PHYSICAL REVIEW B VOLUME 50, NUMBER 7 15 AUGUST 1994-I

Rapid Communications

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Suppression of persistent currents in one-dimensional disordered rings by the Coulomb interaction

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(Received 24 May 1994)

The effects of the Coulomb interaction on persistent currents in disordered one-dimensional rings are investigated numerically. First, the effectiveness of the Hartree-Fock approximation is established on small systems. Then the calculations are performed for systems with 40 electrons in 100 sites. It is found that the amplitude of the average persistent current in the diffusive regime is suppressed as the strength of the Coulomb interaction increases. The suppression of the current is stronger in larger rings than in smaller ones. The enhancement of the current by the electron-electron interaction was not observed in the diffusive regime.

About ten years ago, Büttiker *et al.*[1] suggested that an equilibrium persistent current could exist in a mesoscopic normal-metal ring pierced by a magnetic flux line, if the size of the ring were so small that the coherence of the electrons were maintained in the entire system. Later the existence of persistent currents was confirmed by three experiments. The first experiment[2] was performed on many isolated copper rings, the second one[3] on a single gold ring, and the third one[4] on a $GaAs/Al_xGa_{1-x}As$ semiconductor. In the third experiment the system is in the ballistic regime, and the size of the persistent current is in reasonable agreement with theory: The current is of the order of $I_0=ev_F/L$, where v_F is the Fermi velocity and L is the circumference of the ring. On the other hand, in the previous two experiments the system was in the diffusive regime. In that case, simple theories that neglect the electron-electron interaction had predicted the persistent current to be of the order of $I\simeq I_0/M$ where M is the number of transverse channels.[5–7] However, the persistent current observed was stronger than that, particularly in the second experiment where the magnitude of the current was comparable to the clean case: $I\sim I_0$. We might think that the discrepancy arises from an inadequacy of the approximations employed. However, numerical calculations done by Montambaux and co-workers[8,9] for noninteracting electrons in disordered rings are also unable to explain the large magnitude of the current as seen in the second experiment. Thus it is natural to consider that the discrepancy between theoretical calculations and experimental data is not due to the approximation employed in the theory but due to a defect of the model in which the electron-electron interaction is neglected.

Models that include the electron-electron interaction have been investigated both analytically and numerically. In some analytic calculations[10–12] cooperon diagrams, which contribute most to the flux dependence of the energy, were considered and resulted in a larger current than in the noninteracting case. However, it was found that the effect of higher-order diagrams was to suppress the current.[13] In numerical calculations, the effects of the electron-electron interaction were investigated by exact diagonalization of its Hamiltonian for small-size rings. In the case of a one-dimensional discrete-lattice ring the interaction, which has both long-range[14] and short-range components,[15] is found to suppress the average persistent current. Conversely, starting from a continuum model,[16] it was suggested that the average persistent current was enhanced by the electron-electron interaction. Thus, in both analytical and numerical calculations the role of the electron-electron interaction for persistent currents is controversial.

The difficulty in the present problem is that there is no guiding principle for the analytical calculation. It is not clear which diagrams we should take into account. On the other hand, numerical investigations, where we can obtain results free from analytic approximations, are limited to very small systems. Thus it is desirable to perform numerical calculations for much larger systems. This is what we seek in this paper: to investigate numerically the effects of the Coulomb interaction on the strength of the persistent current in a large sample and to determine whether the results are different from those for smaller rings. In order to study larger systems we use the Hartree-Fock approximation (HFA). We first compare the results of the HFA with exact-diagonalization results for small systems. We find that the HFA gives qualitatively correct results. So we apply the HFA to systems with 100 sites, for which exact diagonalization is impossible.

We consider a one-dimensional disordered lattice ring with N_s sites pierced by a magnetic flux line ϕ in which electrons mutually interact with long-range $(1/r)$ Coulomb repulsion. For simplicity we neglect the spin degrees of freedom of the electrons. We adopt the tight-binding model for

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the kinetic term. The impurity potential is introduced by a random site energy ε_i which has a random uniform distribution with width W ($-W/2 \leq \varepsilon_i \leq W/2$). Thus,

$$\mathcal{H} = -t\sum_{i=1}^{N_s} (e^{i\theta}a_{i+1}^{\dagger}a_i + e^{-i\theta}a_i^{\dagger}a_{i+1}) + \sum_{i=1}^{N_s} \varepsilon_i a_i^{\dagger}a_i + \frac{1}{2}\sum_{i\neq j} \frac{V}{N_s} \frac{1}{\left|2\sin\left[\frac{\pi}{N_s}(i-j)\right]\right|} a_i^{\dagger}a_j^{\dagger}a_j a_i , \quad (1)$$

where a_i ($a_i^{\dagger}$) is an annihilation (creation) operator of a spinless fermion at site i. The (N_s+1) site is identical to the first site. The effect of a flux line (ϕ) piercing a ring is introduced through the phase factor $e^{i\theta}$ which is gained when a electron hops to the neighboring site, thus $\theta = 2\pi\phi/N_s\phi_0$, where $\phi_0 = h/e$. The Coulomb repulsion is parametrized by $V(>0)$.

In the HFA $\mathcal{H}$ is replaced by $\mathcal{H}_{\rm HF}$,

$$\mathcal{H}_{\rm HF} = -t\sum_{i=1}^{N_s} (e^{i\theta}a_{i+1}^{\dagger}a_i + e^{-i\theta}a_i^{\dagger}a_{i+1}) + \sum_{i=1}^{N_s} \varepsilon_i a_i^{\dagger}a_i + \frac{1}{2}\sum_{i,j} \frac{V}{N_s} \frac{(\langle a_j^{\dagger}a_j\rangle a_i^{\dagger}a_i - \langle a_j^{\dagger}a_i\rangle a_i^{\dagger}a_j)}{\left|2\sin\left[\frac{\pi}{N_s}(i-j)\right]\right|} , \quad (2)$$

where $\langle\cdots\rangle$ denotes the expectation value with respect to the self-consistent HF eigenstate $|\Psi\rangle = b_1^{\dagger}b_2^{\dagger}\cdots b_{N_e}^{\dagger}|0\rangle$, and b_n ($b_n^{\dagger}$) is the electron-annihilation (-creation) operator of the nth eigenstate of $\mathcal{H}_{\rm HF}$, and N_e is the total number of electrons. Self-consistency is achieved by iteration. Once the Hamiltonian is solved, the persistent current is calculated by the formula

$$I(\phi) = -\frac{\partial E_g(\phi)}{\partial\phi} , \quad (3)$$

where $E_g(\phi)$ is the ground-state energy for a flux ϕ.

In the following we calculate the current at several values of W/t and V/t. We mostly calculate the current in the diffusive regime. In one dimension the localization length ξ is given by

$$\xi = \frac{105at^2}{W^2} \quad (W \ll 2\pi t), \quad (4)$$

$$\xi = \frac{a}{\ln(W/2et)} \quad (W \gg 2\pi t), \quad (5)$$

where a is the lattice constant.[17–19] The above equations were derived under the condition of the half-filled-band case for the tight-binding model. The system investigated here is not half-filled. However, we use these equations to estimate the localization length, since it is not far from half-filled. We are mainly interested in the diffusive regime and consider the value of W such that $\xi > L = N_s a$.

We first examine the validity of the HFA. For that purpose we calculate the persistent current for systems of 4 electrons in 10 sites by two methods: the exact diagonalization and the HFA. Average over site energy randomness is performed over ten samples.[20] Flux dependence of the persistent current at $W=t$ and for $V=0$ to $20t$ is shown in Fig. 1 for half period, $0 \leq \phi \leq \phi_0/2$; the current is an odd function of ϕ, and it is periodic with period ϕ_0. The current is normalized by the maximum persistent current for a clean ($W=0$) and noninteracting ($V=0$) system, $I_0 = (2et/N_s\hbar)\sin(N_e\pi/N_s)$.[19] In these systems the amplitude of the persistent current is sup-

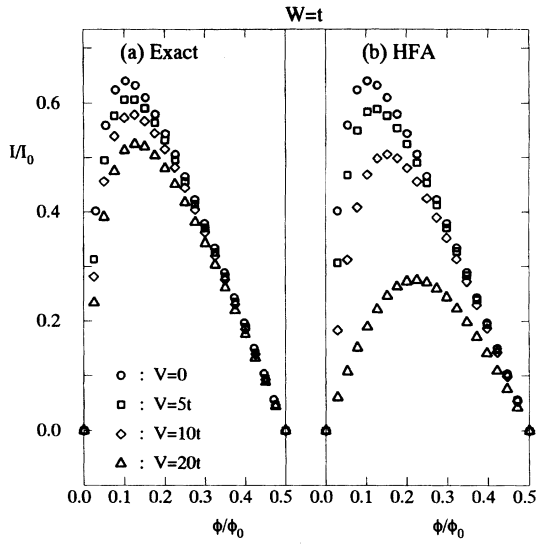

FIG. 1. Current I/I_0 vs flux ϕ/ϕ_0 for a 10-site 4-electron ring at $W=t$, and $V=0$ (circle), $5t$ (square), $10t$ (diamond), and $20t$ (triangle), where $I_0 = (2et/N_s\hbar)\sin(N_e\pi/N_s)$ is the maximum persistent current for a clean, noninteracting system. Panel (a) shows the results by the exact diagonalization and panel (b) shows those by the HFA.

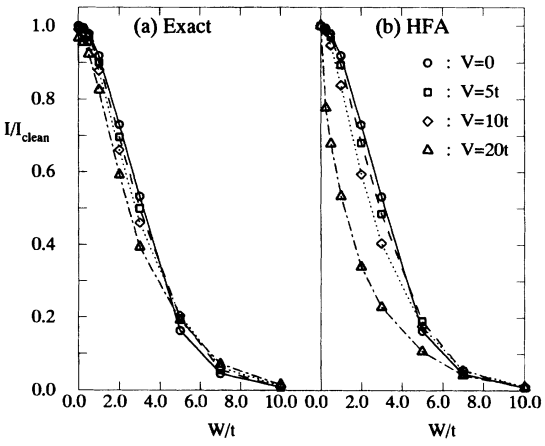

FIG. 2. Current $I/I_{\rm clean}$ vs randomness (W) for a 10-site 4-electron ring (a) by the exact diagonalization and (b) by the HFA for $V=0$ (circle), $5t$ (square), $10t$ (diamond), and $20t$ (triangle), where $I_{\rm clean} = I_0\sin(\pi/2N_s)/\sin(\pi/N_s)$ is the value of the current at $\phi = \phi_0/4$ in the clean, noninteracting system. The lines are guides to the eye.

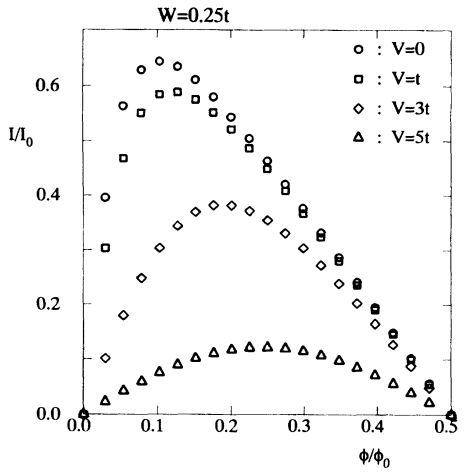

FIG. 3. Current I/I_0 vs flux ϕ/ϕ_0 for a 100-site 40-electron ring in the case of the HFA at $W=0.25t$, and $V=0$ (circle), t (square), $3t$ (diamond), and $5t$ (triangle).

pressed as the Coulomb interaction becomes larger. The result by the exact diagonalization is in agreement with that in Ref. 14 where a system with 5 electrons in 10 sites is investigated. Although the suppression is stronger, we see the HFA gives qualitatively similar behavior. The comparison is done at other values of W also. Figure 2 summarizes the results. The vertical axis shows the magnitude of the current I at $\phi=\phi_0/4$ divided by I_{clean} which is the value of the current at $\phi=\phi_0/4$ in the clean, noninteracting system: $I_{\text{clean}} = I_0\sin(\pi/2N_s)/\sin(\pi/N_s)\simeq I_0/2$.[19] The plot of the noninteracting case (circle) is almost on the curve represented by $\exp[-L/\xi(W)]$. The HFA results reproduce those of the exact

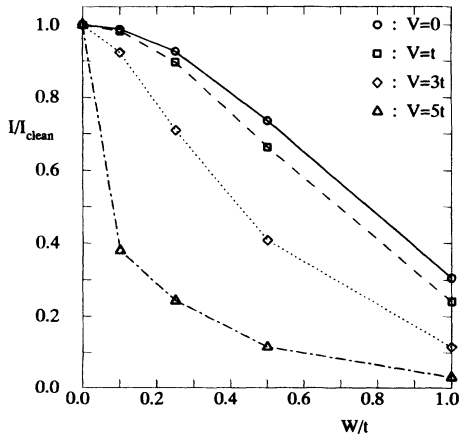

FIG. 4. Current I/I_{clean} vs randomness (W) for a 100-site 40-electron ring by the HFA for $V=0$ (circle), t (square), $3t$ (diamond), and $5t$ (triangle). The lines are guides to the eye.

diagonalization qualitatively: The persistent current is suppressed by the Coulomb interaction in the diffusive regime, $W<3$. It is remarkable that the slight enhancement of the current in the localized regime ($W>3$) is also reproduced.

Now that we have found that the HFA gives qualitatively correct behavior of the persistent current, we investigate larger systems where the exact diagonalization is impossible. Specifically, we consider systems with 40 electrons in 100 sites. Figure 3 shows the flux dependence of the persistent current at $W=0.25t$, and Fig. 4 shows W dependence of the current. In these figures, an average over 10 samples is shown. For this 100-site system the sample dependence is small due to self-averaging. Therefore 10 samples are enough. These results also show the suppression of the current with increase in V. In this system $\xi\simeq L$ at $W\simeq t$, so only the diffusive regime is considered. The noninteracting case is also almost on the curve $\exp[-L/W(\xi)]$. Compared to the 10-site system it is seen that the effect of V is larger in the present larger system.

From the results stated above we can conclude that the Coulomb interaction between electrons cause the reduction of the persistent current in the experimentally relevant diffusive regime. The results found in Refs. 14 and 15 are confirmed for larger systems. In Ref. 14 it was suggested that this suppression was attributed to the Mott-Hubbard transition. If so, it should occur in a clean ($W=0$) system, and in fact it was observed in Refs. 14 and 15. It is also seen in our results, Fig. 2(a). On the other hand, in the HFA the suppression of the current does not occur in a clean sample at any filling and V, since the eigenstates in the case of $V=0$ are still the eigenstates and the ground state is also unchanged. Nevertheless, in a dirty system, the current is suppressed as V increases both in the case of the exact diagonalization and the HFA. Furthermore the Coulomb effect is larger in disordered systems in the diffusive regime. This seems to teach us that the Mott-Hubbard transition is not essential to the suppression of the current in a dirty system.

Our results are in disagreement with those in Ref. 16. That may be due to the difference in models, discrete or continuum, as some people[21,22] pointed out. However, in view of the fact that the system with more lattice points approaches the continuum system, our results that the Coulomb interaction suppress the current more in the larger system cast some doubt to the interpretation of the difference. Another candidate for the reason of the enhancement in Ref. 16 would be truncation of the single electron states adopted there.

We cannot explain the experimental results by our model and calculations. It may be possible that the enhancement of the current will occur in multitransverse channel systems. These systems cannot be investigated by the exact diagonalization because of the limitation in memories. However, we can treat such a system by the HFA. Results of such a calculation will be published in the near future.

In summary, we have established the effectiveness of the HFA for the present model. With this approximation it has become possible to investigate systems with more than 100 sites even in the presence of the Coulomb interaction. We

have found that the Coulomb interaction suppress the persistent current.

One of the authors (D.Y.) thanks the Aspen Center for Physics where part of this work was done. This work was supported by a Grant-in-Aid for Scientific Research on Priority Area "Computational Physics as a New Frontier in Condensed Matter Research" (No. 04231105) from the Ministry of Education, Science and Culture.

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