QUANTUM BISTABILITY, STRUCTURAL TRANSFORMATION, AND SPONTANEOUS PERSISTENT CURRENTS IN MESOSCOPIC AHARONOV-BOHM LOOPS

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Fixed-number-of-electron mesoscopic or macromolecular conducting ring is shown to support persistent currents due to Aharonov-Bohm flux, and the "spontaneous" persistent currents without the flux when structural transformation in the ring is blocked by strong coupling to the externally azimuthal-symmetric environment. In the free-standing macromolecular ring, symmetry breaking removes the azimuthal periodicity which however is further restored at the increasing field. Three-site ring with one or three electrons represent an interesting quantum system which can serve as a qubit (quantum bit of information) and a qugate (quantum logical gate).

1. Introduction

Persistent currents^{1,2,3} have been predicted for mesoscopic conducting loops which do not show the effect of superconductivity. The current appears in presence of magnetic field as a result of Aharonov-Bohm effect⁴, the special role of vector potential in quantum mechanics. As discussed in a review paper⁵, persistent currents are similar to orbital currents in normal metals considered by Teller⁶ in his interpretation of Landau diamagnetism⁷, but specific to the double connected geometry of the conductors (loops, hollow cylinders, etc.). Observation of persistent currents have been done in the indirect^{8,9} as well as in direct^{10,11} experiments showing the single-flux-quantum $\Phi_0 = hc/e$ periodicity in the resistance of thin *Nb* wires⁸ and networks of isolated *Cu* rings⁹, and in the single-loop experiments on metals¹⁰ and semiconductors¹¹.

Further trend in macromolecular persistent currents^{12,13,14} is in the quantum computational perspectives of using Aharonov-Bohm loops as quantum bits of information (qubits) with an advantage of easier (radiation free) manipulation of qubit states, and in the increased decoherence times¹³ as compared to macroscopic "Schrödinger cat" structures (Josephson junctions).

2. Spontaneous persistent current

Nevertheless that the persistent current is related to Aharonov-Bohm effect, at

Figure 1. Examples of occurrence of bistable configuration in a ring. Curve 1: Energy versus flux in a ring of 10 electrons. Curve 2: Energy versus flux in a ring of 11 electrons. The second curve is shifted down for convenience but not rescaled.

special condition (isolated ballistic ring at zero temperature) the current appears at zero Aharonov-Bohm flux as a superposition of degenerate clockwise and counterclockwise current orientations. Fig.1 explains the origin of such "spontaneous" currents as the bistability effect in a ring. Depending on the number of electrons in a loop, energy versus flux can have minimum, or a maximum with a kink at $\Phi = 0$, such that the current which is derivative of energy with respect to flux, $J = -c\partial E/\partial\Phi$, is negative (the diamagnetic effect) or positive (the double-valued paramagnetic effect). Such situation was noticed accidentally by various authors, in particular^{15,16} etc., but have not seemed convincing due to fixed chemical potential configuration studied, and attributed to the effect of Peierls instability in the ring^{17,18,19,20} (with the later paper criticized^{21,22} in regard to the inaccuracy of the mean field approximation). In fact, the fixed-number-of-particle ring with odd number of electrons displays a number of structural instabilities, the Peierls transformation or the Jahn-Teller effect being the most known examples of, or generally, more complex atom rearrangement when the ground state proved degenerate in symmetric configuration. Fig.2 shows the dependence of maximal persistent current, as well as the spontaneous current, on the number of electrons in a ballistic ring (electron mean free path $l = \infty$) modelled as a finite length hollow cylinder with rectangular cross section $L_1 \times L_2$ containing finite number of perpendicular electron channels $N_{\perp} = L_1 L_2 k_F^2 / 2\pi^2$. Mention that the magnitude of the current in a ballistic ring is not ev_F/L , as sometimes suggested (v_F is the Fermi velocity), but rather $J_{max} \sim \frac{ev_F}{L} N_{\perp}^{1/2}$ (see also²). The dependence $J_{max}(N)$ at $T = 0$ is irregular due to addition to the total current of both negative and positive contributions from different electron eigenstates.

Spontaneous current has same order of magnitude as the maximal persistent current, and represents an inseparable part of the Aharonov-Bohm effect in ballistic rings. The structural transformation in the ring following the spontaneous current is investigated in an exact way by considering the ring dynamics in the tight binding approximation in which electrons are hopping between the localization sites (the quantum wells) with certain hopping amplitude τ such that the phase of τ is determined by magnetic flux trapped in the interior of the loop, $\alpha = 2\pi\Phi/N\Phi_0$.

Figure 2. Persistent current versus number of electrons in a ring of cross-sectional dimensions ratio $L : L_1 : L_2 = 10 : 1 : 1$. Upper curve is the max current in units of $J_0 = ev_F/L$, at given N , the dotted curve is the amplitude of first harmonic of $J_{pers}(\Phi)$, and the curve at negative J is the spontaneous persistent current as defined below, also in units of J_0 . Mention that the magnitude of both currents is not of the order of J_0 , as sometimes suggested, but rather $J_0\sqrt{N_\perp}$ where $N_\perp$ is the number of transverse channels in the cross-section of the loop.

N below is the number of sites in the ring. Hamiltonian of the loop in the second quantized form is

$$\begin{aligned}
 H = & \sum_{i=1}^N (\tau_j a_{j\sigma}^+ a_{j+1,\sigma} e^{i\alpha_j} + \text{h.c.} + U \sum_{i=1}^N n_{i\uparrow} n_{i\downarrow} + V \sum_{i=1, \sigma, \sigma'}^N n_{i\sigma} n_{i+1, \sigma'} \\
 & + \frac{1}{2} W \sum_{i=1}^N (\theta_i - \theta_i^0)^2 + \frac{1}{2} K \sum_{j=1}^N (\theta_j - \theta_{j+1})^2
 \end{aligned} \quad (1)$$

where τ_j is the hopping amplitude between two near configurational sites, j and $j+1$,

$$\tau_j = \tau_0 + g(\theta_j - \theta_{j+1}), \quad n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}, \quad (2)$$

and α_j is the Aharonov-Bohm phase (a Peierls substitution for the phase of hopping amplitude)

$$\alpha_j = \frac{2\pi\nu}{N} + (\theta_j - \theta_{j+1})\nu. \quad (3)$$

Here $\nu = \Phi/\Phi_0$, $a_{j\sigma}^+$ is the creation (and $a_{j\sigma}$, the annihilation) operator of electron at site j with spin σ . θ_j with $j = 1, 2, \dots, N$ are the angles of distortion of site locations from their equilibrium positions $\theta_j^0 = 2\pi j/N$ satisfying the requirement $\sum_{j=1}^N \theta_j = 0$, and g is the electron-phonon coupling constant. The interaction (2) reflects the property that the hopping amplitude depends on distance between

the localization positions and assumes that the displacement $\theta_j - \theta_{j+1}$ is small in comparison to $2\pi/N$. U and V are Hubbard parameters of the on-site and intra-site interactions. W is the energy of binding of the loop to the azimuthal symmetric environment (a substrate, for example). The parameters are assumed such that system is not superconductive (e.g., $U > 0$; and anyway, the superconductivity is not allowed for 1d system and it is ruled out for small system). The last term in Hamiltonian (1) is the elastic energy and K is the stiffness parameter of the lattice.

In the smallest loop, the one with three sites ($N = 3$), only two free parameters of the lattice displacement, X_1 and X_2 , remain

$$\theta_1 = X_1 + X_2, \quad \theta_2 = -X_1 + X_2, \quad \theta_3 = -2X_2 \quad (4)$$

which are decomposed to second-quantized Bose operators b_1, b_2 according to

$$X_1 = \left(\frac{3K}{\omega}\right)^{1/4}(b_1 + b_1^\dagger), \quad X_2 = 3\left(\frac{K}{3\omega}\right)^{1/4}(b_2 + b_2^\dagger). \quad (5)$$

In the noninteracting system ($U, V, W, g = 0$), the energy versus ν shows kink with a maximum at $\nu = 0$ in the half filling case, i.e. at the number of electrons n equal to the number of sites N , as well as in a broader range of values of n at larger N . Actually, such dependence is typical for any $N \geq 3$ system for a number of (fixed) values of electron population. The 3-site loop's $J(\Phi)$ dependence is shown in Fig.4.

Figure 3. Spontaneous persistent current versus flux for $\tau_0 = -1$ and various values of Hubbard parameter U : 1 - $U = 0$; 2 - $U = -2$; 3 - $U = 2$; 4 - $U = -5$; 5 - $U = 5$; 6 - $U = -10$; 7 - $U = 10$.

The latter shows discontinuity at $\Phi = 0$ of the same order of magnitude as the standard value of the persistent current. The current at $\Phi = 0$ is *paramagnetic* since energy vs flux has *maximum* rather than minimum at $\Phi = 0$. On-site interaction reduces the amplitude of persistent current near zero flux but doesn't remove its discontinuity at $\Phi = 0$. Therefore, the most strong opponent of the Aharonov-Bohm effect, the electron-electron interaction, leaves it qualitatively unchanged. On the other hand, the electron-phonon interaction flattens the $E(\Phi)$ dependence near the peak value, see Fig.5. At large stiffnesses, K , this flattening remains important only for small magnetic fluxes, much smaller than the flux quantization period $\Delta\Phi = \Phi_0$. Mention that persistent current peak reduces in its amplitude only slightly near $\Phi = 0$. As is seen from Fig.6, electron-phonon interaction splits

Figure 4. Energy vs flux in a loop of noninteracting electrons coupled to lattice with the value of coupling parameter $g = 1$ and various values of the stiffness parameter K : 1 - $K=2$; 2 - $K=3$; 3 - $K=5$; 4 - $K=10$; 5 - $K=20$.

the singularity at $\Phi = 0$ to two singularities at $\Phi = \pm\Phi_{sing}$. Outside the interval $-\Phi_{sing} < \Phi < \Phi_{sing}$, structural transformation is blocked by the Aharonov-Bohm flux. The range of magnetic fluxes between $-\Phi_{sing}$ and Φ_{sing} determines the domain of the developing lattice transformation which signifies itself with the nonzero values of lattice deformations X_1, X_2 . The latter property allows us to suggest that the spontaneous persistent current state (a peak of dissipationless charge transport at, or near, the zero flux) remains at the nonzero Φ when the electron-phonon coupling is not too strong or when the lattice stiffness is larger than certain critical value.

Figure 5. Energy vs flux for a loop with coupling constant $g = 1$ and various values of stiffness K : 1 - $K=2$; 2 - $K=3$; 3 - $K=5$; 4 - $K=10$; 5 - $K=20$.

3. Discussion

In conclusion, we considered Aharonov-Bohm effect in angular-periodic macromolecular structure like, e.g., aromatic cyclic molecule, and found existence of persistent current, and also a spontaneous current when the Aharonov-Bohm flux is not applied to ring. Strong coupling of electron hopping to ion core of the ring-shaped macromolecular structure removes the spontaneous current which nevertheless is restored at (small) magnetic field or when the loop has large stiffness or is strongly bound to external azimuthal periodic environment (a substrate). Degenerate states of the loop at $\Phi = \Phi_0/2$ and at $\Phi = 0$ may serve as components of qubit which are operated by static voltages applied in plane of the loop perpendicular to the

direction of the Aharonov-Bohm flux.

We bring attention to the papers of Gatteschi et al.^{23,24} in which azimuthal-periodic molecular structure (a "ferric wheel" $[Fe(OMe)_2(O_2CCH_2Cl)]_{10}$) exhibited periodic variation of its magnetization in function of magnetic flux and assume that the periodicity with large period can be attributed to persistent currents. The above macromolecular structure is more complex than the one we considered since it contains magnetic ions with strong exchange interactions such that actual magnetic field in the ring may be *larger* than the externally applied field. If this suggestion proves correct, it will open a possibility of engineering the macromolecular structures¹² (qubits and qugates) based on the Aharonov-Bohm effect for purposes of quantum computation. Apart from this, the very existence of the nonzero non-decaying "spontaneous" current in a nonsuperconductive system deserves, to our opinion, a basic physical interest.

References

1. F. Bloch, *Phys. Rev.* **B2**, 109 (1970) and references therein. This paper proved exact periodicity of energy vs magnetic flux with a period hc/e , however with an indefinite amplitude.
2. I. O. Kulik, *JETP Lett.* **11**, 275 (1970).
3. M. Buttiker, Y. Imry and R. Landauer, *Phys. Lett.* **A96**, 365, 1983.
4. Y. Aharonov and D. Bohm, *Phys. Rev.* **115**, 485, 1959.
5. I. O. Kulik, in: *Quantum Mesoscopic Phenomena and Mesoscopic Devices in Microelectronics*, p.259. Eds. I. O. Kulik and R. Ellialtioglu, Kluwer, 2000.
6. E. Teller, *Zs. Physik* **67**, 311 (1931).
7. L. D. Landau, *Zs. Physik*, **64**, 629 (1930).
8. N. B. Brandt, et al., *Sov. J. Low Temp. Phys.*, **8**, 358 (1982).
9. L. P. Levy, et al., *Phys. Rev. Lett.* **64**, 2074 (1990).
10. V. Chandrasekhar, et al., *Phys. Rev. Lett.* **67**, 3578 (1991).
11. D. Mally, et al., *Phys. Rev. Lett.* **70**, 2020 (1993).
12. A. Barone, T. Hakioglu and I. O. Kulik, *Quantum Computation with Aharonov-Bohm Qubits*. E-print cond-mat/0203038 (2002).
13. I. O. Kulik, T. Hakioglu, and A. Barone, *Eur. Phys. J.* **B30**, 219, 2002.
14. I. O. Kulik, in: *Towards the Controllable Quantum States: Mesoscopic superconductivity and spintronics*, p.302. Eds. H. Takayanagi and J. Nitta, World Scientific, 2002.
15. H.-F. Cheung, et al., *Phys. Rev.* **B37**, 6050 (1988).
16. S. Latil, et al., *Phys. Rev.* **B67**, 165420 (2003).
17. I. O. Kulik, et al., *JETP Lett.* **47**, 303 (1988).
18. M. I. Vischer, et al., *Europhys. Lett.* **36**, 613 (1996).
19. Yu. I. Latyshev, et al., *Phys. Rev. Lett.* **78**, 919 (1997).
20. J. Yi, et al., *Phys. Rev. Lett.* **78**, 3523 (1997).
21. B. Nathanson, et al., *Phys. Rev. Lett.*, **80**, 3416 (1998).
22. G. Montambaux, *Phys. Rev. Lett.*, **80**, 3417 (1998).
23. D. Gatteschi, et al. *Science* **265**, 1054 (1994).
24. K. L. Taft, et al., *J. Amer. Chem. Soc.* **116**, 823 (1994).