Orbital Magnetic Ordering in Disordered Mesoscopic Systems

M. Lisowski and E. Zipper
Institute of Physics, University of Silesia
ul. Uniwersytecka 4, 40-007 Katowice, Poland

April 28, 1998

Abstract

We present some model calculations of persistent currents in disordered one- and two-dimensional mesoscopic systems. We use the tight-binding model and calculate numerically the currents in small systems for several values of disorder. Next we fit appropriate analytical formulae, and using them we find self-sustaining currents and critical fields in larger, more realistic systems with different shapes of the Fermi surfaces (FS).

PACS numbers: 71.30.+h; 72.10.-d; 72.90.+y

Keywords: mesoscopic ring, cylinder; self-sustaining, persistent currents; critical field; Fermi surface
1 Introduction

With advances in technology, fabrication of submicron devices has become possible. Such systems exhibit quantum coherence which is the subject of extensive experimental and theoretical studies.

Recently, in a series of papers [1], model considerations of self-sustaining persistent currents in a set of clean mesoscopic metallic rings have been presented. In this paper we investigate whether such currents survive in the presence of scattering driven by impurities and temperature. We will consider a set of concentric mesoscopic rings stacked along a certain axis and a set of concentric two-dimensional (2-D) cylinders. Such samples can be obtained by lithographic methods from metals or semiconductors [2].

2 Quasi One-dimensional Mesoscopic Rings

Let us consider a set of quasi one-dimensional (1-D) metallic mesoscopic rings stacked along $y$ axis threaded by the external magnetic flux $\phi_e$. We assume that each ring possesses the same number of conducting electrons $N_e$ (even or odd). The situation when some of the rings carry an odd number and other carry an even number of electrons has been considered in [1a]. The long range magnetostatic (current-current) interaction between electrons from different
rings is taken into account in the mean field approximation (MFA).

The gauge-invariant tight-binding Hamiltonian for a single ring is of the form:

$$\hat{H}_1 = \sum_{n=1}^{N} \left[ (2t + V_n)c_n^+c_n - te^{i\theta_{n,n+1}}c_{n+1}^+c_n - te^{-i\theta_{n,n+1}}c_n^+c_{n+1} \right],$$  \hspace{1cm} (1)

where $t = \hbar^2/(2mea^2)$ is the hopping matrix element, $a$ is the lattice constant; $c_n^+, c_n$ are the creation and annihilation operators; $N$ is the number of sites in each ring (channel); $\theta_{n,n+1}$ comes from the magnetic flux $\phi$:

$$\theta_{n,n+1} = \frac{e}{h} \int_{r_n}^{r_{n+1}} A \cdot dl = \frac{2\pi}{N} \frac{\phi}{\phi_0} \equiv \theta,$$  \hspace{1cm} (2)

where $A$ is the vector potential, and $\phi_0 = \hbar/e$.

The flux $\phi$ is composed of two parts,

$$\phi = \phi_e + \phi_I, \quad \phi_I = L I(\phi),$$  \hspace{1cm} (3)

i.e., each electron moves in the external magnetic flux $\phi_e$ and in the flux coming from the total current $I$ in the system; $L$ is the selfinductance coefficient.

The disorder is given by a random choice of the on-site potentials $V_n$ from a rectangular distribution of width $W = \kappa t$, $\kappa \geq 0$, and strength $-W/2$ to $W/2$.

In the case of a clean system ($V_n = 0$) we can calculate the current $I$ in the system, diagonalizing the Hamiltonian (1) directly, by using the Fourier transform. We get

$$I(\phi) = M_I I_1(\phi),$$
\[ I_1(\phi) = -\sum_\alpha \frac{\partial E_\alpha}{\partial \phi} = \frac{e\hbar}{Nm_e a^2} \sum_\alpha f_\alpha \sin \left[ \frac{2\pi}{N} \left( \alpha - \frac{\phi}{\phi_0} \right) \right], \quad (4) \]

where \( E_\alpha = 2t \left[ 1 - \cos \frac{2\pi}{N} (\alpha - \phi_\alpha) \right] \), \( f_\alpha \) is the Fermi-Dirac distribution function, \( \alpha \) is the orbital quantum number for an electron going around the ring \((\alpha = 0, \pm 1, \pm 2, \ldots)\); \( M_t = MP \), \( M \) and \( P \) are the numbers of rings along and perpendicular to \( y \) axis respectively \((P \ll N)\).

In this paper we concentrate on a disordered system \((V_n \neq 0)\). The Hamiltonian \( \mathcal{H} \) can be written in the form of a matrix \((N \times N)\):

\[
\mathcal{H}_1 = \begin{pmatrix}
2t + V_1 & -te^{-i\theta_{1,2}} & 0 & 0 \\
-te^{i\theta_{1,2}} & 2t + V_2 & -te^{-i\theta_{2,3}} & 0 \\
0 & -te^{i\theta_{2,3}} & 2t + V_3 & -te^{-i\theta_{3,4}} \\
-te^{-i\theta_{N,1}} & 0 & \cdots & \cdots & -te^{i\theta_{N-1,N}} & 2t + V_{N-1} & -te^{-i\theta_{N-1,N}} & 2t + V_N
\end{pmatrix}
\]

where the base vectors are chosen as follows:
\[
c_1^\dagger |0\rangle = |100...0\rangle \equiv |1\rangle \\
c_2^\dagger |0\rangle = |010...0\rangle \equiv |2\rangle \\
\cdots \\
c_N^\dagger |0\rangle = |000...1\rangle \equiv |N\rangle
\]

\(|0\rangle = |000...0\rangle\) - the vacuum state.

The above matrix we have diagonalized numerically for different \( N \) \((<100)\) and different \( W/t \) using the "Monte Carlo" method \[3\]. We also calculated the current \( I_1(\phi, W/t, T) \) by numerical differentiation; it is presented in Fig. 1 for \( N = 80 \) by symbols \[6\]. We see that the impurity scattering leads to the amplitude reduction and the shift of the maximum of the \( I_1(\phi) \) characteristics. We note \[8\] that elastic scattering has a very similar effect on the
$I_1(\phi)$ as temperature. Whereas a non-zero temperature leads to a redistribution of electrons among the energy levels, collisions lead to a change in the levels themselves. If the average collision time is $\tau$, then the uncertainty in the electron energy is of the order of $\hbar/\tau$, inverse proportional to the elastic scattering mean free path $l_e \sim (t/W)^2$ \cite{3} (the localization length $\xi$ in one dimension). If $\tau$ is not too short, it plays a similar role as the temperature \cite{7}.

Because of the limited capacity of computers and long time needed for computing, it is very difficult to calculate in this way the current $I_1(\phi, W/t, T)$ for $N > 100$. However we want to investigate the possibility of the existance of self-sustaining current in the system with impurities. The phenomenon of such current is a collective effect \cite{10} and can be obtained only if the number of interacting electrons is relatively large, i.e. for large (but still mesoscopic) systems. The selfconsistency formula for the current at $\phi_e = 0$, obtained by the use of Eq. \cite{3}, is of the form:

$$I(\phi, W/t, T) = \frac{\phi}{\mathcal{L}},$$

(6)

where

$$\mathcal{L} = \frac{\mu_0\pi R^2}{l^2} \left( \sqrt{l^2 - R^2} - R \right),$$

(7)

$l = M b$ is the length of the cylinder made of a set of mesoscopic rings, $b$ is the distance between rings; $\mu_0$ is the magnetic permeability of free space.

To get a stable, nontrivial solution of Eq. \cite{3} we need to consider a set
of mesoscopic rings with $N \gg 100$. Even though exact numerical solutions of the current in the presence of impurities were performed for very small samples, they show generic features for all mesoscopic rings [8]. Thus we have fitted an analytical formula to the numerical results of Fig. 1 and we assumed that it can be used for the qualitative analysis of Eq. (6) for larger rings. $I_1$ is periodic in $\phi/\phi_0$, with period 1, and can be expressed as a Fourier sum [3], [9]. The best fitting, denoted in Fig. 1 by solid line, we have obtained for the formula:

$$I_1(\phi, \gamma, T) = \sum_{q=1}^{\infty} \frac{4I_0}{\pi} \left( \frac{L}{2\gamma} + \frac{T}{T^*} \right) \frac{\exp \left[ -q \left( \frac{L}{\gamma} + \frac{T}{T^*} \right) \right]}{1 - \exp \left[ -q \left( \frac{L}{\gamma} + 2 \frac{T}{T^*} \right) \right]} \times$$

$$\times \cos(qk_F L) \sin \left( 2\pi q \frac{\phi}{\phi_0} \right),$$

where $I_0 = e\hbar \sin(k_F a)/(N\xi e a^2)$, $k_F = N\pi/L$, $L = Na$ is the circumference of a ring; $T^* = \Delta/(2\pi^2 k_B)$ is a characteristic temperature that separates the high- and low-temperature regimes, $\Delta = 4\pi t \sin(k_F a)/N$ is the level spacing at zero flux at the Fermi surface (FS), $k_B$ is the Boltzmann constant; $1/\gamma$ is a disorder parameter, $\gamma \approx 10a(t/W)^{3/2} \ln N$.

To account for different values of $\gamma$ ($W/t$) in a set of $M_t$ mesoscopic rings we have performed a quenched average of the current $I(\phi, \gamma, T)$, where disorder was given by a Gaussian distribution with standard deviation $\Delta \gamma = \pm 10% \bar{\gamma}$, $\bar{\gamma}$ is a mean value of $\gamma$. We have obtained a very small decrease in the amplitude of $[I(\phi, \gamma, T)]$, where $[...]$ denotes the quenched average, comparing to the case with the same disorder in each ring.
In the clean system at $T = 0 \, K$ we would have \[3\]:

$$I(\phi) = M_t \sum_{q=1}^{\infty} \frac{2I_0}{\pi q} \cos(qk_FL) \sin\left(2\pi q \frac{\phi}{\phi_0}\right).$$  \hspace{1cm} (9)

Now we are in position to look for the self-sustaining currents. They can be obtained from the self-consistent equation for the total current \([8]\), where the current $I = M_t I_1$ is taken with the quenched average, $I_1$ is given by the formula \([8]\).

The case of a clean system, in the free electron model, has been analysed in [11]. Here we extend earlier studies to include the dependences on disorder and temperature in the tight-binding model with the half-filled band. The results depend on the number of electrons in a single ring.

In the case of an even number of electrons in each ring the current is paramagnetic and the stable solutions of Eq. \([2]\) being the intersections of the curves marked by circle correspond to a spontaneous current $I_s$. They are presented in Fig. 2 for different parameters $\gamma$. In Fig. 3 we also present the temperature dependence of persistent current and we see that both temperature and disorder act almost in the same way.

In the case of an odd number of electrons in each ring the current is diamagnetic for small $\phi$ and the stable solutions of Eq. \([2]\) presented in Fig. 4 correspond to flux trapping, the phenomenon known in superconductors.

The temperature at which the transition to the state with the self-sustaining current occurs is denoted by $T_c$. We see that $T_c$ decreases with increasing
the impurity content and that flux trapping can be obtained only in weakly disordered systems.

3 Two-dimensional Mesoscopic Cylinders

Let us consider now a set of coaxial closely packed two-dimensional (2-D) cylinders [11]. The appropriate tight-binding Hamiltonian for a single cylinder is of the form:

$$\hat{H} = \sum_{m=1}^{M} \sum_{n=1}^{N} \left[ (2t + V_{nm})c_{nm}^+c_{nm} - te^{i\theta_{a,n+1}^m}c_{n+1m}^+c_{nm} + \right.$$

$$\left. - te^{-i\theta_{a,n+1}^m}c_{n+1m}^+c_{nm} - t_b c_{nm+1}^+c_{nm} - t_b c_{nm}^+c_{nm+1} \right],$$

where $t_b = \hbar^2/(2me_b^2)$ is the hopping element in the $y$ direction, $b$ is the lattice constant in the $y$ direction.

In this case to get the current $I$ in a disordered system, we have performed similar procedures to the previous 1-D case. Finally we have obtained:

$$I(\phi, \gamma, T) = P \sum_{m=1}^{\infty} \sum_{q=1}^{\infty} \frac{4I_0(m)}{\pi} \left( \frac{L}{2\gamma} + \frac{T}{T^*} \right) \frac{\exp\left[-q \left( \frac{L}{\gamma} + \frac{T}{T^*} \right)\right]}{1 - \exp\left[-q \left( \frac{L}{\gamma} + \frac{2T}{T^*} \right)\right]} \times$$

$$\times \cos[qk_{F_x}(m)L] \sin\left(2\pi q \frac{\phi}{\phi_0}\right),$$

where $1/\gamma$ is a disorder parameter, $\gamma \sim (t/W)^{3/2} \ln N$;

$$I_0(m) = e\hbar \sin[k_{F_x}(m)a]/(Nm_e a^2), k_{F_x}(m)$$

is the radius of the FS corresponding to the channel $m$ which depends on the shape of the FS.

After performing a quenched average of $I(\phi, \gamma, T)$ over $\gamma (W/t)$ with the Gaussian distribution we can look for self-sustaining currents.
In the clean system at $T = 0 K$ we would have again [8]:

$$I(\phi) = P \sum_{m=1}^{M} \sum_{q=1}^{\infty} \frac{2I_0(m)}{\pi q} \cos(qk_{F_x}(m)L) \sin\left(2\pi q \frac{\phi}{\phi_0}\right). \quad (12)$$

The self-sustaining currents can be obtained from equations (8) and (11).

It is known that for 2-D systems and for 3-D systems with 2-D conduction (an example of such structures are high $T_c$ superconductors in a normal state [10]) persistent currents depend crucially on the strength of the phase correlation between currents of different channels [8], [10] and therefore we have analysed three different cases namely the systems with rectangular, triangular and half-circular FS. The $k_{F_x}(m)$ is then given by

$$k_{F_x}(m) = \pm \frac{\pi}{a} \text{ for } |k_{F_y}(m)| \leq \frac{\pi}{b},$$

$$k_{F_x}(m) = \pm \frac{1}{a} \arccos \left[ -\frac{a^2}{b^2} \cos(k_{F_y}(m)b) \right], \quad (14)$$

and

$$k_{F_x}(m) = \pm \sqrt{\frac{2}{a^2} + \frac{2}{b^2} - k_{F_y}^2(m)} \quad (15)$$

respectively; $k_{F_y}(m) = m\pi/((M+1)b)$. Such shapes of the FS can be obtained in the tight-binding approximation depending on the crystal symmetry and on the band filling.

The most favorable situation is for the rectangular FS (found in bcc crystals for nearly half filled band) where self-sustaining currents $I_s$ are the easiest to obtain and are the largest. In the second case (crystals with simple
cubic symmetry at half filling), it is possible to obtain self-sustaining currents only for weakly disordered systems (ballistic regime) and for the maximal interchannel phase correlation, where $L/l \approx 2 + h/3$, $h$ is a positive integer; Fig. 5. In the third case (found at very low band filling), we have not obtained such currents, for physical values of parameters, because the interchannel correlations are too small [10]. The [$I(\phi)$] characteristics for different shapes of the FS and for $\frac{\tau}{\gamma} = 50000 \text{ Å}$ are presented in Fig. 6.

Self-sustaining currents are a hallmark of a phase coherence. Thus we can introduce, in analogy to superconductors, a notion of a critical field $H_c$ below which the system is in a coherent state. The system is in a coherent state if we get at $\phi_e = 0$ the nonzero crossing of the currents $I(\phi)$ and $\frac{\phi}{L}$ (Eq. (6)). Let us denote by $\phi_{\text{max}}$ the value of $\phi$ at which $I(\phi)$ reaches its maximum value $I_{\text{max}} \equiv I(\phi_{\text{max}})$.

If

$$I(\phi_{\text{max}}) \geq \frac{\phi_{\text{max}}}{L},$$  \hspace{1cm} (16)

we get a non-zero solution. Accepting the interpretation [12] that the critical field $H_c$ in the cylinder is determined by the maximum value of the current $I_{\text{max}}$ one finds from Eq. (16):

$$H_c = \frac{C I_{\text{max}}}{\mu_0 \pi R^2}$$  \hspace{1cm} (17)

The magnitude of $I_{\text{max}}$ depends on temperature, disorder and on the geometry of the FS and can be extracted from Figs. 4, 5.
The critical field $H_c$ as a function of the disorder parameter $1/\gamma$ and temperature $T$ is presented in Figs. 7 and 8 respectively. We see that it decreases with the increasing disorder and likewise decreases with the increasing temperature.

4 Conclusions

In the presented paper we have addressed the question of whether self-sustaining currents in nonsuperconducting rings and cylinders survive in the presence of disorder and finite temperature. The answer to this question is positive. We have performed some model considerations which show that self-sustaining currents can be obtained in weakly disordered systems at temperatures of the order of $1 \, K$ in the systems with strong correlations among the channel currents, i.e. in the systems with the FS having flat regions.

From the presented $I(\phi)$ characteristics we were able to determine the critical field $H_c$, below which the system is in a phase coherent state. We have shown that $H_c$ decreases with increasing disorder and temperature respectively.

5 Acknowledgments

Work was supported by Grant KBN 2P03B 129 14 and partly by Grant KBN PB 1108/P03/95/08. E.Z. acknowledges support from FNRS sabbatical
grant at the University of Liege. She thanks M. Ausloos for stimulating discussions.
References

[1a] D. Wohlleben, M. Esser, P. Freche, E. Zipper, M. Szopa, Phys. Rev. Lett., 66, 3191 (1991); D. Wohlleben, P. Freche, M. Esser, E. Zipper, M. Szopa, Mod. Phys. Lett. B, 6, 1481 (1992).

[1b] M. Szopa, E. Zipper, Int. J. Mod. Phys. B, 9, 161 (1995) and references therein.

[2] Quantum Coherence in Mesoscopic Systems, edited by B. Kramer, Plenum Press, New York 1991.

[3] H. F. Cheung, Y. Gefen, E. K. Riedel, W. H. Shih, Phys. Rev. B, 37, 6050 (1988).

[4] Steven E. Koonin, Computational Physics, The Benjamin/ Cummings Publishing Company, Inc. 1986.

[5] M. Lisowski, E. Zipper, R. Kosimow, Mol. Phys. Rep., 17, 137 (1997).

[6] G. Montambaux and H. Bouchiat, D. Sigeti and R. Friesner, Phys. Rev. B, 42, 7647 (1990).

[7] A. A. Abrikosov, Fundamentals of the Theory of Metals, North-Holland 1988.
[8] H. F. Cheung, Y. Gefen, E. K. Riedel, IBM J. Res. Develop., 32, 359 (1988).

[9] E. K. Riedel, H. F. Cheung, Y. Gefen, Phys. Scripta, T25, 357 (1989).

[10] M. Stebelski, M. Szopa, E. Zipper, Z. Phys. B, 103, 79 (1997); M. Stebelski, M. Lisowski, E. Zipper, Eur. Phys. J. B, 1, 215 (1998).

[11] E. V. Tsiper, A. L. Efros, J. Phys. Cond. Mat., 10, 1053 (1998).

[12] F. Bloch, Phys. Rev., 137, A787 (1965).
Figure Captions

Fig. 1. Persistent currents $I_1$ in a mesoscopic ring as a function of magnetic flux $\phi/\phi_0$ for different values of disorder. Numerical results for different $W/t$ are presented by symbols and analytical results according to formula (8) for different $\gamma$ are plotted by solid lines.

Fig. 2. Persistent currents $[I]/I_0$ as a function of magnetic flux $\phi/\phi_0$ for different parameters $\gamma$, in a set of 1-D mesoscopic rings with even number of conducting electrons $N_e$ in each ring. Self-sustaining spontaneous currents $I_s$ are denoted by circles.

Fig. 3. Persistent currents $[I]/I_0$ as a function of magnetic flux $\phi/\phi_0$ for different temperatures $T$, for the case presented in Fig. 2 with $\gamma = 20000$ Å.

Fig. 4. Persistent currents $[I]/I_0$ as a function of magnetic flux $\phi/\phi_0$ for different parameters $\gamma$, in a set of 1-D mesoscopic rings with odd number of conducting electrons $N_e$ in each ring. Self-sustaining currents $I_s$ denoted by circles correspond to flux trapping.

Fig. 5. Persistent currents $[I]/I_0$ as a function of magnetic flux $\phi/\phi_0$ for
different parameters $\gamma$, in a set of 2-D concentric mesoscopic cylinders with the triangular Fermi surface. Self-sustaining currents $I_s$ (trapped fluxes) are denoted by circles.

Fig. 6. Persistent currents $|I|/I_0$ as a function of magnetic flux $\phi/\phi_0$ for different shapes of the 2-D Fermi surfaces for $\gamma = 50000 \, \text{Å}$. In the inserted figure the shapes of the FS are shown.

Fig. 7. Critical fields $H_c$ as a function of the disorder parameter $\gamma^{-1}$ for the cases presented in figures 4, 5.

Fig. 8. Critical fields $H_c$ as a function of the temperature $T$ for the cases presented in figures 4, 5.
Fig. 1. [M. Lisowski, E. Zipper - Orbital Magnetic Ordering ...]
Fig. 2. [M. Lisowski, E. Zipper - Orbital Magnetic Ordering ...]
Fig. 3. [M. Lisowski, E. Zipper - Orbital Magnetic Ordering ...]
Fig. 4. [M. Lisowski, E. Zipper - Orbital Magnetic Ordering ...]
\[ M = 10000 \]
\[ P = 2000 \]
\[ N = 40000, \ N_e = 20000 \]
\[ a = b = 1 \text{ Å} \]

1. \( \gamma = 20000 \text{ Å} \)
2. \( \gamma = 30000 \text{ Å} \)
3. \( \gamma = 50000 \text{ Å} \)
   \[ T_c \cong 0.40 \text{ K} \]
4. clean system
   \[ T_c \cong 1.36 \text{ K} \]

**Fig. 5.** [M. Lisowski, E. Zipper - Orbital Magnetic Ordering ...]
Fig. 6. [M. Lisowski, E. Zipper - Orbital Magnetic Ordering ...]
Fig. 7. [M. Lisowski, E. Zipper - Orbital Magnetic Ordering ...]
Fig. 8. [M. Lisowski, E. Zipper - Orbital Magnetic Ordering ...]