Broken Time-Reversal Symmetry in Strongly Correlated Ladder Structures

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We provide, for the first time, in a doped strongly correlated system (two-leg ladder), a controlled theoretical demonstration of the existence of a state in which long-range ordered orbital currents are arranged in a staggered pattern, coexisting with a charge density wave. The method used is the highly accurate density-matrix renormalization group technique. This brings us closer to recent proposals that this order is realized in the enigmatic pseudogap phase of the cuprate high temperature superconductors.

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The circulating current phases in correlated electron systems, also called orbital antiferromagnets (OAF), were first considered in the context of excitonic insulators [1], but then discarded in favor of more conventional order. After the discovery of the cuprate high temperature superconductors, they were rediscovered [2,3] and called staggered flux (SF) phases [2]. Many of their properties were discussed, but were forgotten again in the absence of experimental vindication. The discovery of an unusual and robust regime called the pseudogap [4] in these superconductors has changed the picture once more. The pseudogap mimics the momentum dependence of the superconducting gap, but the state itself is not superconducting. In this context, two recent developments have taken place: (i) Attempts have been made to explain this regime in terms of fluctuations of SF order [5] and (ii) a proposal has been made that it is not fluctuations, but a true broken symmetry that is the origin of the pseudogap [6,7]. This ordered state was called the singlet d-density wave (DDW) following Ref. [8] and is the same as the OAF and SF phases. In this Letter, we adopt the density wave (DW) terminology, as it can describe large classes of order parameters with orbital angular momentum. The label d stands for angular momentum 2, as in atomic physics. The conventional charge density wave (CDW) in which charge is modulated in space is its s-wave counterpart with angular momentum zero. The triplet s-wave density wave is what is commonly called a spin density wave. Another breakdown of time reversal symmetry in which the circulating currents obey translational symmetry, as opposed to DDW, has also been pointed out and has been argued to be responsible for the pseudogap phase [9,10].

Although much indirect experimental evidence of DDW can be argued to exist, a direct observation of DDW would be Bragg reflection of neutrons carrying magnetic moments from the staggered arrangement, on the scale of a few Å, of circulating currents. Recent neutron scattering experiments have, however, been controversial [11–14], and more precise and well-characterized experiments are underway to establish this order. Thus, theoretical exploration of microscopic models of correlated electronic systems with controlled methods has acquired urgency. We, therefore, study the simplest geometrical structure in the form of a two-leg ladder [15] that can support staggered orbital currents, as shown in Fig. 1.

Previous studies of DDW order in two-leg ladders have used weak-coupling bosonization/renormalization group (RG) analyses [16–23], density-matrix renormalization group (DMRG) [24] analysis of the t-J model [23] and a half-filled Hubbard-like model [25], or exact diagonalization [26] of the t-t'-J model. At half filling, models with long-range ordered currents have been found both for spinless [16] and spinful [20–22,25] fermions. In contrast, for doped ladders, power-law decay has been found for spinless [17,19] and spinful [18–20] cases. For the t-J ladder, only short-range order was found [23], and the study of the t-t'-J model [26] yielded similar results.

The approach used in the present work is the accurate DMRG method that can be used for arbitrary interaction strength, unlike the weak-coupling bosonization/RG approaches. The results of our calculations are striking. Although common t-J–type models do not exhibit long-ranged DDW order, a separate class of *repulsive* Hamiltonians show robust long-range DDW order even in the presence of *substantial doping*. These have their historical origin in a half-filled SO(5) invariant model on a ladder [27]. At precise half filling, it was shown to exhibit DDW in its phase diagram [21,25]. We shall show that SO(5) invariance is irrelevant by considering coupling constants very far from the "SO(5) parameters" and by substantially doping this model. The real reason for success with this class of models is that it straddles

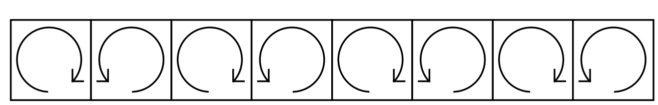

FIG. 1. Circulating plaquette currents on a ladder, characteristic of the DDW phase.

CDW and DSC-like ($d_{x^2-y^2}$-superconductor) states (more precisely rung-singlet states), resulting in a local kinetic exchange between them. This is much like the actual situation in the cuprates in which the DDW phase is an intermediate regime between a multiplicity of complex charge ordered states and DSC [12,21,22,25].

We label the site of a ladder by $\mathbf{i} \equiv (r, l)$, where $r = 1, \ldots, L$ is the rung index and $l = 1, 2$ is the leg index. The current operator between any two sites $\mathbf{i}$ and $\mathbf{j}$, $J_{\mathbf{i},\mathbf{j}}$, is

$$J_{\mathbf{i},\mathbf{j}} = it\sum_{\sigma}(c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma} - c^{\dagger}_{\mathbf{j}\sigma}c_{\mathbf{i},\sigma}), \tag{1}$$

where $c^{\dagger}_{\mathbf{i},\boldsymbol{\sigma}}$ is the creation operator of a fermion with spin σ at site $\mathbf{i}$. We set the lattice spacing to unity.

There are at least two convenient ways of probing DDW order. One approach is to measure the equal-time rung-rung current correlation function in the ground state,

$$C(r, R) = \langle j_{\mathrm{rung}}(R + r/2) j_{\mathrm{rung}}(R - r/2)\rangle, \tag{2}$$

where $j_{\mathrm{rung}}(r) = J_{(r,1),(r,2)}$. In order to minimize the effect of the boundaries of a finite ladder, we should choose R to be the location of the central rung, and we shall denote this correlation function as $C(r)$

An alternative approach is to break the time reversal symmetry explicitly by applying a source $-hj_{\mathrm{rung}}(1)$ on one end of the ladder and measuring the current induced in the sample. The source term for DDW is necessarily complex and a complex DMRG program is needed, which is more demanding on memory and computer time. Nonetheless, we have used both methods for cross checks for every single case discussed in the present Letter. For both methods, we use a finite size algorithm, which is more reliable, performing sweeps to reach convergence [24] .

To orient ourselves, we shall begin with the two-leg t-J ladder, which is defined by the Hamiltonian:

$$H_{tJ} = -t\sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma}(\mathcal{P}c^{\dagger}_{\mathbf{i},\boldsymbol{\sigma}}c_{\mathbf{j},\boldsymbol{\sigma}}\mathcal{P} + \mathrm{H.c.}) + J\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\left(\mathbf{S}_{\mathbf{i}}\cdot\mathbf{S}_{\mathbf{j}} - \frac{n_{\mathbf{i}}n_{\mathbf{j}}}{4}\right), \tag{3}$$

where $n_{\mathbf{i}}$ is the total fermion occupation number at the site $\mathbf{i}$, and $\mathbf{S}_{\mathbf{i}}$ is the spin operator at the corresponding site. $\mathcal{P}$ projects out doubly occupied sites and $\langle \mathbf{i}, \mathbf{j}\rangle$ denotes pairs of nearest neighbor sites. The t-J model is the simplest model that captures some aspects of the high temperature superconductors. Removal of electrons from the system is quantified by the doping parameter $\delta = 1 - \langle n_i\rangle$. In actual experiments, DSC is observed in the range $\delta = 0.05$–0.25; at small values of δ lies the pseudogap regime. In this model, the DDW correlations decay exponentially with a correlation length $\xi = 3$–4 [23]. Additional next-nearest neighbor hopping, augmenting the model, may be supposed to suppress the competing CDW and DSC phases and thus reveal DDW order, but our calculations and those of Ref. [26] do not support this idea.

A more interesting model is the t-J-V-V' model, which is a t-J model augmented by Coulomb repulsion terms V and V' between nearest and next-nearest neighbors:

$$H_{tJVV'} = H_{tJ} + V\sum_{\langle \mathbf{i},\mathbf{j}\rangle}n_{\mathbf{i}}n_{\mathbf{j}} + V'\sum_{\langle\langle \mathbf{i},\mathbf{j}\rangle\rangle}n_{\mathbf{i}}n_{\mathbf{j}}, \tag{4}$$

where $\langle\langle \mathbf{i}, \mathbf{j}\rangle\rangle$ denotes next-nearest neighbor pairs of sites. In order to reduce the effect of open boundaries, a chemical potential term $(V + V')n_{\mathbf{i}}$ is added to the boundary sites. A typical parameter set, given by $J/t = 0.4$, $V/t = 3$, $V'/t = 1$, and $\delta = 0.1$, yields the current correlation function $C(r)$ shown in Fig. 2. We observe what appears to be a bubble of DDW extending up to 20 rungs, and then a sinusoidally modulated exponential decay with $\xi \approx 3$. Thus, although we observe DDW over a moderately long range, there is no macroscopic order. We have probed this model by the second method in which we induce a current by a source at the edge. As shown in Fig. 3, the long-range correlations that are observed at the first infinite-size step disappear after a few sweeps and converge after six sweeps to an exponential decay with a correlation length $\xi \approx 10$. The moderately large bubblelike nature of $C(r)$ and the different values of ξ in these two methods are strong reasons for suspecting proximity to a first order transition to the ordered DDW phase, as the boundary effects seem to nucleate this phase.

Finally, we shall consider a different class of Hamiltonians, in which a pair of electrons across a rung is given an internal structure, much like a molecule. This is an interesting way of generating a set of low energy Hamiltonians [27] that are defined by

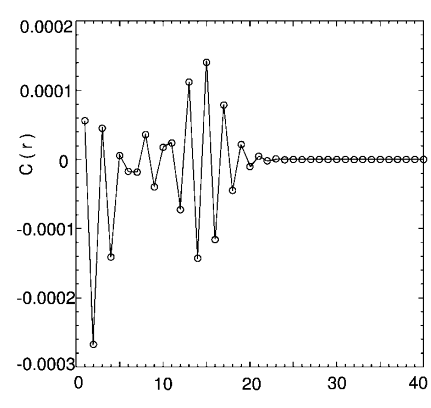

FIG. 2. The correlation function $C(r)$ of the t-J-V-V' model. The parameters are $J/t = 0.4$, $V/t = 3$, $V'/t = 1$, and $\delta = 0.1$. The size of the ladder is 120×2. We kept 800 states and performed 42 sweeps. The vertical scale is chosen in units where $t = 1$.

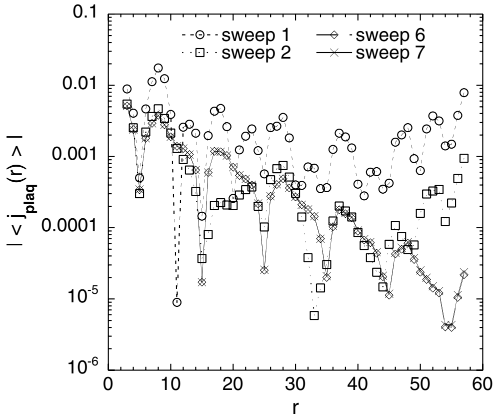

FIG. 3. Absolute value of the current summed around a plaquette, $|\langle j_{\mathrm{plaq}}(r)\rangle|$, as induced by an edge current, $h = 0.01t$, as a function of the distance r from the edge of a 60×2 ladder in the t-J-V-V' model, with the parameters described in the text. Note the convergence as a function of sweeps. The number of states retained was 400 and the results were found to scale with current at this level.

$$H_{tJ_\perp UV_\perp} = -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle\sigma} (c^\dagger_{\mathbf{i},\boldsymbol{\sigma}} c_{\mathbf{j},\boldsymbol{\sigma}} + \mathrm{H.c.}) + \frac{U}{2}\sum_{\mathbf{i}} (n_{\mathbf{i}} - 1)^2 + \sum_r [J_\perp \mathbf{S}_{r,1} \cdot \mathbf{S}_{r,2} + V_\perp (n_{r,1} - 1)(n_{r,2} - 1)]. \tag{5}$$

Note that there are no longer any projection operators $\mathcal{P}$, as in the previous examples, and the problem can be treated for arbitrary interaction strength. In the half-filled case, this Hamiltonian has a precise SO(5) symmetry [27] when $J_\perp = 4(U + V_\perp)$. It also exhibits DDW order [21,25]. As soon as the system is doped, or the parameters are no longer finely tuned, there is no SO(5) symmetry. The weak-coupling phase diagram at half filling obtained from bosonization/RG, as shown in Fig. 4, gives us some guidance as to where to look in our DMRG calculations.

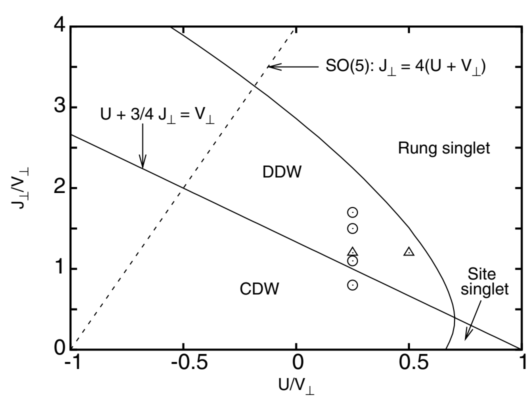

FIG. 4. The weak coupling phase diagram at half filling for $H_{tJ_\perp UV_\perp}$ from a bosonization calculation. The open circles correspond to the parameters in Fig. 5 and the open triangles to those in Fig. 6.

This phase diagram is essentially identical to that of Ref. [22], except that we also show the regime for $U < 0$. Other than the DDW and CDW, there are two relevant states that can be adiabatically continued to resonating valence bond states [28] of the short-range variety [29]—rung singlet ($|\mathrm{rs}\rangle$) and site singlet states ($|\mathrm{ss}\rangle$) [30],

$$|\mathrm{rs}\rangle \propto \prod_r \Big[\Big| \begin{matrix}\uparrow\\ \downarrow\end{matrix} \Big\rangle - \Big| \begin{matrix}\downarrow\\ \uparrow\end{matrix} \Big\rangle \Big]_r, \quad |\mathrm{ss}\rangle \propto \prod_r \Big[\Big| \begin{matrix}\uparrow\downarrow\\ -\end{matrix} \Big\rangle + \Big| \begin{matrix}-\\ \uparrow\downarrow\end{matrix} \Big\rangle \Big]_r.$$

The DDW lies between the CDW and the rung-singlet phases.

We have studied the Hamiltonian in Eq. (4) for a range of parameters and find long-range DDW order in the doped model, which has nothing to do with SO(5) symmetry. Nonetheless, the DDW phase is situated between the CDW and the rung-singlet phases, similar to the weak-coupling bosonization results for half-filled ladders. As a typical example, we have shown in Fig. 5 our results for the rung current as induced by an edge current of tiny magnitude $0.0001t$. The parameters chosen were $U = 0.25$, $t = V_\perp = 1$, $J_\perp = 0.8$, 1.1, 1.5, 1.7, and $\delta = 0.04$. As a response, we see robust long-ranged DDW order in the middle of this range of $J_\perp$ with stripelike features where pairs of holes reside; see, in particular, Fig. 5(c), where we also plot the hole density, and the coexistence with stripe order is especially evident from the antiphase domain wall structure [31]. The induced currents clearly alternate in sign and can be of the order

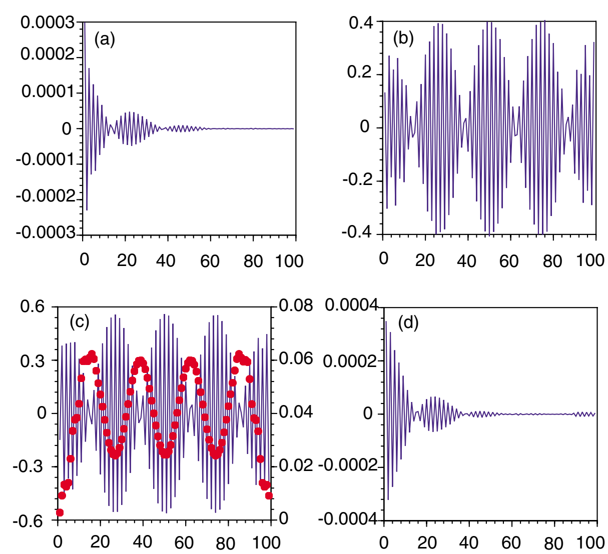

FIG. 5 (color online). Rung current $j_{\mathrm{rung}}(r)$ as a function of the location of the rung r in a t-$J_\perp$-U-$V_\perp$ model at 4% doping on a 100×2 ladder, with parameters $U = 0.25$, $t = V_\perp = 1$, and an edge current of 0.0001. The sequence of figures corresponds to (a) $J_\perp = 0.8$, (b) $J_\perp = 1.1$, (c) $J_\perp = 1.5$, and (d) $J_\perp = 1.7$. In (c), we show the profile of the hole density depicted as solid dots corresponding to the scale on the right. We kept up to 400 states and performed up to eight sweeps. Note the vast differences in the scales of the current strengths.

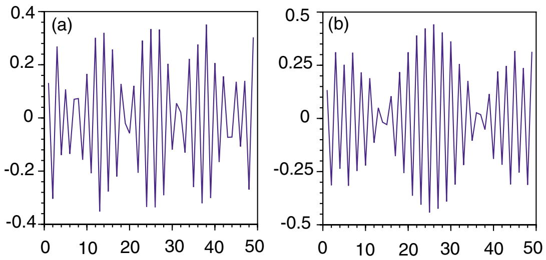

FIG. 6 (color online). Rung current $j_{\rm rung}(r)$ as a function of the location of the rung r in a t-$J_\perp$-U-$V_\perp$ model on a 50×2 ladder, with parameters $t = V_\perp = 1$, $J_\perp = 1.2$, and an edge current of 0.0001. The sequence of figures corresponds to (a) $U = 0.25$ at 8% doping, and (b) $U = 0.5$ at 4% doping. We kept up to 400 states and performed up to eight sweeps.

of unity, in units of t, even though the source current is infinitesimally small. For ladders of lengths 100, 150, and 200, and for parameters of Fig. 5(c), the current amplitudes are, respectively, 0.56, 0.53, and 0.53, consistent with long-range order, though in a numerical calculation it is never possible to rule out a very slow decay. We have studied the d-wave pairing correlations, and find only extremely rapid decay in ladders that exhibit DDW long-range order. This is as expected from previous numerical work on the half-filled system [25], where it was shown that the superconducting correlations decay exponentially in the DDW phase. It is also in accord with the phase diagram in Fig. 4, which shows that the region with strong d-wave superconducting correlations, the "rung-singlet" phase, is distinct from the DDW region. More generally, bosonization leads to the prediction that the phase with strong DDW correlations has only short-ranged pairing correlations. For the case of Fig. 5(c), we have also studied the low-lying excitations about the ground state. We find a robust spin gap, again in accord with general expectations. In Fig. 6, we show the results for $\delta = 0.08$ and for $U = 0.5$. For sufficiently strong doping, roughly between 10% to 20%, DDW is suppressed for these sets of couplings.

In summary, we have shown that there are repulsive microscopic models that exhibit DDW order at finite doping, providing added support for the identification of the pseudogap in the cuprates with this state. Our work also raises the real possibility that an appreciation of the complexity of many novel materials [32] may be impossible without these remarkable broken symmetries, and it is important to search for such complex quantum order in an even wider class of Hamiltonians.

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