Rigorous upper bound for the persistent current in systems with toroidal geometry

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It is shown that the absolute value of the persistent current in a system with toroidal geometry is rigorously less than or equal to $e\hbar N\alpha/4\pi m r_0^2$, where N is the number of electrons, $r_0^{-2}=\langle r_i^{-2}\rangle$ is the equilibrium average of the inverse of the square of the distance of an electron from an axis threading the torus, and $\alpha \leq 1$ is a positive constant, related to the azimuthal dependence of the density. This result is valid in three and two dimensions for arbitrary interactions, impurity potentials, and magnetic fields.

The phenomenon of persistent currents occurs when an electronic system is placed in a magnetic field: at thermal equilibrium, an electric current flows without dissipation of energy. This effect is usually studied in systems which are topologically equivalent to a torus, for example, a metal ring or a hollow cylinder. The interesting quantity is the flow of current through a cross section of the torus.

The persistent current exhibits a variety of behaviors, depending on both the magnetic field and the geometric parameters of the system. A first example is that of a *thin* metal ring, i.e., a ring whose thickness is much smaller than its radius. Mesoscopic versions of this system have received particular attention in the past few years. The experiments[1] have been done in the Aharonov-Bohm configuration, in which a weak magnetic flux threads the ring, without significantly affecting the electron orbits. In this case, the main physical effect is the "twisting" of the boundary conditions on the electron wave function, leading to a persistent current which is a periodic function of the threading flux, with period $\Phi_0=hc/e$.[2] The typical magnitude of the current is ev/L, where v is a characteristic velocity of propagation of an electron, and L is the length of the ring. The current vanishes if the ring is made larger and larger ($L\rightarrow\infty$), so this effect is a purely mesoscopic one.

A different behavior is obtained in a two-dimensional ring, with inner and outer radii R_1 and R_2 ($R_1<R_2$), in the presence of a strong perpendicular magnetic field B such that the magnetic length $\lambda=(\hbar c/eB)^{1/2}\ll R_2-R_1$. This model has been studied by several authors.[3,4] The magnetic field induces currents flowing in opposite directions at the inner and outer edges of the ring. If R_1 and R_2 are macroscopically different, the edge currents do not cancel each other exactly, and one is left with a net current that fluctuates violently as a function of electron number when the Fermi level is in a gap between two Landau levels.[4] A typical value of the order of a fraction of $e\omega_c$ ($\omega_c=eB/mc$ is the cyclotron frequency) has been reported in a numerical study.[4]

In the special limit $R_1\rightarrow 0$, the ring becomes a "punctured disk," and then it has been found[5] (neglecting disorder and interactions) that the net current is quantized in integral multiples of $e\omega_c/4\pi$ when the chemical potential is pinned to one of the Landau levels in the bulk.

In view of the diversity exemplified above, it is remarkable what we show in this paper, that there exists a rigorous upper bound to the persistent current of a system of *arbitrary size and shape,* provided that it is topologically equivalent to a torus. We do not need to assume any symmetry, and we do not put any constraints on the nature of the magnetic field, not even that it be uniform. In essence, our derivation of the upper bound is a sharpening of the argument presented by Bohm,[6] following a suggestion by Bloch, to prove that a *macroscopic* one-dimensional ring cannot carry a finite circulating current at thermal equilibrium. Assuming that the upper bound is a good estimate of the maximum value of the persistent current that can be reached in a given system with an appropriate magnetic field, this result enables us easily to understand the large difference in order of magnitude and geometric dependence of persistent currents in, for example, thin rings and punctured disks. Also, the rigorous upper bound can be useful as a test of the validity of approximate theories of persistent currents.

Let us consider a system of electrons confined within a body of toroidal topology, such as the one shown in Fig. 1. No symmetry is assumed. Let us chose an axis—the z axis—which threads the body, but is otherwise arbitrary. The question of the optimal choice of the z axis will be addressed later. Each half-plane emerging from the z axis

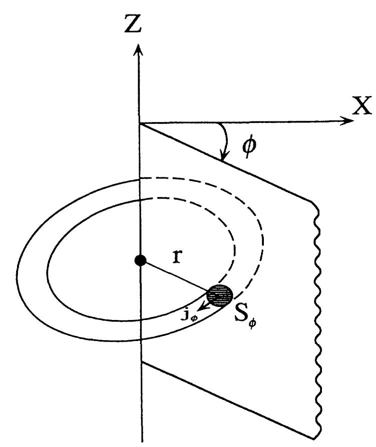

FIG. 1. Cylindrical coordinates for a toroidal body.

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at an angle ϕ $(0<\phi<2\pi)$ cuts a two-dimensional cross section $S(\phi)$ in the body (see Fig. 1).[7] The persistent current is defined as the flux of the current density $\mathbf{j}(\mathbf{r})$ through $S(\phi)$. By virtue of the continuity equation $\nabla\cdot\mathbf{j}(\mathbf{r})=0$, this flux is independent of the choice of ϕ.

We introduce the standard cylindrical coordinates $\mathbf{r}_i=(r_i,z_i,\phi_i)$ to characterize the position of the ith electron in the body. The corresponding momenta are $\mathbf{p}_i=-i\hbar(\partial/\partial r_i,\partial/\partial z_i,r_i^{-1}\partial/\partial\phi_i)$. The Hamiltonian of the system is

$$\hat{H}=\frac{1}{2m}\sum_i\left\{\left[\mathbf{p}_i+\frac{e}{c}\mathbf{A}(\mathbf{r}_i)\right]^2+V(\mathbf{r}_i)\right\}+\frac{e^2}{2}\sum_{i\neq j}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}\ , \tag{1}$$

where $V(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ are *arbitrary* scalar and vector potentials. The exact eigenfunctions $\psi_n(r_1,z_1,\phi_1;\ldots;r_N,z_n\phi_N)$ of $\hat{H}$, with eigenvalue E_n, are completely antisymmetric, and vanish very rapidly (exponentially) outside the boundaries of the body. The average persistent current, at thermodynamic equilibrium, at temperature T, is given by

$$I=\frac{1}{Z}\sum_n e^{-(E_n/kT)}\left\langle\psi_n\left|\int_{S(\phi)}\hat{j}_\phi(\mathbf{r})dr\,dz\right|\psi_n\right\rangle\ , \tag{2}$$

where Z is the partition function, and

$$\hat{j}_\phi(\mathbf{r})=-\frac{e}{2m}\sum_i\{\hat{\Pi}_{i,\phi}\delta(\mathbf{r}-\mathbf{r}_i)+\delta(\mathbf{r}-\mathbf{r}_i)\hat{\Pi}_{i,\phi}\}\ , \tag{3}$$

is the azimuthal component of the current-density operator. The azimuthal component of the kinetic momentum operator is defined as

$$\hat{\Pi}_{i,\phi}=-\frac{i\hbar}{r_i}\frac{\partial}{\partial\phi_i}+\frac{e}{c}A_\phi(\mathbf{r}_i)\ . \tag{4}$$

As we have already remarked, the integral in Eq. (2) is independent of the angle ϕ characterizing the cross section $S(\phi)$ in the (r,z) plane. Using this fact, together with the definition of the current-density operator, Eq. (3), it is easy to verify that

$$I=\langle\hat{I}\rangle\ , \tag{5}$$

where

$$\hat{I}=-\frac{e}{2\pi m}\sum_i\frac{\Pi_{i,\phi}}{r_i} \tag{6}$$

is the current operator, and $\langle\ \rangle$ denotes the usual thermal equilibrium average, with Hamiltonian $\hat{H}$.

The upper bound to I is derived as follows. Consider a gauge transformation

$$\hat{U}_l=\exp\left[i\sum_i f_l(\phi_i)\right]\ , \tag{7}$$

where l is an integer and the function $f_l(\phi)$ is continuous and differentiable in the interval $0\le\phi<2\pi$, and satisfies the boundary condition

$$f_l(\phi+2\pi)=f_l(\phi)+2\pi l\ , \tag{8}$$

in order to preserve the single valuedness of the wave functions. The Hamiltonian is transformed to

$$\hat{H}'=\hat{U}_l\hat{H}\hat{U}_l^{-1}=\hat{H}+\frac{\hbar}{2m}\sum_i\left[\frac{\hat{\Pi}_{i,\phi}}{r_i}f_l'(\phi_i)+f_l'(\phi_i)\frac{\hat{\Pi}_{i,\phi}}{r_i}\right]+\frac{\hbar^2}{2m}\sum_i\left[\frac{f_l'(\phi_i)}{r_i}\right]^2\ , \tag{9}$$

where $f_l'(\phi)=df_l(\phi)/d\phi$. Let F and F' denote the free energies associated with the Hamiltonians $\hat{H}$ and $\hat{H}'$, respectively. They satisfy the well-known inequality[8]

$$F'\le F+\langle\hat{H}'-\hat{H}\rangle\ . \tag{10}$$

But, in this case, $F'=F$ because $\hat{H}$ and $\hat{H}'$ are related by a unitary transformation. Therefore, $\langle\hat{H}'-\hat{H}\rangle\ge 0$. Using Eqs. (3), (5), and (6) to evaluate the average of $\hat{H}'-\hat{H}$, we obtain, after straightforward manipulations, the inequality

$$\frac{\hbar^2}{2m}\left\langle\sum_i\frac{f_l'^2(\phi_i)}{r_i^2}\right\rangle-\frac{lh}{e}I\ge 0\ , \tag{11}$$

which must be satisfied for an arbitrary value of the integer l. Equation (11) can be rewritten for $l\neq 0$ as

$$|I|\le\frac{e\hbar}{4\pi m|l|}\int\rho(\mathbf{x})\left[\frac{f_l'(\phi)}{r}\right]^2 d\mathbf{x}\ , \tag{12}$$

where $\rho(\mathbf{x})$ is the electronic density distribution, and $\mathbf{x}=(r,z,\phi)$ in cylindrical coordinates. Next, we choose the function $f_l(\phi)$ in such a way as to minimize the right-hand side of the inequality. A standard variational calculation leads to the following differential equation for $f_l(\phi)$:

$$\frac{d}{d\phi}[\bar{\rho}(\phi)f_l'(\phi)]=0\ , \tag{13}$$

where we have introduced an "angular density"

$$\bar{\rho}(\phi)\equiv\int_{S(\phi)}\frac{\rho(\mathbf{x})}{r}dr\,dz\ . \tag{14}$$

Solving Eq. (13), with the boundary condition given by Eq. (8), and substituting the solution in Eq. (12), we obtain

$$|I|\le\frac{eh|l|}{2m}\left[\int_0^{2\pi}\frac{d\phi}{\bar{\rho}(\phi)}\right]^{-1}\ . \tag{15}$$

The most stringent bound is obtained when $|l|=1$. Let us now define

$$\frac{1}{r_0^2}\equiv\frac{1}{N}\int\frac{\rho(\mathbf{x})}{r^2}d\mathbf{x}=\frac{1}{N}\int_0^{2\pi}\bar{\rho}(\phi)d\phi\ , \tag{16}$$

which is an average inverse square distance of the electrons from the z axis. The fact that the threading axis does not "touch" the toroidal body guarantees that $1/r_0^2$ is a finite number, because the wave function vanishes exponentially in the regions where $r \rightarrow 0$. In terms of r_0, the upper bound for the current takes the form

$$|I| \leq I_m = \frac{e\hbar N\alpha}{4\pi m r_0^2} , \qquad (17)$$

where

$$\alpha \equiv \left[\frac{1}{4\pi^2} \int_0^{2\pi} \frac{d\phi}{w(\phi)} \right]^{-1} \qquad (18)$$

and

$$w(\phi) \equiv \frac{r_0^2}{N} \bar{\rho}(\phi) \qquad (19)$$

is a rescaled version of $\bar{\rho}(\phi)$ which is normalized to 1 in the interval $0 < \phi < 2\pi$ [see Eq. (16)]. This is the main result of this paper. It is evident from the interpretation of $w(\phi)$ as a normalized probability distribution that

$$\frac{1}{4\pi^2} \int_0^{2\pi} \frac{d\phi}{w(\phi)} \geq 1 , \qquad (20)$$

implying that the positive constant $\alpha \leq 1$. The equality sign holds only when the density distribution is invariant under rotations about the z axis, i.e., when $w(\phi) = 1/2\pi$.

The above argument is also straightforwardly applicable to a strictly two-dimensional ring geometry. The arbitrary axis threading the toroidal body is replaced by an arbitrary point within the hole, and the cylindrical coordinates relative to that axis are replaced by planar polar coordinates relative to this point. The cross section becomes a segment (or a collection of segments) of straight line, and the z coordinate is suppressed. The final result is still given by Eq. (17).

Equation (17) is still dependent on the arbitrary choice of the reference axis. We can completely remove this arbitrariness, by choosing, for any given system, the axis that yields the *most stringent* inequality, i.e., the smallest value of α/r_0^2. Thus, our definition of α/r_0^2 becomes

$$\frac{\alpha}{r_0^2} \equiv \min \left\{ \left[\frac{N}{4\pi^2} \int_0^{2\pi} \frac{d\phi}{\bar{\rho}(\phi)} \right]^{-1} \right\} , \qquad (21)$$

where the minimum is calculated with respect to the set of all axes heading the toroidal body. Qualitatively, the optimal axis is the one which, on the average, remains as far as possible from the body.

It is worth noting that the upper bound on the persistent current depends only on a moment of the electronic density distribution—a relatively "gross" property of a many-electron system. Furthermore, from the form of Eq. (21), it is clear that the value of I_m is not sensitive to too fine details of the density distribution. Essentially, I_m is a geometric parameter. In three-dimensional macroscopic bodies, we expect that approximating the density as a constant within the geometric boundary of the body and zero outside, should lead to an excellent aproximation for I_m. A better estimate of the density distribution can be obtained by solving the Thomas-Fermi or the Kohn-Sham equations.

Let us now consider a few concrete applications of Eq. (17). Suppose that the body is a circular ring of radius R and negligible thickness ("thin ring"). Then the optimal axis coincides with the axis of the ring, and $r_0 \simeq R, \alpha = 1$. The upper bound to the current is in this case is

$$I_m = N \frac{eh}{2mL^2} , \qquad (22)$$

where $L = 2\pi R$ is the circumference of the ring. This tends to 0 for $L \rightarrow \infty$, *so there is no current flowing in a macroscopic thin ring.* It must be noted that Eq. (22) is rigorous for a geometrically thin ring, i.e., it incorporates the effect of electron-electron and impurity scattering exactly. The ring may still be three dimensional as far as the electronic wave function is concerned. No assumption about the form of the density distribution has been used. In the special case of a nondisordered one-channel ring, containing noninteracting electrons with a one-dimensional Fermi velocity v_F, the upper bound reduces to $2ev_F/L$ (the factor 2 arising from spin degeneracy). This value is attained exactly at $T=0$, when the ring is threaded by an Aharonov-Bohm flux $\Phi = hc/2e$ (odd N) or $\Phi = 0^+$ (even N).

As a second example, consider a two-dimensional disk (outer radius R_2) with a central hole of radius R_1, in a strong magnetic field, such that the magnetic length $\lambda \ll R_2 - R_1$. Once again, the optimal axis coincides with the axis of the disk. Since the electronic areal density $n_0 = N/A$ (A is the area of the ring between the inner and the outer edge) is essentially uniform in the bulk of the system, we can calculate $1/r_0^2$ by taking a uniform average of $1/r^2$, which yields the result $1/r_0^2 = 2\pi \ln(R_2/R_1)/A$. Substituting this into Eq. (15), we obtain

$$I_m = \frac{e\hbar}{2m} n_0 \ln \left[\frac{R_2}{R_1} \right] . \qquad (23)$$

The behavior of the upper bound depends only on the aspect ratio R_2/R_1. If $R_1 \sim R_2$ to an accuracy much smaller than R_1 or R_2, we simply recover the thin ring geometry, and the persistent current vanishes. In the limit $R_1 \rightarrow 0$ (or $R_2 \rightarrow \infty$), we obtain the "punctured disk" geometry. The upper bound diverges logarithmically, allowing a large persistent current. (The logarithmic divergence is of course cut off when R_1 becomes comparable to the size of the edge region, in which the approximation of constant density is no longer valid.) In all other cases, the logarithmic factor is a constant of order 1, and the upper bound to the current can be written as $I_m \sim e\hbar/2\pi m a^2$, where a is the average distance between the electrons.

In the interesting case that the filling factor $\nu = 2\pi l^2 n_0$, rather than the areal density, is kept constant in the bulk of the ring, Eq. (23) takes the form

$$I_m = \frac{\nu e \omega_c}{4\pi} \ln \left[\frac{R_2}{R_1} \right] . \qquad (24)$$

In this case the upper bound is proportional to the intensity of the magnetic field, and the persistent current is allowed to grow indefinitely with the latter (N is now not constant). A persistent current of the order of $e\omega_c/4\pi$ [we assume that the geometric parameters are fixed and that $\ln(R_2/R_1)$ is of order unity] is consistent with the results of quantitative calculations of the persistent current in an ideal ring.[4]

All the above examples have cylindrical symmetry, and the value of α is 1. A much more stringent bound can be obtained in situations in which the "angular density" $\bar{\rho}(\phi)$ is a strongly varying function of angle, becoming small at certain values of ϕ. As an example, consider a torus with a narrow constriction, such that the area of the cross section $S(\phi)$ becomes small at some $\phi=\phi_0$. Then, even if the electronic density is nearly uniform, the "angular density" will be small for $\phi\sim\phi_0$ and the value of α will be correspondingly reduced. Another possibility is that the electronic density becomes strongly nonuniform via a process of spontaneous symmetry breaking, such as the formation of a Wigner crystal [we are talking, of course, only of the relevant conduction electrons—see comment (i) below]. In this case the electronic density will be very small on cross sections lying between crystal planes; the value of α and the bound on the persistent current will be reduced to almost zero.

In closing, we make the following remarks. (i) The rigorous upper bound derived in this paper is also applicable to an *effective* Hamiltonian, of the form given in Eq. (1), describing only a *subset* of the electrons in the system (for instance, the conduction electrons in a metal). In this case N and m are replaced by the number and effective mass of the relevant electrons. (ii) Our Hamiltonian (1) does not include the reaction of the electronic currrent on the magnetic field. However, to the extent that this effect can be treated in mean field theory, i.e., by adding a self-consistent correction to the external vector potential, it is clear that the upper bound is not modified by its inclusion. (iii) The upper bound derived in this paper is *not* necessarily applicable to the current carried by a superconducting ring. This is because, in the case of a superconductor, the current-carrying state is not necessarily the true equilibrium state—it can be a metastable state which cannot decay.[9]

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