout the units of $\hbar$ and 2m to be unity. In our case V=0 and the solutions are the plane wave solutions i.e., e^{ikx}, where $k = \sqrt{E}$. Then we adopt a technique that is specially suited to such a serial structure. By the mode matching mechanism we derive a transfer matrix that relates the coefficients of the wave functions at one end to that at the other end of the basic piece. The total transfer matrix is just the product of the transfer matrices of all the basic pieces in order[20].

The transfer matrix of the geometry shown in fig. (1) is

$$T^{(1)} = \begin{pmatrix} 1/t^* & r/t \\ r^*/t^* & 1/t \end{pmatrix} \tag{4}$$

where t is the complex transmission amplitude, r is the reflection amplitude and * de-

notes the complex conjugation. These coefficients can be determined by simply matching the boundary conditions. Using the Griffith boundary conditions at the junction and setting the wavefunction at the free end of the stub to be zero (hard wall boundary condition), we get the transfer matrix due to one such stub as[15]

$$T^{(1)} = \begin{pmatrix} (2 - i\cot(kL))/2 & -(i\cot(kL))/2 \\ \\ (i\cot(kL))/2 & (2 + i\cot(kL))/2 \end{pmatrix} \ , \tag{5}$$

where L is the length of the stub. For a periodic stub structure we have taken length of all the stubs to be equal and they are placed at a length l apart as shown in fig. (2).

The total transfer matrix of N stub system is given by[20]

$$T = T^{(N)} M T^{(N-1)} M T^{(N-2)} M ..... T^{(1)} \ , \tag{6}$$

where

$$M = \begin{pmatrix} e^{ikl} & 0 \\ \\ 0 & e^{-ikl} \end{pmatrix} \ , \tag{7}$$

and T^i is the transfer matrix of the i^{th} stub. Since all stubs are identical we have

$$T^{(1)} = T^{(2)} = ... = T^{(N)} = T_a \ . \tag{8}$$

Defining $T_a M = T_1$, we get

$$T = (T_1)^{N-1} T_a \tag{9}$$

T_1 is not symmetric, but by a similarity transformation it can be brought to a symmetric form. This symmetric matrix can be diagonalized by an orthogonal matrix. Then the multiplication of N matrices become very easy and we obtain the transfer matrix of the

entire chain which again has the form

$$T = \begin{pmatrix} 1/{t_N}^* & r_N/t_N \\ {r_N}^*/{t_N}^* & 1/t_N \end{pmatrix} \ . \tag{10}$$

From this we can find r_N, the total reflection amplitude due to N stubs and t_N, the total transmission amplitude due to N stubs. We have found the complex transmission amplitude t_{N+1} across a periodic structure containing (N+1) scatterers to be

$$1/t_{N+1} = \frac{(1-\tau)e^{ikl}}{\tau\, 2^N\sqrt{\mu}}[\gamma^N - \delta^N] + \frac{1}{t\, 2^{N+1}\sqrt{\mu}}[\rho\,\delta^N - \eta\,\gamma^N] \ , \tag{11}$$

where

$$\mu = \frac{e^{-2ikl}}{t^2} + \frac{e^{2ikl}}{t^{*2}} + 2/\tau - 4 \ ,$$

$$\eta = \frac{e^{ikl}}{t^*} - \frac{e^{-ikl}}{t} - \sqrt{\mu} \ ,$$

$$\rho = \frac{e^{ikl}}{t^*} - \frac{e^{-ikl}}{t} + \sqrt{\mu} \ ,$$

$$\gamma = \frac{e^{ikl}}{t^*} + \frac{e^{-ikl}}{t} + \sqrt{\mu} \ ,$$

$$\delta = \frac{e^{ikl}}{t^*} + \frac{e^{-ikl}}{t} - \sqrt{\mu} \ . \tag{12}$$

Here t is the complex transmission amplitude of a single scatterer (stub or ring) and τ is corresponding transmission coefficient tt^*. The total transmission coefficient T_{N+1} is given by $T_{N+1} = t_{N+1}{t_{N+1}}^*$. From the expression for the total complex transmission amplitude one can obtain the transmission coefficient as well as the density of states,

as discussed later. The total transmission coefficient for N+1 scatterers takes a simple form and is given by[21]

$$1/T_{N+1} = 1 + \frac{sin^2(N\theta)}{sin^2(\theta)}(\frac{1}{\tau} - 1) \ , \tag{13}$$

where, cos(θ)=Re(e^{-ikl}/t). Here θ is the Bloch phase associated with the infinite periodic system. There exists a simple relation between the elastic scattering properties at the Fermi energy and the conduction properties of the sample.The two terminal conductance of an entire network g, measured in units of $e^2/\pi\hbar$ and including the spin is given by g=T, where T is the total transmission coefficient[22].

SERIAL ARRANGEMENT OF STUBS

In the case of a single stub we can readily observe from eqn. (1) oscillations between zero and one in the transmission probability as a function of kL. The wave propagating along the stub is reflected back from the end point of the stub (the wave function vanishes at the end point of the stub) and gives rise to a standing wave inside the stub. This in turn interferes with the propagating wave in the main wire. When the phase shift kL is $n\pi$, we get $\tau = 0$, (total backscattering) and for phase shift of $(n + 1/2)\pi$, we get $\tau = 1$ (total forward scattering). Here τ is the transmission probability across a single stub. As we increase N (the total number of stubs) to say 5, the stub lengths being the same, the sharp drops become extended to forbidden bands. Now we move closer to a periodic structure like the Kronig-Penny model. The band formation can clearly be seen in fig. (5) where we have plotted the total transmission probability as a function of kL for five stubs in series and we have taken L/l=1.0. All the energy

bands are identical with regions of large transmission separated by distinct valleys. This is a very interesting feature characteristic of geometric scattering. If one considers a periodic structure of square wells or delta function potentials and study how the band evolves as a function of the number of scatterers, we then find striking dissimilarity[23]. There for some value of number of scatterers N say N_1 (depending upon the strength of each potential), the first band gap becomes well defined, the other band gaps at higher k (or energy) values are very poorly developed or not developed at all. If we keep on increasing the value of N then for some value of $N = N_2 > N_1$ the second band gap develops but the rest are not. A particular valley gets flatter and deeper as N increases and forms a band gap at some value of number of scatterers. To get the complete band for all values of k we need actually infinite number of potential scatterers. In contrast in the periodic stub structures characterized by geometric scattering finite number of stubs typically of the order of 5 stubs are capable of forming the entire band structure upto infinite energy of incident electron, with wide gaps. This difference arises mainly due to existence of transmission zeros in geometric structures. The transmission zeros do not arise in potential scattering problem with finite scatterers. In the case of geometric structures the transmission coefficient oscillates between zero and one even for arbitrarily large incident energies, whereas in the potential scattering problem the transmission coefficient approaches asymptotically a value of unity as the incident energy is increased.

In a recent study on locally periodic potential, saturation effect has been discussed[24]. This means the transmission probability does not change significantly as the number of barriers is increased. However, their observation is based on the exploration on a limited

energy range and on the use of a gaussian wave packet that washes out the details of the structure. But for the case of periodic square wells and delta function potentials it has been observed that the onset of saturation depends on the energy of the incident particle. For higher energies we have to go to larger values of N to achieve the saturation. In our mesoscopic system we find that the entire band structure for all values of k is well saturated at small value of N. There is not much change as we increase the value of N except that the band edges become sharper and allowed transmission bands accommodate more resonances. This is shown in fig. (6) where again L/l=1.0 and N=10. But as we increase N the transmission probability undergo oscillations from one (unity) to well below one over a narrow region in the allowed bands. Each band for N scatterers contain N ripples or resonances if N is odd, and (N-1) ripples if N is even. But this is true only for the case when L is equal to l. Out of these resonances, one resonance (or unit transmission) corresponds to the total forward scattering state. This resonance always lies at the energy corresponding to the unit transmission of a single stub. All other resonances are of course elementary consequences of quantum mechanical interference due to coherent multiple scattering, and are symmetrically placed around the value of unit transmission corresponding to a single stub. Due to this symmetry we always find odd number of resonances in a given band, irrespective of the total number of scatterers being even or odd. As we increase the number of scatterers (N), the number of spikes (or resonances) increase proportionally within a given band and resonances come close to each other. Width of the each resonance scales as 1/N and hence resonances become sharper as their number increases with N within a given band. This can be seen for $N = 100$ as shown in fig. (7), where again the stub lengths and their separations are

kept the same.

In the above discussion we have restricted to a case where l=L. If we fix L and increase l such that l>L, one can produce more transmission resonances in the allowed bands and make the band edges sharper. The reason is that whenever this intermediate region (or the length l) is such that an integral number of wavelengths of the incident electron fits in exactly, we get a resonance. So, doubling the length l (i.e., l/L=2),within a given band, the number of resonances apart from the unit transmission resonance associated with single stub, double. This increase in the transmitted intensity at certain places in the bands is compensated by decrease in the transmitted intensity at certain places in the gap making the band edges sharper. This effect essentially arises due to the two competing periodicities with period kl and kL (along with their sum, difference and harmonics). This can be seen from fig. (8), where we have plotted the transmission coefficient versus kL for L/l=2.0 and for N=5 stubs. Comparing this fig.(8) with fig. (5) (the case in which N=5 and L/l=1.0), we notice the doubling of resonances and sharper band edge features. In a periodic potential scatterers, say with N delta functions, we always get N-1 resonances in an allowed band and in contrast their number is independent of separation between the scatterers.

In our one channel periodic case the dimensionless conductance g takes a value between one and zero(in the forbidden band) as a function of Fermi energy. The recent work of Leng and Lent[25] should be treated as a generalisation of work to higher dimension(multichannel case). For a multichannel problem the dimensionless two terminal conductance can take a value much higher than unity depending on the fermi energy(or

number of occupied subbands). It is well known that if the ballastic channel in higher dimension is patterned with, constrictions or other obstuctions the quantisation of the conductance is lost and complicated structure for conductance emerges due to quantum intereference and back scattering in the channels(non adiabatic effects). However, if the ballastic channel has a periodically modulated stucture(periodic stubs), the quantisation in conductance is recovered but is no longer a monotonic function of energy. The conductance rather steps up and down between the quantised levels some times going to zero. These new features are sloely related to the periodic multichannel case[25].

SINGLE DEFECT IN SERIAL ARRANGEMENT OF STUBS

Here we shall show how a single defect at the center of the system (in fig. (2)) can totally alter the band structure which keeps on changing abruptly with the strength (length) of the defect. The length of all the stubs are assumed identical except the central one. Again we find the total transfer matrix by multiplying the individual transfer matrices. If the defect stub is twice in length than the other stubs then transmission zeros are produced exactly at the middle of the allowed host bands. It is easy to verify that if a single T junction has a transmission zero at a particular incident energy E, then incorporating this stub in a serial one dimensional geometric structure (ordered or disordered) produces a transmission zero at the same energy irrespective of the position of the stub. This is shown in fig. (9) where we take L/l=1.0 and L_d/l=2.0 where L_d is the length of the defect stub. We have taken four stubs on either side of the defect stub. We clearly observe that this single defect produces transmission zeros in the middle of the allowed host band and also produces resonances at the band edges. If we make length of the defect stub ten times larger than the length of other stubs then we

see five zeros develop within the host band. This is shown in fig. (10) for L/l=1.0 and L_d/l=10.0 with fifty stubs on either side of the defect. Along with the transmission zeros within a given band we also get additional bound states in the forbidden energy band. However, in the transmission analysis of a larger system these bound states cannot be identified. The physics of these bound states will be discussed later in this section. The position of the transmission zeros within a band do not depend in any way on whether the defect is at the center or away from the center. Ofcourse the total transmission in general does depend on the exact position of the defect stub. This result is related to the mathematical fact that transmission matrices do not commute. The total transmission probability is related to the interference pattern arising due to sum of infinite number of Feynman paths which start and end at the two end points of the system[26]. Now by having a single impurity (or impurities) in an otherwise periodic serial structure, all the phases of infinite Feynman paths are altered, as every path has to cross the impurity site at least once. The total sum containing infinite complex amplitudes is hence altered non-trivially and therefore, the total transmission probability is very sensitive to the defect or impurity location. This fact also implies that when the quantum nature of scatterers become important the classical Ohm's law does not hold good [27,28], i.e., the total resistance defined via the transmission coefficient is not the simple sum of individual resistors (or scatterers). Moreover the resistance being non additive is also a non self averaging quantity in that the ensemble averaged fluctuations (over all the realizations of scatterers), in resistance dominates over the mean value of resistance[27,28]. This is directly related to the fact that the resistance (or the transmission coefficient) of a sample is very sensitive to the spatial realization of scatterers. We have shown above that

one can produce a transmission zero in a conduction band at any place with a proper choice of length of single defect stub. Having a zero transmission inside an allowed band can play a very special role in band engeneering technology. For a fixed Fermi energy by varying the length of the single defect stub (which can be varied by applying gate voltage) one can thus induce a metal insulator transition (or switch action).

In recent years some interest has been generated on the possibility of positive energy bound states above the potential barriers (in the continuum) and their effect on the transport properties in quantum wires[29,30]. Classically in the energy regime above the potential barriers the particle motion is unbounded, however, due to quantum mechanical interference bound states can exist in this regime. There are three different physical situations wherein the bound states can arise. The first possibility was proposed by von Neumann and Wigner[19]. In particular they showed that certain spatially oscillating attractive potentials could support bound states above the potential barriers by means of diffractive interference. These bound states coexist with continuum states and hence they are not robust against perturbation. A small perturbation in the potential mixes the bound states with the continuum states. Second class of bound states in classically unbound region can be created in different geometries of quantum wires having a finite cross section[29]. Several geometrical structures like L shaped bent structures, crossed structure and cavity structures have been considered. For example in L shaped bent structures bound states exist, and are localized in the bend. This is due to the fact that near the bend due to availability of larger space the local zero point energy of the electron is reduced considerably as compared to the zero point energy in the side arms away from the bend. Hence the electrons can occupy a state (bound) at the bend which

has an energy lower than the zero point energy of the side arms, thus not able to propagate in the arms. In contrast to the von-Neumann and Wigner state this state does not coexist with the scattering states (sometimes coexistence is possible due to symmetry related reasons). Classically the particle motion is unbounded as the potential everywhere is identically zero. Third possibility arises whereby one can create a bound state in a forbidden energy gap of a periodic host crystal with the help of a single impurity potential[30]. The impurity potential is chosen such that its resonance level lies in the energy gap of the host crystal. Here too bound state is isolated and does not coexist with scattering states. Such bound states have been recently observed in quantum well structures[30]. In the following we explicitly show that the bound state in a continuum can arise in a one dimensional serial structure with a single defect stub. The length of a single defect stub is so chosen that it has a resonant state (unit transmission state) in the forbidden energy gap of the host serial structure. With a few stubs on either side of the defect stub one can spatially localize a state. We have taken the defect stub such that L_d/l=0.75 with only two stubs on either sides of it and L/l=1. For this system we have plotted the transmission coefficient versus kL as shown in fig. (11). In this case of a short chain there is a peak in the transmission in the band gap. However this peak decreases in height as we increase the length of the chain. This is clear from the fig. (12), where we have taken 3 stubs on either sides, with all other parameters remaining the same. If the defect stub is such that it produces a peak in the transmission in the band gap then a localized state will be produced. This is because the particular mode that is allowed in the defect stub is not allowed in the region to the right and left of it. Thus this mode can not propagate to $\pm\infty$ and hence gets trapped.

We can get non-vanishing transmission in the band gap provided the localized state has some spatial extent and does not decay appreciably on either sides of the chain. Then it is capable of contributing to the transmission. The peak becomes shorter if the chain length is increased. This is because the localized state wavefunction amplitude decays exponentially on either sides of the defect scatterer and become very small at the end points, making it unable to couple wavefunctions on either sides of the scatterer (or localized states do not effectively communicate with the end points of the system). For four scatterers on either sides, the peak completely disappears as shown in fig. (13). It is clear that one misses the bound states in transmission analysis of a larger system. However, if one studies the density of states in these systems one can easily locate the bound states which show up as sharp peaks in the gap region. The change in the density of states due to scatterer, at a particular energy is given according to Friedel theorem as $\frac{d\theta}{(\pi dE)}$, where θ is the argument of the complex transmission amplitude[31,32]. Using this formula and with the help of eqn. (11) we have calculated the density of states for the system with four scatterers on either side of the defect stub. Although for this particular system we do not see any peak in the transmission (see fig. (13)) at the localized state energy, however, we see a large peak in the density of states (see fig (14)) at that isolated energy showing the existence of the localized state. Thus we have shown that one can get a positive energy bound state in a continuum for a serial structure by appropriately choosing the length of a defect stub. As the potential everywhere in the network is identically zero the classical motion of a particle is however, unbounded for all energies.

SERIAL ARRANGEMENT OF LOOPS

Now on we will discuss the band formation in serial loop structures both in the presence and in the absence of Aharonov-Bohm flux passing through the center of the loops. We also study in details how the band structure changes with the magnetic flux. The transmission properties of a single loop (as shown in fig. (3)) has been calculated by Xia[15]. The transmission coefficient oscillates as a function of flux ϕ with a period ϕ_0(=hc/e) and is symmetric in the flux ϕ[33]. This is a solid state version of Aharonov-Bohm effect. The transmission coefficient as a function of kL (or energy) exhibits a transmission peak for certain values of kL. This occurs whenever electron energies coincide with the eigen energies of the entire system. In the case of two equal arm lengths the transmission coefficient as a function of kL does not exhibit zeros in the absence of the magnetic field. However, in the presence of the magnetic field through the center of the loop we observe transmission zeros as a function of kL. We now consider a serial structure comprising of many such loops as shown in fig. (4). The two arms of the loop are of equal length L each and the length between the loops is taken to be l. We follow the same procedure as for the serial stubs for calculation of the transmission coefficient. We first consider the situation where the magnetic field is absent. We have plotted (fig. (15)) the transmission versus kL for N=5 loops. The valleys in between unit transmissions develop into wide looking band gaps for the same reason as discussed before for serial stub structures, i.e., the structure moves closer to a periodic structure like the Kronnig Penny model. The number resonances in the conduction band depend on the lengths L and l. The transmission is not zero in the gaps but saturation sets in identically for all gaps. Bands are clearly formed for $N = 5$ as shown in fig. (15) where

L/l=1.0. The bands and the band gaps become more defined as we increase the value of N. It is interesting to note that for a serial loop structure the first allowed conduction band starts right from the energy zero. In contrast, in the serial stub case we always find a forbidden gap around energy zero. This follows from the fact that for an isolated loop the lowest eigenstate in the absence of magnetic field has momentum k=0. Instead of L/l=1.0, if we take l to be smaller such that L/l=100.0(say), with N remaining the same then the band structure shows an effect opposite to that of a serially arranged potentials. We find that the higher band gaps are formed more easily and saturate faster as N increases. This is shown in fig. (16). This happens because if the electron wavelength is larger than separation between loops then multiple reflection between two loops cannot form standing waves. Only high energy electrons with wavelength much smaller than the separation between loops are strongly affected by these regions due to multiple scattering and the effect of periodicity is felt.

We now consider the evolution of the band structure as a function of the magnetic flux in the serial loop structure. In the presence of the magnetic flux through each loop each band splits into two (except the lowest one) and band gap appears at the center of each band. This is shown in fig. (17), where we have taken α = .2 and L/l=1.0 for N=5 loops. This band gap that develops due to the magnetic field can also be made to develop at other places of the band than the center by choosing a different value of L/l. This is seen in fig. (18) where L/l=100.0, α=0.6 and N=20. The band structure evolves continuously as we change the enclosed magnetic flux and the band gap increases continuously with the magnetic flux. In fig. (19) the dashed curve is for N=5.0, L/l=1.0 and α=.4 whereas the solid curve is for N=5.0, L/l=1.0 and α=0.2. The band gap is

seen to be more for the larger magnetic flux. In this way these special band gaps initially keep widening with α upto $\alpha = \pi$ where the transmission is identically zero for all values of kL as evidient from eqn. (2), and then it starts narrowing with α, finally disappearing at $\alpha = 2\pi$. If we increase α further then the same cycle is repeated, with a period ϕ_0. These band gaps appear with the magnetic field because when flux through a loop is non zero then the transmission probability across a single loop show zeros. Each maxima of unit transmission splits into two and a zero develops in between. This is because the magnetic field breaks the time reversal symmetry. For an isolated closed loop (ring) the eigenstates in the absence of magnetic field can be calculated via the boundary condition $e^{i2kL} = 1$, where k is the wave vector and $2L$ is the circumference of the loop. So $k_n = \frac{n\pi}{2L}, n = 0, \pm1, \pm2....$, and the discrete energy states are given by $E_n = \frac{\hbar^2 {k_n}^2}{2m}$. The states with $n = \pm1$ are degenerate.Similarly $n = \pm2$ states are degenerate and so on. Now when we connect perfect leads on two sides, the transmission probability exhibits a peak transmission (T=1) for certain values of kL. This happens whenever the incident electron energy coincides with one of the eigen energies of the system. The deviations from the values of the exact energy states of the closed ring follow from the additional junction scattering due to the leads. Each such peak is degenerate. But once the flux through the isolated closed loop is non-zero this degeneracy is removed and resonance peak splits into two peaks and a zero in the transmission develops in between. The separation between the peaks is periodic in flux reaching the maximum value at $\alpha = \pi$ and the transmission across a single loop is identically zero for all values of kL. In periodic structure the sharp zeros develop into wide looking band gaps and hence one can develop band gaps at the middle of the bands with the help of magnetic field. It

is important to know that as we tune the magnetic field the bands shift their position on the energy axis. The magnetic field destroys the time reversal symmetry and as a consequence degeneracy of the states carrying current clockwise and anticlockwise in the loops is lifted. Depending on the Fermi energy uncompensated current flows in either of the directions. In the case of the isolated ring the persistent current oscillates from one state to the next and the total persistent current is given by a sum due to all occupied levels[34-36]. The current i_n in the loop carried by n^{th} eigenstate with energy $E_n(\phi)$ is proportional to $(-1/c)\frac{\partial E_n(\phi)}{\partial \phi}$. In the case of the periodic loop structure considered here all the odd bands (1,3, etc.) initially narrow as we increase the magnetic field. In these bands the resonances at lower energy shift right on the energy scale and the resonances on the higher energy side of the band shift to the left. This in turn implies that the band exhibits a mixed magnetic behavior, in that the lower energy eigen states carry a diamagnetic current whereas the higher energy eigenstates within these bands carry paramagnetic currents. The even bands (2,4, etc.) always shift to the left on the energy axis initially as we increase magnetic field. This amounts to a fact that all energy eigenstates in an even band carry a paramagnetic current. In fig. (19) we have shown the evolution of second and third bands for two values of the magnetic field. Due to the band formation we expect to observe larger equilibrium magnetic response in the loop structures as compared to isolated rings. Since the total persistent current is due to the sum over all states and the nature of persistent current within a paramagnetic band does not change, i.e., within a given paramagnetic band all the energy levels carry paramagnetic current, by appropriately varying the Fermi level in the band one can obtain larger contribution to the persistent current. As in the case for

a serial stub structures, having a single loop with different dimensions (circumference) from the rest, one can tailor the band structure and one can also create localized states in the continuum. The physics is essentially the same.

CONCLUSIONS

We have analysed the problem of band formation in a periodic multiple stub and loop(in the presence of magnetic flux) configurations, using quantum wave guide theory on networks. Throughout we have restricted ourselves to a single channel free electron network. In these network the scattering is solely due to the geometric nature of the problem. The evolution of band formation as a function of number of scatterers is compared with a conventional one dimensional potential scattering system and several notable differences have been pointed out. A single defect in an otherwise periodic system modifies band properties nontrivially and argued that this fact is a consequence of the existence of zeroes in geometric structures. The sensitivity of the band strucutre to a single defect can be utilised for band tailoring and for quantum device operations. We have also shown that by a proper choice of a single defect one can produce bound states in continuum in the sense of vonNuemann and Wigner. Finally we have also discussed the magnetic properties arising in loop structures in the presence of Aharonov Bohm fulx. In paricular we explained notion of diamagnetic and mixed properties of bands due to orbital currents.

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