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Coherent quantum dynamics of mesoscopic metallic ring with a barrier

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Abstract. In this paper we consider a mesoscopic 1D, ballistic, metallic ring with a potential barrier. We show that the coherent coupling between two distinct quantum states with different winding numbers can lead to a formation of a qubit. We discuss the possible realizations of such a ring, the adjustment of a potential barrier parameters and the possible decoherence sources.

Recently a number of systems, which can be effectively reduced to a two level systems [1], [2], [3], [4], have been examined as candidates for quantum computing hardware. In the present paper we propose a candidate for the quantum qubit, which is based on a mesoscopic metallic ring with a barrier.

Persistent currents in small nonsuperconducting 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 [5], [6]. In other words a normal loop with \( L < L_\phi \) has a nontrivial ground state with a circulating persistent current (PC). In this paper we perform same model calculations on mesoscopic metallic ring which show that quantum tunneling between states with nearly equal energy and opposite PC can lead to a formation of a qubit.

Let us consider the mesoscopic metallic quasi 1D ring of radius \( R \) (\( 2\pi R < L_\phi \)) in the presence of static magnetic flux \( \phi_e, \phi_e = B_e \cdot \pi R^2 \), \( B_e \) is the applied magnetic field perpendicular to the plane of the ring.

The Hamiltonian of the system in the free electron model is

\[
H = \frac{1}{2m_e} (p - eA)^2 + V(x),
\]

where \( x = R\phi, x \in (0, L), A = \frac{\phi}{R} \) and \( m_e \) is the electron mass. \( V(x) \) is the potential energy in the presence of an energy barrier. We assume that a ring is made from a very clean material i.e. we are in the ballistic regime. In the absence of the energy barrier \( V(x) = 0 \) the formulas for the energy levels and the wave functions in a quasi 1D ring are [7]:

\[
E_n = \frac{\hbar^2}{2m_e R^2} \left( n - \phi' \right)^2, \quad \psi_n(x) = \frac{1}{\sqrt{2\pi}} e^{in\frac{\phi}{\phi_0}}, \quad n = 0, \pm 1, \ldots
\]

where \( \phi' = \frac{\phi}{\phi_0}, n \) is the orbital quantum number (winding number) for an electron going around the ring. For very thin ring the selfinductance effect can be neglected and \( \phi = \phi_e, \phi_0 = \frac{\hbar}{e} \).
The system has a set of quantum size energy gaps, the gap at the Fermi surface (FS) at $\phi' = 0.5$ is $\Delta = \frac{\hbar v_F}{k_F}$. Assuming a ring made of a metal (e.g. copper) with $R = 400\,\text{A}$, we get $\Delta \sim 290\,\text{K}$. The energy spectrum as a function of $\phi'$ is shown in Fig. 1 by the dashed lines. At integer and half integer $\phi'$ the states $E_n$ are doubly degenerate, therefore neglecting the spin, each level $E_n$ can be occupied by one or two electrons.

Figure 1. The energy spectrum of a 1D ring as a function of the applied flux $\phi'$.

We can see from Fig. 1, that for $\phi' = 0.5$ and the number of electrons in the ring $N = N_{\text{even}} = 2n_F$ the last occupied level, i.e. the level below the FS, is doubly occupied, whereas for $N = N_{\text{odd}} = 2n_F + 1$ the last level below the FS is occupied by a single electron only. The energy spectrum is periodic with period $\phi' = 1$. We restrict our considerations to $\phi' \in [0, 1]$.

With each energy level we can associate a microscopic current

$$I_n = -\frac{\partial E_n}{\partial \phi} = \frac{e\hbar}{2\pi m_e R^2} \left( n - \phi' \right), \quad n = 0, \pm 1, ...$$

The current is persistent at $kT \ll \Delta$.

In the presence of the energy barrier of finite length $a$ and height $V_0$, the tunneling occurs which mixes the states from the two potential wells. Effectively this is connected with the possibility of an electron wave function phase slip at the barrier. The phase slip rate increases with the height and width of the barrier. 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. This leads to the level splitting of the initial energy levels, which depends on the barrier parameters (the solid line at Fig. 1). Quantum tunneling should thus lead to a qubit i.e. a quantum superposition of the two opposed current states. The Hamiltonian in the second quantization is

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

where the summation is over all pairs of different occupied electronic states, $\delta_{m,n}$ 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 gaps from the FS 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 (3) can be restricted only to two states closest to the FS. Throughout this paper we assume e.g. that \(N = N_{\text{odd}}\) and \(\phi'\) is close to 0.5. Then these states are \(|n_F+1\rangle = |\beta\rangle = (1,0)\) and \(|-n_F\rangle = |\alpha\rangle = (0,1)\) and the Hamiltonian (3) becomes

\[
H = \begin{bmatrix}
E_\alpha & -\frac{1}{2}\delta_{\alpha,\beta} \\
-\frac{1}{2}\delta_{\alpha,\beta} & E_\beta
\end{bmatrix},
\]

where \(E_\alpha = E_{-n_F}\), \(E_\beta = E_{n_F+1}\) and \(\delta_{\alpha,\beta} = \delta_{-n_F,n_F+1}\).

For most values of \(\phi'\) the \(\delta_{\alpha,\beta}\) are small compared with the energy of orbital motion of an electron in the ring. However close to the degeneracy points the \(\delta_{\alpha,\beta}\) term mixes them strongly.

At \(\phi' = 0.5\) the states \(|\beta\rangle\) and \(|\alpha\rangle\) have exactly the same energies

\[
E_\alpha = E_\beta,
\]

but opposite currents

\[
I_\alpha = -I_\beta.
\]

In this case the phase slip rate \(\delta_{\alpha,\beta}/\hbar\) increases at all half integer \(\phi'\).

The quantum tunneling can provide coherent coupling between these two distinct quantum states. The energy after quantum tunneling is the same, but the persistent current is reversed. Quantum tunneling should thus lead to a qubit i.e. a quantum superposition of the two opposed current states. The amplitude of these currents is \(I_0 = \frac{eF}{L}\). Assuming e.g. \(R = 400\,\text{Å}\), for metallic ring \(I_0 \sim 1\,\mu\text{A}\).

In a pseudospin notation (4) can be written as

\[
H = -\frac{1}{2}B_z \hat{\sigma}_z - \frac{1}{2}B_x \hat{\sigma}_x,
\]

where \(\hat{\sigma}_z\) and \(\hat{\sigma}_x\) are Pauli spin matrices.

The energy splitting, which is controlled by the magnetic flux corresponds here to the \(z\) component of the magnetic field

\[
B_z = E_\beta - E_\alpha = \Delta \left[1 - 2\frac{\phi}{\phi_0}\right].
\]

The \(x\) component of the effective magnetic field \(B_x\) describes the tunneling amplitude \(\delta_{\alpha,\beta}\) between the two potential wells. It depends on the height and width of the barrier. The phase slip may occur as a result of a reflection of an electron on a single potential barrier encountered along the ring.

The potential barrier in a mesoscopic ring can be realized in a number of ways. One of them is the ring in which the small fragment of a convex arc have been replaced with a concave one [8]. In this case the resulting potential barrier has a rectangular shape. The potential barrier produces forward and backward scattered electrons with equal energies and opposite currents (Eq. (5), (6)). Another possibility to form the barrier is the local point-like electric gate close to the ring. The electric potential of the gate forms the barrier, the height of which can be modified by the gate voltage. The electric potential barrier can be combined with the geometric one described above. In this case the barrier height and therefore the mixing term \(\delta_{\alpha,\beta}\) can be easily adjusted to the required value. Finally, to obtain a system described by Eq. (7) one can apply a real magnetic field \(B_x\) close to the degeneracy point.
Diagonalizing the Hamiltonian (4) we obtain two energy bands (see Fig. 2)

\[ E_{I,II} = \pm \frac{1}{2} \sqrt{(E_\beta - E_\alpha)^2 + \delta_{\alpha,\beta}^2}. \tag{9} \]

Introducing the "mixing angle" \( \eta = \tan^{-1} \frac{\delta_{\alpha,\beta}}{E_\beta - E_\alpha} \) the eigenstates of Eq. (7) are

\[ |I\rangle = \cos \frac{\eta}{2} |\beta\rangle + \sin \frac{\eta}{2} |\alpha\rangle, \tag{10} \]

\[ |II\rangle = -\sin \frac{\eta}{2} |\beta\rangle + \cos \frac{\eta}{2} |\alpha\rangle. \tag{11} \]

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

\[ E_I - E_{II} = \delta_{\alpha,\beta} \tag{12} \]

and the respective energy eigenstates are

\[ |I\rangle = \frac{1}{\sqrt{2}} (|\beta\rangle + |\alpha\rangle), \]

\[ |II\rangle = \frac{1}{\sqrt{2}} (-|\beta\rangle + |\alpha\rangle). \tag{13} \]

We performed the numerical calculations of the energy levels \( E_{I,II} \) for different sets of the barrier parameters and extracted the magnitude of \( \delta_{\alpha,\beta} \) from it.

**Figure 2.** The energy bands \( E_{I,II} \) as a function of an applied flux \( \phi' \).

Let us estimate the energy splitting \( \delta_{\alpha,\beta} \) of the degenerate states due to the tunneling through the potential barrier of width \( a \ll L \) and height \( V_0 \) \cite{9}. By making use of a transfer matrix method one obtains

\[ \delta_{\alpha,\beta} = \frac{\Delta}{\pi} \arccos \sqrt{T}, \tag{14} \]

where \( T \) is the transmission probability of an electron at the FS. The transmission probability \( T \) as a function of \( V_0 \) and \( a \) is presented in Fig. 3.
The tunneling amplitude depends on the height of the barrier which can be raised or lowered by electronic gating. Assuming e.g. $E_F \sim 1\text{eV}$ one obtains the $\delta_{\alpha,\beta}$ in the range of a few K. The two energy levels given by Eq. (9) for a ring with $V_0 = 1.015\text{eV}$ and $a = 20\text{Å}$ are shown in Fig. 2.

Figure 3. The transmission coefficient $T$ as a function of the potential barrier height $V_0$ and width $a$.

Our model calculations has been performed for a quasi 1D ring. However they are also valid with some modifications for the mesoscopic metallic ring with very small thickness $d$, $d \ll R$ i.e. with a few transverse channels ($M$) [9]. Sharp energy levels $E_n$ will then be replaced by narrow energy bands with $M$ sublevels. However the gaps between these bands will still be large and at low temperature we can approximate thin ring by a quasi 1D ring. In the area of present development of nanotechnology there is a hope that such rings will be produced in the near future.

In this paper we discussed the possibility of making a flux qubit on a nonsuperconducting, mesoscopic, metallic, ballistic quasi 1D ring. Such ring can be effectively reduced to a two-state system and described in the pseudo-spin notation. The term $B_z$ in Eq. (7) can be tuned by the applied flux. The coherent coupling between two distinct quantum states having different winding numbers $n$ is via coherent tunneling through the potential barrier which can be raised or lowered by electrical gating. The off-diagonal term in Eq. (7) can be also accomplished by the real magnetic field $B_x$ perpendicular to the $z$ axis (or in the plane of the ring). With these two external control parameters the elementary single-bit operations i.e. $z$ and $x$ rotations can be performed.

The system discussed in the paper can behave quantum mechanically provided that it is sufficiently decoupled from its environment. Thus the important constraints on the device are dephasing effects due to various decoherence sources. They are mainly caused by material problems such as defects. The magnetic noise in practical currents is smaller than the electrical noise and random fluctuations generated by charged defects. The fluctuations in the barrier and in the magnetic field, necessary to get the degeneracy of the states for $N = N_{\text{odd}}$, can be the source of decoherence. We can estimate the influence of known sources of decoherence, but it is impossible to determine the real decoherence time with certainty, except by measurements. Till now we discussed a single qubit design. Two or more qubits can be coupled by means of the flux that the circulating currents generate [1]. The flux state of the sample can be measured by
a separate magnetometer inductively coupled to the sample. The proposed qubits should be of considerable interest for fundamental studies of quantum coherence in mesoscopic systems.

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