Electron transport through a quantum interferometer: a theoretical study

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Abstract

In the present work, we explore the properties of electron transport through a quantum interferometer attached symmetrically to two one-dimensional semi-infinite metallic electrodes, namely the source and the drain. The interferometer is made up of two sub-rings where individual sub-rings are penetrated by the Aharonov–Bohm (AB) fluxes $\phi_1$ and $\phi_2$, respectively. We adopt a simple tight-binding framework to describe the model, and all the calculations are done based on the single-particle Green’s function formalism. Our exact numerical calculations describe two-terminal conductance and current as functions of the interferometer-to-electrode coupling strength, magnetic fluxes threaded by left and right sub-rings of the interferometer and the difference of these two fluxes. Our theoretical results reveal several interesting features of electron transport across the interferometer, and these aspects may be utilized to study electron transport in AB geometries.

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(Some figures in this article are in colour only in the electronic version.)

1. Introduction

The study of electron transport in quantum confined model systems such as quantum rings, quantum dots, arrays of quantum dots, quantum dots embedded in a quantum ring, etc, has become one of the most fascinating branches of nanoscience and technology. With the aid of present-day nanotechnological progress [1, 2], these simple looking quantum confined systems can be used to design nanodevices, especially in electronic as well as spintronic engineering. The key idea of manufacturing nanodevices is based on the concept of the quantum interference effect [3–5], and it is generally preserved throughout the sample having dimensions smaller than or comparable with the phase coherence length. Therefore, ring-type conductors or two-path devices are ideal candidates to exploit the effect of quantum interference [6]. In a ring-shaped geometry, the quantum interference effect can be controlled in several ways, and most probably, the effect can be regulated significantly by tuning the magnetic flux, the so-called Aharonov–Bohm (AB) flux [7–10], which threads the ring. This key feature motivates us to widely use quantum interference devices in mesoscopic solid-state electronic circuits [11]. Using a mesoscopic ring we can construct a quantum interferometer, and here we will show that the interferometer exhibits several exotic features of electron transport that can be utilized in designing nanoelectronic circuits. To reveal the phenomena, we make a bridge system by inserting the interferometer between two electrodes (the source and the drain), the so-called source–interferometer–drain bridge. Following the pioneering work of Aviram and Ratner [12], theoretical description of electron transport in a bridge system showed much progress. Later, many excellent experiments [13–19] were done in several bridge systems to understand the basic mechanisms underlying electron transport. Although extensive studies of electron transport have already been done both theoretically [7–10, 20–42] and experimentally [13–19], a lot of controversies are still present between the theory and experiment, and complete description of the conduction mechanism in this scale is not very well defined even today. There are several controlling factors that can significantly regulate electron transport in a conducting bridge, and all...
The coupling of the bridging material to the electrodes. The quantum interference effect [we describe the model].

Let us begin with the model presented in figure 1. A quantum interferometer with four atomic sites \((N = 4)\), where \(N\) gives the total number of atomic sites in the interferometer) is attached symmetrically to two semi-infinite one-dimensional (1D) metallic electrodes, namely the source and the drain. The atomic sites 2 and 7 of the interferometer are directly coupled to each other, and accordingly, two sub-rings, left and right, are formed. These two sub-rings are subjected to the AB fluxes \(\phi_1\) and \(\phi_2\), respectively.

Figure 1. Schematic view of a quantum interferometer with four atomic sites \((N = 4)\) attached to two semi-infinite 1D metallic electrodes.

Considering the linear transport regime, the conductance \(g\) of the interferometer can be obtained using the Landauer conductance formula [43–47]

\[
g = \frac{2e^2}{h} \cdot T,
\]

where \(T\) is the transmission probability of an electron across the interferometer. It \((T)\) can be expressed in terms of the Green’s function of the interferometer and its coupling to the side-attached electrodes by the relation [46, 47]

\[
T = \text{Tr} \left[ \Gamma_S G^r \Gamma_D G^a \right],
\]

where \(G^r\) and \(G^a\) are, respectively, the retarded and advanced Green’s functions of the interferometer including the effects of the electrodes. Here \(\Gamma_S\) and \(\Gamma_D\) describe the coupling of the interferometer to the source and the drain, respectively. For the complete system, i.e. the interferometer, source and drain, Green’s function is defined as

\[
G = (E - H)^{-1},
\]

where \(E\) is the injecting energy of the source electron. To evaluate this Green’s function, inversion of an infinite matrix is needed since the complete system consists of the finite size interferometer and 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 interferometer can be effectively written as

\[
G_1 = (E - H_1 - \Sigma_S - \Sigma_D)^{-1},
\]

where \(H_1\) is the Hamiltonian of the interferometer that can be expressed within the non-interacting picture like

\[
H_1 = \sum_j \epsilon_i c_i^j \text{c}^\dagger_i^j + \sum_{<j>} t_{ij} \left( c_i^j \text{c}^\dagger_{i-1}^j + c_i^j \text{c}^\dagger_{i+1}^j \right).
\]

In this Hamiltonian, \(\epsilon_i\) gives the on-site energy for the atomic site \(i\), where \(i\) runs from 1 to 4, \(c_i^j\) \((c_i^j)^\dagger\) is the creation (annihilation) operator of an electron at the site \(i\) and \(j\) is the hopping integral between the nearest-neighbor sites \(i\) and \(j\). For the sake of simplicity, we assume that the magnitudes of all hopping integrals \((t_{ij})\) are identical to \(t\). The phase factor \(\theta_{ij}\), associated with the hopping integral \(t_{ij}\), is due to the fluxes \(\phi_1\) and \(\phi_2\) in the two sub-rings. The phase factors \((\theta_{ij})\) are chosen as \(\theta_{12} = \theta_{23} = \theta_{34} = \theta_{41} = 2\pi \phi / 4 \phi_t\), explores the results, and finally, we conclude our study in section 4.

2. Model and synopsis of the theoretical background

In this presentation, we explore electron transport properties of a quantum interferometer based on the single-particle Green’s function formalism. The interferometer is sandwiched between two semi-infinite one-dimensional (1D) metallic electrodes, namely the source and the drain, and two sub-rings of the interferometer are subjected to the AB fluxes \(\phi_1\) and \(\phi_2\), respectively. A schematic view of the bridge system is depicted in figure 1. A simple tight-binding model is used to describe the system and all the calculations are done numerically, which illustrate conductance–energy and current–voltage \((I–V)\) characteristics as functions of the interferometer-to-electrode coupling strength, magnetic fluxes and the difference of these two fluxes. Several exotic features are observed from this study. These are: (i) semiconducting or metallic nature depending on the coupling strength of the interferometer to the side-attached electrodes, (ii) appearance of anti-resonant states [7–9] and (iii) unconventional periodic behavior of typical conductance/current as a function of the difference of two AB fluxes.

The scheme of the paper is as follows. Following the introduction (section 1), in section 2 we describe the model and theoretical formulation for the calculation. Section 3
\( \theta_{2\Delta} = 2\pi \Delta \phi / 2\phi_0 \), where \( \phi = \phi_1 + \phi_2 \), \( \Delta \phi = \phi_1 - \phi_2 \) and \( \phi_0 = ch/e \) is the elementary flux quantum. Accordingly, a minus sign is used for the phases when the electron hops in the reverse direction. For the two 1D electrodes, a similar kind of tight-binding Hamiltonian is also used, except any minus sign is used for the phases when the electron hops in the reverse direction. For the two 1D electrodes, a similar

The current passing through the interferometer 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 \( V \) by the expression [46]

\[
I(V) = \frac{e}{\pi \hbar} \int_{E_F - eV/2}^{E_F + eV/2} T(E) \, dE, \tag{6}
\]

where \( E_F \) is the equilibrium Fermi energy. Here, we assume that the entire voltage is dropped across the interferometer–electrode interfaces, and it is examined that under such an assumption the \( I-V \) characteristics do not change their qualitative features.

All the results of this paper have been determined at absolute zero temperature, but they should be valid even for some finite (low) temperatures, since the broadening of the energy levels of the interferometer due to its coupling to the electrodes becomes much larger than that of thermal broadening [46]. On the other hand, at the high temperature limit, all these phenomena 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 of phonons, and accordingly, the quantum interference effect vanishes. Our unit system is simplified by choosing \( c = e = \hbar = 1 \).

3. Numerical results and discussion

Before going into the discussion, let us first assign the values of different parameters that are used for our numerical calculation. The on-site energy \( \epsilon_i \) of the interferometer is taken as 0 for all four sites \( i \), and the nearest-neighbor hopping strength \( t \) is set as 3. On the other hand, for two side-attached 1D electrodes the on-site energy \( (\epsilon_0) \) and nearest-neighbor hopping strength \( (t_0) \) are fixed at 0 and 4, respectively. The equilibrium Fermi energy \( E_F \) is set as 0.

Throughout the analysis we present the basic features of electron transport for two distinct regimes of the electrode-to-interferometer coupling.

Case 1: Weak-coupling limit

This limit is set by the criterion \( \tau_S(D) \ll t \). In this case, we choose the values as \( \tau_S = \tau_D = 0.5 \).

Case 2: Strong-coupling limit

This limit is described by the condition \( \tau_S(D) \sim t \). In this regime we choose the values of hopping strengths as \( \tau_S = \tau_D = 2.5 \).

3.1. Interferometric geometry with four atomic \((N = 4)\) sites

3.1.1. Conductance–energy characteristics. In figure 2, we plot conductance \( g \) as a function of the injecting electron energy \( E \) for the interferometer considering \( \phi = 1 \), where (a)–(d) correspond to \( \Delta \phi = 0.2, 0.4, 0.6 \) and 0.8, respectively. The black curves represent the results for the weak-coupling limit, while the results for the strong-coupling limit are shown by the red curves. In the limit of weak-coupling, conductance shows fine resonant peaks for some particular
energies, while \( g \) drops to almost zero for all other energies. At these resonances, conductance reaches the value 2, and therefore, the transmission probability \( T \) becomes unity, since the relation \( g = 2T \) is satisfied from the Landauer conductance formula (see equation (1) with \( e = h = 1 \)). The transmission probability of getting an electron across the interferometer significantly depends on the quantum interference of electronic waves passing through the different arms of the interferometer, and accordingly, the probability amplitude becomes strengthened or weakened. Now all the resonant peaks in the conductance spectra are associated with the energy eigenvalues of the interferometer, and thus it is emphasized that the conductance spectrum reveals itself in the electronic structure of the interferometer. The situation becomes quite interesting as long as the coupling strength of the interferometer to the electrodes is increased from the weak regime to the strong one. In the strong-coupling limit, all the resonances get substantial widths compared with the weak-coupling limit. The contribution to the broadening of the resonant peaks in this strong-coupling limit comes from the imaginary parts of the self-energies \( \Sigma_S \) and \( \Sigma_D \), respectively [46]. Hence, by tuning the coupling strength from the weak to the strong regime, electronic transmission across the interferometer can be obtained for a wider range of energies, while a fine scan in the energy scale is needed to get the electron conduction across the bridge in the limit of weak coupling. These results provide an important signature in the study of \( I-V \) characteristics. Another interesting feature observed in the conductance spectra is the existence of anti-resonant states. The positions of the anti-resonance states can be clearly seen from the red curves, compared with the black curves, since the widths of these curves are too small, where they sharply drop to zero for the respective energy values associated with the different values of \( \Delta \phi \) (see figures 2(a)–(d)). Such anti-resonant states are specific to the interferometric nature of the scattering and do not occur in conventional 1D scattering problems of potential barriers [7–9]. A clear investigation shows that the positions of the anti-resonances on the energy scale are independent of the interferometer-to-electrode coupling strength. Since the widths of these anti-resonance states are too small, they do not provide any significant contribution to the \( I-V \) characteristics.

3.1.2. Typical conductance \( g_{\text{typ}} \) as a function of \( \Delta \phi \). The effect of \( \Delta \phi \), the difference between two AB fluxes \( \phi_1 \) and \( \phi_2 \), on the electron transport through the interferometer is also an important issue in the present context. To visualize it, in figure 3, we display the variation of the typical conductance (\( g_{\text{typ}} \)) as a function of \( \Delta \phi \) for the interferometer in the limit of strong coupling. Figures 3(a)–(d) correspond to the results for \( \phi = 0.2, 0.4, 0.6 \) and 0.8, respectively. The typical conductances are calculated for the fixed energy \( E = 5 \). Very interestingly, we observe that, for a fixed value of \( \phi \), typical conductance varies periodically with \( \Delta \phi \), showing \( 2\phi_0 = 2, \) since \( \phi_0 = 1 \) in our chosen unit) flux-quantum periodicity, associated with the number of atomic sites (2) in the vertical line connecting two sub-rings of the quantum interferometer. This period doubling behavior is completely different from the traditional periodic nature, since in conventional geometries

\[
\text{Figure 3. } g_{\text{typ}} \Delta \phi \text{ curves in the strong-coupling limit for the interferometer with four atomic sites (} N = 4 \text{), where (a) } \phi = 0.2, \text{ (b) } \phi = 0.4, \text{ (c) } \phi = 0.6 \text{ and (d) } \phi = 0.8. \text{ The typical conductances are calculated at energy } E = 5.}
\]

3.1.3. \( I-V \) characteristics. All these features of electron transfer become much more clearly visible when studying the \( I-V \) characteristics. The current \( I \) passing through the interferometer is computed from the integration procedure of the transmission function \( T \) as prescribed in equation (6), which is not restricted to the linear response regime, but is of great significance in determining the shape of the full \( I-V \) characteristics. As illustrative examples, in figure 4, we plot the \( I-V \) characteristics of the interferometer for three different values of \( \phi_2 \), keeping the flux \( \phi_1 \) in the left sub-ring at a fixed value 0.2. The red, blue and black curves
correspond to $\phi_2 = 0, 0.1$ and $0.4$, respectively. In the limit of weak coupling (see figure 4(a)), it is observed that the current exhibits a staircase-like structure with fine steps as a function of the applied bias voltage $V$. This is due to the existence of sharp resonant peaks in the conductance spectrum in this coupling limit, since current is computed by the integration method of the transmission function $T$. With an increase of the bias voltage $V$, the electrochemical potentials on the electrodes are shifted gradually and finally cross one of the quantized energy levels of the interferometer.

Accordingly, a current channel is opened up that provides a jump in the $I-V$ characteristic curve. The most important feature observed in the $I-V$ curves for this weak-coupling limit is that the nonzero value of the current appears beyond a finite bias voltage, the so-called threshold voltage $V_{\text{th}}$. This is quite analogous to the semiconducting nature of a material. Most interestingly, the results predict that the threshold bias voltage of electron conduction can be controlled very nicely by tuning the AB flux $\phi_2$. The situation becomes very different for the strong-coupling case. The results are given in figure 4(b). In this limit, the current varies almost continuously with the applied bias voltage and achieves a much larger amplitude than the weak-coupling case. The reason is that in the limit of strong coupling all the energy levels get broadened, which provides larger current in the integration procedure of the transmission function $T$. Thus, by tuning the strength of the interferometer-to-electrode coupling, we can achieve very large, even an order of magnitude, current amplitude from the very low one for the same bias voltage $V$, which provides an important signature in designing nanoelectronic devices. Contrary to the weak-coupling limit, here the electron starts to conduct as long as the bias voltage is given, i.e. $V_{\text{th}} \to 0$, which reveals the metallic nature. Thus, it can be emphasized that the interferometer-to-electrode coupling is a key parameter that controls the electron transport in a meaningful way. Additionally, the existence of semiconducting or metallic behavior of the interferometer also depends significantly on the AB fluxes $\phi_1$ and $\phi_2$. The nature of all these $I-V$ curves, presented in figure 4, will be exactly similar if we plot the results for different values of $\phi_1$, keeping $\phi_2$ constant.

3.1.4. Typical current amplitude $I_{\text{typ}}$ as a function of $\phi_2$. Now, we focus our attention on the variation of typical current amplitude with either of these two fluxes while the other flux is fixed. To explore this, in figure 5, we show the variation of the typical current amplitude ($I_{\text{typ}}$) with $\phi_2$, considering $\phi_1$ as a constant, where (a) and (b) correspond to $\phi_1 = 0$ and 0.3, respectively. The black and red lines represent the results for the weak- and strong-coupling limits, respectively. Typical current amplitudes are calculated for the fixed bias voltage $V = 1.02$. For both these limiting cases, the typical current amplitude varies periodically with $\phi_2$, exhibiting $\phi_0$ flux-quantum periodicity, as expected. A similar feature is also observed for the $I_{\text{typ}}$ versus $\phi_1$ curves when $\phi_2$ is kept constant. Here, it is also important to note that the variation of $I_{\text{typ}}$ with $\Delta \phi$ is quite similar to that presented in figure 3. The typical current amplitude varies periodically with $\Delta \phi$, showing $2\phi_0$ flux-quantum periodicity, following the $g_{\text{typ}}-\Delta \phi$ characteristics.

With the above description of electron transport for a four-site ($N = 4$) quantum interferometer, we can now extend our discussion to an interferometer with a higher number of atomic sites, i.e. $N > 4$. 

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**Figure 4.** $I-V$ characteristics of the interferometer with four atomic sites ($N = 4$) for a fixed value of $\phi_1 = 0.2$, where the red, blue and black curves correspond to $\phi_2 = 0, 0.1$ and $0.4$, respectively. (a) Weak-coupling limit and (b) strong-coupling limit.

**Figure 5.** $I_{\text{typ}}$ curves in the weak- (black) and strong-coupling (red) limits for the interferometer with four atomic sites ($N = 4$), where (a) $\phi_1 = 0$ and (b) $\phi_1 = 0.3$. The typical current amplitudes are calculated at bias voltage $V = 1.02$. 

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and characteristics are observed as those we saw in the case of a quantum interferometer is given in figure 4. A schematic view of such a quantum interferometer with a large number of atomic sites, compared with our presented mathematical model with here a quantum interferometer with a large number of atomic sites, where we set $N = 15$. The typical conductances are calculated at energy $E = 1.5$. From the spectra, it can be seen that for a fixed value of $\phi$, typical conductance oscillates as a function of $\Delta \phi$, exhibiting $5\phi_0$ flux-quantum periodicity. This phenomenon is completely different from the traditional periodic nature. Comparing the results presented in figures 3 and 7, it is clear that the periodicity of $g_{\text{typ}}-\Delta \phi$ curves depends on the total number of atomic sites in the vertical line connecting the left and right sub-rings of a quantum interferometer. Therefore, by changing the length of the vertical line, periodicity can be changed accordingly.

### 3.2. Interferometric geometry with $N > 4$ atomic sites

To obtain an experimentally realizable system, we consider here a quantum interferometer with a large number of atomic sites, compared with our presented mathematical model with four atomic sites. A schematic view of such a quantum interferometer is given in figure 6, where we set $N = 15$. The vertical line connecting the left and right sub-rings contains five atomic sites, where the individual sub-rings are penetrated by AB fluxes $\phi_1$ and $\phi_2$, respectively. In this interferometric geometry, the phase factors ($\theta_{ij}$’s) are chosen according to our earlier prescription. Along the circumference of the ring $\theta_{ij} = 2\pi \phi/12\phi_0$ and along the vertical line $\theta_{ij} = 2\pi \Delta \phi/5\phi_0$, where $\phi$ and $\Delta \phi$ have identical meanings as before.

For this bigger quantum interferometer ($N = 15$), closely similar features of conductance–energy and $I–V$ characteristics are observed as those we saw in the case of a four-site interferometer. Also, typical current amplitude $I_{\text{typ}}$ shows a variation with $\phi_2$ identical to our previous study. Only the typical conductance $g_{\text{typ}}$ varies in a different way as a function of $\Delta \phi$. As illustrative examples in figure 7, we plot $g_{\text{typ}}-\Delta \phi$ characteristics for the quantum interferometer with $N = 15$ in the limit of strong coupling; figures 7(a) and (b) correspond to $\phi = 0.4$ and 0.8, respectively. Typical conductances are determined at energy $E = 1.5$. From the spectra, it can be seen that for a fixed value of $\phi$, typical conductance oscillates as a function of $\Delta \phi$, exhibiting $5\phi_0$ flux-quantum periodicity. This phenomenon is completely different from the traditional periodic nature. Comparing the results presented in figures 3 and 7, it is clear that the periodicity of $g_{\text{typ}}-\Delta \phi$ curves depends on the total number of atomic sites in the vertical line connecting the left and right sub-rings of a quantum interferometer. Therefore, by changing the length of the vertical line, periodicity can be changed accordingly.

### 4. Closing remarks

To summarize, we have explored electron transport properties through a quantum interferometer using the single-particle Green’s function formalism. We have adopted a simple tight-binding framework to illustrate the bridge system, where the interferometer is sandwiched between two electrodes, namely the source and the drain. We have done exact numerical calculations to study conductance–energy and $I–V$ characteristics as functions of the interferometer-to-electrode coupling strength, magnetic fluxes $\phi_1$ and $\phi_2$ penetrated by left and right sub-rings of the interferometer and the difference of these two fluxes. Several key features of electron transport have been observed that may be useful in manufacturing nanoelectronic devices. The most exotic features are: (i) the existence of semiconducting or metallic behavior, depending on the interferometer-to-electrode coupling strength, (ii) the appearance of anti-resonant states and (iii) unconventional periodic behavior of the typical conductance/current as a function of the difference of two AB fluxes.

Throughout our work, we have addressed the essential features of electron transport through a quantum interferometer with total number of atomic sites $N = 4$. Next, we have extended our discussion to an interferometer having a higher number of atomic sites, where we have set $N = 15$ to achieve an experimentally realizable system. In our model calculations, these typical numbers ($N = 4$ and 15) are chosen...
only for the sake of simplicity. Although the results presented here change numerically with ring size \((N)\), all the basic features remain exactly the same. To be more specific, it is important to note that, in the real situation, experimentally achievable rings have typical diameters within the range \(0.4–0.6 \mu m\). In such a small ring, 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 AB interferometry—that can be operated in moderate magnetic fields [48–52].

This is our first step toward describing electron transport in a quantum interferometer. Here, we have made several realistic approximations by ignoring the effects of electron–electron correlation, electron–phonon interaction, disorder, temperature, etc. Over the last few years, researchers have studied a lot to incorporate the effect of electron–electron correlation into the study of electron transport, yet no such proper theory is well established. Thus the inclusion of electron–electron correlation in the present model is a major challenge to us. The presence of electron–phonon interaction in AB interferometers provides phase shifts of the conducting electrons and, due to this dephasing process, electron transport through an AB interferometer becomes highly sensitive to the AB flux \(\phi\) with an increase of electron–phonon coupling strength [53].

In the present work, we have addressed our results considering that the site energies of all the atomic sites of the interferometer are identical, i.e., we have treated the ordered system. But in the real case, the presence of impurities will affect the electronic structure and, hence, the transport properties. The effect of temperature has already been pointed out earlier, and it has been examined whether the presented results will not change significantly even at finite temperature, since the broadening of the energy levels of the interferometer due to its coupling to the electrodes will be much larger than that of thermal broadening [46]. In conclusion, we would like to mention that we need a further study of such systems that incorporates all these effects.

The importance of this paper mainly lies in (i) the simplicity of the geometry and (ii) the smallness of the size, and our exact analysis may be utilized to study electron transport in AB geometries.

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