Persistent currents in a Möbius ladder: A test of interchain coherence of interacting electrons

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Persistent currents in a Moebius ladder are shown to be very sensitive to the effects of intrachain interactions on the hopping of electrons between chains. Their periodicity as a function of flux is doubled for strong enough repulsive interactions because electrons cannot hop coherently between the chains and have to travel along the full edge of the Moebius ladder, thus encircling the flux twice. The interplay of topology and interactions is shown to lead to interesting finite-size effects on the odd harmonics of the persistent current. [S0163-1829(98)09903-2]

The problem of transport in very anisotropic systems has become one of the central issues in the field of strongly correlated systems. Roughly speaking, it can be stated as follows: Consider an electronic system with transfer integrals much smaller in one direction than in the other(s). Is it possible, and under which conditions, that transport is coherent in the highly conducting direction(s) and incoherent in the other direction at temperatures much smaller than the smallest transfer integrals? This question has recently been raised in several contexts, the most prominent examples being high-T_c superconductors, which are quasi-2D systems,[1,2] and organic superconductors (the Bechgaard salts), which are quasi-1D systems.[3,4] This property is clearly inconsistent with Fermi-liquid theory, and the best candidates to describe such behavior are models of strongly-correlated electrons. Renormalization-group (RG) arguments[5,6] for quasi-1D systems of coupled Luttinger liquids indicate that interchain hopping is a *relevant* perturbation provided the Luttinger-liquid exponent α is smaller than 1. However, an alternative approach drawing an analogy to the problem of coherence in a two-level system coupled to a bath indicates that *coherent* interchain motion may be destroyed for much smaller values of α.[3,7] Evidence in favor of the latter picture based on the analysis of the angular dependence of the magnetoresistance of the Bechgaard salt $(TMTSF)_2PF_6$ has been presented.[3,4] However, the issue remains controversial, and more direct evidence of the effect of correlations on the coherence of motion perpendicular to the chains would be highly desirable.

In this paper, we propose a new approach to study the problem of interchain coherence based on the analysis of persistent currents in a Moebius ladder threaded by an Aharanov-Bohm flux $(\hbar c/e)\Phi$ (see Fig. 1 inset). The persistent current of the system is directly sensitive to the phase coherence of the many-body wave function, and is given at zero temperature by $I(\Phi)=-(e/\hbar)\partial E/\partial\Phi$, where E is the ground-state energy. Gauge invariance[8] implies that $I(\Phi)$ is a periodic function of Φ with period $\phi_0=2\pi$. $I(\Phi)$ can thus be expressed as a Fourier series,

$$I(\Phi)=\sum_{n=1}^{\infty} I_n \sin(n\Phi). \tag{1}$$

Magnetization measurements on normal metal[9] and semiconducting[10] rings typically measure the first few harmonics of $I(\Phi)$, which are in general nonvanishing for a single ring. However, in the Moebius geometry, if the perpendicular hopping integral $t_\perp$ is switched off, electrons will have to go twice around the flux to reach the same site, and the period of the persistent current will be halved to $\phi_0/2$. All the odd harmonics in Eq. (1) must then vanish. Now, for

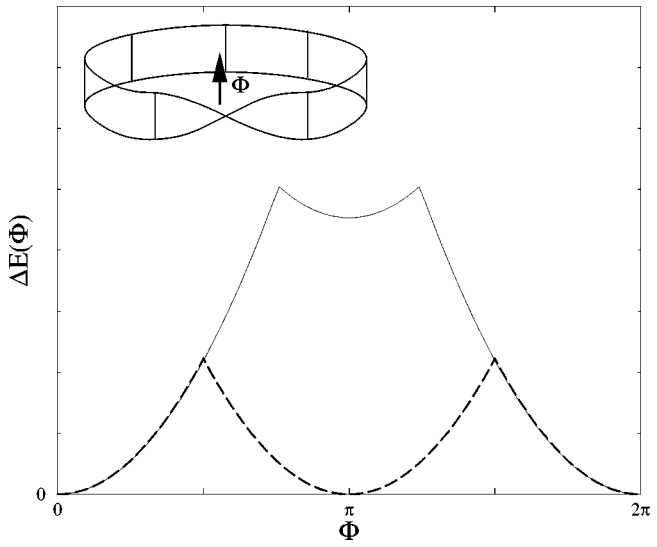

FIG. 1. Generic flux dependence of the ground-state energy of a Moebius ladder. Solid curve: $t_\perp/t=0.2$, dashed curve: $t_\perp/t=0$. Inset: Schematic diagram of a Moebius ladder pierced by a magnetic flux $(\hbar c/e)\Phi$.

an interacting system with $t_\perp \neq 0$, the period is expected to be ϕ_0 as long as coherent motion between the chains is possible, and to become $\phi_0/2$ when the interactions are strong enough to prevent any coherent motion between the chains. The vanishing of the odd harmonics of $I(\Phi)$ in the Moebius geometry would thus be a direct signature of the destruction of interchain coherence.

Rather than considering all of the odd harmonics of $I(\Phi)$ separately, we focus our attention in the following on the energy difference

$$\Delta E = E(\Phi=\pi) - E(\Phi=0) = -\frac{2\hbar}{e}\sum_{n=0}^{\infty}\frac{I_{2n+1}}{2n+1}. \quad (2)$$

The full flux dependence of the ground-state energy for a Moebius ring is shown in Fig. 1. From the discussion above, it is clear that ΔE is in general finite, but must vanish in the absence of coherent interchain tunneling. However, the analysis is less trivial than one might expect due to rather interesting finite-size effects. Let us start with a careful analysis of the noninteracting case. While spin can have important consequences on the nature of the ground state of a system of two coupled chains of interacting electrons,[6] it is not essential for the notion of coherence of Refs. 1 and 7. So, for simplicity, we consider spinless fermions throughout this paper. Spinless fermions on a Moebius ladder with N rungs pierced by a magnetic flux $(\hbar c/e)\Phi$ can be described by a one-dimensional periodic Hamiltonian,

$$H = -t\sum_{i=1}^{2N}(e^{i\Phi/N}c_i^\dagger c_{i+1} + \text{H.c.}) - t_\perp\sum_{i=1}^{2N} c_i^\dagger c_{i+N}, \quad (3)$$

with the usual convention $c_{i+2N} = c_i$. This Hamiltonian is readily diagonalized by a Fourier transform, and the dispersion reads

$$\epsilon_k = -2t\cos(ka + \Phi/N) - t_\perp\cos(Nka) \quad (4)$$

with $k = p(2\pi/2Na)$, p integer. The essential ladder structure of the Moebius ladder is contained in this expression because $\cos(Nka) = \cos(p\pi) = +1$ if p is even and -1 if p is odd. The system thus consists of bonding and antibonding bands with the usual dispersions $\epsilon_k = -2t\cos(ka+\Phi/N) \pm t_\perp$. The difference with a standard ladder is that the wave vectors $k = p(2\pi/2Na)$ are restricted to even and odd values of p for the bonding and antibonding bands, respectively.

Let us consider the periodicity of the ground-state energy of such a system as a function of Φ. If $t_\perp$ is large enough, all the fermions are in the bonding band, and the total energy reads $E(\Phi) = \Sigma_p[-2t\cos(p\pi/N + \Phi/N) - t_\perp]$, where the sum over p is restricted to *even* integers chosen to give the lowest energy for a given Φ. This function is clearly periodic in Φ with period 2π. If $t_\perp = 0$, the bonding and antibonding bands form a single band, and the total energy reads $E(\Phi) = -2t\Sigma_p\cos(p\pi/N + \Phi/N)$, where the integers p can now be both even and odd, and the periodicity of this function is π. For intermediate values of $t_\perp$, the periodicity is 2π except for specific values of $t_\perp$ where it is π. The number of such points scales with the number of particles in the system. To understand this, let us consider the scaled energy difference,

$$\Delta = (-1)^{n-1/2} N \Delta E, \quad (5)$$

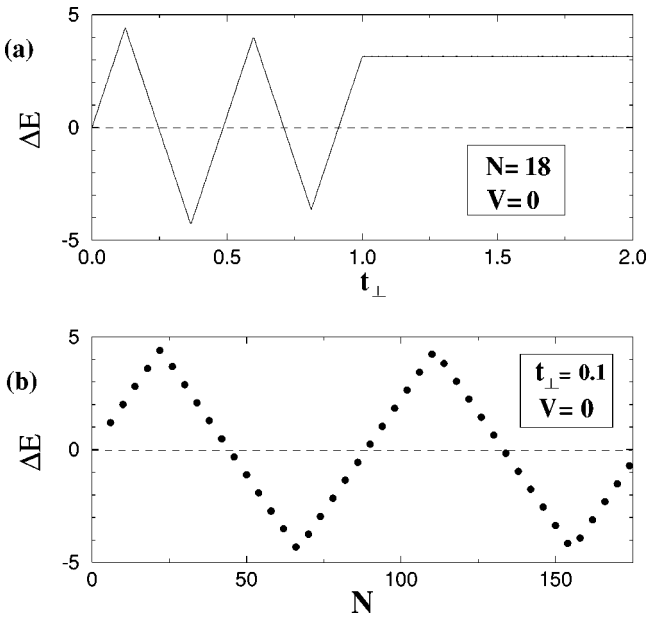

FIG. 2. $\Delta = (-1)^{n-1/2} N[E(\Phi=\pi) - E(\Phi=0)]$ for a noninteracting, quarter-filled system: (a) as a function of $t_\perp$; (b) as a function of the number of rungs N.

where n is the number of particles. In the following, n is restricted to odd values to have a nondegenerate groundstate which makes the analysis slightly simpler, although the results are essentially equivalent for an even number of particles, and the factor $(-1)^{n-1/2}$ has been included to insure that Δ is always positive in the limit $t_\perp \to 0$. As for the curvature at $\Phi = 0$, which gives the Drude weight, one has to multiply by N for 1D systems to get nonvanishing results in the thermodynamic limit. A typical example of the behavior of Δ with $t_\perp$ is depicted in Fig. 2(a). It is clear from the dispersion of Eq. (2) that both $E(\Phi=\pi)$ and $E(\Phi=0)$, and hence Δ, are piecewise linear functions of $t_\perp$. The slope of Δ changes each time a pair of particles goes from the antibonding band to the bonding band, which we know has to occur because the antibonding band is certainly empty for large enough $t_\perp$. Now these transitions do not occur for the same values of $t_\perp$ for $\Phi = \pi$ and $\Phi = 0$. As a result, the slope of Δ alternates between $2N$ and $-2N$ until the antibonding band is empty, in which case it is of course 0. Between changes of slopes, Δ vanishes once, which corresponds to points where the periodicity is π, as for $t_\perp = 0$. Since the particles change bands in pairs, the number of such points is essentially half the number of particles (more precisely $2n+1$ including $t_\perp = 0$ for $4n+1$ particles, and similar formulas for other fillings). The same effect shows up in the behavior of Δ with N: For intermediate values of $t_\perp$, Δ oscillates as a function of size with extrema each time the difference in the particle number between the bonding and the antibonding bands increases by 2 [see Fig. 2(b)]. The points lie on a piecewise linear curve with a slope alternating between $2t_\perp$ and $-2t_\perp$. As a consequence, the periodicity of the ground-state energy for a given $t_\perp$ and for noninteracting fermions is not a well-defined quantity in the thermodynamic limit.

Let us now consider the effect of intrachain interactions on the periodicity of the groundstate energy. To describe

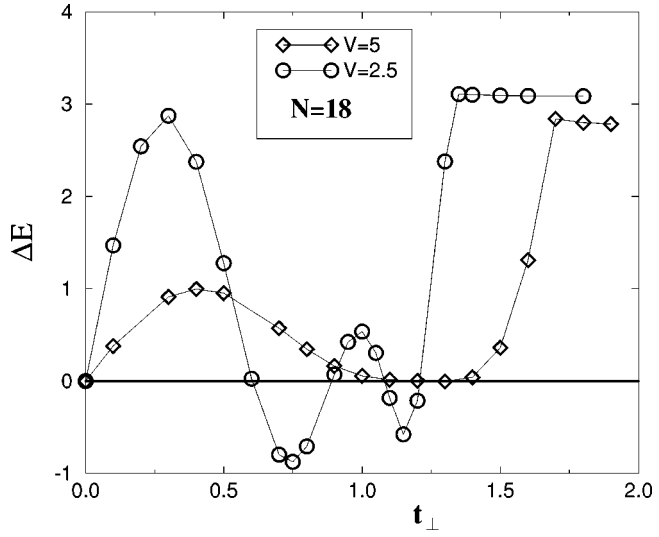

FIG. 3. Δ as a function of $t_\perp$ for $V=2.5$ ($\alpha=0.36$) and $V=5$ ($\alpha=1$) for a quarter-filled system with 18 rungs. All energies are in units of t.

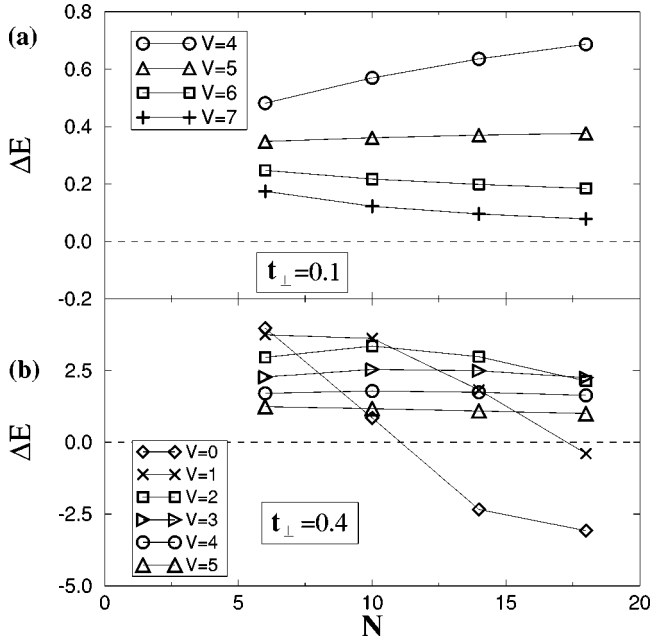

FIG. 4. Δ as a function of the number of rungs N for different values of V and two values of $t_\perp$: (a) $t_\perp=0.1$; (b) $t_\perp=0.4$. All energies are in units of t.

systems with large values of the Luttinger-liquid exponent α, we consider an interaction term of the form

$$H_{\rm int}=\sum_i \left(V n_i n_{i+1}+\frac{2V}{3} n_i n_{i+2}+\frac{V}{2} n_i n_{i+3}\right). \qquad (6)$$

For a quarter-filled system, the exponent α of this model has already been calculated with standard techniques,[11] and it reaches the value 1 for $V/t=5$. Using the Lanczos technique, we have calculated the dependence of Δ on $t_\perp$ for different values of V/t and different sizes up to 36 sites ($N=18$). Typical results are shown in Fig. 3. The effects of intrachain repulsion are rather dramatic. The first oscillation quickly becomes the dominant one, and the first value of $t_\perp$ where Δ vanishes increases significantly: The curve is already strongly affected for $V/t=2.5$ (Fig. 3) with respect to the noninteracting case [Fig. 2(a)]. But more importantly, the oscillations disappear altogether for $V/t=5$, i.e., $\alpha=1$. This critical value turns out to be independent of the size. The origin of the oscillations being that particles go from the antibonding band to the bonding band, this means that these concepts have lost their meaning when α is big enough. In other words, $t_\perp$ is no longer able to produce two separate bands in the low-energy spectrum of the system.

Our discussion of the dependence of Δ on N for interacting systems is limited by the maximum size we can handle with Lanczos, namely, 36 sites ($N=18$) at quarter-filling. For $t_\perp=0.1$, we are limited to the first linear section of Fig. 2(b) where the slope is equal to $2t_\perp$ in the noninteracting case. The slope is considerably reduced by interactions and *changes sign* between $V/t=5$ and $V/t=6$, which means that Δ *decreases* with N [see Fig. 4(a)]. Given the absence of oscillations in Δ as a function of $t_\perp$ for these values of the interaction, it is natural to assume that Δ does not change sign as a function of N either. This leads us to the conclusion that Δ goes to 0 in the thermodynamic limit when $\alpha \geqslant 1$.[12] Significant effects are already present for $\alpha<1$, however. Let us consider for instance $t_\perp=0.4$, for which Δ changes sign between $N=10$ and $N=14$ in the noninteracting case [see Fig. 4(b)]. For the sizes we can reach, Δ already does not change sign for $V/t=2$, and the curve is very flat for V/t as small as 3 ($\alpha=0.46$). It is in fact possible that even in that case Δ goes to 0 with damped oscillations. Obtaining numerical results on larger systems by other methods, e.g., density matrix renormalization group, would be very useful to check this point. Let us note that oscillations would also be present for a regular ladder. However, the periodicity remains equal to ϕ_0 even if $t_\perp$ is switched off. So the Moebius geometry is essential to observe the effects of interactions.

To make contact with current theories of the effect of interactions on interchain hopping, let us first note that the present results strongly suggest that the system has lost any memory of the splitting between bonding and antibonding bands when $\alpha=1$. This is reminiscent of the RG result that $t_\perp$ is an irrelevant perturbation when $\alpha>1$, but we wish to emphasize that this is much stronger: RG arguments are limited to infinitesimal values of $t_\perp$, while our results show that *large* values of $t_\perp$ are still unable to produce a difference between bonding and antibonding states if $\alpha>1$. In fact, we believe that the results of Fig. 3 are the first direct numerical evidence of a strong effect of interactions on hopping between chains because they exhibit a qualitative change without having to go to the thermodynamic limit. In addition, our results concerning the dependence of Δ on N show very dramatic effects for relatively small interactions, i.e., for small values of α where RG arguments just indicate that $t_\perp$ is a relevant perturbation. These conclusions agree qualitatively with those of Refs. 1 and 7, and they are consistent with previous numerical studies of the spectral functions.[13,11]

It is important to contrast the oscillations of Δ described above with the oscillations of the sign of the persistent current with the parity of n,[14] which have already been factored out in Eq. (5); the oscillations of Δ in the Moebius geometry occur as a function of $t_\perp$ even for fixed n. Likewise, the

interaction-induced suppression of Δ predicted here for the Moebius geometry should be contrasted to that predicted in purely 1D systems with spin,[15] since these effects occur for *finite* interaction strength V, while the spin-induced suppression occurs only in the limit of infinite on-site repulsion. The effect of intrachain interactions described here is also to be contrasted to that of interchain interactions, which were found to increase the odd harmonics of the persistent current.[16]

In conclusion, we have shown that interactions between electrons have dramatic effects on their ability to hop coherently from one chain to the other by studying the flux dependence of the ground-state energy—or, equivalently, of the persistent currents—in a Moebius ladder. Importantly, the theoretical quantity Δ that we have studied is related directly to the measurable Fourier components[9,10] of the magnetization of the system. The absence of oscillations of Δ as a function of $t_\perp$ for strong enough interactions is, we believe, the best evidence of an interaction-induced destruction of interchain coherence obtained so far with numerical simulations. Further work along these lines, either numerically by studying larger systems, or experimentally by measuring persistent currents in appropriate mesoscopic devices, should be a promising area for future research.

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