

Scattering Phase Shift Analysis of Persistent Currents in Mesoscopic Aharonov-Bohm Geometries.

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Abstract. – The ensemble average of the persistent currents of Aharonov-Bohm mesoscopic rings is evaluated in a case where the number of electrons rather than the chemical potential is fixed. The difference between the average currents in these two situations is expressed on general grounds in terms of the fluctuation of the scattering phase shift. It is then shown that in the diffusive regime this difference is $(h/2e)$ -periodic and does not depend on the disorder. Possible extensions of the approach used here are emphasized.

The purpose of this letter is the study of persistent currents in disordered mesoscopic metals threaded by an Aharonov-Bohm flux. Although the approach presented here is valid for any disorder, the expression of the current will be derived within the diffusion approximation [1] for which $k_{\ell}l \gg 1$, l being the elastic mean free path.

) The general problem of the existence and behaviour of persistent currents in systems submitted to an Aharonov-Bohm flux was first considered by Bloch [2]. It was subsequently studied by Buttiker, Imry and Landauer [3] who considered also the effect of a slight disorder. These currents were found to be ϕ_0 -periodic ($\phi_0 = h/e$) and to decrease on average exponentially [4] with the size of the system in the presence of elastic scattering. Their recent experimental observation [5] on an assembly of 10^7 disconnected Cooper rings have raised new questions: i) the ensemble average of the current exhibits a $(\phi_0/2)$ -periodicity and ii) the amplitude is much higher than the expected exponential decrease.

The important distinction in this problem between isolated (fixed number of electrons) and nonisolated (fixed Fermi energy) rings was first emphasized by Cheung *et al.* [6]. It was subsequently studied in more details by Bouchiat and Montambaux [7] for slightly disordered systems. They showed numerically that for isolated rings the variation of the Fermi energy with the Aharonov-Bohm flux gives rise to an ensemble-averaged current with $(\phi_0/2)$ periodicity, while in the opposite limit of a nonisolated system it remains periodic

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with ϕ_0 as it should. As discussed by Imry [8], and established recently by Schmid [9] and by Altshuler, Gefen and Imry [10] while this work was completed, this behaviour remains in the diffusive regime. The role of the electron-electron interactions was also considered in this regime [9, 11] to explain the change of periodicity. Noticing that the interactions preserve the local charge density, to take them into account imposes a constraint stronger than the conservation of the total number of electrons.

The assumption of the diffusive regime is of crucial importance. It describes a situation in which the multiple elastic scattering of the electrons can be approximated by a random walk. For mesoscopic samples of length L smaller than the phase coherence length L_ϕ , in spite of the elastic scattering, the electronic wave functions are coherent all over the sample. They are therefore sensitive to the specific configuration of the impurities. This gives rise to anomalously large fluctuations of the electrical conductance [12]. Thermodynamic quantities like for instance the Landau diamagnetic susceptibility are showing anomalous fluctuations as well [13]. It was nevertheless generally believed that unlike transport coefficients average thermodynamic quantities were not sensitive to the diffusive motion of the electrons. Such a statement has to be revisited in order to explain the experimental results on the assembly of isolated rings.

The average over the ensemble of the current for both isolated and nonisolated systems was considered [9, 10] from the thermodynamic point of view in order to relate canonical and grand canonical descriptions. Here, I consider a different approach of the problem. The currents will be described in terms of the on-shell scattering matrix or equivalently the scattering phase shift [14]. This formulation is general and applies not only to persistent currents, but also to systems submitted to a magnetic field. It is also convenient and allows to express in a simple way the difference between the ensemble-averaged current of, respectively, isolated and nonisolated systems in terms of the scattering phase shift.

Consider a mesoscopic metallic ring of volume V with noninteracting electrons, threaded by an Aharonov-Bohm flux. At zero flux the ring is defined by a Hamiltonian H_0 which includes the elastic impurities while in the presence of the flux the Hamiltonian is $H(\phi)$. I assume that H_0 admits delocalized states $|m\rangle$ defined in the volume V and $H(\phi)$ has similar eigenstates $|m'\rangle$. In the limit $V \rightarrow \infty$ of an infinite volume, it is always possible to associate with any solution $|m\rangle$ of energy E of H_0 a solution $|m'\rangle$ of $H(\phi)$ with the same energy. These two stationary eigenstates differ in the asymptotic limit by a phase shift only, so that there exists an operator $S(E, \phi)$ defined by $|m'\rangle = S(E, \phi)|m\rangle$. S is known as the on-shell scattering matrix [15]. More precisely, the operator S_+ describing outgoing waves can be expressed in terms of the resolvent operators $G_0^+(E)$ and $G^+(E)$ respectively associated with H_0 and H by $S_+(z) = G^+(z)[G_0^+(z)]^{-1}$, where z is a complex number. The scattering phase shift $\delta(z)$ is then the real function obtained from S_+ by [15]

$$\delta(z) = \text{Im} \ln \text{Det } S_+(z). \quad (1)$$

Using successively the basis of H_0 and $H(\phi)$ provides for the determinant the equality

$$\text{Det } S_+(z) = \prod_{m, m'} \frac{z - E_m}{z - E'_m}, \quad (2)$$

where E_m and E'_m are, respectively, eigenvalues of H_0 and $H(\phi)$. Finally, taking the derivative of eq. (2) and using the relation $\pi g(E) = -\text{Tr} \text{Im } G_+(E)$ between the density of states per unit energy $g(E)$ and the resolvent gives

$$\pi [g(E, \phi) - g(E, 0)] = \frac{d\delta(E, \phi)}{dE}, \quad (3)$$

which relates the change in density of states due to the flux ϕ to the derivative of the total phase shift $\delta(E, \phi)$.

So far, the results derived above are very general. Consider now the additional constraint provided by the conservation of the number N of electrons in the sample. The chemical potential $\mu(\phi)$ depends now on the flux, and can be written $\mu(\phi) = \mu_0 + \Delta\mu(\phi)$, where μ_0 is the zero-flux contribution which depends on the particular configuration of the impurities. The conservation of the number of particles is then expressed by

$$\int_0^{\mu(\phi)} dE g(E, \phi) = \int_0^{\mu_0} dE g(E, 0) = N. \quad (4)$$

Integrating eq. (3) over the energy and taking eq. (4) into account provides the important equality

$$\pi [n_0(\mu_0) - n_0(\mu(\phi))] = \delta(\mu(\phi), \phi), \quad (5)$$

where $n_0(E)$ is defined as the number of states up to energy E in the absence of flux. This relation is reminiscent of the Friedel sum rule for the perfect screening of a point charge in a metal.

To first order in $\delta\mu(\phi)$, eq. (5) gives

$$\Delta\mu(\phi) = -\frac{1}{\pi g(\mu_0)} \delta(\mu_0, \phi) \quad (6)$$

which relates the change $\Delta\mu(\phi)$ of the chemical potential to the corresponding change of the scattering phase shift. The persistent current $I(\phi)$ can also be expressed in terms of the scattering phase shift [14] by

$$I(\phi) = \frac{1}{\pi} \int_0^{\mu(\phi)} dE \frac{\partial \delta(E, \phi)}{\partial \phi}. \quad (7)$$

It is an odd and periodic function of flux with period ϕ_0 . The total phase shift is therefore an even and ϕ_0 -periodic function of the flux which can be expanded as

$$\delta(E, \phi) = \delta_0(E) + \sum_{n=1}^{\infty} c_n(E) \cos\left(2\pi n \frac{\phi}{\phi_0}\right). \quad (8)$$

The average value over the flux of $\delta(E, \phi)$ is $\delta_0(E)$. Since from eq. (5), one sees⁽¹⁾ that $\delta(\mu_0, 0) = 0$, it implies that $\delta_0(\mu_0) = 0$. Together with eq. (7), it gives to first order in $\Delta\mu(\phi)$

$$I(\phi) = -\sum_{n=1}^{\infty} 2\pi \frac{n}{\phi_0} \sin\left(2\pi n \frac{\phi}{\phi_0}\right) \int_0^{\mu_0} dE c_n(E) + \frac{4}{\pi \phi_0 g(\mu_0)} \sum_{n,n'} c_n(\mu_0) c_{n'}'(\mu_0) n \sin\left(2\pi n \frac{\phi}{\phi_0}\right) \cos\left(2\pi n' \frac{\phi}{\phi_0}\right). \quad (9)$$

⁽¹⁾ In the absence of flux, the scattering impurities introduce also a phase shift. Nevertheless, I do not consider it since it does not contribute to the current given by eq. (7).

The chemical potential μ_0 at zero flux can be written $\mu_0 = \langle \mu_0 \rangle + \delta\mu_0$, where $\langle \mu_0 \rangle$ defines the average over the disorder. To first order in $\delta\mu_0$, the average $\langle I(\phi) \rangle$ of the current is then given by

$$\langle I(\phi) \rangle = \frac{1}{\pi} \int_0^{\langle \mu_0 \rangle} dE \frac{\partial}{\partial \phi} \langle \delta(E, \phi) \rangle - \frac{1}{2\pi^2 g(\langle \mu_0 \rangle)} \frac{\partial}{\partial \phi} \langle \delta^2(\mu_0, \phi) \rangle. \quad (10)$$

The first term in this relation corresponds to nothing but the average current $\langle I_0(\phi) \rangle$ of an open system with fixed chemical potential $\langle \mu_0 \rangle$. In the mesoscopic regime here considered, $\langle I_0(\phi) \rangle$ was shown [4] to decrease like $\exp[-L/l]$. It is moreover periodic with period ϕ_0 as expected. The second term in eq. (10) is new. It results from the conservation of the number of particles (eq. (5)) and the relation it implies between the change $\Delta\mu(\phi)$ of chemical potential and the total scattering phase shift. To obtain its periodicity, it remains now to evaluate the correlation function of the c_n 's within the diffusion approximation which provides the second physical input of the problem. To that purpose, it is worth noticing that from eq. (3) it is possible to relate $\delta(\mu_0, \phi)$ to the variation of the density of states. Therefore, the fluctuation $\langle \delta^2(\mu_0, \phi) \rangle$ which appears in eq. (10) can be expressed as the energy integral of the density of states correlation function $K(E_1, E_2)$. This quantity has been calculated in great details for zero flux by Altshuler and Shklovskii [16]. I rely on these computations and for $T=0$ and nonzero flux it gives

$$\langle \delta^2(\mu_0, \phi) \rangle = - \int dE_1 dE_2 \operatorname{Re} \sum_{n_x} \frac{1}{(E_1 - E_2 + i\hbar D q^2)^2}, \quad (11)$$

where n_x stands for the integers n_x, n_y and n_z , while the transverse wave vectors q_y and q_z are quantized as $q_\mu = (\pi L) n_\mu$. The diffusion constant is $D = v_f l/3$ in three dimensions. The component q_x depends on the flux and to work out this dependence, consider first the correlation function

$$\langle c_n(\mu_0) c'_n(\mu_0) \rangle = \frac{1}{(2\pi\phi_0)^2} \int_{-\pi}^{\pi} d\phi d\phi' \exp \left[i \frac{2\pi}{\phi_0} (n\phi + n'\phi') \right] \langle \delta(\mu_0, \phi) \delta(\mu_0, \phi') \rangle. \quad (12)$$

It corresponds to a generalisation of eq. (11) to the case where the densities of states depend on different values ϕ and ϕ' of the flux. There are two contributions to the diffusion pole. The first one, the diffusion, gives a component of q_x which depends only on $\phi - \phi'$. In the limit $\phi = \phi'$ considered in eq. (11) this contribution to the average current disappears. It describes in fact the zeroth-order harmonic $\delta_0(\mu_0)$ which precisely does not contribute to eq. (10). The second contribution is the Cooperon for which the q_x component is given by $q_x = \pi/L(n + (\phi + \phi')/\phi_0)$, where n is an integer. For $\phi = \phi'$ it gives a nonzero contribution to the average current and allows to rewrite eq. (12) as $\langle c_n(\mu_0) c'_n(\mu_0) \rangle = \delta_{n,n'} \langle c_n^2(\mu_0) \rangle$ which establishes within the diffusion approximation the statistical independence of the harmonics from the scattering phase shift.

In order to calculate now the amplitude of the average current, we have to evaluate $\langle c_n^2(\mu_0) \rangle$. This calculation is closely related to the one presented in [10] for the fluctuation of the chemical potential. Within the same approximation, it gives

$$\langle c_n^2(\mu_0) \rangle = \frac{\sqrt{2}}{8} \int_{-\infty}^{\mu_0/E_c} \frac{du}{\sqrt{|u|}} \exp[-n\sqrt{|u|}] [\cos(n\sqrt{|u|}) + \sin(n\sqrt{|u|})]. \quad (13)$$

In the mesoscopic regime here considered, $\mu_0 \gg E_c$, so that the upper limit of the integral can be taken as infinite. Then, $\langle c_n^2(\mu_0) \rangle$ appears to be *independent of the disorder*, i.e. of E_c . Therefore, from eq. (10), the difference $\langle I(\phi) \rangle - \langle I_0(\phi) \rangle$ is also independent of disorder. This is a periodic function of the flux and the amplitude I_n of the harmonics is given by

$$I_n = -\frac{2i\Delta}{\pi\sqrt{2}\phi_0}, \quad (14)$$

where $\Delta = \hbar^2/(2mk_f L^3)$ is the mean level spacing at the Fermi energy. Introducing the number $M = (k_f L)^2$ of transverse channels and the Bloch expression $I_0 = ev_f/L$ for the current of a one-dimensional ring without disorder, eq. (15) rewrites $I_n = -i/(4\pi^2\sqrt{2})(I_0/M)$.

The main results derived above are now summarized:

i) The conservation of the number of particles in an isolated system gives a general relation (eq. (5)) between the variation with the flux of the chemical potential and the total scattering phase shift. Then the difference $\langle I(\phi) \rangle - \langle I_0(\phi) \rangle$ of the ensemble-averaged currents for, respectively, a closed and an open system is simply expressed as the flux derivative of the fluctuation of the scattering phase shift.

ii) This fluctuation has been calculated within the diffusion approximation, by considering the Cooperon contribution. It shows that $\langle I(\phi) \rangle - \langle I_0(\phi) \rangle$ is a periodic function of the flux with period $\phi_0/2$. The harmonics I_n are independent of both disorder and n and given by eq. (14).

iii) A derivation similar to the one leading to eq. (3) could have been worked out in the absence of magnetic flux, in order to relate the scattering phase shift $\delta(E)$ to the fluctuation $\delta g(E) = g(E) - \langle g(E) \rangle$ of the density of states. Then, $\pi\langle \delta^2(\mu_0) \rangle$ appears to be the fluctuation of the number of levels below the Fermi energy as was calculated by Altshuler and Shklovskii [16]. Their result gives $\langle \delta^2(\mu_0) \rangle \sim (\mu_0/E_c)^{3/2} \gg 1$. The average persistent current therefore appears to play a role similar to the conductance fluctuations in the presence of a magnetic field, the latter providing a measure of $\langle \delta^2(E_c) \rangle$. An «ergodic» hypothesis is currently admitted according to which different values of the magnetic field correspond to different realisations of the impurity configuration. From eq. (13), one has $\langle \delta^2(\mu_0, \phi) \rangle = 1$, therefore much smaller than $\langle \delta^2(\mu_0) \rangle$. It seems therefore that this hypothesis does not apply for the case of persistent currents.

These results coincide with those derived in ref. [9, 10] but are at odd with numerical results obtained by Montambaux *et al.* [17] in the diffusive regime, who found a dependence on the disorder proportional to $\sqrt{M_e}$, where $M_e = M/L$. Moreover, although the above results recover the $(\phi_0/2)$ -periodicity observed experimentally [5], the amplitude of the current is orders of magnitude smaller than the experimental value. The reason for this has probably to do with the diffusion approximation rather than with the assumptions leading to eq. (10). A quantitative explanation would involve other mechanisms. It would therefore be interesting to consider related problems in the presence of a true magnetic field applied on the electrons.

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