Quantum Transport in Bridge Systems

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Abstract. We study electron transport properties of some molecular wires and an unconventional disordered thin film within the tight-binding framework using Green's function technique. We show that electron transport is significantly affected by quantum interference of electronic wave functions, molecule-to-electrode coupling strengths, length of the molecular wire and disorder strength. Our model calculations provide a physical insight to the behavior of electron conduction across a bridge system.

1. Introduction

Recent advances in nanoscience and technology have made feasible to growth nanometer sized systems like, quantum wires [1-3], quantum dots [4-7], molecular wires [8], etc. Quantum transport in such systems provides several novel features due to their reduced dimensionality and lateral quantum confinement. The geometrical sensitivity of low-dimensional systems makes them truly unique in offering the possibility of studying quantum transport in a very tunable environment. In the present age, designing of electronic circuits using a single molecule or a cluster of molecules becomes much more widespread since the molecules are the fundamental building blocks for future generation of electronic devices where electron transmits coherently[9-10]. Based on the pioneering work of Aviram and Ratner [11] where an innovative idea of a molecular electronic device was predicted for the first time, the development of a theoretical description of molecular devices has been pursued. Later, many experiments [12-16] have been carried out in different molecular bridge systems to justify the basic mechanisms underlying such transport. Though there exists a vast literature of theoretical as well as experimental study on electron transport in bridge systems, but yet the complete knowledge of conduction mechanism in such systems is not very well established even today. Many significant factors are there which can control the electron transport across a bridge system, and all these effects have to be taken into account properly to characterize such transport. For our illustrative purposes, here we mention very briefly some of them as follows. (I) The molecular coupling with side attached electrodes and the electron-electron correlation [17] provide important signatures in the electron transport. The understanding of the molecular coupling to the electrodes under non-equilibrium condition is a major challenge in this particular study. (II) The molecular geometry itself has a typical role. To emphasize it, Ernzerhof et al. [18] have predicted several model calculations and provided some new interesting results. (III) The quantum interference effect [19-27] of electron waves passing through a bridge system probably the most important aspect for controlling the electron transport, and a clear idea about it is needed to reveal the transport mechanism. (IV) The dynamical fluctuation in the small-scale devices is another important factor which plays an active role and can be manifested through the measurement of shot noise, a direct consequence of the quantization of charge. It can be used to obtain information on a system which is not available directly through the conductance measurements, and is generally more sensitive to the effects of electron-electron correlations than the average conductance [28-29]. Beside these, several other factors are there which may control the electron transport in a bridge system.
There exist several \textit{ab initio} methods for the calculation of conductance \cite{30-40} through a molecular bridge system. At the same time, tight-binding model has been extensively studied in the literature, and it has also been extended to DFT transport calculations \cite{41-42}. The study of static density functional theory (DFT) \cite{43-44} within the local-density approximation (LDA) to investigate the electron transport through nanoscale conductors, like atomic-scale point contacts, has met with great success. But when this similar theory applies to molecular junctions, theoretical conductances achieve much larger values compared to the experimental predictions, and these quantitative discrepancies need extensive and proper study in this particular field. In a recent work, Sai \textit{et al.} \cite{45} have predicted a correction to the conductance using the time-dependent current-density functional theory since the dynamical effects give significant contribution in the electron transport, and illustrated some important results with specific examples. Similar dynamical effects have also been reported in some other recent papers \cite{46-47}, where authors have abandoned the infinite reservoirs, as originally introduced by Landauer, and considered two large but finite oppositely charged electrodes connected by a nanojunction. In this dissertation, we reproduce an analytic approach based on the tight-binding model to characterize the electron transport properties through some bridge systems, and utilize a simple parametric approach \cite{48-55} for these calculations. The model calculations are motivated by the fact that the \textit{ab initio} theories are computationally much more expensive, while the model calculations by using the tight-binding formulation are computationally very cheap, and also provide a physical insight to the behavior of electron conduction through such bridge systems.

This dissertation can be organized in this way. Following the introductory part (Section 1), in Section 2 we illustrate very briefly the methodology for the calculation of transmission probability, conductance and current through a finite size conductor attached to two metallic electrodes by using Green's function formalism. Section 3 describes electron transport in some molecular wires. In Section 4, we focus our study on electron transport through a unconventional disordered thin film in which disorder strength varies smoothly from layer to layer with the distance from its surface. Finally, we conclude our results in Section 5.

2. Theoretical Description

This section follows the methodology for the calculation of the transmission probability ($T$), conductance ($g$) and current ($I$) through a finite size conductor attached to two one-dimensional semi-infinite metallic electrodes by using Green's function technique. Let us refer to Fig. 1, where a finite size conductor is attached to two metallic electrodes, viz, source and drain through the lattice sites S and S.

![Fig. 1: Schematic view of a finite size conductor attached to two metallic electrodes, viz, source and drain through the lattice sites S and S.](image)

At sufficient low temperature and bias voltage, we use the Landauer conductance formula \cite{56-57} to calculate the conductance $g$ of the conductor which can be expressed as,

$$g = \frac{2e^2}{\hbar} T$$  

(1)
where $T$ becomes the transmission probability of an electron through the conductor. It can be expressed in terms of the Green's function of the conductor and its coupling to the two electrodes by the relation [56-57],

$$T = \text{Tr} \left[ \Gamma_s G^r \Gamma_d G^a \right]$$

(2)

where $G^r_e$ and $G^a_e$ are respectively the retarded and advanced Green's functions of the conductor including the effects of the electrodes. The parameters $\Gamma_s$ and $\Gamma_d$ describe the coupling of the conductor to the source and drain respectively, and they can be defined in terms of their self-energies. For the complete system i.e., the conductor with the two electrodes the Green's function is defined as,

$$G = (E - H)^{-1}$$

(3)

where $E$ is the injecting energy of the source electron. Evaluation of this Green's function requires the inversion of an infinite matrix as the system consists of the finite conductor and the two semi-infinite electrodes. However, the entire system can be partitioned into sub-matrices corresponding to the individual sub-systems and the Green's function for the conductor can be effectively written as,

$$G_e = (E - H_e - \Sigma_s - \Sigma_d)^{-1}$$

(4)

where $H_e$ is the Hamiltonian of the conductor which can be written in the tight-binding model within the non-interacting picture like,

$$H_e = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{ij} t (c_i^\dagger c_j + c_j^\dagger c_i)$$

(5)

where $\epsilon_i$'s are the site energies and $t$ is the hopping strength between two nearest-neighbor atomic sites in the conductor. Similar kind of tight-binding Hamiltonian is also used to describe the two semi-infinite one-dimensional perfect electrodes where the Hamiltonian is parametrized by constant on-site potential $\epsilon_0$ and nearest neighbor hopping integral $t_0$. In Eq. 4, $\Sigma_s^{\dagger} = h_{Sc} g_{Sc} h_{Sc}^{\dagger}$ and $\Sigma_d^{\dagger} = h_{Dc} g_{Dc} h_{Dc}^{\dagger}$ are the self-energy operators due to the two electrodes, where $g_{Sc}$ and $g_{Dc}$ correspond to the Green's functions of the source and drain respectively. $h_{Sc}$ and $h_{Dc}$ are the coupling matrices and they will be non-zero only for the adjacent points of the conductor, S and S as shown in Fig. 1, and the electrodes, respectively. The matrices $\Gamma_s$ and $\Gamma_d$ can be calculated through the expression,

$$\Gamma_{S(D)} = i \left[ \Sigma_{S(D)} - \Sigma_{S(D)}^{a} \right]$$

(6)

where $\Sigma_{S(D)}$ and $\Sigma_{S(D)}^{a}$ are the retarded and advanced self-energies respectively, and they are conjugate with each other. Datta et al. [58] have shown that the self-energies can be expressed like as,

$$\Sigma_{S(D)} = \Lambda_{S(D)} - i \Delta_{S(D)}$$

(7)

where $\Lambda_{S(D)}$ are the real parts of the self-energies which correspond to the shift of the energy eigenvalues of the conductor and the imaginary parts $\Delta_{S(D)}$ of the self-energies represent the broadening of these energy levels. This broadening is much larger than the thermal broadening and this is why we restrict our all calculations only at absolute zero temperature. All the informations about the conductor-to-electrode coupling are included into these two self-energies as stated above.
and are described through the use of Newns-Anderson chemisorption theory [48-49]. The detailed description of this theory is available in these two references. By utilizing the Newns-Anderson model, we can express the conductance in terms of the effective conductor properties multiplied by the effective state densities involving the coupling. This allows us to study directly the conductance as a function of the properties of the electronic structure of the conductor within the electrodes. The current passing across the conductor is depicted as a single-electron scattering process between the two reservoirs of charge carriers.

The current \( I \) can be computed as a function of the applied bias voltage \( V \) through the relation [56],

\[
I(V) = \frac{e}{\pi} \int_{E_F-eV/2}^{E_F+eV/2} T(E,V)dE
\]

where \( E_F \) is the equilibrium Fermi energy. For the sake of simplicity, we assume that the entire voltage is dropped across the conductor-electrode interfaces and this assumption doesn't greatly affect the qualitative aspects of the \( I - V \) characteristics. Such an assumption is based on the fact that, the electric field inside the conductor especially for short conductors seems to have a minimal effect on the conductance-voltage characteristics. On the other hand, for quite larger conductors and high bias voltages the electric field inside the conductor may play a more significant role depending on the internal structure and size of the conductor [58], but yet the effect is quite small.

3. Quantum Transport in Molecular Wires

In this section, we narrate electron transport properties of some molecular wires consisting with polycyclic hydrocarbon molecules. These molecules are named as benzene, napthalene, anthracene and tetracene respectively. The transport properties in the molecular wires are significantly affected by the (i) quantum interference effects, (ii) molecule-to-electrode coupling strength, and (iii) length of the molecular wire, and here we discuss our results in these aspects.

3.1. Model

Fig. 2: Molecular model for the four different polycyclic hydrocarbon molecules. The molecules are benzene (one ring), napthalene (two rings), anthracene (three rings) and tetracene (four rings) respectively. These molecules are attached to the electrodes, at the \( \alpha - \alpha \) positions called the cis configuration, and at the \( \beta - \beta \) positions called the trans configuration via thiol (SH) groups.
In Fig. 2, we show the model of the four different polycyclic hydrocarbon molecules. To reveal the quantum interference effects, we consider two different arrangements of the molecular wires. In one case, the molecules are attached to the electrodes at the $\alpha-\alpha$ sites (see the first column of Fig. 2). This is so-called the cis configuration. In the other case, the electrodes are attached to these molecules at the $\beta-\beta$ sites, as presented in the second column of Fig. 2. This particular arrangement is so-called the trans configuration. In actual experimental set-up, the electrodes made from gold (Au) are used and the molecule coupled to the electrodes through thiol (SH) groups in the chemisorption technique where hydrogen (H) atoms remove and sulfur (S) atoms reside. To describe the polycyclic hydrocarbon molecules here we use the similar kind of non-interacting tight-binding Hamiltonian as illustrated in Eq. 5.

3.2. Results and Discussion

Here we describe all the essential features of the electron transport for the two distinct regimes. One is so-called the weak coupling regime, defined by the condition $\tau_{S(D)} << t$. The other one is so-called the strong-coupling regime, denoted by the condition $\tau_S \approx t$, where $\tau_S$ and $\tau_D$ correspond to the hopping strengths of the molecule to the source and drain respectively. For these two limiting cases we take the values of the different parameters as follows: $\tau_s = \tau_d = 0.5$, $t = 2.5$ (weak-coupling) and $\tau_s = \tau_d = 2$, $t = 2.5$ (strong-coupling). Here we set the on-site energy $\varepsilon_0 = 0$ (we can take any constant value of it instead of zero, since it gives only the reference energy level) for the electrodes, and the hopping strength $t_0 = 4$ in the two semi-infinite metallic electrodes. For the sake of simplicity, we set the Fermi energy $E_F = 0$.

Let us begin our discussion with the variation of the conductance $g$ as a function of the injecting electron energy $E$. As representative examples, in Fig. 3, we plot the $g-E$ characteristics for the molecular wires in which the molecules are attached to the electrodes in the trans configuration. Figures 3(a), (b), (c) and (d) correspond to the results for the wires with benzene, naphthalene, anthracene and tetracene molecules respectively. The solid and dotted curves represent the results in the weak and strong molecule-to-electrode coupling limits respectively.

![Fig. 3: $g-E$ characteristics of the molecular wires in the trans configuration, where (a), (b), (c) and (d) correspond to the wires with benzene, naphthalene, anthracene and tetracene molecules respectively. The solid and dotted curves represent the results in the weak and strong molecule-to-electrode coupling limits respectively.](image-url)
approaches the value 2, and therefore, the transmission probability $T$ goes to unity since we have the relation $g = 2T$ from the Landauher conductance formula (see Eq. 1 with $e = h = 1$ in the present description). These resonance peaks are associated with the energy eigenvalues of the single hydrocarbon molecules, and therefore we can say that the conductance spectrum manifests itself the electronic structure of the molecules. Now in the strong molecule-to-electrode coupling limit, all the resonances get substantial widths, which emphasize that the electron conduction takes place almost for all energy values. Such an enhancement of the resonance widths is due to the broadening of the

$$g - E$$

with $E$ being the energy of the molecular levels, as shown in Fig. 4.

![Fig. 4](image)

**Fig. 4:** $g - E$ characteristics of the molecular wires in the cis configuration, where (a), (b), (c) and (d) correspond to the wires with benzene, naphthalene, anthracene and tetracene molecules respectively. The solid and dotted curves represent the results in the weak and strong molecule-to-electrodes coupling limits respectively.

molecular energy levels in the limit of strong molecular coupling, where the contribution comes from the imaginary parts of the self-energies $\Sigma_s$ and $\Sigma_d$[56] as mentioned earlier in the previous section.

To illustrate the quantum interference effects on electron transport, in Fig. 4, we plot the conductance-energy $(g - E)$ characteristics for the molecular wires where the molecules are attached

$$I - V$$

with $V$ being the voltage, as shown in Fig. 5.

![Fig. 5](image)

**Fig. 5:** $I - V$ characteristics of the molecular wires in the trans configuration, where the solid, dotted, dashed and dot-dashed curves correspond to the results for the wires with benzene,
napthalene, anthracene and tetracene molecules respectively. (a) weak-coupling limit and (b) strong-coupling limit.

to the electrodes in the cis configuration. Figures 4(a), (b), (c) and (d) correspond to the results of the wires with benzene, napthalene, anthracene and tetracene molecules respectively. The solid and dotted lines indicate the same meaning as in Fig. 3. These results predict that, some of the conductance peaks do not reach to unity anymore, and get much reduced value. This behavior can be understood in this way. During the motion of the electrons from the source to the drain through the molecules, the electron waves propagating along the different possible pathways can get a phase shift among themselves according to the result of quantum interference. Therefore, the probability amplitude of getting the electron across the molecules either becomes strengthened or weakened. This causes the transmittance cancellations and provides anti-resonances in the conductance spectrum. Thus it can be emphasized that the electron transmission is strongly affected by the quantum interference effects and hence the molecule to electrodes interface structures.

The scenario of the electron transfer through the molecular junction becomes much more clearly visible by investigating the current-voltage \( I-V \) characteristics. The current through the molecular

![Image](https://example.com/image.png)

Fig. 6: \( I-V \) characteristics of the molecular wires in the cis configuration, where the solid, dotted, dashed and dot-dashed curves correspond to the results for the wires with benzene, napthalene, anthracene and tetracene molecules respectively. (a) weak-coupling limit and (b) strong-coupling limit.

systems can be computed by the integration procedure of the transmission function \( T \) (see Eq. 8), where the function \( T \) varies exactly similar to the conductance spectra, differ only in magnitude by the factor 2, since the relation \( g = 2T \) holds from the Landauer conductance formula (Eq. 1). To reveal this fact, in Fig. 5 we plot the current-voltage characteristics for the molecular wires in which the molecules attached to the electrodes in the trans configuration. Figures 5(a) and (b) correspond to results for the weak- and strong-coupling limits respectively. The solid, dotted, dashed and dot-dashed curves represent the variations of the currents with the bias voltage \( V \) for the molecular wires consisting with benzene, napthalene, anthracene and tetracene molecules respectively. In the weak molecular coupling, the current exhibits staircase-like structure with fine steps as a function of the applied bias voltage. This is due to the existence of the sharp resonance peaks in the conductance spectra in this limit of coupling, since the current is computed by the integration method of the transmission function \( T \). With the increase of the applied bias voltage, the electrochemical potentials on the electrodes are shifted gradually, and finally cross one of the
quantized energy levels of the molecule. Therefore, a current channel is opened up and the current-voltage characteristic curve provides a jump. The other important feature is that the threshold bias voltage of the electron conduction across the wire significantly depends on the length of the wire in this weak-coupling limit. On the other hand, for the strong molecular coupling, the current varies almost continuously with the applied bias voltage and achieves much large amplitude than the weak-coupling case. This is because the resonance peaks get broadened due to the broadening of the energy levels in the strong-coupling limit which provide much larger current amplitude as we integrate the transmission function $T$ to get the current. Thus by tuning the molecule-to-electrode coupling, one can achieve very high current from the very low one. For this strong-coupling limit, the electron starts to conduct as long as the bias voltage is applied, in contrary to that of the weak-coupling case, for all these molecular wires. Thus we can say that, for this strong molecular coupling limit, the threshold bias voltage of the electron conduction is almost independent of the length of the molecular wire.

The effects of the quantum interference on electron transport can be much more clearly understood from the current-voltage characteristics plotted in Fig. 6. In this case, the molecular wires are attached to the electrodes in the cis configuration, where Figs. 6(a) and (b) correspond to the results for the weak- and strong-coupling limits respectively. The solid, dotted, dashed and dot-dashed curves represent the same meaning as in Fig. 5. Our results show that, for these wires the current amplitudes get reduced enormously compared to the results obtained for the wires when the molecules are attached with the electrodes in the trans configuration. This is solely due to the quantum interference effects among all the possible pathways that the electron can take. Therefore, we can predict that designing a molecular device is significantly influenced by the quantum interference effects i.e., the molecule to electrodes interface structures.

In conclusion of this section, we have introduced a parametric approach based on the tight-binding model to investigate the electron transport properties in some polycyclic hydrocarbon molecules attached to two semi-infinite one-dimensional metallic electrodes. This technique may be utilized to study the electronic transport in any complicated molecular bridge system. The conduction of electron through the hydrocarbon molecules is strongly influenced by the molecule-to-electrode coupling strength, length of the molecule, and the quantum interference effects. This study reveals that designing a whole system that includes not only the molecule but also the molecule-to-electrode coupling and the interface structures are highly important in fabricating molecular electronic devices.

4. Quantum Transport in a Thin Film

Here we explore a novel feature of electron transport in a unconventional disordered thin film where disorder strength varies smoothly from its surface. In the present age of nanoscience and technology, it becomes quite easy to fabricate a nano-scale device where charge carriers are scattered mainly from its surface boundaries [59-68], and not from the inner core region. It is completely opposite to that of a traditional doped system where the dopant atoms are distributed uniformly along the system. For example, in shell-doped nanowires the dopant atoms are spatially confined within a few atomic layers in the shell region of a nanowire. In such a shell-doped nanowire, Zhong and Stocks [60] have shown that the electron dynamics undergoes a localization to quasi-delocalization transition beyond some critical doping. In other very recent work [62], Yang et al. have also observed such a transition in edge disordered graphene nanoribbons upon varying the strength of edge disorder. From extensive studies of electron transport in such unconventional systems, it has been suggested that the surface states [69], surface scattering [70] and the surface reconstructions [71] may be responsible to exhibit several diverse transport properties. Motivated with these systems, here we focus our study of electron transport in a special type of thin film, in which disorder strength varies smoothly from layer to layer with the distance from its surface. This system shows a peculiar behavior of electron transport where the current amplitude increases with
the increase of the disorder strength in the limit of strong disorder, while it decreases in the weak disorder limit. On the other hand, for the traditional disordered thin film i.e., the film subjected to uniform disorder, the current amplitude always decreases with the increase of the disorder strength.

4.1. Model

Let us refer to Fig. 7, where a thin film is attached to two metallic electrodes, viz, source and drain. In this film, disorder strength varies smoothly from the top most disordered layer (solid line) towards the bottom layer, keeping the lowest bottom layer (dashed line) as disorder free. The electrodes are symmetrically attached at the two extreme corners of the bottom layer. Both this film and the two side attached electrodes are described by the similar kind of tight-binding Hamiltonian as prescribed in Eq. 5. Now to achieve our required unconventional thin film, we choose the site energies ($\varepsilon_i$'s in Eq. 5) randomly from a “Box” distribution function such that the top most front layer becomes the highest disordered layer with strength $W$, and the strength of disorder decreases smoothly towards the bottom layer as a function of $W/(N_l - m)$, where $N_l$ gives the total number of layers and $m$ represents the total number of ordered layers from the bottom side of the film. On the other hand, in the conventional disordered thin film, all the layers are subjected to the same disorder strength $W$. Here, we concentrate our study on the determination of the typical current amplitude which is obtained from the relation,

$$I_{op} = \sqrt{\langle I^2 \rangle_{W,V}}$$

where $W$ and $V$ correspond to the impurity strength and the applied bias voltage respectively.

4.2. Results and Discussion

All the numerical calculations we present here are performed for some particular values of the different parameters, and all the basic features remain also invariant for some the other parametric values. The values of the required parameters are as follows. The coupling strengths of the film to the electrodes are taken as $\tau_s = \tau_d = 1.5$, the nearest-neighbor hopping integral in the film is fixed to $t = 1$. The on-site potential and the hopping integral in the electrodes are set as $\varepsilon_0 = 0$ and $t_0 = 2$ respectively. In addition to these, here we also introduce another three parameters $N_x$, $N_y$ and $N_z$ to specify the system size of the thin film, where they correspond to the total number of lattice sites.
along the $x$, $y$ and $z$ directions of the film respectively. In our numerical calculations, the typical current amplitude ($I_{typ}$) is determined by taking the average over the disordered configurations and bias voltages (see Eq. 9). Since in this particular model the site energies are chosen randomly, we compute $I_{typ}$ by taking the average over a large number (60) of disordered configurations in each case to get much accurate result. On the other hand, for the averaging over the bias voltage $V$, we set the range of it from -10 to 10. In this presentation, we focus only on the systems with small sizes since all the qualitative behaviors remain also invariant even for the large systems. Figure 8 represents the variation of the typical current amplitude ($I_{typ}$) as a function of disorder ($W$) for some typical thin films with $N_x=10$, $N_y=8$ and $N_z=5$. Here we set $m=1$, i.e., only the lowest bottom layer of the unconventional disordered thin film is free from any disorder. The solid and dotted curves correspond to the results of the smoothly varying and complete disordered thin films respectively. A remarkably different behavior is observed for the smoothly varying disordered film compared to the film with complete disorder. In the later system, it is observed that $I_{typ}$ decreases rapidly with $W$ and eventually it drops to zero for the higher value of $W$. This reduction of the current is due to the fact that the eigenstates become more localized [72] with the increase of disorder, and it is well established from the theory of Anderson localization [73]. The appreciable change in the variation of the typical current amplitude takes place only for the unconventional disordered film. In this case, the current amplitude decreases initially with $W$ and after reaching to a minimum at $W=W_c$ (say), it again increases. Thus the anomalous behavior is observed beyond the critical disorder strength $W_c$, and we are interested particularly in this regime where $W > W_c$. In order to illustrate this peculiar behavior, we consider the smoothly varying disordered film as a coupled system combining two sub-systems. The coupling exists between the lowest bottom ordered layer and the other disordered layers. Thus the system can be treated, in other way, as a coupled order-disorder separated thin film. For this coupled system we can write the Schrodinger equations as: $(H_o - H_1)\psi_o = E\psi_o$ and $(H_d - H_2)\psi_d = E\psi_d$. Here $H_o$ and $H_d$ represent the sub-Hamiltonians of the ordered and disordered regions of the film respectively, and $\psi_o$ and $\psi_d$ are the corresponding eigenfunctions. The terms $H_1$ and $H_2$ in the above two expressions are the most significant and they can be expressed as: $H_1 = H_{od}(H_d - E)^{-1}H_{do}$ and $H_2 = H_{do}(H_d - E)^{-1}H_{od}$. $H_{od}$ and $H_{do}$ correspond to the coupling between the ordered region and the disordered region [60-61]. From these mathematical expressions, the anomalous behavior of the electron transport in the film can be described clearly. In the absence of any interaction between the ordered and disordered regions, we can assume the full system as a simple combination of two independent sub-systems.

Fig. 8: $I_{typ}$ vs. $W$ for the two different types of thin films with $N_x=10$, $N_y=8$ and $N_z=5$. Here we set $m=1$. The solid and dotted curves correspond to the smoothly varying and complete disordered films respectively.
Therefore, we get all the extended states in the ordered region, while the localized states are obtained in the disordered region. In this situation, the motion of an electron in any one region is not affected by the other. But for the coupled system, the motion of the electron is no more independent, and we have to take the combined effects coming from both the two regions. With the increase of disorder, the scattering effect becomes dominated more, and thus the reduction of the current is expected. This scattering is due to the existence of the localized eigenstates in the disordered regions. Therefore, in the case of strong coupling between the two sub-systems, the motion of the electron in the ordered region is significantly influenced by the disordered regions. Now the degree of this coupling between the two sub-systems solely depends on the two parameters $H_1$ and $H_2$, those are expressed earlier. In the limit of weak disorder, the scattering effect from both the two regions is quite significant since then the terms $H_1$ and $H_2$ have reasonably high values. With the increase of disorder, $H_1$ decreases gradually and for a very large value of $W$ it becomes very small. Hence the term $(H_o - H_1)$ effectively goes to $H_o$ in the limit $W \to 0$, which indicates that the ordered region becomes decoupled from the disordered one. Therefore, in the higher disorder regime the scattering effect becomes less significant from the ordered region, and it decreases with $W$. For the low regime of $W$, the eigenstates of both the two effective Hamiltonians, $(H_o - H_1)$ and $(H_d - H_2)$, are localized. With the increase of $W$, $H_1$ gradually decreases, resulting in much weaker localization in the states of $(H_o - H_1)$, while the states of $(H_d - H_2)$ become more localized. At a critical value of $W = W_c$ (say) ($\approx$ band width of $H_o$), we get a separation between the much weaker localized states and the strongly localized states. Beyond this value, the weaker localized states become more extended and the strongly localized states become more localized with the increase of $W$. In this situation, the current is obtained mainly from these nearly extended states which provide the larger current with $W$ in the higher disorder regime.

To illustrate the size dependence of the film on the electron transport, in Fig. 9 we plot the variation of the typical current amplitude for some typical thin films with $N_x = 12$, $N_y = 10$ and $N_z = 6$. For these films we take $m = 2$, i.e., two layers from the bottom side of the smoothly varying disordered film are free from any disorder. The solid and dotted curves correspond to the identical meaning as in Fig. 8. For both the unconventional and traditional disordered films, we get almost the similar behavior of the current as described in Fig. 8. This study shows that the typical current amplitude strongly depends on the finite size of the thin film.

In summary of this section, we have provided a numerical study to exhibit the anomalous behavior of electron transport in a unconventional disordered thin film, where the disorder strength varies smoothly from its surface. Our numerical results have predicted that, in the smoothly varying disordered film, the typical current amplitude decreases with $W$ in the weak disorder regime.
($W < W'_c$), while it increases in the strong disorder regime ($W > W'_c$). On the other hand for the conventional disordered film, the current amplitude always decreases with disorder. In this present investigations, we have also studied the finite size effects which reveal that the typical current amplitude strongly depends on the size of the film. Similar type of anomalous quantum transport can also be observed in lower dimensional systems like, edge disordered graphene sheets of single-atom-thick, surface disordered finite width rings, nanowires, etc.

5. Concluding Remarks

In this dissertation, we have demonstrated the quantum transport properties in different types of bridge systems like, molecular wires and thin films. The physics of electron transport through these nanoscale systems is surprisingly rich. Many fundamental experimentally observed phenomena in such systems can be understood by using simple arguments. In particular, the formal relation between conductance and transmission coefficients (the Landauer formula) has enhanced the understanding of electronic transport in the bridge system. We have investigated the electron transport properties of some molecular bridge systems and unconventional disordered thin films within the tight-binding framework using Green's function technique and tried to explain how electron transport is affected by the quantum interference of the electronic wave functions, molecule-to-electrode coupling strengths, length of the molecular wire and disorder strength. Our model calculations provide a physical insight to the behavior of electron conduction in these bridge systems.

First, we have studied the electron transport in some molecular wires consisting with some polycyclic hydrocarbon molecules. Most interestingly, it has been observed that the transport properties are significantly influenced by the molecular coupling strength to the side attached electrodes, quantum interference effects and length of the molecule. Our study has emphasized that the molecule to electrodes interface structures are highly important in fabricating molecular electronic devices. Secondly, we have investigated the electron transport in a unconventional disordered thin film. Most remarkably, we have noticed that the typical current amplitude increases with the disorder strength in the strong disorder regime, while it decreases with the strength of disorder in the weak disorder regime. This particular study has suggested that the carrier transport in an order-disorder separated mesoscopic device may be tailored to desired properties through doping for different applications.

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