Multi-terminal quantum transport through a single benzene molecule: Evidence of a Molecular Transistor

Santanu K. Maiti\textsuperscript{1,2}

\textsuperscript{1}Theoretical Condensed Matter Physics Division, Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata-700 064, India
\textsuperscript{2}Department of Physics, Narasinha Dutt College, 129 Belilious Road, Howrah-711 101, India

We explore multi-terminal quantum transport through a benzene molecule threaded by an Aharonov-Bohm flux $\phi$. A simple tight-binding model is used to describe the system and all the calculations are done based on the Green’s function formalism. With a brief description of two-terminal quantum transport, we present a detailed study of three-terminal transport properties through the benzene molecule to reveal the actual mechanism of electron transport. Here we numerically compute the multi-terminal conductances, reflection probabilities and current-voltage characteristics in the aspects of molecular coupling strength and magnetic flux $\phi$. Most significantly we observe that, the molecular system where the benzene molecule is attached to three terminals can be operated as a transistor, and we call it a molecular transistor. This aspect can be utilized in designing nanoelectronic circuits and our investigation may provide a basic framework to study electron transport in any complicated multi-terminal quantum system.

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I. INTRODUCTION

The rapid development in nanofabrication techniques have enabled us to measure current through molecular wires, even through a single isolated molecule attached to two measuring electrodes. Electronic transport through molecular systems have attracted much more attention since these are the fundamental building blocks for future generation of electronic devices. In 1974, Aviram and Ratner\textsuperscript{[1]} first studied theoretically the electron transport through a molecular bridge. In their work they have calculated two-terminal conductance based on the Landauer conductance formula\textsuperscript{[2]}. Following this pioneering work, several experiments have been done through different molecules placed between two electrodes with few nanometer separation. Though, to date a lot of theoretical\textsuperscript{[3, 4, 5, 6, 7, 8, 9]} as well as experimental works\textsuperscript{[10, 11, 12, 13]} on two-terminal electron transport have been done addressing several important issues, but a very few works are available on multi-terminal quantum systems\textsuperscript{[14, 15, 16, 17, 18, 19, 20, 21]} and still it is an open subject to us. Büttiker\textsuperscript{[22]} first addressed theoretically the electron transport in multi-terminal quantum systems following the theory of Landauer two-terminal conductance formula. Full quantum mechanical approach is needed to study electron transport in molecular systems. The transport properties are characterized by several significant factors like as the quantization of energy levels, quantum interference of electronic waves associated with the geometry of the bridging system adopts within the junction and other different parameters of the Hamiltonian that are used to describe a complete system.

Several \textit{ab initio} methods are used to study electron transport\textsuperscript{[23, 24, 25, 26, 27, 28]} through molecular systems. At the same time, tight-binding model has extensively been studied in the literature and it has also been extended to DFT transport calculations\textsuperscript{[29, 30, 31]}. The study of static density functional theory (DFT)\textsuperscript{[32]} 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 larger values compared to the experimental predictions and these quantitative discrepancies need detailed study in this particular field. In a recent work, Sai et al.\textsuperscript{[32]} have predicted a correction to the conductance using the time-dependent current-density functional theory since the dynamical effects give significant contribution to the electron transport, and demonstrated some key results with specific examples. Quite similar dynamical effects have also been reported in some other recent papers\textsuperscript{[33, 34]}, 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 the present paper, we reproduce an analytic approach based on a simple tight-binding model to characterize the electron transport properties through a benzene molecule placed between the macroscopic contacts. A simple parametric approach\textsuperscript{[35, 36, 37, 38, 39, 40, 41, 42]} is presented for the calculations and it is 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 worth insight to the problem.

The aim of this work is to describe multi-terminal electron transport through a single benzene molecule threaded by an Aharonov-Bohm (AB) flux $\phi$. We do exact numerical calculation based on the Green’s function formalism to reveal the actual mechanism of electron transport. With a very brief description of electron transport in two-terminal system, we express elabo-
rately the three-terminal transport properties of the benzene molecule. Here we numerically compute the conductances, reflection probabilities and current-voltage characteristics as functions of the molecule-to-lead coupling strength and threaded magnetic flux $\phi$. Most interestingly we predict that the benzene molecule attached to three leads can be used as a transistor, and we can call it as a molecular transistor. These three leads are quite analogous to emitter, base and collector as defined in conventional transistor.

The scheme of the paper is as follow. With the brief introduction (Section I), in Section II, we describe the model and the theoretical formulations for our calculations. Section III presents the significant results, and finally, we conclude our results in Section IV.

II. MODEL AND THE SYNOPSIS OF THE THEORETICAL BACKGROUND

A. Two-terminal molecular system

Let us start by referring to Fig. 1 where a benzene molecule, threaded by a magnetic flux $\phi$, is attached symmetrically to two semi-infinite one-dimensional (1D) metallic leads, viz, lead-1 and lead-2.

To calculate two-terminal conductance ($g$) of the benzene molecule, we use the Landauer conductance formula $[43, 44]$. At much low temperatures and bias voltage it can be expressed as,

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

where, $T$ gives the transmission probability of an electron across the molecule and it is related to the reflection probability $R$ by the expression $R = 1 - T$. In terms of the Green’s function of the molecule and its coupling to the leads, the transmission probability can be written in the form $[43, 44]$,

$$T = \text{Tr}[\Gamma_1G_M^r\Gamma_2G_M^a]$$

where, $\Gamma_1$ and $\Gamma_2$ describe the coupling of the molecule to the lead-1 and lead-2, respectively. Here, $G_M^r$ and $G_M^a$ are the retarded and advanced Green’s functions, respectively, of the molecule including the effects of the leads. Now, for the full system i.e., the molecule and two leads, the Green’s function is expressed as,

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

where, $E$ is the energy of the injecting electron. Evaluation of this Green’s function needs the inversion of an infinite matrix, which is really a difficult task, since the full system consists of the finite size molecule and the two semi-infinite 1D leads. However, the full system can be partitioned into sub-matrices corresponding to the individual sub-systems and the Green’s function for the molecule can be effectively written in the form $[43, 44]$,

$$G_M = (E - H_M - \Sigma_1 - \Sigma_2)^{-1}$$

where, $H_M$ corresponds to the Hamiltonian of the benzene molecule. Within the non-interacting picture, the Hamiltonian of the molecule can be expressed like,

$$H_M = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{<ij>} t \left( c_i^\dagger c_j e^{i\theta} + c_j^\dagger c_i e^{-i\theta} \right)$$

Here, $\epsilon_i$ and $t$ correspond to the site energy and nearest-neighbor hopping strength, respectively. $c_i^\dagger$ ($c_i$) is the creation (annihilation) operator of an electron at the site $i$ and $\theta = \pi\phi/3\phi_0$ is the phase factor due to the flux $\phi$ enclosed by the molecular ring. A similar kind of tight-binding Hamiltonian is also used, except the phase factor $\theta$, to describe the leads where the Hamiltonian is parametrized by constant on-site potential $\epsilon'$ and nearest-neighbor hopping integral $t'$. The hopping integral between the lead-1 and the molecule is $\tau_1$, while it is $\tau_2$ between the molecule and the lead-2. In Eq. (4), $\Sigma_1$ and $\Sigma_2$ are the self-energies due to the coupling of the molecule to the lead-1 and lead-2, respectively, where all the information of the coupling are included into these self-energies.

The current passing through the molecule can be regarded as a single electron scattering process between the two reservoirs of charge carriers. The current-voltage relationship can be obtained from the expression $[43, 44]$,

$$I(V) = \frac{e}{\pi\hbar} \int_{-\infty}^{\infty} (f_1 - f_2) T(E) \, dE$$

where, $f_{1(2)} = f(E - \mu_{1(2)})$ gives the Fermi distribution function with the electrochemical potential $\mu_{1(2)} = E_F \pm eV/2$. $E_F$ is the equilibrium Fermi energy. Usually, the electric field inside the molecule, especially for small molecules, seems to have a minimal effect on the $g$-$E$ characteristics. Thus it introduces a very little error if we assume that the entire voltage is dropped across the molecule-lead interfaces. On the other hand, for larger molecules and higher bias voltage, the electric field inside the molecule may play a more significant role depending on the size and structure of the molecule $[45]$, though the effect becomes quite small.

![FIG. 1: (Color online). Two-terminal quantum system where a benzene molecule, threaded by a magnetic flux $\phi$, is attached symmetrically to two semi-infinite one-dimensional metallic leads, viz, lead-1 and lead-2.](image-url)
B. Three-terminal molecular system

The schematic view of a three-terminal quantum system is presented in Fig. 2, where a benzene molecule is attached to three semi-infinite leads, viz, lead-1, lead-2 and lead-3. These leads are coupled to the molecule asymmetrically i.e., the path differences between them are not identical to each other and they (three leads) are quite analogous to the emitter, base and collector as defined in traditional macroscopic transistor. The actual scheme of connections with the batteries for the operation of the molecule as a transistor is depicted in Fig. 3, where the voltages in the lead-1 and lead-2 are applied with respect to the lead-3.

In order to calculate the conductance in this three-terminal quantum system, we use Büttiker formalism, an elegant and simple way to study electron transport through multi-terminal mesoscopic systems. In this formalism we treat all the leads (current and voltage leads) on an equal footing and extend the two-terminal linear response formula to get the conductance between the terminals, indexed by $p$ and $q$, in the form \[ g_{pq} = \frac{2e^2}{h} T_{pq} \] where $T_{pq}$ gives the transmission probability of an electron from the lead-$p$ to lead-$q$. Here, the reflection probabilities are related to the transmission probabilities by the equation $R_{pp} + \sum_{q \neq p} T_{qp} = 1$, which is obtained from the condition of current conservation \[43\]. Now, similar to Eq. (2), the transmission probability $T_{pq}$ can be expressed in terms of the molecule-lead coupling matrices and the effective Green’s function of the molecule as \[43\],

\[
T_{pq} = \text{Tr} \left[ \Gamma_p G_M^r \Gamma_q G_M^a \right]
\] (8)

In the presence of multi leads, the effective Green’s function of the molecule becomes (extension of Eq. (1) \[43\]),

\[
G_M = \left( E - H_M - \sum_p \Sigma_p \right)^{-1}
\] (9)

where, $\Sigma_p$ is the self-energy due to the coupling of the molecule to the lead-$p$ and the sum over $p$ runs from 1 to 3. $H_M$ is the molecular Hamiltonian (see Eq. (5)).

Finally, as an extension of two-terminal devices, we can write the current $I_p$ for the lead-$p$ in the form \[43\],

\[
I_p(V) = \frac{e}{\pi \hbar} \sum_{q} \int_{-\infty}^{\infty} T_{pq}(E) \left[ f_p(E) - f_q(E) \right] dE
\] (10)

In this presentation, all the results are computed only at absolute zero temperature. These results are also valid even for some finite (low) temperatures, since the broadening of the energy levels of the benzene molecule due to its coupling to the leads becomes much larger than that of the thermal broadening \[43\]. On the other hand, at high temperature limit, all these features completely disappear. This is due to the fact that the phase coherence length decreases significantly with the rise of temperature where the contribution comes mainly from the scattering on phonons, and therefore, the quantum interference effect vanishes. For the sake of simplicity, we take the unit $c = e = h = 1$ in our present calculations.
III. RESULTS AND DISCUSSION

To illustrate the results, let us begin our discussion by mentioning the values of the different parameters used for the numerical calculations. In the benzene molecule, the on-site energy $\epsilon_i$ is fixed to 0 for all the sites $i$ and the nearest-neighbor hopping strength $t$ is set to 3. While, for the side-attached leads the on-site energy ($\epsilon'$) and the nearest-neighbor hopping strength ($t'$) are chosen as 0 and 4, respectively. The Fermi energy $E_F$ is taken as 0.

Throughout the study, we narrate our results for the two limiting cases depending on the strength of the coupling of the molecule to the leads. Case I: $\tau_{1(2,3)} << t$. It is the so-called weak-coupling limit. For this regime we choose $\tau_1 = \tau_2 = \tau_3 = 0.5$. Case II: $\tau_{1(2,3)} \sim t$. This is the so-called strong-coupling limit. In this particular limit, we set the values of the parameters as $\tau_1 = \tau_2 = \tau_3 = 2.5$.

In the forthcoming sub-sections we will describe the characteristic properties of electron transport both for the two- and three-terminal molecular systems and our exact study may give some significant insight to the electron transport in any multi-terminal quantum system.

A. Two-terminal molecular system

1. Conductance-energy characteristics

As illustrative examples, in Fig. 4 we present the variation of two-terminal conductance $g$ and reflection probability $R$ as a function of the injecting electron energy $E$. The results for the weak-coupling limit are shown in (a) and (b), while (c) and (d), correspond to the variation for the limit of strong molecular coupling. The flux $\phi$ is fixed at 0. In the limit of weak-coupling, conductance exhibits sharp resonant peaks (Fig. 4(a)) for some particular energies, while it vanishes almost for all other energies. It emphasizes that a fine tuning in the energy scale is necessary to get electron conduction across the molecule. At the resonances, the conductance reaches the value 2, and therefore, the transmission probability $T$ goes to unity, since the relation $g = 2T$ is satisfied from the Landauer conductance formula (see Eq. 1 with $e = h = 1$ in our present description). All these resonant peaks are associated with the energy eigenvalues of the benzene molecule, and hence, we can predict that the conductance spectrum manifests itself the electronic structure of the molecule. Following this conductance spectrum, the variation of the reflection probability ($R$) (Fig. 4(b)) can be clearly explained. It shows sharp dips ($R = 0$) for some fixed energies where the conductance gets the value 2. At these resonant energies $T = 1$ which provides $R = 0$, since for the two-terminal quantum system $R$ is related to the transmission probability $T$ by the equation $R = 1 - T$. For all other energies $R$ becomes 1, which reveals that for these cases no electron conduction takes place through the molecule. The behavior of electron transport becomes quite interesting as long as the molecular coupling is increased. In the strong-coupling limit, all the resonant peaks get substantial widths (Fig. 4(c)) compared to the weak-coupling limit. The contribution to the broadening of the resonant peaks appears from the imaginary parts of the self-energies $\Sigma_1$ and $\Sigma_2$, respectively [43]. From the conductance spectrum it is observed that the electron conduction through the molecular bridge takes place almost for all energies, and therefore, in the strong molecular coupling, fine tuning in the energy scale is not required to get electron conduction across the molecule. A similar effect of the molecular coupling is also observed in the $R$-$E$ spectrum (Fig. 4(d)). It is noticed that almost for the entire energy range the reflection probability does not reach to unity anymore, which allows electron transmission, and, specifically for the four typical energies, it ($R$) drops exactly to zero which indicates ballistic transmission through the molecular wire.

2. Effects of magnetic flux $\phi$

To visualize the effects of magnetic flux $\phi$ on electron transport, in Fig. 5 we display the variation of two-terminal conductance (reddish yellow line) and reflection probability (blue line) as a function of $\phi$. The results are computed for the typical energy $E = 0$ in the limit of strong molecular coupling. Both the conductance and reflection probability vary periodically with $\phi$ showing $\phi_0 (= 1$, in our chosen unit) flux-quantum periodicity. In the presence of magnetic flux, the $g$-$E$ spectrum gets modified significantly due to the additional phase shift among the electronic waves traversing through different arms of the molecular ring and one can control the ele-
tron transmission through the molecular wire in a meaningful way. Most significantly we see that, for the typical flux $\phi = \phi_0/2$, the conductance exactly vanishes, and therefore $R$ becomes 1, which reveals zero transmission. This feature can be implemented as follow. The probability amplitude of getting an electron from the lead-1 to lead-2 across the molecular ring depends on the quantum interference of the electronic waves passing through the upper and lower arms of the ring. For the symmetrically connected molecule (lengths of the upper and lower arms of the molecular ring are identical to each other) which is threaded by a magnetic flux $\phi$, the probability amplitude of getting an electron across the molecule becomes exactly zero ($T = 0$) for the typical flux, $\phi = \phi_0/2$. This is due to the result of the quantum interference among the two waves in the two arms of the molecular ring, which can be shown through few simple mathematical steps. Thus, quantum interference effect plays a crucial role in the study of electron transport in a molecular bridge system which can be controlled by changing the lead-molecule interface geometry as well as by changing the AB flux $\phi$ passing through the molecule.

3. Current-voltage characteristics

All the basic features of electron transfer through the molecule become much more clearly visible by investigating the current-voltage characteristics. The current $I$ is determined by the integration procedure of the transmission function $T$ (see Eq. (3)), where the function $T$ varies exactly similar to the conductance spectra, differ only in magnitude by the factor 2, since the equation $g = 2T$ is satisfied from the Landauer conductance formula (Eq. (1)). As representative examples, in Fig. 5 we display the variation of current with the bias voltage $V$ for the benzene molecule considering $\phi = 0$. The result for the weak-coupling limit is shown in (a), while for the case of strong-coupling it is presented in (b). In the weak-coupling case, the current shows staircase like structure with sharp steps as a function of the applied bias voltage $V$. This is due to the presence of fine resonant peaks in the conductance spectrum (Fig. 4(a)), as the current is computed from the integration procedure of the transmission function $T$. The electrochemical potentials in the leads cross one of the molecular energy levels as we increase the bias voltage, and accordingly, it provides a jump in the current-voltage spectrum. Addition to this, it is also important to note that the non-zero value of the current appears beyond a finite value of $V$, the so-called threshold voltage $V_{th}$. The behavior of $I-V$ characteristics changes significantly in the limit of strong molecular coupling (Fig. 4(b)). The step-like feature almost disappears and the current varies quite continuously with the bias voltage $V$. Not only that, it (I) also achieves very large current amplitude compared to the weak-coupling case. This enhanced current amplitude can be noticed clearly by observing the area under the $g-E$ curve presented in Fig. 4(c). Here the non-zero value of the current is observed for very small value of the bias voltage $V$ i.e., $V_{th} \rightarrow 0$. Finally, from these $I$-$V$ spectra (Figs. 4(a) and (b)) it can be manifested that the molecule-to-lead coupling strength has a significant influence in the determination of the current amplitude as well as the threshold bias voltage $V_{th}$, which may provide several key features in designing molecular electronic devices.
B. Three-terminal molecular system

Following the above brief description of electron transport in the two-terminal molecular system, now we focus our results in detail for the three-terminal molecular system, and here we will show how such a simple system can be utilized as an electronic transistor.

1. Conductance-energy characteristics

In the three-terminal molecular system, several anomalous features are observed in the conductance-energy spectra as well as in the variation of reflection probability with the energy \( E \). As representative examples, in Fig. 7 (Color online), Three-terminal conductance \( g_{pq} \) and reflection probability \( R_{pp} \) as a function of the energy \( E \) of the benzene molecule with \( \phi = 0 \). The red and green curves correspond to the results for the weak-coupling limit, while the blue and reddish yellow lines represent the results for the limit of strong coupling.

![Conductance-energy characteristics](image)

FIG. 7: (Color online). Three-terminal conductance \( g_{pq} \) and reflection probability \( R_{pp} \) as a function of the energy \( E \) of the benzene molecule with \( \phi = 0 \). The red and green curves correspond to the results for the weak-coupling limit, while the blue and reddish yellow lines represent the results for the limit of strong coupling.

In order to describe the dependence of magnetic flux \( \phi \) on conductances and reflection probabilities, in Fig. 8 we plot the results for the three-terminal molecular system in the limit of strong-coupling. The first column corresponds to the conductance (\( g_{pq} \)), while the second column represents the results for the reflection probability (\( R_{pp} \)). All the results are done for the typical energy \( E = 0 \) and they show different complex spectra. The conductances and reflection probabilities vary periodically exhibiting \( \phi_0 (=1) \) flux-quantum periodicity. From our results we see that, at \( \phi = \phi_0/2 \), the conductances \( g_{12} (g_{21}) \) and \( g_{23} (g_{32}) \) drop exactly to zero i.e., \( T_{12} = T_{23} = 0 \). While, \( g_{13} (g_{31}) \) gets the value 2 for this typical value of \( \phi \). This vanishing transmission probability at \( \phi = \phi_0/2 \) will not always appear for the other choices of the energy \( E \) in our asymmetrically connected three-terminal molecular system. On the other hand, here it is important to note that, for our symmetrically connected two-terminal molecular system the transmission probability always vanishes for the flux \( \phi = \phi_0/2 \), since for this typical value of \( \phi \), a \( \pi \) phase shift takes place among the waves traversing through the upper and lower arms of the molecular ring which provides zero transmission amplitude.

2. Effects of magnetic flux \( \phi \)

Finally, we describe the current-voltage characteristics: Transistor operation

3. Current-voltage characteristics: Transistor operation

The current \( I_p \) passing through any lead-p is obtained by integration procedure of the transmission function \( T_{pq} \).
FIG. 8: (Color online). Three-terminal conductance $g_{pq}$ (reddish yellow) and reflection probability $R_{pp}$ (blue) in the limit of strong-coupling as a function of $\phi$ of the benzene molecule with $E = 0$.

FIG. 9: (Color online). Current $I_1$ as a function of $V_{13}$ ($= V_1 - V_3$) for constant $V_{12}$ ($= V_1 - V_2$) for the three-terminal molecular system in the limit of strong-coupling with $\phi = 0$. The red, magenta, blue and green curves correspond to $V_{12} = 0.2, 0.4, 0.6$ and 0.8, respectively.

FIG. 10: (Color online). Current $I_2$ as a function of $V_{23}$ ($= V_2 - V_3$) for constant $V_{12}$ for the three-terminal molecular system in the limit of strong-coupling with $\phi = 0$. The red, green, blue and magenta curves correspond to $I_1 = 0.09, 0.36, 0.73$ and 0.92, respectively.

FIG. 11: (Color online). Current $I_2$ as a function of $V_{23}$ for constant $I_1$ for the three-terminal molecular system in the limit of strong-coupling with $\phi = 0$. The red, green, blue and magenta curves correspond to $I_1 = 0.09, 0.36, 0.73$ and 0.92, respectively.

In the form $I_p = \sum_q g_{pq} (V_p - V_q) \equiv \sum_q g_{pq} V_{pq}$, where $V_{pq} = (V_p - V_q)$ is the voltage difference between the lead-$p$ and lead-$q$.

In Fig. 9 we plot the current $I_1$ in the lead-1 as a function of $V_{13}$ for constant $V_{12}$ in the limit of strong-molecular coupling considering $\phi = 0$. The red, magenta, blue and green curves correspond to the currents for $V_{12} = 0.2, 0.4, 0.6$ and 0.8, respectively. From the results it is observed that, for a constant voltage difference between the lead-1 and lead-2, the current $I_1$ initially rises to a large value when $V_{13}$ starts to increase from zero value, and after that, it ($I_1$) increases very slowly with the rise of $V_{13}$ and eventually saturates. On the other hand, for a constant lead-1 to lead-3 voltage difference, the current $I_1$ increases gradually as we increase $V_{12}$, which is clearly described from the four different curves in Fig. 9. Quite similar behavior is also observed in the variation of the current $I_2$ as a function of $V_{23}$ for constant $V_{12}$. The

more precise, we can write the current expression for the three-terminal molecular device where one of the terminals serves as a voltage as well as a current probe. 

In Fig. 9, we plot the current $I_1$ in the lead-1 as a function of $V_{13}$ for constant $V_{12}$ in the limit of strong-coupling considering $\phi = 0$. The red, magenta, blue and green curves correspond to $V_{12} = 0.2, 0.4, 0.6$ and 0.8, respectively. From the results it is observed that, for a constant voltage difference between the lead-1 and lead-2, the current $I_1$ initially rises to a large value when $V_{13}$ starts to increase from zero value, and after that, it ($I_1$) increases very slowly with the rise of $V_{13}$ and eventually saturates. On the other hand, for a constant lead-1 to lead-3 voltage difference, the current $I_1$ increases gradually as we increase $V_{12}$, which is clearly described from the four different curves in Fig. 9. Quite similar behavior is also observed in the variation of the current $I_2$ as a function of $V_{23}$ for constant $V_{12}$. The

results are shown in Fig. 10 where the currents are cal-
culated for the strong-coupling limit in the absence of any magnetic flux $\phi$. The red, magenta, blue and green lines represent the currents for $V_{23} = 0.4$, 0.8, 1.2 and 1.6, respectively. Comparing the results plotted in Figs. [9] and [10] it is clearly observed that the current in the lead-2 is much higher than the current available in the lead-1 for the entire voltage range. This is solely due to the effect of quantum interference among the electronic waves passing through different arms of the molecular ring, and, we can manifest that for a fixed molecular coupling, the current amplitude significantly depends on the positions of the different leads.

At the end, we illustrate the results plotted in Fig. [11] where the variation of the current $I_2$ is shown as a function of $V_{23}$ for the constant current $I_1$. The currents ($I_2$) are calculated for the strong-coupling limit considering $\phi = 0$, where the red, green, blue and magenta curves correspond to fixed $I_1 = 0.09$, 0.36, 0.73 and 0.92, respectively. For a constant $V_{23}$, current through the lead-2 increases gradually as we increase the current $I_1$ which is clearly visible from the four different curves in this figure. These current-voltage characteristics are quite analogous to a macroscopic transistor. Thus, in short, we can predict that this three-terminal molecular system can be operated as a transistor and we may call it a molecular transistor. Like a conventional macroscopic transistor, the three different terminals of the molecular transistor can be treated as emitter, base and collector. Here, the important point is that, since all these three terminals are equivalent to each other, any one of them can be considered as an emitter or base or collector. Not only that, for this molecular transistor as there is only one type of charge carrier, which is electron, the conventional biasing method is not required. These features provide several key ideas which motivate us to develop a molecular transistor rather than the traditional one.

All the above current-voltage characteristics for the three-terminal quantum system are studied only for the limit of strong molecular coupling. Exactly similar features, except the current amplitude, are also observed for the case of weak-coupling limit, and in the obvious reason here we do not plot these results once again.

**IV. CONCLUDING REMARKS**

To summarize, we have explored multi-terminal electron transport through a benzene molecule threaded by a magnetic flux $\phi$. The molecular system is described by a simple tight-binding Hamiltonian and all the calculations are done through the Green’s function approach. We have numerically calculated the conductances, reflection probabilities and current-voltage characteristics as functions of the molecular coupling strength and magnetic flux $\phi$. Following a brief description of electron transport in two-terminal molecular system, we have illustrated in detail the behavior of electron transport in three-terminal molecular system. Very interestingly we have seen that the three-terminal benzene molecule can be operated as an electronic transistor, and we call it as a molecular transistor. These three terminals are analogous to the emitter, base and collector as defined in traditional transistor. All these features of electron transport may be utilized in fabricating nano-electronic devices and our detailed investigation can provide a basic theoretical framework to characterize electron transport in any complicated multi-terminal quantum system.

Instead of a benzene molecule if we consider a small mesoscopic ring and attach it asymmetrically to three different terminals then it can also be operated as a transistor. Only the results presented here change numerically with the ring size, but all the basic features remain exactly invariant. To be more specific, it is important to note that, in real situation the experimentally achievable rings have typical diameters within the range 0.4-0.6 $\mu$m. In such a small ring, unrealistically very high magnetic fields are required to produce a quantum flux. To overcome this situation, Hod et al. have studied extensively and proposed how to construct nanometer scale devices, based on Aharonov-Bohm interferometer, those can be operated in moderate magnetic fields $[47, 48, 49, 50]$.

In the present paper we have done all the calculations by ignoring the effects of the temperature, electron-electron correlation, etc. Due to these factors, any scattering process that appears in the molecular ring would have influence on electronic phases, and, in consequences can disturb the quantum interference effects. Here we have assumed that, in our sample all these effects are too small, and accordingly, we have neglected all these factors in this particular study.

The importance of this article is mainly concerned with (i) the simplicity of the geometry and (ii) the smallness of the size.

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