Persistent current for interacting electrons: a simple Hartree-Fock picture

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Abstract

The average persistent current $\langle I \rangle$ of diffusive electrons in the Hartree-Fock approximation is derived in a simple non-diagrammatic picture. The Fourier expansion directly reflects the winding number decomposition of the diffusive motion around the ring. One recovers the results of Ambegaokar and Eckern, and Schmid. Moreover one finds an expression for $\langle I \rangle$ which is valid beyond the diffusive regime.

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The physics of persistent currents in mesoscopic isolated rings pierced by an Aharonov-Bohm flux $\phi$, has attracted a lot of interest on the description of the thermodynamic properties of mesoscopic metals, both in the non-interacting picture or in the presence of electron-electron interactions. The description of the interactions is a complicated task: although several attempts have been made to describe the role of the interactions in one-dimensional or few-channel rings, with the help of analytical arguments or numerical calculations [1], the diffusive nature of the electronic motion, which is probably essential in the experiments on metallic rings with finite thickness [2–4], has been treated only in two series of papers by Ambegaokar and Eckern and Schmid [5,6]. They calculated the average persistent current in the Hartree-Fock approximation where the interaction is treated perturbatively in a diagrammatic picture. Although this calculation provides an average current smaller that experimentally observed [2], one can believe that it contains the essential physical ingredient namely weakly interacting diffusive electrons. Thus it may be interesting to simplify as much as possible the calculation in order to possibly generalize it, or to compare it with numerical calculations. In the above papers, the average persistent current is calculated with a diagrammatic technique where the diffusive motion is described by a Cooperon pole with a wave vector quantized by periodic boundary conditions. Then, by Poisson summation, this sum over diffusive modes is transformed into a sum over harmonics with periodicity $\phi_0/2$ where $\phi_0$ is the flux quantum.

In this short note, we propose a simple derivation where the average current is directly related to the return probability for a diffusive particle. Then this return probability is expanded according to the winding number of the diffusive motion around the ring, which gives directly access to the harmonics expansion of the current. Moreover, we obtain a general expression which can be used beyond the diffusive regime.

Consider a quasi-one dimensional ring of perimeter $L$ and of transverse section $S$, in which the motion is supposed to be diffusive along the perimeter and uniform along the transverse section.

The first step is to write the total energy $E_T$ in the Hartree-Fock approximation:
\[ E_T = E_T^0 + \sum_{i,j} \int U(\mathbf{r} - \mathbf{r}')|\psi_j(\mathbf{r}')|^2|\psi_i(\mathbf{r})|^2 d\mathbf{r} d\mathbf{r}' \]

\[ - \sum_{i,j} \delta_{\sigma_i, \sigma_j} \int U(\mathbf{r} - \mathbf{r}')\psi^*_j(\mathbf{r}')\psi_j(\mathbf{r})\psi^*_i(\mathbf{r})\psi_i(\mathbf{r}') d\mathbf{r} d\mathbf{r}' \]

where \( E_T^0 \) is the total energy in the absence of interaction. In the lowest order in the interaction parameter, the states \( \psi_i \) are the states of the non-interacting system. The summation \( \sum_{i,j} \) is over filled energy levels. \( \sigma_i \) is the spin of a state \( \psi_i \).

Considering that the Coulomb interaction \( U(\mathbf{r} - \mathbf{r}') \) is screened in the metallic regime, it is replaced by \( U(\mathbf{r} - \mathbf{r}') = U\delta(\mathbf{r} - \mathbf{r}') \) where \( U = 4\pi e^2/q_{TF}^2 \) and \( q_{TF} \) is the Thomas-Fermi wave vector. Replacing the interaction in eq.1 by a \( \delta \) function is certainly correct as long as the Thomas-Fermi wave length is smaller than the mean free path \( l_e: q_{TF} l_e \gg 1 \). The interaction being now considered as \( \delta \)-like, it is quite easy to see that the Fock term has the same structure as the Hartree term. Introducing the local density \( n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2 \), the total energy can be rewritten:

\[ E_T = E_T^0 + U \int n^2(\mathbf{r}) d\mathbf{r} - \frac{U}{2} \int n^2(\mathbf{r}) d\mathbf{r} \]  

The Fock term is half the Hartree contribution because of the constraint on the spin and its sign is opposite because of exchange of particles. The local density \( n(\mathbf{r}) \) can be expressed in terms of the Green function: \( n(\mathbf{r}) = -(1/\pi) \int_{\epsilon_F}^{\epsilon_F} ImG^R(\mathbf{r}, \mathbf{r}, \omega)d\omega \) so that the average current is given by:

\[ \langle I_{e-e}(\phi) \rangle = \left\langle -\frac{\partial E_T}{\partial \phi} \right\rangle \]

\[ = -\frac{U}{4\pi^2} \frac{\partial}{\partial \phi} \int_{\epsilon_F}^{\epsilon_F} \int_{0}^{\epsilon_F} \langle G^R(\mathbf{r}, \mathbf{r}, \omega)G^A(\mathbf{r}, \mathbf{r}, \omega') \rangle d\omega d\omega' d\mathbf{r} \]

where \( G^R \) (\( G^A \)) is the retarded (advanced) Green function. The product \( \langle G^R(\mathbf{r}, \mathbf{r})G^A(\mathbf{r}, \mathbf{r}) \rangle \) simply expresses the probability to go from some point \( \mathbf{r} \) to itself \[8\]. More precisely, for a particle at energy \( E \) \[8,10\]:

\[ P(E, \omega) = \frac{1}{2\pi \rho_0} \langle G^R(\mathbf{r}, \mathbf{r}, E + \omega/2)G^A(\mathbf{r}, \mathbf{r}, E - \omega/2) \rangle \]  

is the Fourier transform of the return probability \( P(E, t) \) after a time \( t \):

\[ \text{3} \]
Because of disorder average, this return probability is independent of the position \( r \). The current can now be expressed directly in terms of \( P(E, t) \). Neglecting the energy dependence \( (P(E, t) = P(t)) \), one gets:

\[
\langle I_{e-e}(\phi) \rangle = -\Omega U \rho_0 \frac{2}{\pi} \frac{\partial}{\partial \phi} \int_0^{\infty} \frac{P(t, \phi)}{t^2} dt
\]

\( \Omega = LS \) is the volume. Since the relation (4) is exact, the expression (6) is quite general and is valid beyond the diffusive regime. In the classical approximation for the diffusive regime \( (l_e \ll L) \), the diffusion probability is the solution of a classical diffusion equation

\[
D \Delta P = \frac{\partial P}{\partial t}
\]

where \( D \) is the diffusion coefficient taken here at the Fermi level, \( D = v_F l_e/3 \). It is given by

\[
P_{ct}(r, r', t) = \frac{1}{(4\pi Dt)^{d/2}} e^{-|r-r'|^2/4Dt}
\]

In the geometry of a quasi-one-dimensional ring, the return probability can thus be expanded according to the winding number of the diffusive motion:

\[
P(t, \phi) = \frac{1}{S \sqrt{4\pi Dt}} \sum_m e^{-\frac{m^2 \phi^2}{4Dt}} [1 + \cos(4\pi m \varphi)]
\]

where \( \varphi = \phi/\phi_0 \). The second term, of importance here, results from the phase interference between time-reversed paths in the semi-classical approximation, each path accumulating a phase \( \pm 2\pi m \varphi \) \([1],[2]\). In zero flux, the return probability is twice the classical one. This expansion according to the winding number gives directly the Fourier decomposition of the current:

\[
\langle I_{e-e}(\phi) \rangle = \sum_m I_m \sin(4\pi m \varphi)
\]

with

\[
I_m = \frac{8mU \rho_0}{\phi_0 \sqrt{4\pi E_c}} \int_0^{\infty} e^{-\frac{m^2}{4E_c t}} \frac{dt}{t^{5/2}}
\]
We have introduced the Thouless energy $E_c = \hbar D/L^2$. Defining a dimensionless winding number $w$ by $w^2 = m^2/4E_c t$, $I_m$ can be simply rewritten as

$$I_m = \frac{64 U \rho_0 E_c}{m^2 \sqrt{\pi} \phi_0} \int_0^\infty w^2 e^{-w^2} dw$$

$$= 16 \frac{U \rho_0 E_c}{\phi_0} \frac{m^2}{w^2} (11)$$

which is the result of Ambegaokar and Eckern [5] and Schmid [6].

We finish with the calculation of the current at finite temperature $T$ where two Fermi factors $f(\epsilon)$ have to be introduced in eq.4. Doing the standard substitution $\int f(\epsilon) g(\epsilon) d\epsilon = 2i\pi \sum \omega_n g(i\omega_n)$ where $\omega_n = (2n + 1)\pi T$, the average current at finite $T$ is straightforwardly given by:

$$\langle I_{e-e} \rangle = -\Omega U \rho_0 \frac{2}{\pi} \frac{\partial}{\partial \phi} 4\pi^2 T^2 \sum_{\omega_n, \omega_n'} P(i\omega_n - i\omega_n')$$

$$= -\Omega U \rho_0 \frac{2}{\pi} \frac{\partial}{\partial \phi} \int \frac{\pi^2 T^2}{(\sinh \pi T t)^2} P(t, \phi) dt (12)$$

By introducing the same dimensionless winding number $w$ as above, the harmonics $I_m$ are given by

$$I_m(T) = I_m(0) \frac{4}{\sqrt{\pi}} \int_0^\infty dw w^2 e^{-w^2} \left( \frac{\pi \theta_m}{4w^2} \right)^2 \frac{1}{\cosh \left( \frac{\pi \theta_m}{4w^2} \right)} (13)$$

where $T_m = E_c/m^2$ is the effective temperature associated with the winding number $m$ and $\theta_m = T/T_m$. Although the integrand is quite different, this temperature dependence is identical to the one found by Ambegaokar and Eckern [5]. It directly expresses the current in terms of a temperature square average of a winding number.

In conclusion, we have calculated the average persistent current in the first order of the Hartree-Fock approximation. By writing the current directly in terms of the winding number decomposition of the return probability, we have avoided the use of the diagrammatic calculation and directly found the harmonic expansion of the current. Although this calculation is reminiscent of the semiclassical description of the spectral correlations and of the average current of non-interacting particles in the canonical ensemble [12], it does not use any semiclassical sum rule, since here the correlation function of interest can be exactly written in...
terms of the return probability without any approximation. Moreover, we have written an expression for the average current (eqs.6,12) which is valid beyond the diffusive regime and may be used for example in the ballistic regime where interesting magnetic response have also been observed [13].
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