Electron-electron interactions in one- and three-dimensional mesoscopic disordered rings: a perturbative approach

Michel Ramin, Bertrand Reulet and Hélène Bouchiat

Laboratoire de Physique des Solides, associé au CNRS
Bât. 510, Université Paris–Sud, 91405, Orsay, France.

Abstract

We have computed persistent currents in a disordered mesoscopic ring in the presence of small electron-electron interactions, treated in first order perturbation theory. We have investigated both a contact (Hubbard) and a nearest neighbour interaction in 1D and 3D. Our results show that a repulsive Hubbard interaction produces a paramagnetic contribution to the average current (whatever the dimension) and increases the value of the typical current. On the other hand, a nearest neighbour repulsive interaction results in a diamagnetic contribution in 1D and paramagnetic one in 3D, and tends to decrease the value of the typical current in any dimension. Our study is based on numerical simulations on the Anderson model and is justified analytically in the presence of very weak disorder. We have also investigated the influence of the amount of disorder and of the statistical (canonical or grand-canonical) ensemble.
Since the experimental discovery \cite{1,2,3} of persistent currents in phase-coherent mesoscopic rings pierced by a magnetic flux, a great deal of theoretical work has been devoted to the understanding of the order of magnitude of these currents, which is difficult to explain within a single electron theory. Both the amplitude of the average current measured in a many-rings experiment \cite{1}, and the typical current measured in single ring experiments \cite{2,3} are found to be, at least in the diffusive regime, between 1 and 2 orders of magnitude larger than their expectations \cite{4,5,6,7,8,9}. In order to explain this discrepancy between experiment and theory, several authors have studied the influence of electron-electron (e-e) interactions on the persistent currents. Since the work of Altshuler and Aronov \cite{10} based on diagrammatic theory, it has been indeed known that transport properties of quantum coherent disordered systems are affected by e-e interactions. Inspired by these results, Ambegaokar and Eckern \cite{11} have shown that the presence of short-range interactions gives rise to a contribution to the average persistent current, whose sign depends on the sign of the interactions. The low flux current is found to be paramagnetic for repulsive and diamagnetic for attractive interactions. It has also been suggested that the typical value of the current could be strongly enhanced by interactions and disorder independent \cite{12,13}. In contrast with these results which are valid for 3D disordered rings in the diffusive regime, numerical 1D exact diagonalisations have found that the current is decreased in the presence of repulsive nearest neighbour interactions \cite{14}. The case of long range Coulomb interactions has also been investigated \cite{15,16}, with the result that the current is decreased for a very weakly disordered ring and increased at higher disorder. However from these studies performed in 1D it is very difficult to anticipate the behavior of a realistic 3D multichannel ring, which is very difficult to handle exactly numerically.

These considerations have motivated the present work where we have studied the influence of a small e-e interactions, on disordered rings in 1D and 3D. We have compared the cases of a pure contact Hubbard and a first neighbour interaction. The e-e interaction is treated within first order of perturbation on the Anderson model as follows:
\[ \mathcal{H} = \sum_{i,j} \left[ t_{ij} c_i^\dagger c_j + c.c. \right] + \sum_i w_i c_i^\dagger c_i \]  

(1)

with \( t_{ij} = \exp \left( 2i\pi \Phi / \Phi_0 (x_i - x_j) / L_x \right) \), where \( i \) and \( j \) are nearest neighbours, and where \( w_i \) is the onsite disorder potential uniformly distributed in the interval \([-W/2, W/2]\). This hamiltonian is exactly diagonalized in the presence of disorder.

We first consider the one-band Hubbard model, characteristic of contact interactions described by the hamiltonian \( \mathcal{H}_{int} = U \sum_i n_{i\uparrow} n_{i\downarrow} \) with \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) and \( U > 0 \) for repulsive interactions. The first order correction to the energy of a \( N \) electrons state reads:

\[
\begin{align*}
\delta E(2p) &= \sum_{\alpha,\beta=1}^p U(\alpha, \beta) \quad \text{if } N = 2p \\
\delta E(2p + 1) &= \delta E(2p) + \sum_{\alpha=1}^p U(\alpha, p + 1) \quad \text{if } N = 2p + 1
\end{align*}
\]

(2)

Here \( U(\alpha, \beta) \) describes the interaction energy between electrons in the states \( \alpha \) and \( \beta \) which are single electron eigenstates of the Anderson hamiltonian.

\[ U(\alpha, \beta) = U \sum_i |\psi_\alpha(i)|^2 |\psi_\beta(i)|^2 \]

(3)

where \( \psi_\alpha(i) \) denotes the value of the one-electron wavefunction at the site \( i \). We can also write the correction to the ground state with \( 2p \) electrons in the form:

\[ \delta E(2p) = U \sum_i n_{p}^2(i) \]

(4)

where \( n_p(i) = \sum_{\alpha=1}^p |\psi_\alpha(i)|^2 \) is the electronic density at the site \( i \) with the first \( p \) eigenstates occupied by only one electron. Expression (4) is very similar to the result obtained by Argaman and Imry [17]. We deduce the correction to the current given by:

\[ \delta I(N) = -\frac{\partial \delta E(N)}{\partial \Phi} \]

(5)

and compute the canonical (C) and grand-canonical (GC) average of this current in 3D in the diffusive regime (the averaging is done over the filling, between 1/4 and 3/4 of the spectrum). In the GC case, only configurations with an even number of electrons contribute. In fig. \[ \] these quantities are compared to the average C and GC currents without interactions. We...
can see that, unlike the non-interacting case, both statistics give identical results for $\langle \delta I \rangle$ which has the same paramagnetic sign (in zero flux) as the canonically average current in the absence of interactions. Furthermore, the effect of interactions is to enhance the current, which is in agreement with analytical results [11]. From the first order correction to the energy, it is also possible to compute the quantity $\langle \delta(I^2(N)) \rangle = 2\langle I(N)\delta I(N) \rangle$ which is the first order correction in $U$ to the typical current $\langle I^2 \rangle$. We observe in fig. 1b that $\langle I \delta I \rangle$, in both C and GC statistics, is always positive and of the order of $\sqrt{\langle I^2 \rangle \langle \delta I^2 \rangle}$, which means that there is a strong correlation between the current of $N$ electrons and the correction to this current for the same number of electrons. We have made this calculation for different values of the disorder. The first harmonics of average and typical currents are presented in fig. 2 as a function of the disorder $W$. We observe that $\langle I_2 \rangle$, $\langle \delta I_2 \rangle$, $\sqrt{\langle I^2 \rangle}$ and $\sqrt{\langle I_1 \delta I_1 \rangle}$ decrease as $W^{-2} \propto l_e$, the mean free path. This dependence of $\langle \delta I_2 \rangle$ with the disorder is in complete agreement with analytical calculations [11]. Nevertheless, as already pointed out [8], the disorder dependence of the C average $\langle I_2 \rangle$ for this small ring disagrees with analytical predictions [5–7]. In conclusion we have found that the effect of a contact interaction results in an increase of both average and typical currents. In the following we demonstrate this result analytically in the weak disorder limit. Eigenstates of the Anderson Hamiltonian in 1D without disorder are plane waves of the type $\psi_{n,\Phi}(x) = \exp(i2\pi(n - \Phi/\Phi_0)x/L)/\sqrt{L}$. In the presence of a very weak disorder, the degeneracy occurring at $\Phi = 0$ and $\Phi = \Phi_0/2$ is lifted, resulting in the following wavefunctions:

\begin{align*}
\psi_{n,\Phi}^+(x) &= \sqrt{2/L} \cos[2\pi(n - \Phi/\Phi_0)x/L + \chi_n] \\
\psi_{n,\Phi}^-(x) &= \sqrt{2/L} \sin[2\pi(n - \Phi/\Phi_0)x/L + \chi_n]
\end{align*}

(6)

where $\chi_n$ is a phase factor which depends on the particular realisation of the disorder. We can easily deduce the following value of $\delta E(2p)$:

$$\delta E(2p) = \begin{cases} 
(p^2 + \frac{1}{4})/L & \text{for } (\Phi = 0 \text{ and } p = 2N) \text{ or } (\Phi = \Phi_0/2 \text{ and } p = 2N + 1) \\
\frac{p^2}{L} & \text{otherwise}
\end{cases}$$

(7)

The resulting $\delta I(\Phi)$ presents an antisymmetric paramagnetic peak in the vicinity of $\Phi = 0$ (resp. $\Phi_0/2$) for an even (resp. odd) number of electron pairs, in agreement with the
symmetry property of the 1D electron spectrum, according to which: \( I(N, \Phi) \sim I(N + 1, \Phi + \Phi_0 / 2) \), valid in the limit \( N \gg 1 \). This behavior gives rise to a current contribution \( \delta I \) which has the same sign as in the absence of interactions (i.e. paramagnetic in zero flux for \( 2p \) electrons) in agreement with our numerical findings (see fig. 3a).

In comparison with the Hubbard model we also considered the short-range nearest-neighbours interactions studied by Bouzerar et al. \[14\]. The corresponding hamiltonian reads:

\[
\mathcal{H}_{\text{int}} = U \sum_i c_i^+ c_i c_{i+1}^+ c_{i+1}.
\]

Two terms appear now in the first order correction to the energy: a direct and an exchange term, so that the final correction reads:

\[
\delta E(2p) = U \left( 2 \sum_i n_p(i) n_p(i + 1) - \sum_i \sum_{\alpha,\beta=1}^p \psi_\alpha^*(i) \psi_\beta(i) \psi_\alpha(i + 1) \psi_\beta^*(i + 1) \right)
\] (8)

Note that unlike the case of ref. \[14\], here spin has been taken into account. However we have found that the exchange term is always much smaller than the direct one, which means that the expression obtained for spinless electrons would only differ by a factor two from what we have calculated.

In 1D, we find a current contribution which, for each value of the number of electron pairs (which varies from \( \frac{1}{4}L \) to \( \frac{3}{4}L \), \( L \) being the length of the ring) is opposite in sign to the current in the absence of interaction, in agreement with ref. \[14\]. The resulting average current gives rise to a diamagnetic contribution (see fig. 3b).

On the other hand in 3D, the same type of interaction gives rise to an average paramagnetic contribution to the current, which is shown in fig. 3a for different values of the disorder. We observe like previously that the current does not depend on the statistics considered, but its amplitude is much larger than the value obtained for a contact interaction. The dependence of the average current on disorder is also very weak in contrast with the results obtained for the Hubbard interaction (see fig. 2a). If we now study the results obtained for the corrections to the typical current in 3D we see that for most values of the flux and for ballistic and diffusive regimes \( \langle I\delta I \rangle \) is negative for the C statistics except in the vicinity of \( \Phi = 0 \) and \( \Phi = \Phi_0 / 2 \) where it is slightly positive. In the GC ensemble \( \langle I\delta I \rangle \) is always negative (see for instance fig. 3 obtained in the diffusive regime). The typical current is thus
diminished in the presence of first neighbour interactions both in 1D and 3D. The variation of the first harmonics versus disorder are presented in fig. 2. We observe that \( \langle \delta I_2 \rangle \) generally does not vary very much with disorder.

We have also performed an analytical computation of \( \delta E(2p) \) (as previously discussed in the Hubbard case) for a 1D ring in the limit of very weak disorder, and obtained for the first order energy correction:

\[
\delta E(2p) = \begin{cases} 
[f_1(p) + f_2(p)]/L & \text{for } (\Phi = 0 \text{ and } p = 2N) \text{ or } (\Phi = \Phi_0/2 \text{ and } p = 2N + 1) \\
 f_1(p)/L & \text{otherwise}
\end{cases} 
\]  

with

\[
f_1(p) = 2p^2 - \left( \frac{\sin p\pi/L}{\sin \pi/L} \right)^2 \quad \text{and} \quad f_2(p) = \frac{1}{2} \cos 2p\pi/L
\]

(9)

Note the strong dependence of \( \delta E(p) \) on the filling: the sign of \( \cos 2p\pi/L \) determines the flux dependence of \( \delta E(2p) \) and consequently the sign of \( \delta I(N, \Phi) \). When \( p \) varies between \( \frac{1}{4}L \) and \( \frac{3}{4}L \), \( \cos 2p\pi/L \) is negative. It results from this that \( \delta I(\Phi) \) presents an antisymmetric diamagnetic peak near \( \Phi = 0 \) (\( \Phi_0/2 \)) for an even (odd) number of electron pairs. In the weak disorder limit this calculation can be generalised to a multichannel ring. In that case we can separate the contribution of the interactions to the persistent current into its longitudinal and transverse part. The longitudinal component can, depending on the filling, lead to diamagnetism; however, the transverse part of the interaction always gives rise to paramagnetism, since it is identical to the Hubbard contribution. This explains why the total contribution is paramagnetic. Nevertheless, note that the case of anisotropic interactions may lead to the opposite conclusion. So we have obtained a confirmation of our numerical results which show that a first neighbour interaction gives a diamagnetic contribution to the average current in 1D, and also tends to decrease the value of the typical current. Only this last result remains valid in 3D, where the average current is paramagnetic.

From our perturbative study of the influence of e-e interactions on the persistent current in a disordered ring, we have shown that a repulsive Hubbard interaction enhances the typical value of the persistent current in any dimension. It also contributes to the average current
with a paramagnetic sign in zero field. These extra both typical and average contributions
to the current decrease with disorder just like the single electron quantities. There is thus no
evidence that the Hubbard interaction could attenuate the sensitivity of the currents upon
disorder.

A nearest neighbour interaction, on the other hand, tends to decrease the value of the
typical current, while the sign of the average contribution depends however on the dimen-
sionality of the ring: it is diamagnetic in 1D and paramagnetic in a multichannel ring, with
very small disorder dependence. These differences between Hubbard and nearest neighbour
interactions in the one dimensional limit \cite{18} have also been found analytically.

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FIGURES

FIG. 1. (a): flux dependence of C and GC corrections to the average current, compared to their values without interactions. (b): C and GC corrections to the typical current compared to the typical C current without interactions. All curves are calculated for a $30 \times 4 \times 4$ ring, for a contact (Hubbard) interaction with $W = 2$ and $U = 1$.

FIG. 2. Dependence of different harmonics of the correction to average or typical current on disorder. The effect of Hubbard (subscript "H") or nearest neighbour (subscript "NN") interactions are compared with the average and typical currents without interaction (all of them for a $30 \times 4 \times 4$ ring with $U = 1$). (a): second harmonics of the average current with Hubbard, nearest neighbour or no interaction. (b): first harmonics of the typical current with or without Hubbard interactions. (c): first harmonics of the typical current with or without nearest neighbour interactions.

FIG. 3. Flux dependence of $\delta I$ for a Hubbard (a) or nearest neighbour (b) interactions for all the even fillings of a 1D ring of length $L = 16$, from $\frac{1}{4}L$ to $\frac{3}{4}L$. The circles correspond to the average within the same range.

FIG. 4. (a): flux dependence of $\langle \delta I \rangle$ for a nearest neighbour interaction for three amplitudes of disorder, in the C ensemble in 3D. (b): flux dependence of (negative) C and GC corrections to the typical current compared to the typical C value, for a $30 \times 4 \times 4$ ring with nearest neighbour interactions, with $W = 3$ and $U = 1$. 
