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Influence of spin on the persistent current of strongly interacting electrons

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Abstract

The lowest eigenenergies of a few, strongly interacting electrons in a one-dimensional ring are studied in the presence of an impurity barrier. The persistent current I, periodic in an Aharonov-Bohm flux penetrating the ring, is strongly influenced by the electron spin. The impurity does not remove discontinuities in I at zero temperature. The total electron spin of the ground state oscillates with the flux. Strong electron-electron interaction enhances I, albeit not up to the value of the clean ring which itself is smaller than I for free electrons. I disappears on a temperature scale that depends exponentially on the electron density. In the limit of very strong interaction, the response to small fluxes is diamagnetic.

1. Introduction

The appearance of persistent currents is a consequence of the coherent electron motion in a ring [1]. In contrast to transport currents this is an equilibrium property also of non-superconducting electrons in small rings enclosing an Aharonov–Bohm flux. The persistent current is observable at sufficiently low temperatures [2] even in the presence of disorder [3, 4]. Only sophisticated SQUID-techniques allow to separate the equilibrium magnetization from the externally applied field. Much larger magnitudes were found for the currents I than theoretically predicted [5,6]. Non-interacting electrons can explain neither the magnetization observed in 10⁷ rings [3] nor in single rings [4].

Contributions from electron—electron interaction, estimated on the Hartree—Fock level [7], improve the single electron estimates though the results are not yet conceived as being completely satisfying. Additionally, at reduced dimensionalities or

electron densities, as it appears in semiconducting rings [2], a mean field description becomes unreliable [8,9].

The persistent current of interacting, spinless electrons on a one-dimensional (1D) clean ring has been studied within a Luttinger liquid model [10]. The question of how far interaction modifies the magnitude of the current in a clean ring has been discussed controversially [10,11]. The sign of the magnetic response is found to be the same as for spinless non-interacting electrons.

The influence of the strong Coulomb interaction in a disordered ring has not yet been clarified. In a continuous ring, the interaction is predicted to enhance the current [11], while reduced currents, even below their value in the absence of interaction, were found in a lattice model where spin has been ignored [12].

A new, interesting question in the presence of interaction is how far the electron spin is important. This has been investigated up to now only for a clean Hubbard model [13]. Spinless impurity

scatterers and a constant vector potential conserve the total electron spin. Energy levels with different spins are not mixed by the impurities and can intersect when the flux changes. Only energy levels of the same spin repel each other. It is not clear as to how far random matrix theory can be applied even within the blocks of given total spins [14]. A generalization of the concept of the Thouless energy [15] is presumably needed in the presence of electron–electron interaction.

In the present work, interacting electrons with spin are investigated on a 1D, continuous ring which contains an impurity barrier. Strong correlations, found at moderately low electron densities, can be included by the present approach. Like in the context of quantum dots [9, 16], classical, Wigner crystallized electrons are taken as the starting point for which quantum corrections are calculated using group theoretical means.

The sign of the susceptibility to small fluxes will be shown to be not only dependent on the parity of the electron number but also on the strengths of impurity and interaction. The total spin values in the ground state can periodically vary with flux. At very strong interaction, the response turns out to be always diamagnetic. Backscattering from the impurity reduces the probability for the electrons to circulate around the ring which reduces the magnitude of the current. The electron spin can cause the persistent current to increase with increasing interaction strength. The interaction changes the energy level spectrum considerably and therefore the temperature scale for the persistent current to disappear compared to non-interacting or spinless electrons.

2. Model

The model describing N interacting electrons on a quasi-one-dimensional ring penetrated by an Aharonov-Bohm flux $\phi h/e$ (ϕ is the number of flux quanta) is in polar coordinates,

$$H = B \sum_{j=1}^{N} \left(-i \frac{\partial}{\partial \theta_{j}} - \phi \right)^{2} + \frac{1}{2} \sum_{i,j'} w(|\theta_{j} - \theta_{j'}|) + \sum_{i} v(\theta_{j}),$$
 (1)

where $B = h^2/2mL^2$ is the rotational constant of a mass m on the ring of circumference L. For simplicity, only one repulsive impurity barrier, $v(\vartheta)$, is assumed to be present with a range shorter than the mean electron separation a = L/N. The range of the repulsive interaction $w(|\vartheta|) \ge 0$ is assumed to be larger than the width of the ring. An example would be the Coulomb interaction

$$w(|\vartheta|) = 2\pi e^2 / \varepsilon L \sqrt{\vartheta^2 + b^2}$$
 (2)

in a ring of transversal width $bL/2\pi \ll L$. The curvature of the ring can be neglected if $N\gg 2\pi$.

For low densities, $a \gtrsim a_{\rm B} = \varepsilon \hbar^2/me^2$ (ε is the dielectric constant), the electrons form a 'Wigner molecule', due to the rapid decay of the kinetic energy compared to the repulsion (2). The impurity prohibits free overall rotation and well defined electron sites on the ring become energetically favourable. At very large a, the ground state is independent of the individual spin orientations and 2^N -fold degenerate. Increasing densities remove this degeneracy. The ensuing energy splittings Δ are due to tunnelling and proportional to the rates for the classically forbidden transitions of electrons exchanging positions. The resulting low energy excitation spectrum can be obtained within the pocket state approximation (PSA) [16].

3. Pocket state approximation

The approximation consists in truncating the Hilbert space of N-electron wave functions to a finite set of 'pocket' basis states $\{|p\rangle\}$ $(1 \le p \le N!)$. Each pocket state has one pronounced maximum in configuration space $(2\pi)^N$. The locations of the maxima of $|\langle \vartheta_1, \dots, \vartheta_N | p \rangle|$ and $|\langle \vartheta_1, \dots, \vartheta_N | p' \rangle|$ differ in a permutation of their coordinates. The eigenstates of Eq. (1) with lowest energies are approximated by linear combinations of the $\{|p\rangle\}$, according to the eigenvectors of the matrix $H_{pp'} \equiv \langle p|H|p'\rangle$. The transformation behaviour under permutations of the coordinates $\{\theta_1, \ldots, \theta_N\}$ fixes uniquely the total spin S of the respective Fermion eigenstate. The off-diagonal elements of $H_{pp'}$ describe the exchange processes of electron positions.

The set of symmetrized linear combinations $\mathcal{O}_{\Gamma}\{|p\rangle\}$ makes the Hamiltonian matrix block diagonal. Here \mathcal{O}_{Γ} is a projector onto states that transform according to the irreducible representation Γ of the group of permutations of N elements. Only those blocks are needed and must be diagonalized which belong to Fermion states of a total electron spin S. This leads to

$$n_S = \frac{(2S+1)N!}{(N/2+S+1)!(N/2-S)!}$$

lowest energy levels $E_S(\phi)$ to given spin $S = \{ \{ \begin{smallmatrix} 0 \\ 1/2 \end{smallmatrix} \}, \ldots, \frac{1}{2} N \}$ [16].

PSA is valid if Δ is small compared to the energies associated with other processes, for instance phonon-like excitations in the Wigner crystal. The electron 'molecule' in a quantum dot shows exponentially decreasing Δ with increasing a while the vibrational energies decrease only according to a power law [17]. PSA is justified at low densities to determine low energy excitations.

In the present problem rotational excitations have to be considered additionally, they determine persistent currents. Without disorder, they scale with the rotational constant $\hbar^2/(2Nm(L/2\pi)^2)$ = B/N of N electron masses. Rotations by $\Delta \theta = 2\pi a/L$ correspond to cyclic permutations of the electrons and can be incorporated into the pocket state calculation. Its validity requires that the lowest energies of long-wavelength phonons should be larger than rotational excitations

$$h\Omega = 2\pi \frac{e^2}{\varepsilon a_{\rm B}} \frac{a_{\rm B}}{L} \sqrt{\frac{a_{\rm B}}{a}} \gg \frac{B}{N}$$

$$\Leftrightarrow s \gg \frac{h}{NmL} \iff \sqrt{\frac{a}{a_{\rm B}}} N^2 \gg \pi \tag{3}$$

where s is the sound velocity [18] in the electron molecule. Condition (3) is on the safe side to estimate the applicability of the PSA because the impurity barrier leaves $\hbar\Omega$ almost unchanged while it reduces Δ .

4. Exchange processes

In the 1D square well potential the most relevant off-diagonal entries $H_{pp'}$ describe the exchange of

adjacent electrons [16]. Other matrix elements are exponentially small. In the ring (1) the importance of the process of circulating electrons depends on their number and on the strength of the impurity barrier. I assume here three types of off-diagonal entries $H_{pp'}$, $p \neq p'$. They are illustrated in Fig. 1:

i. The matrix element t describes the pair exchange of adjacent electrons on the ring. It leads to the splitting of the lowest vibrational multiplet into levels of different total spins. The stronger the electron–electron interaction is, the more it is difficult for the electrons to pass one another and the smaller is |t|. It depends also on the width of the ring (cf. Eq. (2)) and on the electron density. All of the t's are assumed to be equal, except the following.

ii. The exchange of two electrons located on either side of the (repulsive) impurity is described by u. In addition to the Coulomb repulsion, the particles have to tunnel through a barrier, therefore |u| < |t|. Absence of the impurity corresponds to u = t and a large impurity makes u vanishing. Neither u nor t depend on the flux.

iii. The (collective) ring exchange transferring all electrons cyclically by $\Delta \theta_j = \pm 2\pi a/L$ is described by $r \propto e^{\pm 2\pi i\phi}$. It contains the same phase factor that the one electron wave function acquires by turning its coordinate $\theta_j \to \theta_j + 2\pi$ once around the loop.

An upper limit for |r| can be deduced from the requirement that r should not cause splittings of energies larger than the rotational constant for

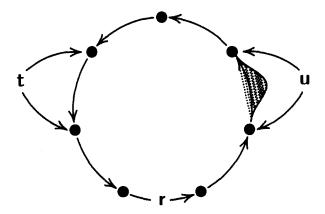


Fig. 1. Illustration of the exchange processes associated with the tunneling integrals r, t and u (see text).

a circulating mass Nm

$$|r| < \begin{cases} 2 \\ 1 \end{cases} \frac{N}{8\pi^2} B \quad \text{for} \quad N \begin{cases} \text{even,} \\ \text{odd.} \end{cases}$$
 (4)

Apart from corrections of order $\mathcal{O}(1/N)$ (4) can be expressed in terms of the Fermi velocity v_F

$$|r| < \begin{cases} 2 \\ 1 \end{cases} \frac{\hbar}{2\pi} \frac{v_{\rm F}}{L}. \tag{5}$$

A finite impurity barrier has to be passed by one of the electrons during the ring exchange. This reduces |r| compared to Eqs. (4) or (5). The persistent current, given as a derivative with respect to ϕ , is mainly determined by r.

The dependencies and the ranges of t, u and r are summarized in Table 1. Being tunneling integrals they are negative (r < 0 for $\phi = 0$). Their number reflects the three relevant parameters in this problem: The strengths of the interaction and the impurity, and the circumference of the ring.

The transport and pinning properties of a one-dimensional Wigner crystal in the presence of an impurity barrier have been studied in detail [18]. The obtained non-trivial renormalizations of the barrier at zero and at finite temperatures [19] are consequences of phonon like excitations in the Wigner crystal which for spinless electrons are the leading contributions and are of low energy in infinite systems. In the present consideration, vibrational excitations are neglected and thus, for consistency, the influence of the strength of the e-e interaction on r is ignored. The results are not valid at temperatures as high as the vibrational energies.

Table 1
Magnitudes of the dominant tunneling integrals within the pocket state description

Parameter	Depends on the	Is small for	Maximum value
r	impurity	strong impurity	$NB/(2\pi)^2$
t	interaction	strong interaction	$ t \gg r $
и	impurity	strong impurity	u = t

5. Estimating |t|, |u|, |r|

The dependence of the tunneling integrals t and u on the electron density a^{-1} and on the height V_0 of the impurity barrier, can be estimated within the WKB approximation [16] for $b \ll 2\pi/N$

$$|t| \sim \exp(-c_1 \sqrt{a/a_{\rm B}}), |u| \sim t \exp(-c_2 \sqrt{a/a_{\rm B}} V).$$
 (6)

Here $V=V_0/(e^2/\epsilon a)$ is the height of the barrier on the scale of the Coulomb energy, and $c_1=(1/\pi\sqrt{2})\int_0^{2\pi}\mathrm{d}\theta(|(\pi/\theta)-1|)^{-1/2}=1+(\pi+\ln(3+\sqrt{8}))/\sqrt{8}=2.734$ and $c_2=1+(\pi-\ln(3+\sqrt{8}))/\sqrt{8}=1.487$ are constants determined by the Coulomb interaction (2). The reduction of |r| can be estimated perturbatively for small V_0 .

$$|r| \sim N(B/2\pi - V_0)/2\pi$$
. (7)

Eq. (7) shows that |r| is necessarily reduced in the presence of disorder. Experimentally, |r| is mainly related to the amplitude of the current oscillations with flux and t mainly to the temperature dependence as described in the following section.

6. Results

The eigenvalues $E_S(\phi)$ that correspond to the total electron spin S can be determined analytically for $S = \frac{1}{2} N$ (spin polarized states), and for N = 3.

$$E_{S=N/2}(\phi) = (-1)^N 2|r|\cos 2\pi\phi + (N-1)|t| + |u|$$
(8)

corresponds to the energies of spinless electrons. Their persistent current is given as $I = -\partial E_S(\phi)/\partial (\frac{h}{e}\phi) = (-1)^N (2e/\hbar)|r|\sin 2\pi \phi$ which is (also in presence of the impurity) periodic in the flux quantum h/e. The impurity reduces the amplitude |r| of the current oscillations (cf. Eq. (7)) as compared to the value for one electron circulating with the Fermi velocity, cf. Eq. (5).

The eigenvalues for N=3, $S=\frac{1}{2}$ are

$$\begin{split} E_{S=1/2}^{(1)}(\phi) &= |r|\cos 2\pi\phi - \sqrt{3(|r|\sin 2\pi\phi)^2 + (t-u)^2}\,, \\ E_{S=1/2}^{(2)}(\phi) &= |r|\cos 2\pi\phi + \sqrt{3(|r|\sin 2\pi\phi)^2 + (t-u)^2}\,. \end{split}$$

(9)

Many qualitative features can be seen already from the results (8) and (9). The difference (t - u) leads to the repulsion between levels of same spin and t separates levels of different spins in energy. For large |t| (weak interaction) the ground state energy is $E_{S=1/2}^{(1)}(\phi)$. The response to small fluxes, $(\partial^2 E_{S=3/2}^{(1)}(\phi)/\partial \phi^2)|_{\phi=0} = -|r|((2\pi)^2 + 12/|t-u|)$ < 0 is paramagnetic, as for three non-interacting electrons. If |t| < |r| (strong interaction) the ground state becomes spin polarized and shows now diamagnetic response to $(\partial^2 E_{S=3/2}^{(1)}(\phi)/\partial \phi^2)|_{\phi=0} = 8\pi^2 |r| > 0$. In the presence of a given impurity, |r| remains constant when the interaction is increased while |u| and |t| (> |u|) both are reduced (cf. Table 1 and Eq. (6)) and the steepness $-\partial E_{\rm S}(\phi)/\partial \phi$ raises.

In the absence of disorder (t = u) the interaction influences the magnitude and even the sign of I if |t| < |r|. The ground state does not follow a whole segment of the parabola $E_S(\phi)$ but switches with changing flux to adjacent pieces of parabolas belonging to other spins. Only the persistent current of spinless electrons (within the approximation considered here) is unaffected by the electron–electron interaction [11]. Increasing t = u increases the distances between the levels, leaving their ϕ -dispersion almost unchanged. This, eventually, makes I independent of a weak interaction $|t| \gg |r|$.

The eigenvalues for $N \ge 4$ electrons (Figs. 2 and 3) obtained by numerical diagonalizations of Hamiltonian matrices in the pocket state basis confirm these features. Figs. (a) refer to 'typical' situations where neither interaction nor disorder dominates. In the Figs. (b), the electron—electron interaction is increased compared to (a), leaving the impurity unchanged. Figs. (c) show the energy levels in the presence of a high impurity barrier but weak interaction.

Weak interactions lead to pronounced contributions of higher harmonics to the flux periodicity, see Figs. (a) and (b), due to the level repulsion (cf. Ref. [6]). A very strong interaction $|t| \ll |r|$, however, brings the spin polarized state $S = \frac{1}{2}N$ at $\phi = \frac{1}{4}(1-(-1)^N)$ close to the ground state. The h/e-flux-periodicity (8) of the former is not affected by the impurities. This leads to a non-vanishing h/e contribution at strong interaction even after impurity averaging, in contrast to the

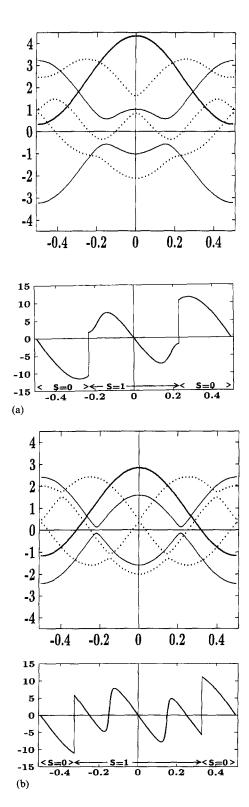
purely h/2e-periodic current of an odd number of non-interacting electrons.

The low energy of the spin polarized state causes a diamagnetic response to small fluxes (cf. Eq. (8)) for $|t| \ll |r|$ and N odd ($\phi \approx 0$). This behaviour is in contrast to the paramagnetic susceptibility of an odd number of non-interacting electrons. But also an even number of electrons respond diamagnetically if interacting strongly, because the persistent current approaches h/Ne-periodicity if $t = u \to 0$, as it is found for the 1D-Hubbard model for $U \to \infty$ [20]. The energy minimum at $\phi \approx N/2N = \frac{1}{2}$, Eq. (8) induces an equivalent minimum around $\phi \approx 0$.

In general, the sign of the magnetic susceptibility depends not only on particle number but also on the disorder and the strength of the interaction. The long time variations observed in the experiment [2] can be explained by fluctuating electron numbers but also by changes in the impurity configuration. In the limit of both weak disorder and interaction $|t| \gtrsim |u| \gg |r|$, the sign of the response becomes equal to that of ballistic electrons on a 1D ring which is diamagnetic only if N-2 divided by 4 is an integer (including N=2), otherwise paramagnetic [21].

The temperature dependence of the persistent current differs considerably from non-interacting or spinless electrons. I vanishes if the temperature exceeds the width of the level multiplet, which is of the order of $\max\{|r|, N|t|\}$, because the trace of the matrix $H_{pp'}$ is independent of ϕ . The persistent current of interacting electrons with spin vanishes therefore on an energy scale Δ that varies exponentially with the electron density, cf. (6), while both, the energy Ω related to the sound velocity in the Wigner crystal, and the Fermi velocity vary only like power laws with a^{-1} . The former would be relevant to spinless, the latter to non-interacting electrons.

The impurity cannot smoothen out the discontinuities of the persistent current at zero temperature at certain values of ϕ , in contrast to spinless electrons. Levels with different spins can intersect and the magnitude of the current jumps, mostly also its sign. Simultaneously, the values of the ground state spins alternate. The experimental observation of these oscillations would be interesting.



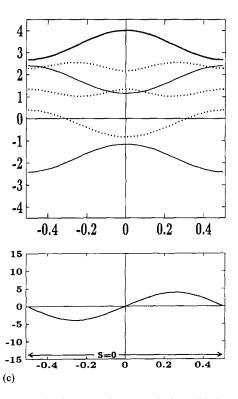
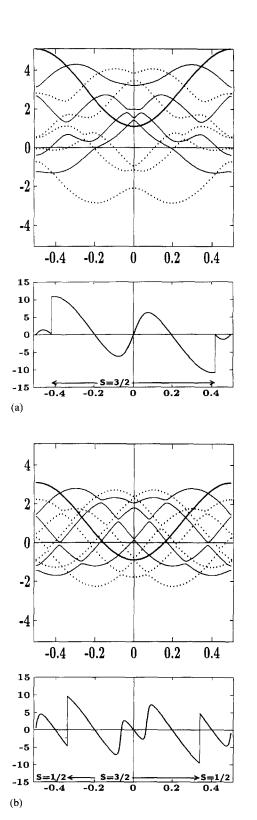


Fig. 2. Energy levels versus the magnetic flux $\phi h/e$ for N=4 electrons. Thick solid lines: S=2, dotted lines: S=1, thin solid lines: S=0. Parameters are (a): |r|=1, t=-3/4, u=-1/12; (b): |r|=1, t=-1/4, u=-1/12; (c): |r|=1/3, t=-1, u=-1/3 (see text and Fig. 1). Figures (b) correspond to strong interaction and Figures (c) to strong impurity. Below each figure $-\partial E_0(\phi)/\partial \phi$ of the ground state energy E_0 is plotted which is proportional to the persistent current at zero temperature.

Only for very weak electron-electron interaction $|t| \gg |r|$ the ground state spin remains constant, S = 0 or $S = \frac{1}{2}$, Figs. c.

Disorder reduces the current for two reasons. At first, the magnitude |r| is reduced directly according to Eq. (7). The increasing repulsion between levels of same spin causes additionally flattened dispersions in ϕ which reduces the current. An increasing interaction does not influence the former but reduces significantly the level repulsion and thus the second reason for current suppression. This can be seen by comparing the Figs. (a) and (b). The level repulsion is reduced because $|t| \to 0$ forces also u to vanish. In qualitative agreement with [11, 22], I claim that in the presence of an impurity the



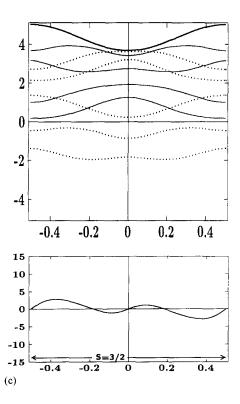


Fig. 3. Same as Fig. 2 for the same parameters but for N=5 electrons. Thick solid lines: S=5/2, thin solid lines: S=3/2, dotted lines: S=1/2.

persistent current increases with increasing electron-electron interaction, though not up to the value expected for the clean ring. This increase requires, however, the electron spin.

7. Summary and conclusion

The eigenenergies of a continuous, 1D ring (1) that contains few, strongly interacting electrons have been analyzed in the presence of impurity barrier and Aharonov–Bohm flux $\phi h/e$ considering explicitly the electron spin. Correlated, localized many-electron states have been used to determine the low energy excitations. The electron density and the circumference of the ring are assumed to be sufficiently small so that phonons of the Wigner electron 'molecule' can be ignored. Circular ring symmetry is only used for some of the estimates, the results do not depend on this assumption.

Spin carring electrons differ qualitatively from spinless electrons in their persistent current I (cf. Eq. (8)). Impurities do not smoothen the current at zero temperature if the electron-electron interaction is strong. The interaction can increase I by reducing the repulsions between levels of same spin-the spectrum becomes less rigid. This effect must be distinguished from the current suppression due to the reduced transmittivity of the impurity barrier which is not neutralized by strong e-e-interactions. Therefore the current does not reach the value $I \sim 2ev_{\rm F}/L$ found in the absence of both interaction and disorder. The current remains periodic in once the flux quantum for any N. Very strong interaction makes the sign of the response to small fluxes always diamagnetic. This can help to explain the unexpected recent experimental finding [23] of the diamagnetic response of an ensemble of semiconducting rings. The temperature scale on which the persistent current is destroyed depends exponentially on the electron density. This again is in contrast to the case of non-interacting or spinless electrons.

The h/Ne-periodicity of the persistent current found in the limit of infinitely strong interaction is similar to that of a 1D Hubbard ring [13, 20]. However, the suppression of the current, obtained in the lattice model with increasing interaction between spinless electrons [12], is not always confirmed in the continuous model that includes the spin.

It should be noted that magnetic impurities change the qualitative results presented here only if the rate for spin flip transitions happen to be comparable to the level repulsions caused by the fluctuations of the impurity potential so that the spin states become highly mixed. A weak spin flip scattering is even implicitly assumed to ensure the system to remain in its ground state while the applied flux is (slowly) swept through.

Systematic experimental studies of the dependence of the persistent current on (i) the electron density, (ii) the height of a hindering tunneling barrier on the ring and (iii) the temperature would be extremely desirable. Furthermore, it would be pleasing to observe the electronic ground state spins to oscillate with flux. The most promising experimental set up could be the semiconducting

ring that allows to regulate the barrier by a gate, as it has been used in Ref. [2].

Note added in proof: After completion of the present work, the Author became aware of an article by R. Römer and A. Punnoose [Phys. Rev. B 52 (1995) 14809] where the Hubbard model has been treated in the presence of disorder by renormalization group techniques, including spin. This lattice model shows increasing currents with increasing strength of the interaction above a certain strength for the disorder.

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