Theoretical study of electronic properties for pristine and alloyed double metal rings

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Abstract. The present work is a theoretical study of the electronic properties of pristine and alloyed double metal rings threaded by magnetic flux in the presence of transverse flux. The system that takes into account in the study is consisting of two rings connected in parallel, with the same type of atomic sites for pristine double metal ring, and with two different types of atomic sites for an alloyed double metal ring. The tight-binding method was used to calculate the energy spectrum and persistent current in presence of transverse flux. Our results show that the transverse flux causes bending of the persistent current and increase in current amplitude at the pristine double metal ring, while it leads to asymmetry at alloyed double metal ring. The energy gap is not affected by the transverse flux.

1. Introduction

Over the last few decades, the phenomenon of a persistent current (PC) in mesoscopic ring systems has received much attention because it has an important role in understanding quantum coherence in such ring systems. The quantum orbital motion of electrons in ring structures threaded of a magnetic field creates quantum interference phenomena such as the Aharonov-Bohm (AB) effect and persistent currents. The PC does not decay with time and even in existence of disorder [1, 2]. Big persistent currents have many important applications in nanoelectronics such as the fabrication of a superconducting qubit [3, 4].

The seed work of the PC in a normal metal ring was first suggested by Büttiker et al. in 1983 [5] and Büttiker in 1985 [6]. The experimental basis of PC originated after few years when Levy et al. considered an ensemble of $10^7$ independent copper rings [7]. Later, several experimental studies were then carried out to demonstrate the presence of the PC in the conducting rings [8-10] and calculated energy spectrum of semiconducting rings [11]. Therefore, a lot of topical recognition have been described in new condensed matter publications. Amongst these, simple mesoscopic ring [12-16], an array of mesoscopic rings [17], mesoscopic cylinder [18-20], Möbius strip [21] and Möbius-type graphene [22]. In these studies, persistent currents have been calculated with respect to temperature [23, 24], electron–phonon interaction [25], electron correlation [26], Rashba and Dresselhaus spin-orbit interactions [27, 28] electric field [29].

The tight-binding method is the simplest quantum mechanical approximation to the electronic structure of molecules and solids. The tight-binding calculations offer an appealingly direct and clear picture of chemical bonding. In many works, the tight-binding method used to calculate the PC. Maiti studied the PC and low-field magnetic susceptibility by tight-binding method for single mesoscopic ring and cylinders [20]. Patra and Maiti investigated the PC in a quasi-periodic Fibonacci ring in presence of RSO and DSO interactions by using tight-binding method [30]. Xu et al. studied the energy spectrum and PC of triangle silicene rings (TSRs) within the tight-binding method [31].

Not only experimental measurements have contributed to the subject of PC, but also theoretical approaches. Computational studies are well-known for playing an important role in understanding physical, chemical, and biological phenomena of molecules [32]. Furthermore, in last decade it has also been possible to design noble metals in several two-dimensional and three-dimensional nanostructures.
The design of noble metals in different nanostructures prepares for understanding their electronic and structural properties, in addition to the possibility of using them in various electronic applications [35, 36].

In this work, we present an analytical method for studying the electronic properties of pristine and alloyed double metal rings exposed to an AB flux in presence of transverse flux. The electronic properties such as the energy spectrum and PC are calculated by the tight-binding Hamiltonian.

2. Theoretical model

The considered system is illustrated in Fig. 1. Alloyed double metal ring (ADMR) is subjected to Aharonov-Bohm flux, a lower ring consists of one type of atomic sites different from atomic sites in the upper ring.

Fig. 1. Alloyed double metal ring, threaded by Aharonov-Bohm flux $\Phi$ in presence of transverse flux $\Phi_t$, a lower ring consists of one type of atomic sites different from atomic sites in upper ring.

The tight binding Hamiltonian of the system is given by,

$$H = E_{up} \sum_i a_i^+ a_i + E_{lo} \sum_j b_j^+ b_j - t_{up} \sum_i \left( a_i^+ a_{i+1} e^{i(\phi_{up} + \varphi_{up})} + h.c. \right)$$

$$- t_{lo} \sum_j \left( b_j^+ b_{j+1} e^{i(\phi_{lo} - \varphi_{lo})} + h.c. \right)$$

$$- V \sum_{i \neq j} (a_i^+ b_j + b_j^+ a_i),$$

where $E_{up}$ and $E_{lo}$ are the on-site energies of upper and lower rings, respectively, $t_{up}$ and $t_{lo}$ represent nearest-neighbor hopping strengths of upper and lower rings, respectively. While $V$ represents inter-ring coupling strength. $a_i^+$ ($a_i$) and $b_j^+$ ($b_j$) represent the creation (annihilation) operators for an electron at the atomic sites in upper and lower ring, respectively. The phase factors of Aharonov-Bohm flux and transverse flux are $\phi_{\alpha} = \frac{2\pi}{N_{\alpha} \Phi_0}$ and $\varphi_{\alpha} = \frac{\pi}{N_{\alpha} \Phi_0}$, where $\alpha = up, lo$. $\Phi$ is the magnetic flux produced by magnetic field applied in the perpendicular direction at the plane of the ADMR, which called Aharonov-Bohm flux. While $\Phi_t$ is the magnetic flux presented by magnetic field applied in the radial direction, which called transverse flux. $\Phi_0 = h/e$ represents the elementary flux quantum, the number of atomic sites in each ring is $N_{\alpha}$, which will be equal in both rings ($N_{\alpha} = N_{up} = N_{lo}$).

2.1. Energy spectrum

In order to calculate the energy dispersion relation for ADMR, let us begin with Hamiltonian (1). By using Fourier transforms can be rewritten Eq. (1) in k-space,

$$H = \sum_k a_k^+ a_k (E_{up} - 2t_{up} \cos q_{up} \alpha) + \sum_k b_k^+ b_k (E_{lo} - 2t_{lo} \cos q_{lo} \alpha)$$

$$- V \sum_k (a_k^+ b_k e^{ika} + b_k^+ a_k e^{-ika}),$$

(2)
where \( q_{up}a = \frac{2\pi}{N_{up}}(n + \frac{\Phi}{\Phi_0} + \frac{1}{2}\Phi) \) and \( q_{lo}a = \frac{2\pi}{N_{lo}}(n + \frac{\Phi}{\Phi_0} - \frac{1}{2}\Phi) \). The quantized values of wavevector \( k \) are given by \( \frac{2\pi n}{Na} \), where \( a \) is the lattice spacing, \( n \) is an integer and it is restricted within the range: \( -N/2 \leq n < N/2 \) [37]. The Eq. 2 can be written as a matrix,

\[
H = \sum_k (a_k^\dagger b_k^\dagger) \begin{pmatrix} E_{up} - 2t_{up} \cos q_{up}a & -Ve^{ika} \\ -Ve^{-ika} & E_{lo} - 2t_{lo} \cos q_{lo}a \end{pmatrix} (a_k b_k)
\]

(3)

The dispersion relations of ADMR can be given by,

\[
E = \frac{(A + B) \pm \sqrt{(A - B)^2 + 4V^2}}{2}
\]

(4)

where \( A = E_{up} - 2t_{up} \cos q_{up}a \) and \( B = E_{lo} - 2t_{lo} \cos q_{lo}a \)

2.2. Persistent current

At absolute zero temperature (\( T = 0 \) K), the PC with fixed number of electrons \( N_e \) is given by

\[
I_n = -\frac{\partial E_0}{\partial \Phi}
\]

(5)

where \( E_0 \) is the ground-state energy of studied system [28]. Once we get the energy eigenvalues as a function of flux \( \Phi \), we can easily calculate PC for discrete energy eigenstates. It is simply the first order derivative of energy with respect to the flux. Therefore, for an \( n \)-th eigenstate we can write the expression for the current as,

\[
I_n = \frac{1}{2} \left( X_{up} + X_{lo} \right) \pm \frac{ \left( X_{up} - X_{lo} \right) (A - B) }{ \sqrt{(A - B)^2 + 4V^2} }
\]

(6)

Where

\[
X_{up} = t_{up} \frac{4\pi}{N_{up}\Phi_0} \sin \frac{2\pi}{N_{up}} \left( n + \frac{\Phi}{\Phi_0} + \frac{1}{2}\Phi \right)
\]

(7)

\[
X_{lo} = t_{lo} \frac{4\pi}{N_{lo}\Phi_0} \sin \frac{2\pi}{N_{lo}} \left( n + \frac{\Phi}{\Phi_0} - \frac{1}{2}\Phi \right)
\]

(8)

where, +ve or -ve sign in the current expression appears depending on the choice of \( n \) i.e., in which subband the energy level exists, with \( n = 0, \pm 1, \pm 2, ... \). At absolute zero temperature, total PC for a certain filling \( N_e \) is obtained by taking the sum of discrete contributions from the lowest \( N_e \) energy eigenstates, i.e. \( n = 0 \) for \( N_e = 1 \) and \( n = 0, \pm 1 \) for \( N_e = 3 \), and correspondingly for even \( N_e \) [37]. Therefore, the total PC can be written as,

\[
I_T = \sum_{n=1}^{N_e} I_n
\]

(9)

3. Results and discussion

All energies and coupling strengths between subsystems were measured in units of \( t_{lo} = 1 \) where \( c = e = h = 1 \). All calculations achieved for non-interacting systems of electrons.

3.1. Energy spectrum

The energy spectrum of PDMR and ADMR plotted as a function of the magnetic flux in Figs. 2-4 for different factors at zero temperature. The number of atomic sites in each ring is selected \( N_{up} = N_{lo} = 10 \), this means that the total size of ADMR is \( N = N_{up} + N_{lo} = 20 \).

The results with presence of transverse magnetic flux are presented. Firstly, the PDMR with one type of atoms is considered. The inter-ring coupling strength opens gap between the upper and lower bands with
magnitude $2V$, thus avoiding intersections at $\Phi = 0$, as presented in Fig. 2(a). The magnitude of energy gap is not affected by the transverse flux, as shown in Figs. 2(b) and 2(c) at $\Phi_t = 2$ and 3, respectively. In Fig. 3, the bottom of lower band for several values of transverse flux $\Phi_t = 1, 2, 3$ positioned at the values of AB flux $|\Phi| = 0.5, 1, 1.5$, respectively. Meaning that the transverse flux adjusts the values of allowed quasimoment by magnitude $\frac{\Phi_t}{2}$ from through relation $q = \frac{2\pi}{N} (n + \frac{\Phi}{\Phi_0} + \frac{1}{2} \frac{\Phi_t}{\Phi_0})$. The intersections at $E = -0.9, -0.6, -0.2$ depend on transverse flux at $\Phi_t = 1, 2, 3$.

Secondly, the energy spectrum of ground state ($n=0$) for ADMR with two different types of atoms ($E_{lo} = -E_{up} = 1$) is presented in Fig. 4. The energy spectrum has non-monotonously behaves. The upper and lower band do not crossing in case $\Phi_t = 1$ on all rang $\Phi$, but in case $\Phi_t > 1$ note cross two bands at certain value of $\Phi$ depending on the value of transverse flux. At $\Phi_t = 2$, the energy bands cross at $\Phi = 1.6, 3.4$ and -6.4, while the range of crossing increases of value $\Phi_t = 3$ at $\Phi = 1, 4$ and 6.

3.2. Persistent current

Firstly, we discuss the PC at $E_{lo} = E_{up} = 1$, which means that the two rings have same type of atoms. The PC as a function of magnetic flux in presence of transverse flux at $\Phi_t = 1$ for several values of inter-ring coupling strength $V = 0.2, 0.4, 0.6$ is presented in Fig. 5. The amplitude of PC increases as inter-ring coupling strength increases due to rise the probability of electron hopping from one ring to another.

The PC greatly affected by the transverse flux as shown in Fig. 6 at $V = 0.2$ for several values of $\Phi_t = 1, 2, 3$. The curvature of PC will increase by increasing $\Phi_t$. In addition to, the amplitude of PC is increase by increasing transverse flux.

Secondly, we discuss the PC at ADMR with $E_{lo} = -E_{up} = 1$, which means that the two rings have two different types of atoms. In Fig. 7, the amplitude of PC is asymmetry around $I(\Phi) = 0$ when the transverse flux $\Phi_t = 1$. Noteworthy, the periodicity of PC is shifted by order 0.5 into negative scale, therefore the periodic range from -1.5 to 0.5. In Fig. 8, the asymmetry in PC spectrum increases when the transverse flux rises. This behavior can be obviously understood from non-monotonous behavior of energy spectrum in Fig. 4.
Figure 2. Energy spectrum for ground state ($n=0$) in case PDMR at $t_{up} = t_{lo} = 1$, $E_{lo} = E_{up} = 1$, $v=0,0.2,0.4$ at (a) $\Phi_t = 1$, (b) $\Phi_t = 2$ and (c) $\Phi_t = 3$.

Figure 3. Energy spectrum for ground state ($n=0$) in case PDMR at $t_{up} = t_{lo} = 1$, $E_{lo} = E_{up} = 1$, $V=0$ at $\Phi_t = 1,2,3$.

Figure 4. Energy spectrum for ground state ($n=0$) in case ADMR at $t_{up} = t_{lo} = 1$, $E_{lo} = -E_{up} = 1$, $V=0$ at $\Phi_t = 1,2,3$. 

**Figure 5.** Persistent current as a function of magnetic flux in case PDMR with \( N=10, E_{lo} = E_{up} = 1, t_{lo} = 1, t_{up} = 1 \), transverse flux \( \Phi_t = 1 \) for several values of inter-ring coupling \( V = 0.2, 0.4, 0.6 \). The number of electrons are (a) \( N_e = 6 \) and (b) \( N_e = 7 \).

**Figure 6.** Persistent current as a function of magnetic flux in case PDMR with \( N=10, E_{lo} = E_{up} = 1, t_{lo} = 1, t_{up} = 1, \nu = 0.2 \). For several values of transverse flux \( \Phi_t = 1, 2, 3 \). The number of electrons are (a) \( N_e = 6 \) and (b) \( N_e = 7 \).

**Figure 7.** Persistent current as a function of magnetic flux in case ADMR with \( N=10, E_{lo} = -E_{up} = 1, t_{lo} = 1, t_{up} = 1 \), transverse flux \( \Phi_t = 1 \) for several values of inter-ring coupling \( V = 0.2, 0.4, 0.6 \). The number of electrons are (a) \( N_e = 6 \) and (b) \( N_e = 7 \).
Figure 8. Persistent current as a function of magnetic flux in case ADMR with N=10, $E_{lo} = -E_{up} = 1$, $t_{lo} = 1$, $t_{up} = 1$, $v = 0.2$. For several values of transverse flux $\Phi_t = 1,2,3$. The number of electrons are (a) $N_e = 6$ and (b) $N_e = 7$.

4. Summary

To summarize, the energy spectrum and PC of PDMR and ADMR were examined in dependence on the magnetic flux with presence of transverse flux. At PDMR, the inter-ring coupling strength opens gap between the upper and lower bands by $2V$, but this gap not affected by the transverse flux. The transverse flux controls the values of allowed quasimoment by $\Phi_t$. At ADMR, the energy spectrum has non-monotonously behavior. The curvature and amplitude of PC greatly affect by increasing transverse flux at PDMR. While in ADMR, the transverse flux lead to asymmetry in the PC and shift the periodicity by 0.5 towards negative direction. Therefore, these systems may be used to develop metal rings used to generate persistent currents and some nanoelectronic applications.

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