Persistent Currents in Helical Structures

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Abstract

Recent discovery of mesoscopic electronic structures, in particular the carbon nanotubes, made necessary an investigation of what effect may helical symmetry of the conductor (metal or semiconductor) have on the persistent current oscillations. We investigate persistent currents in helical structures which are non-decaying in time, not requiring a voltage bias, dissipationless stationary flow of electrons in a normal-metallic or semiconducting cylinder or circular wire of mesoscopic dimension. In the presence of magnetic flux along the toroidal helical structure, our calculations suggest that circular persistent currents in these structures have two components with periodicities of Φ_0 and Φ_0/s (s is an integer specific to any geometry), which results in a total circular persistent current oscillations with Φ_0 periodicity.

Aharonov - Bohm (AB) Effect

It is commonly believed that current in a normal (non-superconducting) metal can only flow if the voltage is applied to the sample, and that current transport is necessarily related to the Joule heat dissipation inside the sample. Aharonov and Bohm showed that contrary to the conclusion of classical electrodynamics, there exists effects of the potentials on the charged particles, even in the region where all fields vanish. This effect has quantum mechanical origin because it comes from the interference phenomenon. The well-known manifestation of the Ahoronov-Bohm effect is the periodical persistent currents in the normal metal rings and mesoscopic rings threaded by a magnetic flux.

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Persistent currents in mesoscopic rings

Persistent currents in mesoscopic systems was first predicted by one of the authors[2] [1] and later discovered by Buttiker [2] et al. If we consider a one dimensional ring of circumference $L_r = 2\pi r = N\Delta$ where N is the number of lattice points and Δ is the lattice spacing, in the presence of magnetic flux (Φ) applied at the center of the ring, we can write the Hamiltonian in tight-binding approximation as

$$H_e = -t_0 \sum_{n=1}^{N} \left(a_n^+ a_{n+1} e^{i\alpha} + h.c. \right), \tag{1}$$

where t_0 is the hopping amplitude between the nearest-neighbours for an undistorted lattice, the operators a_n (a_n^+) annihilates (creates) an electron at site n and α is the corresponding phase change which can be expressed in terms of AB flux (Φ)

$$\alpha = \frac{e}{\hbar c} \int_n^{n+1} \mathbf{A} \cdot d\mathbf{l} = 2\pi \frac{\Phi}{N\Phi_0}, \tag{2}$$

where $\Phi_0 = hc/e \simeq 4.1 \times 10^{-7}$ G cm^2 is the flux quantum.

The corresponding eigenvalue spectrum and the persistent currents (variation of free energy with the magnetic flux) are both periodic in Φ with a period of Φ_0. If we ignore spin of the electron, ground state energy and the total current flowing along the ring can be written as

$$\begin{aligned} E(\Phi) &= \sum_n \epsilon_n(\Phi) \\ &= -2t_0 \sum_n \cos\left[\frac{2\pi}{N}\left(n + \frac{\Phi}{\Phi_0}\right)\right], \quad (3) \\ I(\Phi) &= \sum_n I_n(\Phi) = -c \sum_n \frac{d\epsilon_n(\Phi)}{d\Phi} \end{aligned}$$

$$= -I_0 \sum_n \sin\left[\frac{2\pi}{N}\left(n + \frac{\Phi}{\Phi_0}\right)\right], \quad (4)$$

where $I_0 = 4c\pi t_0/N\Phi_0$ is the current amplitude, and the summation is carried out over number of electrons, N_e, for each value of flux.

Persistent Currents in Helical Structures

Existence of transverse persistent currents in double-connected mesoscopic rings, in the presence of both longitudinal and transverse flux, was shown in [3, 4]. Similarly, in this paper we considered a set of identical and connected mesoscopic rings with circumference $L_r = 2\pi r$ and each having N lattice points with lattice spacings of $\Delta_1 = L_r/N$. We also assumed our helical structure has L periods with a periodicity of N rings as in Fig. 1. So, we have a toroid of circumference $L_t = 2\pi R$ containing LN number of rings which are uniformly separated by $\Delta_2 = L_t/LN$ along the circumference of the toroid. In the presence of magnetic fluxes $\Phi(\alpha)$ and $\Phi(\beta)$, which are applied at the center of the rings and at the center of the toroid, we propose two models.

First Helical Model

In order to have helical symmetry, we allow only circular and vertical hoppings (no cross-hoppings) in and between the rings respectively. Assuming

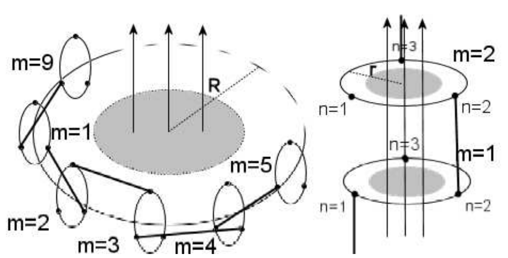

Figure 1: Left: Toroid of $LN = 3*3 = 9$ rings are connected by vertical hoppings and $\Phi(\beta)$ is applied at the center. Right: Each ring has $N = 3$ sites and $\Phi(\alpha)$ is applied at the center.

the tight-binding model for electron transport, system Hamiltonian can be written as

$$\begin{aligned} H &= -t_1 \sum_{m=1}^{LN}\sum_{n=1}^{N}\left(a^+_{mn}a_{m,n+1}e^{i\alpha} + h.c.\right) \\ &- (t_3 - t_1)\sum_{m=1}^{LN}\sum_{n=1}^{N}\left(a^+_{mn}a_{m,n+1}e^{i\alpha} + h.c.\right)\delta_{m_N,n} \\ &- t_2 \sum_{m=1}^{LN}\left(a^+_{m,m_N+1}a_{m+1,m_N+1}e^{i\beta} + h.c.\right), \end{aligned} \quad (5)$$

where t_1 is the hopping amplitude between the nearest-neighbour atoms in the ring, t_3 is the circular hopping amplitude which connects two vertical hoppings and t_2 is the vertical hopping amplitude in between the rings. The operators a_{mn} (a^+_{mn}) annihilates (creates) an electron at ring m and site n. m_N represents $m(mod\, N)$, α and β are the corresponding phase changes of lattice points in between sites in a particular ring and different rings in the toroid respectively. They can be expressed in terms of AB flux (Φ)

$$\alpha = 2\pi\frac{\Phi(\alpha)}{N\Phi_0}\ ,\ \beta = 2\pi\frac{\Phi(\beta)}{LN\Phi_0}. \quad (6)$$

System Hamiltonian can be diagonalized by discrete Fourier transformation of the operator a_{mn} as

$$a_{mn} = \frac{1}{\sqrt{LN}}\sum_{k,q} b_{qk}e^{i(kn\Delta_1 + qm\Delta_2)}, \quad (7)$$

where $k = \frac{2\pi}{N\Delta_1}n$ and $n = 0, 1, 2, ..., N-1$ and $q = \frac{2\pi}{LN\Delta_2}m$ and $m = 0, 1, 2, ..., LN-1$. In diagonal form, Hamiltonian becomes

$$\begin{aligned} H &= -2\sum_{q,k} b^+_{qk}b_{qk}\left\{t_1\cos(k\Delta_1 + \alpha)\right. \\ &+ \frac{t_3 - t_1}{N}\cos(k\Delta_1 + \alpha) \\ &+ \left.\frac{t_2}{N}\cos(q\Delta_2 + \beta)\right\}, \end{aligned} \quad (8)$$

with periodic energy spectrum in Φ with a period of Φ_0 which are given by

$$\begin{aligned} \epsilon_{mn}(\Phi) &= -2\left(t_1 + \frac{t_3 - t_1}{N}\right)\cos\left[\frac{2\pi}{N}\left(n + \frac{\Phi}{\Phi_0}\right)\right] \\ &- 2\frac{t_2}{N}\cos\left[\frac{2\pi}{LN}\left(m + \frac{\Phi(\beta)}{\Phi_0}\right)\right]. \end{aligned} \quad (9)$$

Total persistent currents along the rings (circular) and the toroid (longitudinal) are perpendicular to each other and they are also periodic in Φ with a period of Φ_0. Ignoring the spin of electrons, they are given by summation over number of electrons, N_e, for each value of flux as

$$I_{circ}(\Phi(\alpha)) = \sum_{m,n} \frac{d\epsilon_{mn}(\Phi)}{d\Phi(\alpha)}$$
$$= -I_0 \sum_{m,n} \left(t_1 + \frac{t_3 - t_1}{N}\right) \sin\left[\frac{2\pi}{N}\left(n + \frac{\Phi(\alpha)}{\Phi_0}\right)\right], \tag{10}$$

$$I_{long}(\Phi(\beta)) = -c \sum_{m,n} \frac{d\epsilon_{mn}(\Phi)}{d\Phi(\beta)}$$
$$= -I_0 \frac{t_2}{LN} \sum_{m,n} \sin\left[\frac{2\pi}{LN}\left(m + \frac{\Phi(\beta)}{\Phi_0}\right)\right], \tag{11}$$

where $I_0 = 4c\pi/N\Phi_0$ is the current amplitude.

Second Helical Model

In order to satisfy necessary boundary conditions for the geometry of the toroid (ring $(m = LN + 1)$ should coincide with ring $(m = 1)$), we fix the first ring in position and rotate rest $(LN - 1)$ of them by some angle specific to any geometry, $2\pi s/LN$, as shown on the left in Fig. 2 where s is an integer. In this model, we considered all possible circular and cross hoppings in and between the rings respectively as shown on the right in Fig. 2.

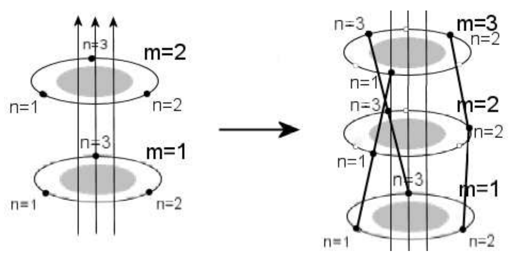

Figure 2: Left: Connected rings in the first model with $\Phi(\alpha)$ applied at the center. Right: Rotated rings by angle $2\pi s/LN$ for $s = 1$

In the tight-binding approximation, system Hamiltonian becomes

$$H = -t_1 \sum_{m=1}^{LN} \sum_{n=1}^{N} \left(a^+_{mn} a_{m,n+1} e^{i\alpha} + h.c.\right)$$
$$-t_2 \sum_{m=1}^{LN} \sum_{n=1}^{N} \left(a^+_{mn} a_{m+1,n} e^{i\beta} e^{i\frac{s\alpha}{L}} + h.c.\right), \tag{12}$$

where t_1 is the hopping amplitude between the nearest-neighbour atoms in the ring and t_2 is the cross-hopping amplitude between rings. The operators a_{mn} (a^+_{mn}) annihilates (creates) an electron at ring m and site n. α and β are the corresponding phase changes between sites in a particular ring and different rings in the toroid respectively and they are given by Eq. 6.

Similar transformation of operators as in Eq. 7 yields diagonal Hamiltonian as

$$H = -2 \sum_{q,k} b^+_{qk} b_{qk} \{t_1 \cos(k\Delta_1 + \alpha) + t_2 \cos\left(q\Delta_2 + \beta + \frac{s\alpha}{L}\right)\}, \tag{13}$$

where $k = \frac{2\pi}{N\Delta_1} n$ and $n = 0, 1, 2, ..., N-1$ and $q = \frac{2\pi}{LN\Delta_2} m$ and $m = 0, 1, 2, ..., LN-1$. Eigenvalues of this Hamiltonian are periodic in Φ with a period of Φ_0 in general and they are given by

$$\epsilon_{mn}(\Phi) = -2t_1 \cos\left[\frac{2\pi}{N}\left(n + \frac{\Phi(\alpha)}{\Phi_0}\right)\right]$$
$$-2t_2 \cos\left[\frac{2\pi}{LN}\left(m + \frac{\Phi(\beta)}{\Phi_0} + \frac{s\Phi(\alpha)}{\Phi_0}\right)\right]. \tag{14}$$

Corresponding total persistent currents along the rings and the toroid (circular α and longitudinal β currents) which have periodicity in Φ with a period of Φ_0 are perpendicular to each other and given by summation over number of electrons, N_e, for each value of flux as

$$I_{circ}(\Phi(\alpha)) = -I_0 \sum_{m,n} \left\{t_1 \sin\left[\frac{2\pi}{N}\left(n + \frac{\Phi(\alpha)}{\Phi_0}\right)\right] + t_2 \frac{s}{L} \sin\left[\frac{2\pi}{LN}\left(m + \frac{\Phi(\beta)}{\Phi_0} + \frac{s\Phi(\alpha)}{\Phi_0}\right)\right]\right\}, \tag{15}$$

$$I_{long}(\Phi(\beta)) = -I_0 t_2 \frac{s}{L} \sum_{m,n} \sin\left[\frac{2\pi}{LN}\left(m + \frac{\Phi(\beta)}{\Phi_0} + \frac{s\Phi(\alpha)}{\Phi_0}\right)\right]. \tag{16}$$

Discussion and Conclusion

The geometric structure determines the electronic structure and thus the characteristics of the persistent current oscillations. The electronic structure calculated from the tight-binding model are given in Eq. 9 and Eq. 14.

In the first model, both circular and longitudinal currents which are due to $\Phi(\alpha)$ and $\Phi(\beta)$ are periodic in Φ with a periodicity of Φ_0 and they are flowing in perpendicular directions. Eq. 10 and Eq. 11 are in agreement with Eq. 4 in the limits when $N \rightarrow 1$ and $t_2 \rightarrow 0$ together with $t_1 = t_3$ respectively. However, in the second model since we consider electron transport with cross hoppings, Eq. 12, in contrast to vertical hoppings in the first model, Eq. 5, this couples two different symmetries. This coupling yields extra component to the total circular current, which have periodicity of Φ_0/s, Eq. 15. Since s is a positive integer, total circular persistent currents have periodicity of Φ_0 as expected. In the special case, for $s = LN$, all cross-hoppings are indeed now vertical hoppings and we recover the result of first model together with circular currents which have periodicity of Φ_0.

Extra component of circular persistent currents appears since because including cross-hoppings preserves helical symmetry in the second model with compared to first model in which helicity is not totally present. These currents are vanishingly small in the limit of large number of rings, $L \rightarrow \infty$, as expected. Note that, extra circular current component is due only to $\Phi(\alpha)$ and the presence of $\Phi(\beta)$ results only in longitudinal persistent currents along the toroid. Our both model results are also in complete agreement with Lin [5] et al., in which they showed perpendicular $\Phi(\beta)$ through the carbon nanotube toroidal structures results in persistent current oscillations with periodicity of Φ_0. To conclude, our calculations suggest that circular persistent currents in structures with helical symmetry have two components with periodicity of Φ_0 and Φ_0/s which results in a total circular persistent current oscillations with Φ_0 periodicity.

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