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Persistent Currents in Interacting Systems: Role of the Spin

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Abstract. — Persistent currents flowing through disordered mesoscopic rings threaded by a magnetic flux are investigated. Models of fermions with on-site interactions (Hubbard model) or models of spinless fermions with nearest neighbor interactions are considered on 2D cylinders with twisted boundary conditions in one direction to account for a magnetic flux. Self-consistent Hartree-Fock methods are used to treat the electron-electron interaction beyond first order. We show that the second harmonic of the current (which is relevant in the diffusive regime) is *strongly suppressed* by the interaction in the case of spinless fermions while it is *significantly enhanced* in the Hubbard model. Our data also strongly suggest that the reduction (increase) of this harmonic is related to a strong increase (reduction) of the spatial fluctuations of the charge density.

The observations of mesoscopic currents in very pure metallic nano-structures was done in pioneering experiments [1–3]. In the first case the experiment dealt with the average current of a system of 10^7 disconnected rings in the diffusive regime while in the second a single ring was used. Although the existence of such persistent currents in small metallic rings was predicted long ago [4–6] the magnitude of the observed currents is still a real challenge to theorists. There is a general belief that the interaction plays a crucial role in enhancing the current. But, so far, the role of the interaction in disordered systems is still unclear. Treating interaction and disorder on equal footings is a difficult task. Previous work [7, 8] has shown by exact diagonalizations (ED) of small clusters that, for strictly 1D systems of spinless fermions, the effect of a *repulsive* interaction is to increase further the localization of the electrons and hence to decrease the value of the current. Using a Hartree-Fock approach, Kato *et al.* [16] have obtained a qualitatively good agreement with the exact calculations. On the other hand, Giarmarchi *et al.* [9] have pointed out that, for the 1D Hubbard model, *i.e.* when spin is included, the interaction enhances the persistent current. In this case, the increase of the current is closely related to the *decrease* of the spatial fluctuations of the charge density or, equivalently,

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to the smoothing out of the charge density as it occurs in the 1D Hubbard model with repulsive interaction. This emphasizes the important role of the spin in 1D systems.

In higher dimensions the role of the spin is still unclear. First order calculations for which spin is irrelevant have shown that the persistent currents are increased by the interactions [11]. More recently, Ramin *et al.* [13] have numerically shown that the first order Hartree-Fock (HF) correction to the second harmonic of the persistent current was in agreement with the analytical treatment [11]. Hence, for both the spinless fermion model with nearest-neighbor interactions and the Hubbard model, the second harmonic is enhanced. However, in this treatment it is found that a nearest neighbour interaction tends to decrease the value of the typical current while a repulsive extended Hubbard interaction enhances it. In some previous work, Exact Diagonalizations (ED) calculations have been compared to a Self-consistent Hartree-Fock (SHF) treatment of the interaction. For the small clusters (4×4 clusters) which could be handled we have found a good agreement between the two sets of data [19]. This direct comparison with the exact results has therefore established some degree of reliability of the self-consistent Hartree-Fock approximation at least in the diffusive regime. In this paper, we use both HF and SHF treatments of the interaction between particles which enables us to treat much larger systems. The SHF treatment takes into account high order terms in the interaction and, simultaneously, deals with quantum interference effects due to the disorder somehow exactly. It is important to note that this method is different from the usual perturbative approach [11] where the corrections to the current due to the interacting term are calculated perturbatively. In contrast to their approach, our procedure includes a resummation of higher order terms through a self-consistency relation, which turns out to become essential at moderate interaction. Nevertheless, an exact connection with some diagrammatic expansion is a tedious problem and this issue probably deserves further study. Note that our study also applies in principle to single or multi-ring experiments. From a theoretical point of view, the difference simply relies in the absence or presence of particle number fluctuations. In the following, we shall assume that the number of electron of the ring is fixed.

This paper is organized as follows: first, we compare, for both spinless and Hubbard models, the first order correction (in the interaction) and the SHF correction to the second harmonic of the persistent currents. We show that, in the case of spinless fermions, the two methods stay in good agreement only for rather small values of the interaction parameter but a complete disagreement appears for moderate values. In contrast, in the Hubbard case, the agreement between the two approaches is rather good. Secondly, we present evidences that this *decrease* (*increase*) of the persistent currents is directly related to the *increase* (*decrease*) of the spatial fluctuations of the charge density from site to site as the interaction is switched on. Thirdly, the effect of the electron repulsion on the second harmonic is shown to increase with the system size.

The Hamiltonian is defined on a $L \times L$ lattice with periodic boundary conditions in one direction (*e.g.* x direction) and reads:

$$\mathcal{H} = \mathcal{H}_K + \mathcal{H}_{\text{int}} + \mathcal{H}_{\text{des}}. \quad (1)$$

$\mathcal{H}_K = \sum_{i,j} t_{ij} c_i^\dagger c_j$ is the usual kinetic part containing the flux dependence, $t_{ij} = \frac{1}{2} \exp\{i \frac{2\pi\Phi}{L}(i_x - j_x)\}$ if i and j are nearest neighbor sites and 0 otherwise. \mathcal{H}_{int} is the interacting part and \mathcal{H}_{des} is the term due to the disorder,

$$\mathcal{H}_{\text{des}} = \sum_i w_i n_i \quad (2)$$

where n_i is the local density operator at site i and w_i are on-site energies chosen randomly in $[-W/2, W/2]$. When spin is included, $n_i = n_{i\uparrow} + n_{i\downarrow}$ and the kinetic term contains an additional

sum over the spin indices. In the spinless fermion case the electron repulsion is given by

$$\mathcal{H}_{\text{int}}^{\text{S}} = \frac{1}{2} \sum_{i,j} V_{ij} n_i n_j, \quad (3)$$

where $V_{i,j}$ of strength $V = |V_{ij}|$ only connects nearest neighbor sites (screened interaction). Lastly, the Hubbard interaction is defined by

$$\mathcal{H}_{\text{int}}^{\text{H}} = U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (4)$$

In the SHF approximation, the interaction part of the spinless fermion model reduces to

$$\mathcal{H}_{\text{int}}^{\text{S}} = - \sum_{i,j} \delta t_{ij} c_i^\dagger c_j + \sum_i \delta w_i n_i - \frac{1}{2} \sum_{i,j} V_{ij} (\langle n_i \rangle_0 \langle n_j \rangle_0 - |\langle c_j^\dagger c_i \rangle_0|^2) \quad (5)$$

where $\langle \rangle_0$ stands for the expectation value in the ground-state wavefunction. The expression above contains two terms: an Hartree term proportional to $\delta w_i = \sum_{j \neq i} V_{ij} \langle n_j \rangle_0$ which comes out as an extra on-site disorder potential and a Fock term proportional to $\delta t_{ij} = V_{ij} \langle c_j^\dagger c_i \rangle_0$ which is an extra hopping amplitude. The quantities $\langle n_j \rangle_0$ and $\langle c_j^\dagger c_i \rangle_0$ are calculated self consistently so that the SHF Hamiltonian itself depends on the filling factor, the disorder strength *etc.* Similarly, in this approximation $\mathcal{H}_{\text{int}}^{\text{H}}$ becomes

$$\mathcal{H}_{\text{int}}^{\text{H}} = U \sum_i (\langle n_{i\uparrow} \rangle_0 n_{i\downarrow} + \langle n_{i\downarrow} \rangle_0 n_{i\uparrow} - \langle n_{i\downarrow} \rangle_0 \langle n_{i\uparrow} \rangle_0). \quad (6)$$

Since we are interested in the paramagnetic phase we shall assume $\langle n_{i\downarrow} \rangle_0 = \langle n_{i\uparrow} \rangle_0$. In this case the spin \uparrow and \downarrow are decoupled so that one can write $\mathcal{H}_{\text{int}}^{\text{H}} = \sum_\sigma \mathcal{H}_{\text{int}}^\sigma$ where

$$\mathcal{H}_{\text{int}}^\sigma = U \sum_i \langle n_{i\sigma} \rangle_0 n_{i\sigma} - \frac{1}{2} \langle n_{i\sigma} \rangle_0^2. \quad (7)$$

The current is defined as the derivative of the total energy *versus* flux

$$I(\Phi) = - \frac{\partial E(\Phi)}{\partial \Phi} \quad (8)$$

where $E(\Phi)$ is the total energy. The current is a periodic function of Φ of period 1 (Φ is measured in units of Φ_0) and thus can be expanded as a Fourier series,

$$I(\Phi) = \sum_n I_{hn} \sin(2\pi n\Phi) \quad (9)$$

where I_{hn} are the harmonics of the current. The solution of the previous set of non-linear self-consistent equations are obtained numerically on small clusters by an iterative procedure for arbitrary values of Φ and arbitrary disorder realizations. The various physical quantities are then averaged over disorder. The disorder average denoted by $\langle \rangle_{\text{dis}}$ in the following corresponds typically to an average over at least 1000 configurations of the disorder.

It is now well established that the ensemble average (over filling or disorder) suppresses the first harmonic of the current [18,19]. This fact was indeed observed in multi-ring experiments where the current was found to be $\Phi_0/2$ periodic. We have explicitly checked that the first

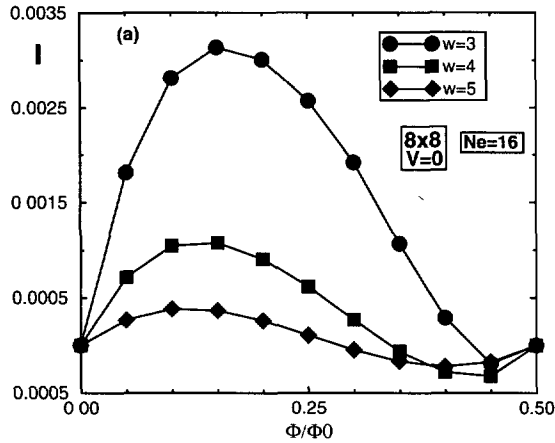


Fig. 1. — Total averaged current $I(\Phi)$ versus Φ (non interacting fermions) for a 8×8 system and for different values of the disorder parameter W , N_e is the total number of electrons. An average over 1000 disorder configurations has been done.

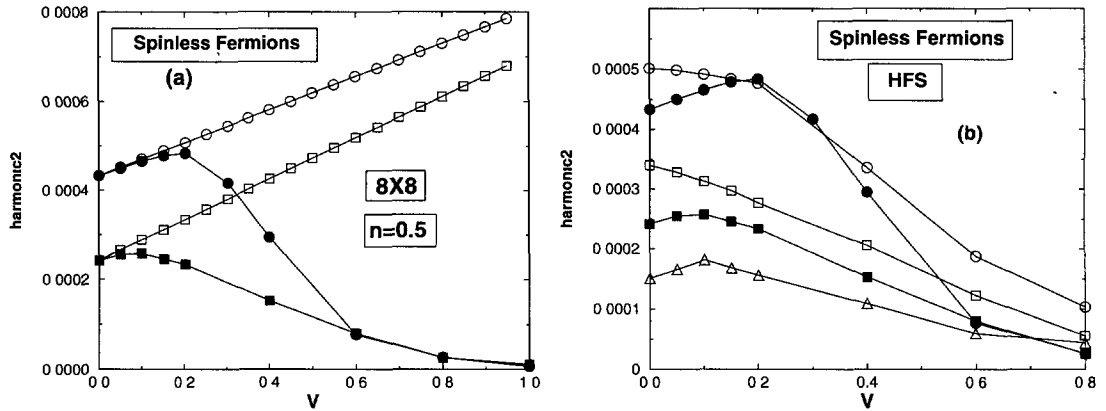


Fig. 2. — $\langle I_{h2} \rangle_{dis}$ as a function of V calculated within the SHF method for spinless fermions on a 8×8 cylinder. An average over 1000 disorder configurations has been done. a) Comparison between first order HF (open symbols) and SHF results (full symbols) at half-filling. Circles correspond to $W = 3$ and squares to $W = 4$. b) SHF results at half-filling (full symbols) and quarter filling (open symbols). Circles correspond to $W = 3$, squares to $W = 4$ and triangles to $W = 5$.

harmonic is suppressed for sufficiently large disorder. We show in Figure 1 the dependence of the total averaged current $\langle I(\Phi) \rangle_{dis}$ versus flux for different values of the disorder parameter. We observe from that figure that the current is $\Phi_0/2$ periodic for sufficiently large values of the disorder parameter ($W/t \geq 4$ for a system of size 8×8). This is a simple way to estimate the cross-over from the ballistic to the diffusive regime.

As noted previously, the self-consistency relations can take care of high order effects in the interaction. It is therefore necessary, as a preliminary study, to investigate the role of the self-consistency by comparing the SHF results to the simple first order calculations (referred to hereafter as HF). In Figure 2a $\langle I_{h2} \rangle_{dis}$ for spinless particles is plotted as a function of V . The calculations have been done at half-filling on a 8×8 cylinder. The HF contribution

is of course linear in V . As expected, we observe for small values of the interaction a perfect agreement between the SHF and the HF calculations. Indeed, the slope at $V = 0$ of the SHF results is actually given by the HF data. However, for increasing V the SHF calculation shows a strong reduction of the current whilst the HF predicts an increase. We also observe that the region of agreement between HF and SHF is reduced as the disorder increases. In other words, this means that, as the strength of the interaction increases, the effect of higher order terms becomes more and more dominant and thus a first order calculation is not sufficient. We will see later on that this reduction is related, as in the 1D case, to an increase of the spatial fluctuations of the charge density. The influence of the filling factor and of the disorder strength on $\langle I_{h2} \rangle_{\text{dis}}$ versus V is shown in Figure 2b. This figure shows that the repulsive interaction is detrimental to the persistent currents which are drastically suppressed for a wide range of parameters. Note that, at quarter filling, $\langle I_{h2} \rangle_{\text{dis}}$ starts immediately to decrease with V contrary to the behavior observed at half-filling.

Similar conclusions can also be reached from a direct investigation of the complete distributions of the first and second harmonics obtained in the SHF method (Figs. 3a and b) Note that these distributions contain more information than the above expectation values which correspond only to their first moments. In absence of interaction, we clearly observe that the distribution of the first harmonic is perfectly symmetric ($\langle I_{h1} \rangle_{\text{dis}} = 0$) in agreement with Figure 1. The effect of the spinless interaction on I_{h1} consists only on reducing the width of the distribution. That is why we focus on the conjugated effect of interaction and disorder on I_{h2} only. The case of the second harmonic is completely different. Indeed, in absence of interaction the distribution is strongly asymmetric, $\langle I_{h2} \rangle_{\text{dis}}$ is finite (current is $\Phi_0/2$ periodic). When we switch on the interaction, the effect is dramatic, for $V/t = 0.8$ the distribution gets perfectly symmetric ($\langle I_{h2} \rangle_{\text{dis}}$ is suppressed by the interaction) and the width of the distribution is significantly reduced.

In contrast to the spinless model, the Hubbard model exhibits a completely different behavior, as seen in Figure 4 showing the relative increase of $\langle I_{h2} \rangle_{\text{dis}}$ as a function of the Hubbard repulsion U . Interestingly enough, both SHF and HF calculations predict an increase of the current. It is also interesting to notice that the first order calculation gives reliable results regarding the effect of the interaction. However, the first order calculations always predict larger values of the currents. In Figure 3c, we also show the effect of the Hubbard interaction on the distribution of I_{h2} due to the interaction (SHF). The shape of the distribution remains asymmetric and $\langle I_{h2} \rangle_{\text{dis}}$ is increasing with the interaction as shown previously.

At this point, these results already suggest that the nature of the interaction plays a crucial role: in the spinless case the currents are strongly reduced by the interaction in contrast to a Hubbard repulsive interaction which enhances the currents. Secondly, we have shown that, in the spinless fermions case, higher order terms become rapidly dominant even for relatively small values of the interaction strength. Hence a first order approach is not sufficient.

Let us now try to develop a physical picture that could help to understand the role of the spin. We shall argue that the enhancement (reduction) of the persistent currents is related to the reduction (increase) of the fluctuations of the charge density n_i from site to site. One way of observing this effect on the charge density consists in plotting the distribution of the local density $\langle n_i \rangle_0$. For that purpose, we shall consider here a 10×10 system and assume that the $\langle n_i \rangle_0^k$ (where the subscript k labels the various realizations of the disorder) are independent variables. The distribution of the charge densities can then be defined as

$$P(\rho) = \frac{1}{N_{\text{dis}} L^2} \sum_{k=1}^{N_{\text{dis}}} \sum_{\iota} \delta(\langle n_{\iota} \rangle_0^k - \rho) \quad (10)$$

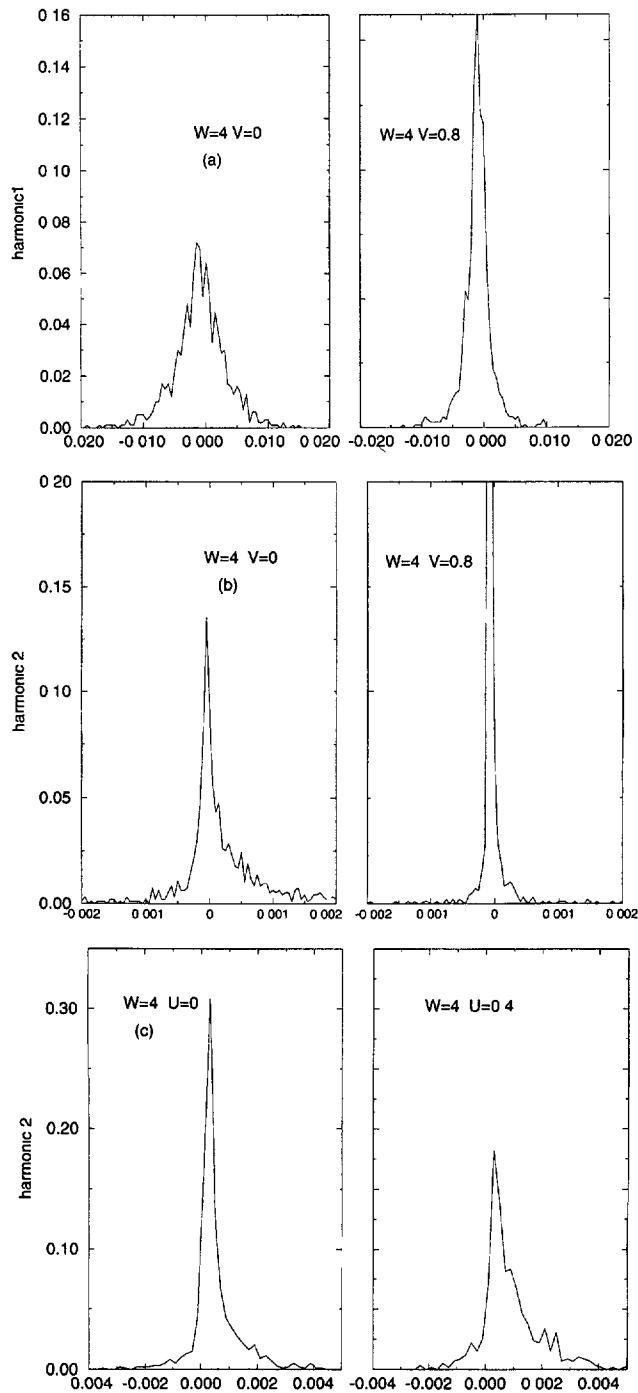


Fig. 3. — Distribution of the first and second harmonic calculated for a 8×8 system at half-filling. The disorder parameter is fixed ($W/t = 4$) We have considered 1 000 configurations of disorder. a) I_{h1} in the spinless fermion case ($V/t = 0$ and 0.8), b) I_{h2} in the spinless fermion case ($V/t = 0$ and 0.8), c) I_{h2} in the Hubbard case ($U/t = 0$ and $U/t = 0.4$).

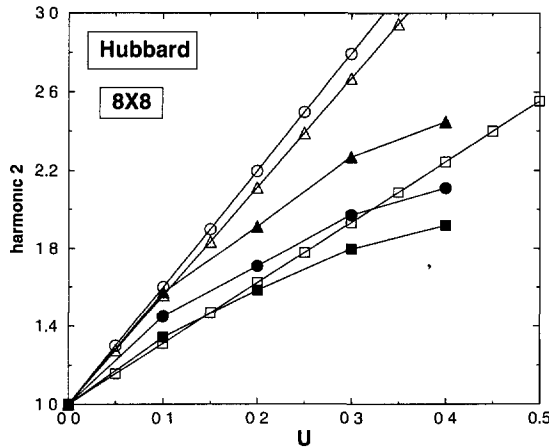


Fig. 4. — Ratio $\langle I_{h2} \rangle_{dis}(U, W) / \langle I_{h2} \rangle_{dis}(0, W)$ as a function of U calculated in the Hubbard model within both HF (open symbols) and SHF (full symbols) methods on a 8×8 cylinder. An average over 1 000 disorder realizations have been performed. Circles correspond to $W = 3$ at quarter-filling, squares to $W = 3$ at half-filling and triangles to $W = 4$ at half-filling.

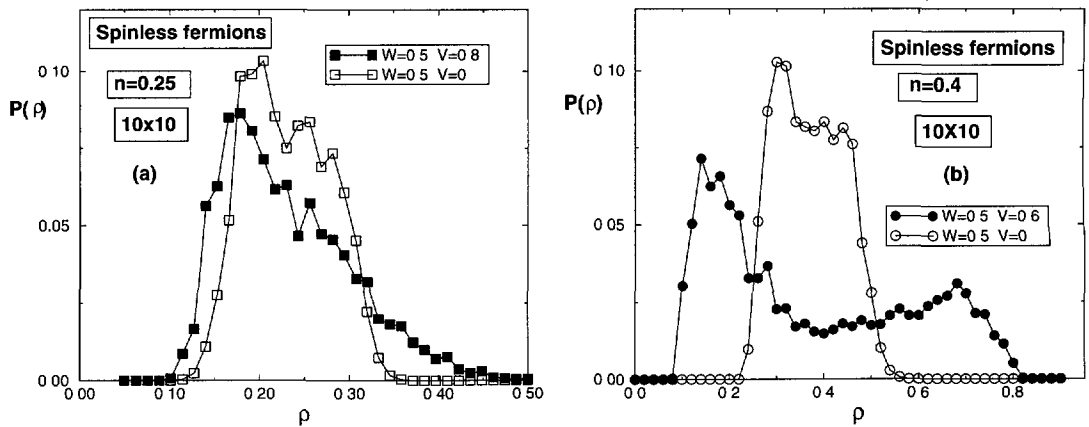


Fig. 5. — Distribution $P(\rho)$ in the case of spinless fermions. The calculations have been done at quarter filling $n = 0.25$ (a) and $n = 0.4$ (b) on a 10×10 cylinder. We have averaged over 30 configurations of the disorder. The values of V and W are given in the figure.

where L is the length of the system ($L = 10$) and N_{dis} is the number of disorder configurations. As usual, the local densities $\langle n_i \rangle_0^k$ are calculated self-consistently. Note that, for a sufficiently large system, we expect the distribution to become independent of the choice of the disorder configurations.

For spinless fermions, we have plotted in Figures 5a, b the distribution $P(\rho)$ calculated on a 10×10 cylinder for two different fillings. We clearly observe that, with the interaction, both the shape of the distribution change and the width of the distribution increases. These effects are strongly emphasized in Figure 5b in which two peaks appear, showing a tendency towards the formation of a charge density wave as we approach commensurability ($n = 0.5$). Note that such an instability is clearly unphysical for a metal and could be easily removed

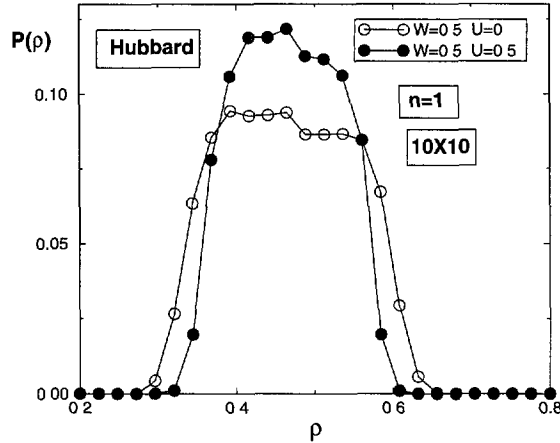


Fig. 6. — Distribution $P(\rho)$ in the Hubbard case. The calculations have been done at half-filling ($n = 1$) on a 10×10 cylinder. We have considered 30 configurations of the disorder. The values of U and W are given in the figure.

by preventing perfect nesting of the Fermi surface (for example, by including hopping terms at larger distances). However, the effect of the interaction to broaden the distribution $P(\rho)$ seems to be independent of the precise details of the band structure and is generic for any filling. In contrast, in the case of the Hubbard model (Fig. 6), we observe the opposite effect: the distribution shrinks around the average value as the interaction is switched on.

Let us now turn to more qualitative results. The width of the distribution (assuming independent variables for different configurations of the disorder) $\delta\rho$ is given by

$$\delta\rho = \frac{1}{N_{\text{dis}}} \sum_{k=1}^{N_{\text{dis}}} \sqrt{\frac{1}{L^2} \sum_z \langle \langle n_i \rangle_0^k - n \rangle^2} \quad (11)$$

where $n = N_e/L^2$ is the filling (N_e is the number of electrons). We have studied the effect of the interaction on $\delta\rho$ as a function of V (spinless fermions) or U (Hubbard model) for different values of the disorder strength W and different fillings. In Figure 7a $\delta\rho(V, W)$ is plotted at half-filling as a function of the parameter V (spinless fermions). Here we clearly observe an increase of the width $\delta\rho$ of the distribution for increasing V . Very crudely, this effect seems to depend only on the combined parameter V/W . In contrast, in the Hubbard case shown in Figure 7b, we observe a reduction of $\delta\rho(U, W)$ as U increases. In Figures 8a, b we have plotted the relative variations of the width of the distribution $\delta\rho(V, W)/\delta\rho(0, W)$ and $\delta\rho(U, W)/\delta\rho(0, W)$ as a function of the interaction parameters V and U for various densities. We observe that the effects described above become stronger for larger fillings *i.e.* when the interaction between the particles becomes more effective. Note however that, in the case of the spinless fermion model, this behavior is unrelated to the commensurability since densities $n = 0.25$ and $n = 0.4$ have been chosen, clearly away from half-filling ($n = 0.5$). In Figures 8 we see that, in the spinless case, the width has increased by almost a factor 4 for $V = 0.8$ and $N_e = 40$. In the Hubbard case the reduction of $\delta\rho(U, W)$ is 25% larger compared to half-filling. Our present study then strongly suggests that a reliable explanation of the observed large persistent currents must somehow take into account the spin of the particles.

We finish our discussion by a study of the influence of the system size on our results. In Figure 9 we have plotted the relative increase of the current $\langle I_{h2} \rangle_{\text{dis}}(U, W)/\langle I_{h2} \rangle_{\text{dis}}(0, W)$

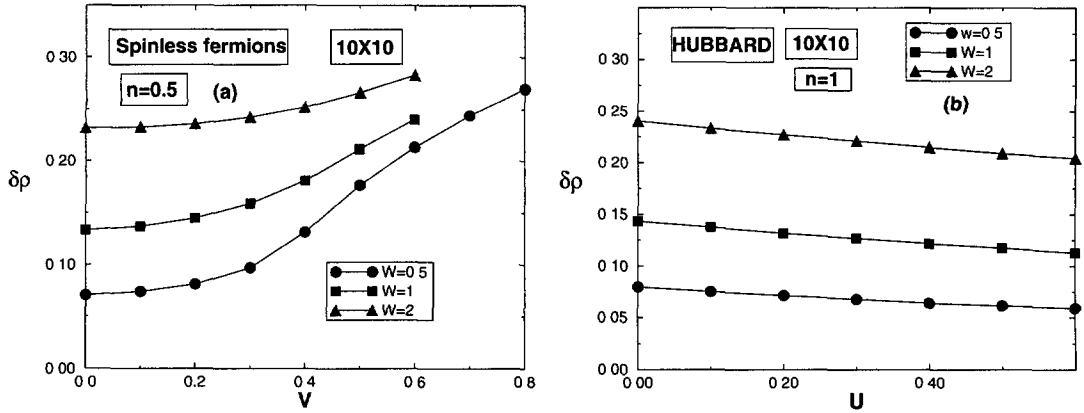


Fig. 7. — Effect of the interaction on the width $\delta\rho(V, W)$ at half-filling as a function of the interaction parameter (U or V). The calculations have been done on a 10×10 cylinder and 30 configurations of the disorder have been considered. The values of W are given in the figure. a) Spinless fermion model; b) Hubbard model.

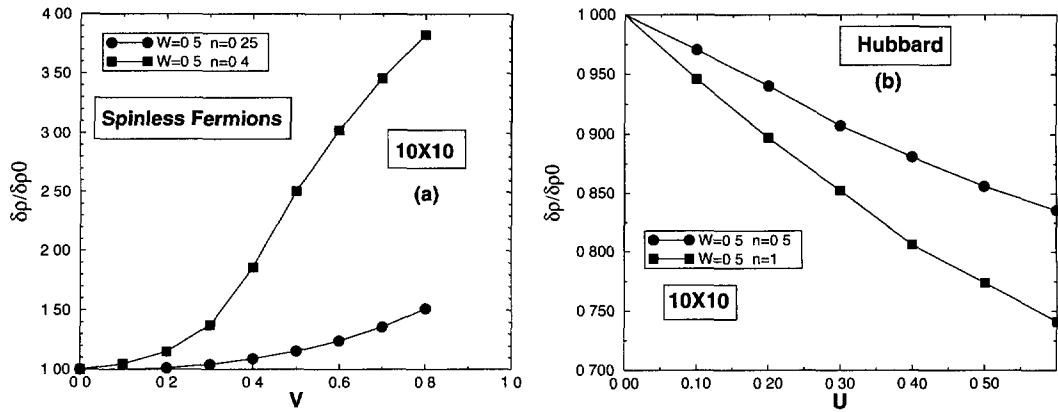


Fig. 8. — Ratio $\delta\rho(V, W)/\delta\rho(0, W)$ as a function of the interaction parameter (U or V) for different filling factors (the filling is indicated on the plot) and values of W . The calculations have been done on a 10×10 cylinder with 30 configurations of the disorder. a) Spinless fermion model ($n = 0.25$ and $n = 0.5$); b) Hubbard model ($n = 0.5$ and $n = 1$).

versus U at fixed density but for different system sizes. This figure clearly indicates that, as the size of the system increases, the effects induced by the interaction become stronger. We also expect that this is also true when the connectivity of the lattice increases (*i.e.* going from 2D to real 3D rings). Although a systematic accurate study as a function of the sample size is not feasible, our data for the Hubbard model for, let say $U = 0.4$, are not inconsistent with the magnitude of the currents observed in the experiments.

In conclusion, we have shown that, in the spinless fermion model, the effect of a moderate interaction leads to a drastic reduction of the magnitude of the current, contrary to what is expected from first order calculations. For the first time, we have established that, in 2D, taken into account the spin degrees of freedom is crucial to explain the enhancement of the current due to the interaction, similarly to the 1D case. Although the calculations presented in this paper

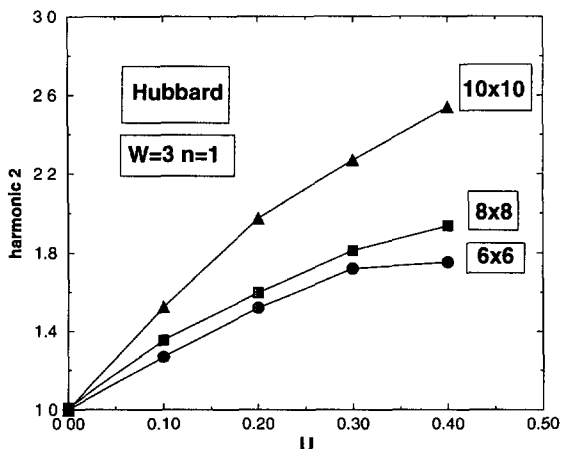


Fig. 9. — Ratio $\langle I_{h2} \rangle(U, W)_{\text{dis}} / \langle I_{h2} \rangle(0, W)_{\text{dis}}$ as a function of U (Hubbard case) calculated within the SHF method. The calculations have been done on 6×6 (circles), 8×8 (squares) and 10×10 (triangles) cylinders at half-filling ($n = 1$) and for $W = 3$. 1 000 realizations of the disorder have been used.

deal with rather small 2D clusters, we expect that, for larger systems and higher connectivity (*e.g.* in 3D) and in the presence of an Hubbard interaction, the impurity scattering will become even less effective to localize the electrons. Although a systematic study as a function of the sample size is still out of reach of present day computers, our data of the Hubbard model at intermediate U (around 0.4) are not inconsistent with the magnitude of the current observed in the experiments. Our study suggests that the SHF approach provides a relatively good tool to study, on equal footings, the effects of the interaction and of the disorder.

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