Recovery of the persistent current induced by the electron-electron interaction in mesoscopic metallic rings

G. Chiappe
Departamento de Física, Universidad de Buenos Aires, Ciudad Universitaria, Pabellón I, 1428 Capital Federal, Buenos Aires, Argentina

J.A. Vergés and E. Louis
Departamento de Física Aplicada, Universidad de Alicante, Apartado 99, E-03080 Alicante, Spain.

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Abstract

Persistent currents in mesoscopic metallic rings induced by static magnetic fields are investigated by means of a Hamiltonian which incorporates diagonal disorder and the electron-electron interaction through a Hubbard term ($U$). Correlations are included up to second order perturbation theory which is shown to work accurately for $U$ of the order of the hopping integral. If disorder is not very strong, interactions increase the current up to near its value for a clean metal. Averaging over ring lengths eliminates the first Fourier component of the current and reduces its value, which remains low after interactions are included.

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The theoretical prediction concerning the existence of persistent currents in isolated rings in the presence of static magnetic fields \[1\] has recently been experimentally demonstrated \[2\]. As a consequence of the boundary conditions imposed by the magnetic field, both the current and the free energy are periodic functions of the magnetic flux threading the loop \(\Phi\) with a fundamental period \(\Phi_0 = \hbar/e\). In clean (ideal) metallic loops at zero temperature, this current is expected to be nearly \(ev_F/L\), where \(L\) is the perimeter of the loop. Impurities are thought to decrease this current in an amount \(l/L\), where \(l\) is the mean free path. A persistent current periodic in the magnetic flux with period \(\Phi_0\) was reported in \[2\]. However, the value of this current resulted to be \((0.3 - 2.0)ev_F/L\), that is, with no apparent correction due to disorder (impurities) and two or three orders of magnitude higher than predicted by theoretical analyses. On the other hand, magnetization measurements on an ensemble of \(10^7\) Cu loops \[3\] suggested a persistent current of about \(3 \times 10^{-3} ev_F/L\), periodic in the magnetic flux with a period \(\Phi_0/2\). The latter result is believed to be a consequence of the large number of rings \[4,5\]: averaging eliminates the first Fourier component of the current although the second survives.

The large current found in a single isolated ring has prompted several theoretical studies aiming to find a mechanism which could compensate the effect of impurities \[5–13\]. In particular it has been suggested that e-e interactions may tend to homogenize the system, offsetting the reduction in the current promoted by disorder. Calculations by means of spinless fermions models indicate that e-e interactions reduce the value of the persistent current \[6–8\], or show increased currents in unrealistic regions of the parameter space \[6\]. On the other hand, recent analysis of the effect of a Hubbard term \((U)\) indicate that the interaction compensates in part the detrimental effect of disorder \[9–12\]. In particular renormalization group and exact calculations \[9,10\] show that the Drude stiffness of the disordered system increases with \(U\). This result is in line with calculations of the full current by means of a first order perturbation treatment of the Anderson-Hubbard Hamiltonian \[11,12\]; we note, however, that first order perturbation theory may strongly overestimate the effects of the interactions.
In this work we present the results of a study of persistent currents in one dimensional metallic rings by means of the Anderson-Hubbard Hamiltonian. Correlation is included up to second order perturbation theory \[^{[14]}\], which is shown to work very accurately for the rather small values of $U$ which apply for a metallic band. The Hamiltonian used in this work is:

$$\begin{align*}
H &= \sum_{l\sigma} \epsilon_l c_{l\sigma}^\dagger c_{l\sigma} - t \sum_{\langle lm \rangle \sigma} \left[ e^{2\pi i \Phi / L} c_{l\sigma}^\dagger c_{m\sigma} + H.c. \right] \\
&\quad \quad + U \sum_l n_{l\uparrow} n_{l\downarrow},
\end{align*}$$

(1)

where the on-site energies, $\epsilon_l\sigma$, are chosen randomly between $-W/2$ and $W/2$. $U(>0)$ is the on-site Coulomb repulsion, $t$ the hopping integral between nearest neighbor sites, and $L$ the number of sites. The results herewith discussed correspond to one electron per site (half-filling) which is adequate to describe metallic systems. In the following we will take $t = 1$ and all lengths will be given in units of the lattice constant. Second order perturbation theory is implemented as follows. Single particle excitations are included in all orders of perturbation theory (Hartree selfconsistency) \[^{[15]}\] whereas two particle excitations will be included in second order (Fig. 1). Only paramagnetic solutions are considered. It should be noted that this approach could likely be valid to describe the Anderson phase of this system (small $U$) \[^{[16]}\]. Actually, a transition to a Hubbard-like phase is expected for large $U$ \[^{[16]}\] which cannot be described within the second order perturbation theory utilized in this work. Note, however, that in the present systems $U$ is always smaller than half the bandwidth.

The persistent current will be calculated from:

$$I(\Phi) = -\frac{1}{2\pi} \frac{\partial E_g(\Phi)}{\partial \Phi},$$

(2)

where $E_g(\Phi)$ is the ground state energy for a flux $\Phi$.

To facilitate the choice of $W$, we have calculated the localization length from the decay of the Drude weight with the system size at $U = 0$. The Drude weight $D$ is given by:

$$D = \frac{L}{4\pi^2} \left( \frac{\partial^2 E_g(\Phi)}{\partial \Phi^2} \right)_{\Phi = \Phi_m},$$

(3)
where $\Phi_m$ is the location of the minimum of the ground state energy. We have carried out simulations for $L = 4−512$, keeping constant the product $L \times \text{number of realizations} (16384)$. The results can be very accurately fitted by exponential functions $D(L) \propto \exp(-(L/\xi)$ for the three $W$ shown in Fig. 2. The resulting values for the localization length, $\xi$, are 110, 29 and 7 for $W=1$, 2 and 4, respectively. The accuracy of these results is supported by the fact that similar scaling laws were obtained for other magnitudes. For instance $<I^2>^{1/2}$ averaged over the magnetic flux, is very accurately fitted by $<I^2>^{1/2} \propto \exp(-(L/\xi))/L$, with $\xi = 28.4$ for $W=2$, in excellent agreement with the previous result. Our numerical results for $\xi$ agree very well with the well-known expression obtained at the mid-band for small disorder [7], $\xi = 105/W^2$ ($W << 2\pi$); in fact this formula gives 105, 26 and 6.6, for $W = 1$, 2 and 4, respectively, to be compared with the results given above. We note that for rings of $L \approx 100$, $W=1,2$ will represent two cases in which the localization length is of the order or significantly smaller than the length $L$ of the ring.

The accuracy of second order perturbation theory was checked by comparing results for $I(\Phi)$ obtained by means of perturbation theory with those of exact calculations (Lanczos method) for rings of $L = 8$ and several values of $W$ and $U$ (Fig. 3). We note that for $U$ up to 1.5 the agreement is excellent. Instead the agreement for larger $U$ is poor and the numerical results obtained by means of perturbation theory are not shown in the Figure. In particular, the second order results show abrupt changes in the current (near $\Phi = 0$ and/or 0.5) which we associate to changes in the nature of the wavefunction (Anderson to Hubbard-like); these abrupt changes in the current were used as an indication of the failure of second order perturbation theory when larger rings were investigated. The results of Fig. 3 do also illustrate a key point of the effects of $U$. As the exact results show, for small values of the e-e interaction an increase in the current is observed (the effect of $U$ increases with $W$, for instance a factor of 7 increase in $I$ is obtained when an interaction of $U = 2$ is switched in a chain of $L=8$ and $W=8$). Further increases in $U$ reduce the current below its value for $U = 0$, and for $U = \infty$ the current vanishes no matter the degree of disorder. These results can be understood in terms of clear physical grounds [8]. For small $U$ the e-e
interaction homogenizes the disordered system promoting a delocalization of the electronic states and, subsequently, an increase of the current. When $U$ is increased above a given value, the scattering mechanism added by the e-e interaction dominates and the current starts to decrease, becoming zero for an interaction of infinite strength. Previous analyses of these systems did not consider this question in detail.

Figure 4 shows the results for rings of length $L=100$. In order to facilitate the comparison with the experimental data for a single metallic loop, the results of a single realization are shown. The results for the ordered ring and $U=0$ are also shown as a reference. We first note that for $U=0$ the current for $W=1$ is much larger than for $W=2$. This is a consequence of the fact that $\xi/L$ is 1.1 for $W=1$ and 0.29 for $W=2$. Electron-electron interactions increase the magnitude of the persistent current very significantly. Although this increase is relatively more important for $W=2$ (up to a factor of 7 for the represented results), the current is still well below the value corresponding to the ordered system. Instead for $W=1$, the current for $U=1.5$ gets rather close to that of the ordered system, in qualitative agreement with the experimental results.

It should be pointed out that we have never obtained currents higher than that of the ordered system, as apparently observed in the experiments on single rings. In our opinion, e-e interactions can never increase the current beyond that of the ordered ring, as these interactions are by themselves a source of scattering (see above).

One of the most intricate issues concerning persistent currents in mesoscopic rings is the way in which averages are performed. This is of particular significance when plausible explanations for experiments such as the one performed on $10^7$ metallic rings have to be found. Here, in order to facilitate the investigation of the effects of the e-e interaction, we have adopted the simple approach of averaging over the rings length. This kind of average has not been considered previously, despite of the fact that the actual lengths of the rings investigated in Ref. should show considerable dispersion. Fig. 5 reports the persistent currents obtained by averaging those for rings of lengths $L=100$ and $102$ (five realizations each). We first note that the persistent current is a periodic function of the magnetic flux on the scale of half a flux quanta ($\Phi_0$), as already predicted by other
authors. The reason for this halving of the period is, in this case, very simple; in fact the two rings, being half-filled, have an even or odd number of electrons per spin, and, thus, their resulting currents are out of phase in $\Phi_0/2$. On the other hand, the amplitude of the current is significantly smaller than in the case of a single ring. Although as in the case of a single ring the e-e interaction increases the current, this remains well below the value corresponding to the ordered system. More extensive averaging may reduce further the amplitude of the current, albeit, as discussed in [4], it should remain finite.

In conclusion, we have presented an investigation of persistent currents in mesoscopic metallic rings by means of a model Hamiltonian which includes diagonal disorder and a Hubbard term. We have proved that second order perturbation theory works very accurately for the low values of the strength of the e-e interaction ($U$) which are adequate in the present systems. Our results show that for small $U$ the current is increased up to near the value corresponding to the non-interacting case, in line with the common believe which assumes that the interaction should homogenize the disordered system. Instead, for large values of $U$, the e-e interaction acts as a scattering mechanism that reduces the current, which decays to zero in the $U = \infty$ limit. These results may explain the large currents observed in isolated metallic rings. We have also shown that averaging over ring length promotes a halving of the period of the current and a strong reduction of its amplitude (not substantially increased by the e-e interaction), in line with the experimental information obtained on $10^7$ Cu loops.

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*Permanent address: Instituto de Ciencia de Materiales, Consejo Superior de Investigaciones Científicas, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

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[19] Note that although the qualitative behavior of the current versus $U$ was correctly described in [7], the actual increments in its amplitude were much lower than those obtained here, likely due to the spinless fermions model and/or the small rings investigated in [7]. On the other hand, the maximum in the current versus $U$ is not accounted for by means of renormalization group equations which do not incorporate $4k_F$ impurity scattering [8], as discussed in [10]. We finally note that this maximum was already observed in the behavior of the localization length for the Anderson-Hubbard Hamiltonian [18].
FIGURE CAPTIONS

Fig.1: Feynman diagram included in the second order perturbation theory utilized in this work.

Fig.2: Scaling of the Drude weight ($D$) with the length of the ring ($L$) in the non-interacting case ($U=0$) and for several values of the disorder parameter. $W=0.01$ (circles), 1 (squares), 2 (up triangles) and 4 (down triangles).

Fig.3: Persistent currents in rings of length $L = 8$, half-filling and $W=4$ as a function of the magnetic flux threading the ring. $U= 0$ (thin continuous line). Exact results (thick lines): $U= 1, 1.5, 3$ and 4, dotted, continuous, dashed, and chain lines, respectively. Second order perturbation theory results: $U= 1$ (circles) and 1.5 (triangles).

Fig.4: Persistent current in rings of $L=100$ and half-filling as a function of the magnetic flux threading the ring. a) $W=1$ and $U=0$ and 1 (continuous and dashed thick lines, respectively). The results for the ordered chain (thin continuous line) are also shown (for $U=0$). b) $W=2$ and $U=0, 1$ and 2 (continuous, dashed and dot-dashed thick lines, respectively). The e-e interaction was treated in second order perturbation theory (see text).

Fig.5: Persistent current in metallic rings as a function of the magnetic flux threading the ring. The results correspond to the average of those obtained for two rings of $L=100$ and 102 (5 realizations each), both at half filling. Results for $W=1$ and $U=0$ and 1 (continuous and dashed lines, respectively) are shown.
