Persistent currents in distorted quantum ring

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Abstract. Persistent currents in distorted narrow mesoscopic rings threaded by the magnetic flux of the Aharonow Bohn type are investigated. It is shown that the ring distortions can be modelled by an appropriate potential term. The cases with a single and multiple distortions are considered. The single distortion opens a gap in the electron energy spectrum of a ring and decreases the amplitude of persistent currents. It is shown that in the ring with multiple distortions, under some geometrical conditions, there is an enhancement of the persistent current and some of the electronic states remain degenerated. The possible application of the model to the formation of a qubit is discussed.

1. Introduction

During the last 20 years, persistent currents (PC) in mesoscopic rings have attracted significant interest both theoretically and experimentally [1-4]. PC in small quantum rings threaded by a magnetic flux are a manifestation of quantum coherence in a submicron system. If the ring circumference $L$ is smaller than the phase coherence $L_\phi$ the electron wave function may extend coherently over $L$ even in the presence of elastic scatterers. In other words a normal loop with $L < L_\phi$ has a nontrivial ground state with a circulating PC.

In this paper we present theoretical study of persistent currents in the quantum ring. We consider a narrow ring with two distortions of uniform cross section lying on a plane (Fig. 1). We show that quantum tunneling between states with nearly equal energy and PC can lead to a formation of a qubit.

The paper is organized as follows. In Sec. 2, we write down and discuss the Schrödinger equation for one electron in the ring with two distortionss in the presence of a magnetic flux. We show that the curvature of distorted ring enters into the Schrödinger equation via a geometrical potential term [5]. We demonstrate that the factorization of the wave function leads to two separate eigen-equations in transverse and longitudinal directions. In Sec. 3 we analyze a distorted quantum ring consisting of eight constant-curvature segments and we find the energy spectrum of such a ring. We show that the geometrical potential $V_g$ opens gaps in the electron energy spectrum with the exception of the case when distortions are symmetrically placed. Next, in section 4 we perform analytical calculations and computer simulations to analyze the effect of distortions on the persistent currents. We show that in the case of a small one-dimensional ring the presence of distortions significantly changes the currents and especially how the currents are affected by various configuration of distortions. In Sec. 5 we show that distorted quantum ring can be useful for quantum computing hardware. Conclusions are presented in Sec. 6.
2. Model of a distorted ring - Hamiltonian

Let us consider the electron of an effective mass $m_e$ rigidly bounded to a distorted quantum ring by a potential $V_\xi (\xi$ is the characteristic width of $V_\xi$) in the presence of static magnetic flux $\Phi$ threading the ring. Following the reasoning of [5] and [6] we shall introduce a curvilinear coordinate system of the ring based on the curve $K$

$$R(s, q) = r(s) + qn(s),$$

where $s$ is the arc length parameter and $q$ is the coordinate along the normal $n(s)$.

We consider (see [5, 7]) $V_\xi$ to be dependent only on $q$ coordinate

$$V_\xi (q) = \begin{cases} 0, & |q| < \frac{\xi}{2} \\ \infty, & |q| \geq \frac{\xi}{2} \end{cases}$$

We assume that the system is well insulated from the environment - it can be put in a shield that screens it from the unwanted radiation.

The motion of the electron obeys Schrödinger equation which has the form

$$\frac{1}{2m_e} \left( \hat{p} - \frac{e}{c} A \right)^2 \psi + V_\xi (x) \psi = E\psi,$$

where $\hat{p}$ is the electron momentum operator, $A(r) = \frac{1}{2} [B, r]$ is the vector potential and $x \in (0, L)$. It can be rewritten (using the gauge $\text{div}(A) = 0$) as

$$\frac{1}{2m_e} \left( -\hbar^2 \Delta - \frac{e^2}{c^2} A\hat{p} + \frac{e^2}{c^2} A^2 \right) \psi + V_\xi (x) \psi = E\psi,$$

The Laplacian $\Delta$ in curvilinear coordinates $s$ and $q$ is

$$\Delta_{s,q} = \frac{1}{h} \frac{\partial}{\partial s} h \frac{\partial}{\partial s} + \frac{1}{h} \frac{\partial}{\partial q} h \frac{\partial}{\partial q},$$

where $h = 1 - k(s) q$ depends upon the curvature $k(s) = \frac{1}{r(s)}$.

After several transformations and substitutions (following the approach proposed in [5, 6])
the wave function in Eq. (4) is converted to a form \( \tilde{\psi}(s,q) \) which can be decomposed by \( \psi(s,q) = \psi_l(q) \psi_L(s) \). It leads to the separations of Eq. (4) into equations

\[
-q^2 \psi_L + V_L \psi_L = E_L \psi_L,
\]

\[
-q^2 \psi_L + V_L \psi_L = E_L \psi_L,
\]

where \( V_L = \frac{\hbar^2 k_2^2(s)}{2m} \). First of them, describing the transverse confinement of electron in the ring, depends on the particular shape of the potential \( V_L \), the second, describing the longitudinal motion of the electron in the ring, does not depend on the detailed behavior of the potential \( V_L \) but depends on \( V_g \). In this paper we make the assumptions that \( \xi \ll r_2 \) and that the electrons occupy only the lowest subband of the transverse confinement and their position is not important. In the rest of the paper we consider only Eq. (7) and we omit the index \( \ell \) (\( \psi_L(s) = \psi_L(s) \)).

We work in a gauge for the vector potential in which the field does not appear explicitly in the Hamiltonian but enters the calculation via the flux-modified boundary conditions

\[
\psi(L) = \psi(0) e^{i2\pi \frac{\psi}{\Phi_0}}, \quad \frac{\partial \psi(L)}{\partial s} = \frac{\partial \psi(0)}{\partial s} e^{i2\pi \frac{\psi}{\Phi_0}}.
\]

### 3. Effect of the distortion on the electron energy spectrum

As we showed in Fig. 1. our distorted ring consists of eight smoothly connected arcs. The two long segments have the same radius \( r_1 \), each of the distorted segments consists of three short arcs of the radius \( r_2 \) where \( V_g = V_0 \) is constant. The relations between \( \alpha, \beta \) and \( \varphi \) are

\[
\alpha = 2 \arcsin \left[ \frac{\sin \left( \frac{\varphi}{2} \right) (r_1 - r_2)}{2r_2} \right], \quad \beta = \frac{\varphi}{2} + \frac{\alpha}{2}.
\]

The minimal possible value of \( r_2 \) for a given \( r_1 \) and \( \varphi \) is given by \( r_2^{\min} = \frac{\sin(\varphi/2)r_1}{2+\sin(\varphi/2)} \).

We can write Eq. (7) for the two distorted segments and two long segments as

\[
-q^2 \psi_L + V_0 \psi_L = E_L \psi_L \quad \text{for} \quad 0 < s < l,
\]

\[
-q^2 \psi_L + V_0 \psi_L = E_L \psi_L \quad \text{for} \quad l + a < s < 2l + a,
\]

\[
-q^2 \psi_L + V_0 \psi_L = E_L \psi_L \quad \text{for} \quad l < s < l + a,
\]

\[
-q^2 \psi_L + V_0 \psi_L = E_L \psi_L \quad \text{for} \quad 2l + a < s < 2l + a + b = L,
\]

where \( l = (2\beta + \alpha) r_2 \) is the total length of the three short segments (the same for both distortions), \( L = (2\pi - 2\varphi) r_1 + 2l \) is the total length of the curve \( K \), \( V_0 = \frac{\hbar^2}{2m} \left( \frac{1}{r_2^2} - \frac{1}{r_1^2} \right) \) and \( a, b \) are distances between the two blocks of the distorted segments.

The general solution of Eqs. (10) and (11) reads

\[
\psi_1 = b_1 e^{ik_1s} + b_2 e^{-ik_1s},
\]

\[
\psi_2 = c_1 e^{ik_2s} + c_2 e^{-ik_2s},
\]

\[
\psi_3 = d_1 e^{ik_1s} + d_2 e^{-ik_1s},
\]

\[
\psi_4 = f_1 e^{ik_2s} + f_2 e^{-ik_2s},
\]
where \( k_1 = \sqrt{\left(2m_e/h^2\right)(E_\ell + V_0)} \) and \( k_2 = \sqrt{\left(2m_e/h^2\right)E_\ell} \). The wave functions \( \psi_i, i = 1, \ldots, 4 \) are connected at \( s = l \) via \( \psi_1(l) = \psi_2(l) \), \( s = l + a \) via \( \psi_2(l + a) = \psi_3(l + a) \), \( s = 2l + a \) via \( \psi_3(2l + a) = \psi_4(2l + a) \) (plus the same requirements of continuity for its derivatives) and \( s = 0, L \) via Eqs. (8). Using the transfer matrix method [8] we obtain from these boundary conditions equation for the energy spectrum. For unbound states \( E_\ell > 0 \) we have

\[
2 \cos \Theta - \left[ \frac{3}{2} + \frac{k_1^2}{4k_2^2} + \frac{k_2^2}{4k_1^2} \right] \cosh [k_2(b + a)] \cos (2k_1l) + \left[ \frac{k_1}{k_2} + \frac{k_2}{k_1} \right] \sin (2k_1l) \sinh [k_2(b + a)] - \\
- \left[ \frac{1}{2} - \frac{k_1^2}{4k_2^2} - \frac{k_3^2}{4k_1^2} \right] \{ \cos (2k_1l) \cosh [k_2(b - a)] + \cos [k_2(b + a)] - \cosh [k_2(b - a)] \} = 0, \quad (16)
\]

and for bound states \(- V_0 < E_\ell < 0 \)

\[
2 \cos \Theta - \left[ \frac{3}{2} - \frac{k_1^2}{4k_2^2} - \frac{\kappa^2}{4k_1^2} \right] \cosh [\kappa(b + a)] \cos (2k_1l) + \left[ \frac{k_1}{\kappa} - \frac{\kappa}{k_1} \right] \sin (2k_1l) \sinh [\kappa(b + a)] - \\
- \left[ \frac{1}{2} + \frac{k_1^2}{4k_2^2} + \frac{\kappa^2}{4k_1^2} \right] \{ \cos (2k_1l) \cosh [\kappa(b - a)] + \cos [\kappa(b + a)] - \cosh [\kappa(b - a)] \} = 0, \quad (17)
\]

where \( \kappa = -ik_2 = \sqrt{\left(2m_e/h^2\right)(-E_\ell)} \) and \( \Theta = 2\pi \frac{\Phi}{\Phi_0} \).

Figure 2. Electron energy levels [in arbitrary units] as a function of magnetic flux in quantum ring of the length \( L \approx 2527 \, [\text{Å}] \) with different degrees of distortions for \( \varphi = \frac{\pi}{8} \) and \( a = 750 < b \approx 1499 \, [\text{Å}] \).
Figure 3. Electron energy levels [in arbitrary units] as a function of magnetic flux in quantum ring of the length $L \approx 2527$ [Å] with different degrees of distortions for $\varphi = \frac{\pi}{8}$ and $a = b \approx 1099$ [Å] (distortions are symmetrically placed).

Figure 4. The energy spectrum [in arbitrary units] as a function of $a$ (distance between distortions in Å) in quantum ring of the length $L \approx 2527$ [Å] with different degrees of distortions for $\varphi = \frac{\pi}{8}$ and $\frac{\Phi}{\Phi_0} = \frac{1}{2}$. 
In Fig. 2 we show the calculated energy as a function of magnetic flux with different degrees of both distortions. In perfect quantum ring the electron energy levels are intersecting parabolas. Geometrical potential provides open gaps in the energy spectrum at the points of intersection of the parabolas. The energy gap increases for more distorted ring except for some special cases. When the two distortions are symmetrically placed (Fig. 3) the energy gap for $\Phi = \frac{1}{2}$ vanishes for each energy levels and we obtain doubly degenerate states. This effect is independent on the degree of distortions. Furthermore, as we shown in Fig. 4, for high energy levels we have also other degeneracies for different distances between distortions. The number of degeneracies increases and amount to $2n - 1$ for the level $n$. We obtain also one or two bound states of energy $-V_0 < E_{\ell} < 0$ depending on the radius of distortions and the distance between them.

4. Effect of the distortion on the persistent current

In our model we assume that the number of spinless electrons $N$ is fixed. With each energy level we can associate a microscopic current

$$I_n = -\frac{\partial E_n}{\partial \phi} = \frac{e\hbar}{2\pi m R^2} \left( n - \frac{\Phi}{\Phi_0} \right), \quad n = 0, 1, \ldots$$

where $n$ is the orbital quantum number (winding number) for an electron going around the ring.

![Figure 5](image_url)

**Figure 5.** Persistent current in the ring at $T = 0$, $\varphi = \frac{\pi}{8}$ and $N = 3$ for different degrees of distortions and distances between them.

In Fig. 5 we present numerical calculations of the PC in the distorted ring with the energy spectrum determined from Eq. (16). We show the influence of two distortions on the persistent currents of three electron states $N = 3$ at $T = 0$. The distortion of the ring changes the current amplitude due to the opening of energy gaps at the points of intersection. Notice that the
amplitude of the oscillations decreases and it becomes smoother with larger distortion in the case \( a \neq b \). For symmetricalaly placed distortions \( a = b \) we observe saw tooth shape of the current with significantly higher amplitude.

5. Qubits

In the presence of the distortion of finite length \( l \) and degree \( \frac{\Phi}{\Phi_0} \), the tunneling occurs which mixes the states from both sides of the potential well. Effectively this is connected with the possibility of an electron wave function phase slip at the potential well. The phase slip rate is proportional to the degree and width of the distortion. The phase slip is more likely to occur close to the degeneracy points of the energy spectrum and then the eigenstates which are the superposition of flux states with different winding numbers can be formed. It causes the level splitting of the initial energy levels. Quantum tunneling should thus lead to a qubit i.e. a quantum superposition of the two opposed current states \([9, 10]\).

The Hamiltonian in the second quantization is

\[
H = \sum_{m \neq n} \left[ \frac{\hbar^2}{2m_e R^2} \left( n - \frac{\Phi}{\Phi_0} \right)^2 |n\rangle \langle n| - \frac{1}{2} \hbar \omega_{m,n} (|n\rangle \langle m| + |m\rangle \langle n|) \right]
\]

where \( \omega_{m,n} \) is the phase slip rate between states \(|m\rangle \) and \(|n\rangle \).

The energy states with \(|n| < n_F\) are fully occupied and form the "Fermi sea". The energy states for \(|n| > n_{F+1}\) are separated by large energy gap \( \Delta (\Delta = \hbar v_F l \text{ and } v_F \text{ is the electron velocity at the Fermi Surface}) \) and at \( kT \ll \Delta \) are fully empty. Thus the only states which can take part in the tunnelling are the states in the immediate neighbourhood of the FS and we can consider a mesoscopic ring as a two-state quantum system. In this case the summation in (19) can be restricted to two states closest to the FS. If we assume e.g. that \( N = N_{\text{odd}} \) and \( \frac{\Phi}{\Phi_0} \) close to \( \frac{1}{2} \) these states are \(|n_{F+1}\rangle = |\mu\rangle\) and \(|-n_F\rangle = |\nu\rangle \) \([9]\) and the Hamiltonian (19) becomes

\[
H = \left[ \begin{array}{cc} E_\nu & -\frac{1}{2} \hbar \omega_{\nu,\mu} \\ -\frac{1}{2} \hbar \omega_{\nu,\mu} & E_\mu \end{array} \right]
\]

where \( E_\nu = E_{-n_F}, E_\mu = E_{n_{F+1}}, \omega_{\nu,\mu} = \omega_{-n_F,-n_{F+1}} \)

Diagonalizing the hamiltonian (20) we obtain two energy bands

\[
E_{I,II} = \pm \frac{1}{2} \sqrt{\left( E_\mu - E_\nu \right)^2 + \hbar^2 \omega_{\nu,\mu}^2}. \tag{21}
\]

Introducing the "mixing angle" \([2]\), \( \eta = \tan^{-1} \frac{\hbar \omega_{\nu,\mu}}{E_\mu - E_\nu} \) the eigenstates of Eq. (20) are

\[
|I\rangle = \cos \frac{\eta}{2} |\mu\rangle + \sin \frac{\eta}{2} |\nu\rangle, \tag{22}
\]

\[
|II\rangle = -\sin \frac{\eta}{2} |\mu\rangle + \cos \frac{\eta}{2} |\nu\rangle. \tag{23}
\]

At the degeneracy point \( E_\mu = E_\nu, \eta = \frac{\pi}{2} \) the energy splitting is

\[
E_I - E_{II} = \hbar \omega_{\nu,\mu} \tag{24}
\]

and the respective energy eigenstates are symmetric and antisymmetric superpositions of states with opposite PC

\[
|I\rangle = \frac{1}{\sqrt{2}} (|\mu\rangle + |\nu\rangle), \tag{25}
\]
|II⟩ = \frac{1}{\sqrt{2}} ( |μ⟩ + |ν⟩ ) . \quad (25)

By making use of a transfer matrix method one obtains

$$\hbar \omega_{ν,μ} = \frac{Δ}{\pi} \arccos \sqrt{T}$$

where \( T \) is the transmission probability of an electron at the FS.

In case of the quantum ring with one single deformation the tunneling amplitude depends on its height and width which can be realized in many ways, for example by mechanical pressing. When we have more than one distortion (two in our case) we have an additional degree of freedom because the tunneling amplitude depends also on the distance between the distortions. Changing the distance between deformations we can smoothly adjust the gap and consequently the phase slip rate \( \omega_{ν,μ} \) to a desired value.

6. Conclusions

We have investigated persistent currents in a quantum ring with two distortions. We derived the Schrödinger equation and we have shown that the ring curvature enters into Hamiltonian through a geometrical potential term and causes the meaningful changes in the electron energy spectrum and persistent currents. It was found that the presence of distortions opens gap in the energy spectrum which depends on the degree of the distortions and distance between them. In case of symmetricaly placed distortions the degeneracy reappears at \( \frac{Φ}{Φ_0} = \frac{1}{2} \) and the energy levels are again intersecting. As was shown in Section 4, for some distances between the distortions we obtain also the strongest persistent currents. For these cases the persistent current as a function of the magnetic field looks similar to the persistent current in a perfect undistorted ring at \( T = 0 \).

Finally, we have considered quantum distorted ring as two level quantum system that can be potentially useful for quantum communication. It was found that we have an additional degree (distance between the distortions) of freedom which can be manipulated to obtain a qubit of a desired properties.

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