Possibility of long-range order in clean mesoscopic cylinders

M. Lisowski, E. Zipper, and M. Stebelski
Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland
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A microscopic Hamiltonian of the magnetostatic interaction is discussed. This long-range interaction can play an important role in mesoscopic systems leading to an ordered ground state. The self-consistent mean-field approximation of the magnetostatic interaction is performed to give an effective Hamiltonian from which the spontaneous, self-sustaining currents can be obtained. To go beyond the mean-field approximation the mean-square fluctuation of the total momentum is calculated and its influence on self-sustaining currents in mesoscopic cylinders with quasi-one-dimensional and quasi-two-dimensional conduction is considered. Then, by the use of the microscopic Hamiltonian of the magnetostatic interaction for a set of stacked rings, the problem of long-range order is discussed. The temperature T^* below which the system is in an ordered state is determined. [S0163-1829(99)03311-1]

I. INTRODUCTION

One of the most exciting areas of physics is the study of mesoscopic electronic systems, i.e., metal or semiconductor samples that are sufficiently small and at sufficiently low temperature, such that inelastic electron-phonon scattering is reduced and the electron propagates as a phase coherent wave throughout the entire sample.[1]

Recently in a series of papers[2,3] we discussed a possibility of spontaneous persistent currents in relatively clean (ballistic regime) metallic or semiconducting systems of cylindrical geometry.

It was shown in the mean-field approximation (MFA) that the inclusion of the magnetostatic interaction among electrons can lead to an ordered ground state with spontaneous self-sustaining orbital currents that run without support of external magnetic field.

In our investigations we considered a collection of many mesoscopic rings with a thickness $d \ll R$ (R is the radius of the ring) stacked along z axis and the three-dimensional (3D) mesoscopic cylinder of very small thickness.[4]

In this paper we want to give some justification to the calculation mentioned above, because there was no microscopic theory of this phenomenon till now. We will examine a microscopic Hamiltonian for the magnetostatic (current-current) interaction and show that the self-consistent MFA of it gives the effective Hamiltonian H^{MF} leading to self-sustaining currents. We also show that magnetostatic interaction is long range and therefore the criteria of the MFA are met.

The orbital magnetic interaction and its static version, the magnetostatic coupling, has been discussed previously by Pines and Nozieres[5] and has been shown to be small in macroscopic metallic samples. However, this interaction should be reexamined in mesoscopic systems where the presence of energy gaps in the energy spectrum changes qualitatively its physical properties leading, e.g., to persistent currents driven by the static magnetic flux ϕ at low temperatures.[6] Persistent currents create orbital magnetic moments and their interaction can lead to interesting coherent collective phenomena, which bear some resemblance to ferromagnetism and to superconductivity.[2,7]

To go beyond the MFA and discuss fluctuations we follow the ideas developed by Bloch.[8] He discussed the problem of quantum coherence in a macroscopic, metallic ring manifested, e.g., by the thermodynamically stable flux trapping at zero external magnetic field. He covers in his paper different long-range characteristics of the normal and the superconductive state of a metal.

Irrespective of the specific dynamical properties of the systems he shows that the general criteria for flux trapping are closely related to the mean-square fluctuation of the total momentum and depend strongly on the dimensionality of the system.

We will show, using Bloch's formulas that if we reduce the dimensions of a macroscopic cylinder made of a normal metal or semiconductor to mesoscopic dimensions, the system exhibits coherent properties absent in macroscopic samples. We will formulate the criteria under which flux trapping can be obtained in mesoscopic cylinders with quasi-one-dimensional (quasi-1D) and quasi-2D conduction. In particular, we will discuss the mean-square fluctuation of the total momentum—the decisive quantity for the characterization of the properties of the system. We show that it is smaller in mesoscopic systems than in the corresponding macroscopic ones thus favoring quantum coherence.

Finally, using the microscopic Hamiltonian we discuss the possibility of the long-range order in a mesoscopic cylinder made of a set of mesoscopic rings. We calculate the correlation length and the characteristic temperature under which the system is in a magnetically ordered state.

II. MAGNETOSTATIC INTERACTION

The general formula for the magnetostatic interaction is of the form

$$H_{mgt} = -\frac{\mu_0}{8\pi}\int d^3\mathbf{r}\, d^3\mathbf{r}'\, \frac{\mathbf{J}(\mathbf{r})\cdot\mathbf{J}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \tag{1}$$

where $\mathbf{J}(\mathbf{r}) = e\mathbf{p}(\mathbf{r})/m_e$, $\mathbf{J}(\mathbf{r})$ is the current density, $\mathbf{p}(\mathbf{r})$ is the momentum of an electron.

Let us assume that the currents run in a set of M_z mesoscopic rings of small thickness deposited along the z axis. We can write

$$\mathbf{J}(\mathbf{r}) = \sum_{m/1}^{M_z} I_m \oint_{C_m} \delta^3(\mathbf{r} - \boldsymbol{\xi}_m(s)) d\boldsymbol{\xi}_m, \tag{2}$$

where C_m is given by a parametric equation for an electron going around the circumference of a ring, and $\boldsymbol{\xi}_m = \boldsymbol{\xi}_m(s)$, s is the coordinate along the circumference of the ring, I_m is the current in the mth ring.

We obtain

$$H_{mgt} = -\frac{1}{2}\sum_{m/1}^{M_z} \sum_{m'/1}^{M_z} \mathcal{L}_{mm'} I_m I_{m'}, \tag{3}$$

where

$$\mathcal{L}_{mm'} = \frac{\mu_0}{4\pi} \oint_{C_m} \oint_{C_{m'}} \frac{d\boldsymbol{\xi}_m d\boldsymbol{\xi}_{m'}}{|\boldsymbol{\xi}_m - \boldsymbol{\xi}_{m'}|}, \quad \mathcal{L}_{mm'} = \mathcal{L}_{m'm}. \tag{4}$$

Thus we have obtained the interaction Hamiltonian of the currents from different rings. In this derivation we neglected the self-inductance effects in each single ring. It can easily be seen that they are small.

The interaction constant $\mathcal{L}_{mm'}$ depends on the sample geometry; here it has to be calculated for the rings deposited along the z axis at distance $z_{mm'} = z_m - z_{m'}$.

The result is[9]

$$\mathcal{L}_{mm'} = \mu_0 R\left[\left(\frac{2}{h_{mm'}} - h_{mm'}\right)K - \frac{2}{h_{mm'}}E\right], \tag{5}$$

where

$$h_{mm'}^2 = \frac{4R^2}{4R^2 + z_{mm'}^2}, \tag{6}$$

$$K = \int_0^{\pi/2} \frac{d\theta}{(1 - h^2 \sin^2\theta)^{1/2}}, \quad E = \int_0^{\pi/2} (1 - h^2 \sin^2\theta) d\theta, \tag{7}$$

K and E are the elliptical integrals of the I and II kind, respectively.

The z dependence of the coupling constant $\mathcal{L}$ is presented in Fig. 1. We see that the interaction (3) is a long-range interaction. For small z it falls down slowly proportionally to $\mu_0 R \ln(R/z-2)$, for large z it falls down faster proportionally to $1/z^3$. The interaction constant depends only on R and on the relative distance of the centers of the rings.

As the currents I_m can run only in the clockwise or anticlockwise direction the Hamiltonian (3) has the form of the Ising Hamiltonian. It can be also expressed via the momenta p_m, $p_{m'}$ from different rings.

For the ring geometry we get

$$I_m = \frac{e}{2\pi R m_e} p_m, \tag{8}$$

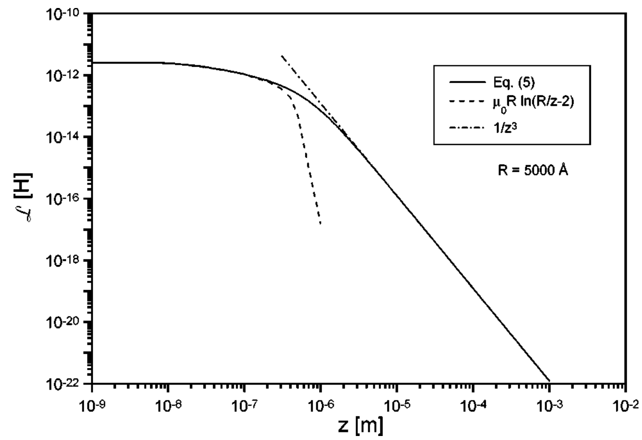

FIG. 1. The interaction constant $\mathcal{L}$ as a function of distance z between the ring centers.

$$p_m = \sum_{n/1}^{N^R} p_{nm},$$

where N^R is a number of conducting electrons in a single ring.

H_{mgt} given by Eq. (3) can be rewritten in the form

$$H_{mgt} = -\frac{e^2}{2m_e^2}\sum_{m/1}^{M_z} \sum_{m'/1}^{M_z} g_{mm'} p_m p_{m'}, \tag{9}$$

$$g_{mm'} = \frac{1}{4\pi^2 R^2}\mathcal{L}_{mm'}.$$

If we add to H_{mgt} the kinetic energy term and if we assume that the external magnetic field parallel to the z axis is applied to the system, we obtain Hamiltonian H:

$$H = \frac{1}{2m_e}\sum_{m/1}^{M_z} \sum_{n/1}^{N^R} p_{nm}^2 - \frac{e^2}{2m_e^2}\sum_{m/1}^{M_z} \sum_{m'/1}^{M_z} g_{mm'} p_m p_{m'}, \tag{10}$$

where $p_{nm} = p_{nm}^0 - eA_e$; p_{nm}^0 is the momentum of the nth electron in mth ring. A_e is the vector potential of an external magnetic field that points in the x direction measured along the ring.

The first term in Eq. (10) represents the kinetic energy of electrons in the external magnetic field, the second term represents the orbital magnetic interaction; due to the negative sign it favors states with large total momentum in competition with the kinetic energy.

III. MEAN-FIELD APPROXIMATION OF MAGNETOSTATIC COUPLING

We have seen in Sec. II that the magnetostatic coupling is a long-range interaction. This indicates, in particular, that thermodynamic fluctuations of the current will be strongly supressed.[10]

Let us perform a self-consistent MFA of the interaction (9); such an approximation is known to be good for a long-range interaction:

$$H_{mgt}=-\frac{e^2}{2m_e^2}\sum_m p_m \sum_{m'} g_{mm'}p_{m'} \equiv -\frac{e}{2m_e}\sum_m p_m A_I(z_m), \tag{11}$$

$$A_I(z_m)=\frac{e}{2m_e}\sum_{m'} g_{mm'}p_{m'}, \tag{12}$$

$$BC \to B\langle C\rangle + \langle B\rangle C - \langle C\rangle\langle B\rangle,$$

$$H_{mgt}=-\frac{e}{2m_e}\sum_m [2p_m\langle A_I(z_m)\rangle - \langle p_m\rangle\langle A_I(z_m)\rangle], \tag{13}$$

where the first term in Eq. (13) has been obtained by use of the symmetry relation (4), $\langle A_I(z_m)\rangle=(e/2m_e)\Sigma_{m'}g_{mm'}\langle p_{m'}\rangle \equiv A_I$, where we assumed that $\langle p_m\rangle \equiv \langle p\rangle$ is the same for all rings, and hence from Eq. (8) $\langle I_m\rangle \equiv \langle I\rangle$.

Assuming that our stack of M_z rings forms a long cylinder of length l we can calculate the vector potential A_I. We get

$$A_I=\mu_0 R\frac{M_z\langle I\rangle}{2l}. \tag{14}$$

Calculating the current $\langle I\rangle$ with a total vector potential $A=A_e+A_I$ we get

$$\langle I\rangle=\frac{e}{2\pi R m_e}(\langle p\rangle - N^R e A_I). \tag{15}$$

Inserting Eq. (15) into (14) we obtain the self-consistent equation for A_I:

$$A_I=\frac{\mu_0 e M_z}{4\pi l m_e}(\langle p\rangle - N^R e A_I), \tag{16}$$

from which we get

$$eA_I=\frac{\eta}{1+\eta N^R M_z}M_z\langle p\rangle, \tag{17}$$

where

$$\eta=\frac{\mu_0 e^2}{4\pi l m_e}.$$

Inserting $\langle p\rangle$ from Eq. (17) into Eq. (13) we obtain the Hamiltonian H [Eq. (10)] in the self-consistent mean-field approximation:

$$H^{MF}=\frac{1}{2m_e}\sum_{m/1}^{M_z}\sum_{n/1}^{N^R}(p_{nm}-eA_I)^2+\frac{\phi_I^2}{2\mathcal{L}}, \tag{18}$$

where $\mathcal{L}=\mu_0\pi R^2(\sqrt{l^2-R^2}-R)/l^2$, $\quad \phi_I=2\pi R A_I$.

The Hamiltonian (18) was the basis of our previous investigations[2] of spontaneous self-sustaining currents [see Eqs. (50) and (51)]. Its derivation from the long-range current-current interaction serves as a justification of the use of the Hamiltonian (18) to investigate magnetic properties of mesoscopic systems.

It has been generally believed that the MFA should work well for long-range forces. However, it has been shown in Ref. 11 that the above statement is correct if an additional condition is fulfilled. The authors defined there the quantity S:

$$S=\frac{\left(\sum_{m'}\mathcal{L}_{mm'}\right)^2}{\sum_{m'}\mathcal{L}_{mm'}^2}, \tag{19}$$

where $\mathcal{L}_{mm'}$ is the interaction constant. They proved that MFA is correct if $S \gg 1$.

We have calculated S with $\mathcal{L}_{mm'}$ given by Eq. (5) for the following set of parameters: $b \equiv z_{m,m+1}=10$ Å, $R=5000$ Å, $M_z \sim 10^3$. We have obtained $S\sim 10^5$; it means that the MFA should work well in the case considered by us.

IV. SUMMARY OF THE BLOCH'S RESULTS

We are going now to investigate the possibility of flux trapping in mesoscopic cylinders using the ideas developed by Bloch.[8] The general criteria for flux trapping are closely related to mean-square fluctuations and give a natural way to describe the system in terms of the two-fluid model. At first we briefly recall Bloch's results.

Let us consider a system of N particles with mass m and charge e, contained in a ring with radius R and radial width $d \ll R$. We assume that the magnetic field parallel to z axis is caused by a current around the ring, so the vector potential $A=\phi/(2\pi R)$ points in the x direction.

The total momentum in the x direction is given by

$$P_x=\sum_{n/1}^{N} p_n^0, \tag{20}$$

where p_n^0 represents the momentum of the nth particle ($n=1,2,\ldots,N$).

The Hamiltonian of the particles is of the form

$$H=\frac{(P_x-NeA)^2}{2Nm_e}+H', \tag{21}$$

where H' contains the kinetic energy of the motion in the y and z direction and of the relative motion in the x direction as well as any additional terms that arise from interactions and characterize the specific dynamical properties of the system.

From the symmetries and periodic boundary conditions[8] we get the eigenvalues of P_x:

$$P=n\frac{\hbar}{R}=(N\nu+\mu)\frac{\hbar}{R}, \tag{22}$$

where n, ν are arbitrary integers, and μ is likewise an integer such that

$$-\frac{N}{2}<\mu\leq\frac{N}{2}.$$

Eigenenergies of the system are given by

$$E_{\mu\nu q}=\frac{\hbar^2 N\left(\nu-\phi'+\frac{\mu}{N}\right)^2}{2m_e R^2}+E'_{q\mu}, \tag{23}$$

where q represents the system of additional quantum numbers necessary in addition to $P(\nu,\mu)$ in order to fully characterize the state of the system; $\phi'=\phi/\phi_0$, $\phi_0=h/e$.

Using Eq. (23) we can calculate the free energy from the particles. The flux-dependent part of the total free energy is

$$F(\phi')=F_1(\phi')+F_2(\phi'), \tag{24}$$

where $F_1(\phi')$ is a periodic function of ϕ' with period 1,

$$F_1(\phi')=-k_BT\ln Z_1(\phi'), \tag{25}$$

$$Z_1(\phi')=\sqrt{\frac{\pi}{N\gamma}}\left(1+2\sum_{g/1}^{\infty} a_g e^{-(\pi g)^2/N\gamma}\cos 2\pi g\phi'\right), \tag{26}$$

$$a_g=\sum_{\mu} z_\mu e^{-2\pi i g\mu/N}, \tag{27}$$

$\gamma=\hbar^2/(2m_eR^2k_BT)$; z_μ is the statistical weight of the state $E'_{q\mu}$,

$$\sum_{\mu} z_\mu=1, \quad z_\mu\geqslant 0; \tag{28}$$

$$F_2(\phi')=\frac{\hbar^2\phi'^2}{2e^2\mathcal{L}}, \tag{29}$$

where $F_2(\phi')$ is the energy stored in the magnetic field, $\mathcal{L}$ is the self-inductance of the ring.

Thermodynamically stable flux trapping is determined by those values of ϕ' for which $F(\phi')$ has a minimum. To achieve it a strong variation of $F_1(\phi')$ is necessary to prevent the dominance of $F_2(\phi')$, which has minimum at $\phi'=0$.

Let us consider now three special cases that elucidate how different states of matter can be described in this model. The information about specific properties of the system is contained in the quantities z_μ.

a. z_μ is independent of μ, i.e., $z_\mu=1/N$. After some algebra we arrive at

$$Z_1(\phi')=\sqrt{\frac{\pi}{N\gamma}}\left(1+2\sum_{g/1}^{\infty} e^{-(\pi g)^2N/\gamma}\cos 2\pi g N\phi'\right). \tag{30}$$

The general periodicity in $\phi'=1$ is accompanied here by a far shorter period $\phi'=1/N$, which is vanishingly small for large N. Besides the amplitude of the oscillation is small at any realistic temperature leading to a very small variation of $F_1(\phi')$ and hence to the absence of stable flux trapping. This situation corresponds to the case where the system exhibits no long-range order and is characteristic of the normal state of a metal.

b. $z_\mu=\delta_{\mu 0}$. From Eq. (26) we find

$$Z_1(\phi')=\sqrt{\frac{\pi}{N\gamma}}\left(1+2\sum_{g/1}^{\infty} e^{-(\pi g)^2/N\gamma}\cos 2\pi g\phi'\right), \tag{31}$$

which has the periodicity with $\phi'=1$. However, in order to get a stable flux trapping for $\phi'\neq 0$ we need

$$N\gamma=\frac{N\hbar^2}{2m_eR^2k_BT}\gg 1, \tag{32}$$

which is satisfied at low temperatures T. Then $F_1(\phi')$ can well dominate the part $F_2(\phi')$ in Eq. (24). The pronounced minima of $F(\phi')$ occur at $\phi'=\nu$ and are equivalent with stable flux trapping. This case corresponds to a condensed ideal Bose gas where all particles have momentum $p=\nu\hbar/R$.

c. $z_\mu=\frac{1}{2}(\delta_{\mu 0}+\delta_{\mu(N/2)})$. The partition function is of the form

$$Z_1(\phi')=\sqrt{\frac{\pi}{N\gamma}}\left(1+2\sum_{g/1}^{\infty} e^{-(2\pi g)^2/N\gamma}\cos 4\pi g\phi'\right). \tag{33}$$

This expression has the periodicity in ϕ' with $\phi'=1/2$, i.e., with $\phi=h/2e$. This case exhibits the property that $N/2$ pairs all have the same momentum $p=\nu\hbar/R$ and corresponds to the long-range order characteristic of a superconductor at temperatures in which the condition (32) is satisfied.

To consider other, more general cases one assumes that the total momentum P can admit the values given by Eq. (22) with $\mu\neq 0$, but with a sharp maximum around $\mu=0$. The formula for $Z_1(\phi')$ has then the form

$$Z_1(\phi')=\sqrt{\frac{\pi}{N\gamma}}\left(1+2\sum_{g/1}^{\infty} e^{-(\pi g)^2/[N\gamma(1-\rho)]}\cos 2\pi g\phi'\right), \tag{34}$$

where

$$\rho=\frac{\langle(\Delta P)^2\rangle}{Nm_ek_BT}, \quad 0\leqslant\rho\leqslant 1, \tag{35}$$

$\langle(\Delta P)^2\rangle$ is the mean-square fluctuation of momentum P around the set of values $\phi' N\hbar/R$, where ϕ' is an integer multiple of the period, and ρ can be called a relative fluctuation;

$$\langle(\Delta P)^2\rangle=\frac{\hbar^2}{R^2}\langle(\Delta\mu)^2\rangle=-m_ek_BT\sum_{\alpha} p_\alpha\frac{\partial f(p_\alpha)}{\partial p_\alpha}, \tag{36}$$

where $\langle(\Delta P)^2\rangle=\langle P^2\rangle-\langle P\rangle^2$; $f(p_\alpha)$ is the mean number of particles with momentum $p_\alpha=\hbar(\alpha-\phi')/R$, $\alpha=0,\pm 1,\pm 2,\ldots$

Equation (34) covers the special cases discussed before. Case *a* corresponds to the situation where all values of μ are equally probable, which leads to $\rho\to 1$; $Z_1(\phi')$ becomes then independent of ϕ' with the exclusion of flux trapping. Cases *b* and *c* correspond to $\rho=0$ and thus describe the systems in the coherent state with no fluctuations.

The intermediate case

$$0<\langle(\Delta P)^2\rangle<Nm_ek_BT, \tag{37}$$

or equivalently, $0<\rho<1$, still results in a pronounced variation of $F_1(\phi')$ as long as

$$N\gamma(1-\rho)\gg 1. \tag{38}$$

It means that stable flux trapping can be expected as soon as $\langle(\Delta P)^2\rangle$ is found to be smaller than the maximal value of mean-square fluctuation of P.

V. FLUX TRAPPED IN MESOSCOPIC CYLINDERS

We will perform now, using Bloch's formalism, some model calculations of flux trapped in mesoscopic hollow cylinders of radius R, length l, and wall thickness d $(d\ll R)$ made of a normal metal or semiconductor. Such cylinders can be treated as a multichannel system with M_z channels in the length and M_r channels in the thickness of the cylinder $(M\equiv M_zM_r)$, with the total number of conducting electrons $N=N^RM$. We will study the systems with quasi-1D and quasi-2D conduction. It is known that coherent response in mesoscopic cylinders can be obtained[12,4] for systems with large phase correlation of currents from different channels, which is related to the shape of the Fermi surface (FS). The most favorable situation is for systems with quasi-1D conduction, i.e., with a flat FS parallel to axes of the wave vector **k**. There exists then a perfect correlation among the channel currents and the magnetic response is the strongest. Such FS can be obtained in bcc crystals,[13] in low-dimensional organic conductors with the overlap of the orbitals mainly in one direction, and when a cylinder is made of a set of M quasi-1D rings stacked along the z axis by, e.g., the lithographic method. Such multiple quantum chains can be mapped into a system with the flat (rectangular) FS.

In the case of quasi-2D conduction our cylinder can be constructed from a set of M_r 2D coaxial cylinders (e.g., multiwall carbon nanotubes and cylinders made of a material with layered structure).

To simulate different shapes of the 2D FS (Refs. 4 and 14) we can use the equation

$$k_F^u=k_{F_x}^u+k_{F_z}^u, \tag{39}$$

where u is an integer number.

For $u=2$ we get the circular FS, for $u\geq 12$ the rectangular one, and for $2<u<12$ the rectangular FS with rounded corners. For the circular FS the currents from different channels add almost without correlation, the correlation increases with increasing the curvature of the FS, i.e., with increasing u.

Let us consider at first a set of M quasi-1D rings stacked along the z axis (or in general a cylinder with quasi-1D conduction). Let us assume that the magnetic field is caused by persistent currents from all rings. Thus we meet conditions from the Bloch's paper and our mean-field Hamiltonian H^{MF} [Eq. (18)] leads to the free energy given by Eq. (24) with

$$F_1(\phi')=MF_1^R(\phi'), \tag{40}$$

where $F_1^R(\phi')$ is the free energy of a single ring.

In general an external magnetic flux ϕ_e parallel to the z axis can be also applied to the system but we are mainly interested in the self-sustaining flux at $\phi_e=0$.

The necessary condition for coherent behavior has the form

$$N^R\gamma\equiv\frac{\Delta_0}{k_BT}\gg 1, \tag{41}$$

where $\Delta_0=\hbar^2N^R/(2m_eR^2)$, Δ_0 is the quantum size energy gap at the FS.

Let us calculate the momentum P defined as in Eq. (22) for three different model cases.

(1) If the number of electrons N^R in each ring is odd we find

$$P=N\nu\frac{\hbar}{R}\quad\text{for}\quad(\nu-\tfrac{1}{2})<\phi'<(\nu+\tfrac{1}{2}),\quad \nu=0,1,\ldots, \tag{42}$$

which corresponds to the case b with $z_\mu=\delta_{\mu 0}$ and $\rho=0$. Calculating the minimum of the total free energy [Eq. (24)] at $\phi_e=0$ and at $T\ll\Delta_0/k_B$ we get the value of the flux trapped ϕ'^t in the cylinder:[2]

$$\phi'^t_{odd}=\frac{\nu}{1+\kappa}, \tag{43}$$

where

$$\kappa=\frac{4\pi^2m_eR^2}{e^2\mathcal{L}N}\quad\text{and}\quad|\nu|\leq\tfrac{1}{2}(1+\kappa^{-1}).$$

Equation (43) reveals the influence of the finite-size effect—the flux trapped is quantized in units less than ϕ_0.[15] For macroscopic samples $\kappa\to 0$ and $\phi'^t_{odd}=\nu$.

(2) If the number of electrons N^R in each ring is even, the momentum P is

$$P=N(\nu+\tfrac{1}{2})\frac{\hbar}{R}\;\;\text{for}\;\;(\nu-\tfrac{1}{2})<\phi'<(\nu+\tfrac{1}{2}),\quad \nu=0,1,\ldots, \tag{44}$$

which corresponds to $z_\mu=\delta_{\mu(N/2)}$ and stable values of trapped flux are

$$\phi'^t_{even}=\frac{\nu+\frac{1}{2}}{1+\kappa},\quad |\nu+\tfrac{1}{2}|<\tfrac{1}{2}(1+\kappa^{-1}). \tag{45}$$

For macroscopic samples $\phi'^t_{even}=\nu+\frac{1}{2}$, which corresponds to stable minima of the free energy at half-integral values of ϕ_0.

We see that a system under consideration exhibits thermodynamically stable persistent currents and flux trapped at temperatures $T\ll\Delta_0/k_B$. This condition is easily satisfied for mesoscopic rings at $T\leq 1$ K (e.g., for $R\sim 1$ μm, $\Delta_0/k_B\sim 12.5$ K); it is, however, unrealistic for macroscopic samples (for $R\sim 1$ cm, $\Delta_0/k_B\sim 10^{-3}$ K).[16]

Our treatment is not only for identical rings. We have performed the calculations for a set of rings in which the number of electrons N^R changes in the range $N^R=\overline{N^R}\pm\Delta N^R$, $\Delta N^R=10$. We have considered two kinds of changes: (i) N^R fluctuates from $\overline{N^R}$ to $\overline{N^R}\pm 2n$, $n=1,2,3,4,5$—the influence of such fluctuation on the persistent current is very small. (ii) N^R changes from $\overline{N^R}$ to $\overline{N^R}$

$\pm(2n-1)$—the influence of this kind of changes on the current is fairly large (see below).

In the presented paper we study mainly the systems with the diamagnetic reaction on small magnetic flux ϕ. The rings with odd N^R give a diamagnetic current whereas those with even N^R give a paramagnetic current. We have found that the diamagnetic reaction and trapped flux can still be obtained if about 20% of rings carry an even number of conducting electrons.

(3) Finally, we may also consider the model case where roughly half of the rings have an even number of electrons and half of the rings have an odd number of electrons. It corresponds to case *c*, where $z_\mu = \frac{1}{2}(\delta_{\mu 0} + \delta_{\mu(N/2)})$ and the minima of the free energy occur with the twice smaller period. We have not discussed this situation here in details because the total current in this case is paramagnetic.[2]

We now go beyond the MFA and consider fluctuations around the set of P values discussed above. We assume that the total momentum P in a cylinder given by Eq. (22) can admit the values with $\mu \neq 0$ and/or $\mu \neq N/2$ but with a maximum at $\mu = 0$ and/or $\mu = N/2$. This assumption leads to the partition function $Z_1(\phi')$ given by Eq. (34) and the criteria for quantum coherence manifesting themselves in the flux trapping are ultimately related to the magnitude of the mean-square fluctuation of momentum P. The condition for coherent behavior takes then the form

$$\frac{\Delta_0(1-\rho)}{k_B T} \gg 1, \tag{46}$$

and we see that the fluctuations decrease the energy gap. Equation (34) covers also as a special case a situation characteristic of a normal state of a metal (no flux trapping) in which all values of μ can be found, with equal probability, in the formula for P.

Stable flux trapping can be expected as soon as $\langle(\Delta P)^2\rangle$ is found to be a small fraction below $N m_e k_B T$, called by Bloch the equipartition value. In the following we will calculate $\langle(\Delta P)^2\rangle$ from Eq. (36) and relate its magnitude to the coherent behavior of the sample.

The mean number of electrons with momentum $p_{\alpha m}$, $f(p_{\alpha m})$ is given by the Fermi-Dirac distribution function:

$$f(p_{\alpha m}) \equiv f(E_{\alpha m}(\phi)) = \frac{1}{e^{(E_{\alpha m}-\mu_c)/k_B T}+1}, \tag{47}$$

where μ_c is calculated from the condition

$$N = M_r \sum_{m/1}^{M_z} \sum_{\alpha/0,\pm 1}^{\pm\infty} f(E_{\alpha m}(\phi)). \tag{48}$$

The electron energy eigenvalues, calculated by the use of periodic boundary conditions in the x direction and cyclic boundary conditions in the z direction:

$$E_{\alpha m} = \frac{1}{2m_e}\left[\left(\frac{\hbar}{R}\alpha - eA\right)^2 + \hbar^2 k_z^2(m)\right], \quad A = \frac{\phi}{2\pi R}, \tag{49}$$

$$\phi = \phi_e + \phi_I, \tag{50}$$

with ϕ the total flux contained in the cylinder, $\phi_I = \mathcal{L} I(\phi)$, where

$$I(\phi) = \frac{e\hbar}{2\pi m_e R^2} M_r \sum_{m/1}^{M_z} \sum_{\alpha/0,\pm 1}^{\pm\infty} (\alpha - \phi') f(E_{\alpha m}(\phi)), \tag{51}$$

and after expansion in the Fourier series,[4]

$$I(\phi) = \frac{4eak_BT}{\pi\hbar} M_r \sum_{m/1}^{M_z} \sum_{g/1}^{\infty} k_{F_x}(m) \times \frac{\exp\left(-\frac{2\pi^2 g k_B T}{\Delta_0(1-\rho)}\right)}{1-\exp\left(-\frac{4\pi^2 g k_B T}{\Delta_0(1-\rho)}\right)} \cos[2\pi g R k_{F_x}(m)] \times \sin(2\pi g \phi'),$$

where a is the lattice constant, and according to Eq. (39) $k_{F_x}(m) = k_F[1-(k_z(m)/k_F)^u]^{1/u}$, $k_z(m) = m\pi/l$, $m = 1,2,\ldots,M_z$.

Equations (50) and (51) form a set of self-consistent equations for the current. The question of existence of self-sustaining, persistent currents is reduced to the problem of whether these equations have stable, nonvanishing solutions at $\phi_e = 0$.

Notice that the dispersion relation (49) is modified by the presence of the flux ϕ_I coming from the currents and has to be calculated in a self-consistent way. We show below that ϕ_I produces a dynamic gap in the system and therefore increases coherence.

The values of $\langle(\Delta P)^2\rangle$ for different shapes of the FS and for $R \simeq 10^4$ Å$/(2\pi)$, $M_z = 10\,000$, $M_r = 100$ at $T = 15$ K are presented in Table I.

For the rectangular FS, corresponding to quasi-1D conduction, we assumed that it lies in the middle of an energy gap Δ_0 for an electron going along the circumference of the cylinder. We see that the magnitude of $\langle(\Delta P)^2\rangle$ (or the corresponding relative fluctuation ρ) decreases with increasing the curvature of the FS. The difference between the normal and the coherent state of a mesoscopic cylinder is reflected in the magnitude of $\langle(\Delta P)^2\rangle$.

In the ideal, limiting case corresponding to $\langle(\Delta P)^2\rangle = 0$ [case (1)] the system is fully coherent, i.e., $N = N_c$, where N_c is the number of electrons in a coherent state.

Finite values of $\langle(\Delta P)^2\rangle$ can be interpreted by use of the two-fluid model[8,7] as being proportional to $N_n = N - N_c$, N_n is the number of particles in the normal state. We can write $\langle(\Delta P)^2\rangle = N_n m_e k_B T$.

The maximal values of $\langle(\Delta P)^2\rangle$ given by Eq. (36) will be obtained for macroscopic values of R where the replacement of the sums over α by integrals is permitted. This gives us $\langle(\Delta P)^2\rangle = N m_e k_B T$ or $N = N_n$ and the system is in a normal phase. However, for mesoscopic cylinders such replacement is not allowed and the presence of finite-size energy gaps leads to $N_n < N$, which means that a part of the electrons is in a coherent state. The presence of coherent electrons results in persistent currents, the amplitude of which depends on the shape of the FS.

TABLE I. The relative mean-square fluctuations of the total momentum P, $\rho = \langle (\Delta P)^2 \rangle / N m_e k_B T$, in a system made of 2D coaxial cylinders with $N = 10\,001 \times 10^6$ conducting electrons (lattice constant $a = 1$ Å, $b = 5$ Å) at temperature $T = 15$ K, in the magnetic flux ϕ_e and $\phi = \phi_e + \phi_I$, respectively, for different shapes of the Fermi surface. ϕ_I has been calculated for each ϕ_e in the self-consistent way, assuming the number of interacting coaxial cylinders $M_r = 100$. N_n represent the total number of "normal" electrons in the system. The number of coherent electrons is $N_c = N - N_n$.

Shape of the FS	ϕ_e / ϕ_0	ϕ / ϕ_0	ρ^{ϕ_e}	ρ^{ϕ}	$N_n{}^{\phi_e} \times 10^6$	$N_n{}^{\phi} \times 10^6$
Half-circular	0.000	0.000	0.9851	0.9851	9852.22	9852.22
($u = 2$)	0.100	0.088	0.9968	0.9944	9969.15	9944.78
Rectangular with	0.000	0.000	0.0695	0.0695	0695.52	0695.52
rounded corners	0.100	0.017	0.1207	0.0709	1207.51	0708.92
($u = 6$)						
Rectangular	0.000	0.000	0.0688	0.0688	0687.00	0687.00
($u = 12$)	0.100	0.016	0.1195	0.0700	1195.00	0700.00
	0.250	0.041	0.5725	0.0767	5727.00	0768.00

Persistent currents driven by an external flux ϕ_e vanish if we switch the external field off. However, the presence of the flux ϕ_I coming from the magnetostatic interaction can lead to persistent self-sustaining currents or, in other words, to trapped flux. In general persistent currents can be paramagnetic or diamagnetic. Paramagnetic self-sustaining currents correspond to spontaneous currents,[4] and diamagnetic self-sustaining currents correspond to flux trapping.[7] In the following we will study mainly the diamagnetic solutions.

In order to discuss the influence of ϕ_I on the coherent properties of mesoscopic cylinders we calculate an energy gap at the FS for electrons going around the circumference of the cylinder (and for $\phi < \phi_0/2$). Using Eq. (49) we find

$$\Delta_F \equiv E_{\alpha_F+1,m} - E_{\alpha_F,m} = \Delta_0 \left(1 - 2\phi_e' + 2\frac{\mathcal{L}|I|}{\phi_0} \right). \tag{52}$$

Δ_F contains a term

$$\Delta_d \equiv \Delta_0 \frac{\mathcal{L}|I|}{\phi_0}, \tag{53}$$

Δ_d is the dynamic part of an energy gap that should increase coherence in the sample.

That this is really the case we can see from the comparison of the first and second columns in Table I. We see that the mean-square fluctuation $\langle (\Delta P)^2 \rangle$ when calculated with the dispersion relation pertinent for normal electrons, namely, with $\mathcal{E}_{\alpha m} = [(\hbar\alpha/R - eA_e)^2 + \hbar^2 k_z^2(m)]/(2m_e)$ is larger than $\langle (\Delta P)^2 \rangle$ calculated with the dispersion relation (49), modified by the presence of self-consistent flux ϕ_I. Thus the presence of the magnetostatic coupling decreases fluctuations and the number of normal electrons in the sample. This is also seen in Fig. 2 where the temperature smearing of the distribution function calculated with the self-consistent flux is smaller than that calculated with ϕ_e. We also checked that, as should be expected, the mean-square fluctuation $\langle (\Delta P)^2 \rangle$ decreases with an increase in the number of interacting channels.

This type of analysis bears some resemblance to the two-fluid description of a superconductor.[17] For free electrons with the dispersion relation $\mathcal{E}_\alpha$ the electron density can be written as

$$n = -\frac{2\hbar^2}{3m_e V} \sum_{\mathbf{k}} \mathbf{k}^2 \frac{\partial f(\mathcal{E}_{\mathbf{k}})}{\partial \mathcal{E}_{\mathbf{k}}}. \tag{54}$$

Defining similarly the density of normal electrons in a superconductor, with a dispersion relation $E_{\mathbf{k}} = \sqrt{\mathcal{E}_{\mathbf{k}}^2 + \Delta^2}$, as

$$n_n = -\frac{2\hbar^2}{3m_e V} \sum_{\mathbf{k}} \mathbf{k}^2 f'(E_{\mathbf{k}}) \tag{55}$$

and the density of superelectrons as

$$n_c = n - n_n, \tag{56}$$

we get the two-fluid description.

We are going to discuss now the influence of fluctuations on self-sustaining currents. In Fig. 3 we present the currents given by Eqs. (50) and (51) at $\phi_e = 0$, for different shapes of the FS and for different values of ρ. The fluctuations decrease the current, but self-consistent solutions can still be obtained for Fermi surfaces with flat regions ($u = 6$ and $u = 12$). However, as should be expected, the value of self-consistent current (flux) is smaller for the case with fluctua-

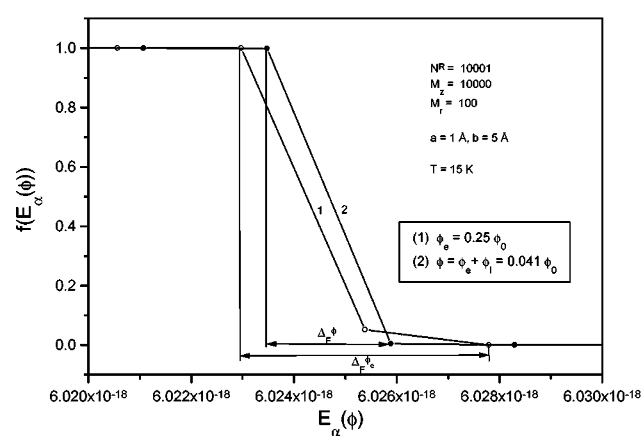

FIG. 2. The Fermi-Dirac distribution function $f(E_\alpha)$ versus energy E_α, for the cylinder made of a set of quasi-1D mesoscopic rings, in the magnetic flux ϕ_e and $\phi = \phi_e + \phi_I$, respectively. ϕ_I has been calculated in the self-consistent way for parameters as in the figure.

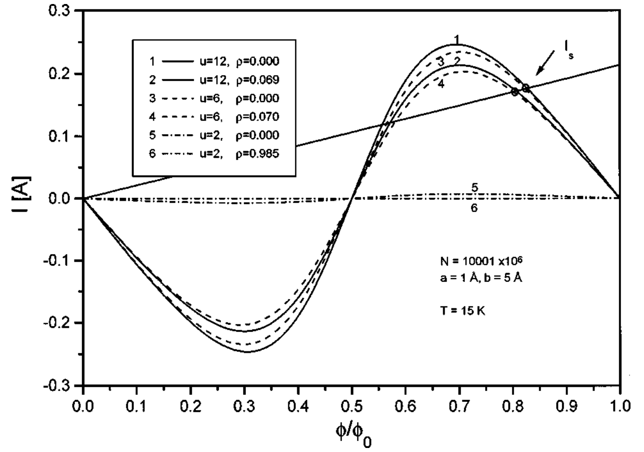

FIG. 3. Persistent currents I as a function of magnetic flux ϕ/ϕ_0 in quasi-2D mesoscopic cylinders with different shapes of the Fermi surfaces, with and without fluctuations. Self-sustaining currents I_s.

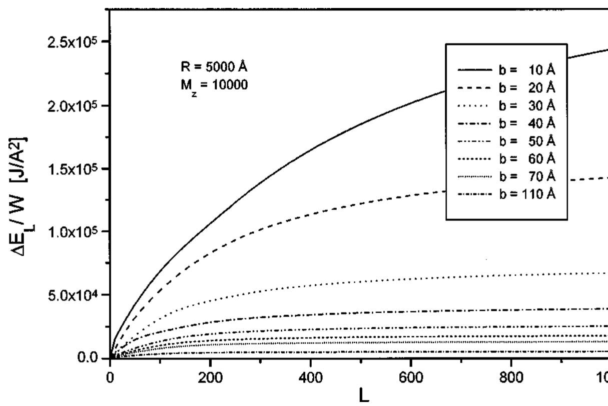

FIG. 4. The energy change $\Delta E_L/W$, where $W=\frac{1}{2}(e\hbar N^R/2\pi m_e R^2)^2$, as a function of the number of magnetic moments L for different values of $b\equiv z_{m,m+1}$.

tions included. For $u=2$ we do not get flux trapping because the number of coherent electrons is too small.

Finally, to get more insight into the properties of our system we discuss, using the microscopic Hamiltonian (3), the possibility of long-range order in a cylinder made of a set of mesoscopic rings. In the literature one finds the statements that phase transitions and long-range order are impossible in quasi-1D systems. It is true for systems in the thermodynamic limit with short-range interactions. However, one can look for the conditions for an ordered state for a large but finite number of interacting entities.[18]

Let us consider a set of M_z rings described by the Ising-like Hamiltonian (3). In the ground state all currents run parallel. Let us construct a new configuration by reversing the direction of L currents ($L\ll M_z$) in s ($1\leqslant s\ll M_z$) different places in the chain of rings. The energy change will be denoted by $s\Delta E_L(M_z)$, and the change in the free energy is

$$\Delta F=s\Delta E_L(M_z)-T\Delta S=s[\Delta E_L(M_z)-k_BT\ln M_z]. \tag{57}$$

If $\Delta F>0$ then the ordered configuration is stable. This condition is equivalent to

$$\xi_T\equiv e^{\Delta E_L/k_BT}>M_z, \tag{58}$$

where ξ_T has the sense of a (dimensionless) correlation range. If Eq. (58) is fulfilled the system is ordered in the sense that the correlations extend over all its length.

Let us discuss the possibility of long-range order for the case considered by us. The energy $\Delta E_L(M_z)$ is of the form

$$\Delta E_L(M_z)=\frac{1}{2}\left(\frac{e\hbar N^R}{2\pi m_e R^2}\right)^2\sum_{n/1}^{L}\sum_{m-m'/L+1}^{M_z-n}\mathcal{L}(m-m'). \tag{59}$$

The L dependence of $\Delta E_L(M_z)$ is presented in Fig. 4. We see that $\Delta E_L(M_z)$ increases with L and decreases with $b\equiv z_{m,m+1}=z_{m+1}-z_m$. The smallest energy change is obtained when reversing a direction of a single current in several different places. In Fig. 5 we present the M_z dependence of ΔE_1. We see that ΔE_1 increases with M_z for small M_z and then saturates.

We are in position now to calculate the temperature T^* at which the crossover from an ordered to disordered state occurs:

$$T^*=\frac{\Delta E_1(M_z)}{k_B\ln M_z}. \tag{60}$$

The calculations performed for the following set of parameters: $M_z=10^4$, $M_r=1$, $R=5000$ Å, $b=10$ Å gave us $T^*\sim 0.14$ K. It means that at $T<T^*$ the system exhibits a long-range order in the sense that the correlation range is longer than the sample size. The temperature T_c calculated in the MFA for the above set of parameters is $T_c\sim 0.216$ K.[2]

We see that T^* obtained by the use of the Ising model is of the same order as T_c obtained with the MFA. It means that long-range interactions encountered in our system strongly supress fluctuations. If we assume that each ring has a small number of transverse channels M_r then, e.g., for $M_r\sim 3$, $T^*\sim 1$ K.

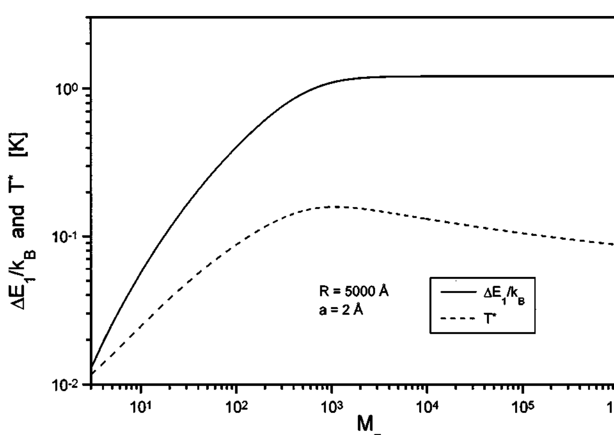

FIG. 5. The energy change ΔE_1 and the temperature T^* as a function of the number of channels M_z in a single cylinder.

It has to be stressed, e.g., that finite value of T^* for our system is a finite-size effect. Indeed, as we can see from Eq. (60) and Fig. 5 $T^* \rightarrow 0$ for $M_z \rightarrow \infty$.

VI. DISCUSSION AND CONCLUSIONS

In the presented paper we discussed the magnetostatic coupling of electrons in mesoscopic systems and its approximations. This interaction is known to be weak in macroscopic samples; however, it seems it can play an important role in mesoscopic samples due to very peculiar properties of mesoscopic systems in the magnetic field.

It is possible to induce persistent currents (or in other words orbital magnetic moments) in mesoscopic ring by the static magnetic field. The magnetic interaction of orbital magnetic moments can lead to magnetically ordered ground state. This possibility has been discussed in a number of papers[2,11] using the mean-field approximation, which states that each electron moves in an external magnetic field and the field coming from all currents in a system. The obtained two self-consistent equations for the current can lead to spontaneous self-sustaining current at zero external field. We neglected here the Zeeman energy of the electron spins because it turns out to be very small compared to the orbital energies. The influence of spins has been discussed in Ref. 19.

In this paper we have presented the microscopic Hamiltonian which is responsible for the internal magnetic field—the magnetostatic (current-current) interaction. The strength of the interaction depends strongly on the sample geometry. For the stack of mesoscopic rings deposited along certain axis we get the long-range interaction with the coupling constant depending only on the radii of the rings and on the relative distance of its centers.

We have shown that the self-consistent MFA of the current-current interaction, gives the effective Hamiltonian H^{MF} leading to self-sustaining currents. Its derivation from the long-range interaction serves as a justification of the use of the Hamiltonian (18) to investigate magnetic properties of mesoscopic systems. The MFA is known to be the best for systems with long-range forces [if the condition (19) is fulfilled], thus we should expect that it leads to reasonable results in the considered case.

To obtain the full Hamiltonian describing our system one should add to the Hamiltonian given by Eq. (10) the Coulomb interaction and the interaction with impurity potential. It was recently shown that the Coulomb interaction does not influence persistent currents in clean systems,[20] whereas it enhances the current in diffusive regime.[21] In a work by Pascaud and Montambaux[22] the experiments that permit us to test the role of Coulomb interaction have been suggested.

In the model calculations presented in this paper we did not consider the effect of impurities in order not to obscure the whole subject with too many details. The influence of disorder on self-sustaining currents has been analyzed in Ref. 3. We found that disorder decreases persistent currents but self-sustaining currents can still be obtained for relatively clean samples (ballistic regime).

To go beyond the MFA we have considered the influence of fluctuations, calculated by the use of Eq. (36), on the properties of a mesoscopic cylinder. We have shown that these fluctuations are smaller in mesoscopic systems than in macroscopic ones because of the quantum size energy gaps. On the top of it the magnetostatic coupling modifies a dispersion relation and creates a dynamic gap that leads to further reduction of the fluctuations. Thus in mesoscopic systems coherent and normal electrons coexist and the system can be described by the two-fluid model where the fluctuations are proportional to the amount of normal electrons. Self-sustaining currents run by coherent electrons survive fluctuations in systems with FS having flat regions; however, their magnitude is reduced.

Having the microscopic Hamiltonian for electrons interacting by magnetostatic coupling [Eq. (3)] we have discussed, for a set of stacked rings, the possibility of long-range order. Phase transitions and long-range order are possible in the strict mathematical sense only for systems in the thermodynamic limit. For finite (but still large) systems discontinuities of thermodynamic quantities and infinite range correlations are not necessary. ''Discontinuities'' have finite widths and correlation ranges may be as large as the system itself, regardless of the behavior in the thermodynamic limit.[18] What is more, finite systems can show interesting effects that will be wiped away in the thermodynamic limit. This is the situation in the presented paper where, at temperatures $T \leqslant T^* \sim 0.1-1$ K the set of mesoscopic rings (or, in general, the mesoscopic cylinder with quasi-1D conduction) can exhibit the long-range order, but $T^* \rightarrow 0$ for $M_z \rightarrow \infty$.

The statistical properties of the system following from Eq. (3) will be presented in a subsequent paper.

ACKNOWLEDGMENTS

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