Robust *D*-Wave Pairing Correlations in a Hole-Doped Spin-Fermion Model

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(Received 8 October 2001; published 17 April 2002)

Pairing correlations are studied numerically in a hole-doped spin-fermion model. Simulations performed on up to 12 × 12 clusters provide indications of D-wave superconductivity away from half-filling comparable to those of the 2D t-J model. The pairing correlations are the strongest in the direction *perpendicular* to the dynamic stripes that appear in the ground state at some densities. An optimal doping, where correlations are maximized, was observed at ~25% doping with an estimated $T_c \sim 100-200$ K, in qualitative agreement with high-T_c cuprates' phenomenology, while pairing correlations are suppressed by static stripe inhomogeneities.

DOI: 10.1103/PhysRevLett.88.187001 PACS numbers: 74.20.De, 74.20.Rp, 74.72.–h

The nature of high temperature superconductors is an important open problem in the area of strongly correlated electrons [1]. In this context, models for cuprates have been extensively used to search for superconductivity (SC) arising from a purely electronic mechanism. In spite of this effort, the current situation is still confusing, with a few positive reports of ground-state SC in electronic models using truly unbiased many-body techniques. Recently, a simple spin-fermion model (SFM) has been proposed for cuprates [2]. The main advantage of the SFM is its simplicity for numerical studies, while still keeping a realistic, unbiased, and nontrivial character. Previous studies have already shown that several of its properties, such as magnetic incommensurability, a density-of-states pseudogap at the chemical potential, and the shape of the Fermi surface, resemble experimental data for high-T_c cuprates [2]. In addition, upon hole doping, the ground state exhibits charge incommensurability caused by hole-rich stripes [2]. Our goal is to study for the first time the pairing correlations of this phenomenological model, and determine the role that charge stripes play in the pairing process. To our surprise, relatively robust pairing correlations in the D-wave channel were detected, in the presence of dynamical stripes.

The SFM is constructed as an interacting system of electrons and spins, mimicking phenomenologically the coexistence of charge and spin degrees of freedom in the cuprates [3]. Its Hamiltonian is given by

$$H = -t \sum_{\langle \mathbf{ij} \rangle \alpha} (c^{\dagger}_{\mathbf{i}\alpha} c_{\mathbf{j}\alpha} + \mathrm{H.c.}) + J \sum_{\mathbf{i}} \mathbf{s_i} \cdot \mathbf{S_i} + J' \sum_{\langle \mathbf{ij} \rangle} \mathbf{S_i} \cdot \mathbf{S_j} , \qquad (1)$$

where $\mathbf{s_i} = \sum_{\alpha\beta} c^{\dagger}_{\mathbf{i}\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{i}\beta}$ is the spin of the mobile electron, $\mathbf{S_i}$ is the localized spin at site $\mathbf{i}$, $\langle \mathbf{ij} \rangle$ denotes nearest-neighbor (NN) lattice sites, t is the NN-hopping amplitude for the electrons, $J > 0$ is an antiferromagnetic (AF) coupling between the spins of the mobile and localized degrees of freedom, and $J' > 0$ is a direct AF coupling between the localized spins. The rest of the notation is standard. The density $\langle n \rangle = 1 - x$ of itinerant electrons is controlled by a chemical potential μ. The unit of energy will be $t = 1$. J' and J are fixed to 0.05 and 2.0, respectively, values shown to be realistic in previous investigations [2,4]. The presence of a nonzero J' is *crucial* to stabilize the stripes found in Ref. [2] due to the competition of nearly degenerate phases, an effect also observed in manganites [5]. These stripes exist on a bounded region of the J-J' plane. The temperature is mainly fixed to a low value, $T = 0.01$, shown to lead to the correct high-T_c phenomenology [2]. Although focusing on cuprates, the present study has potential implications for heavy-fermion (HF) systems as well, since Eq. (1) is known in that context as the Kondo lattice model [5,6].

To simplify the numerical calculations, avoiding the sign problem, the localized spins are assumed to be classical (with $|S_{\mathbf{i}}| = 1$). This approximation is not drastic, and it was already discussed in detail in Ref. [2]. Studies performed as part of this effort (not shown) reproduced qualitatively the ferromagnetic and spiral regimes of the 1D Kondo lattice at $J' = 0$ [6], showing that classical spins may be a qualitatively useful approximation for HF models as well. Equation (1) will be analyzed using a Monte Carlo (MC) method (for details see Ref. [5]). To study superconducting properties, pair correlation functions, $C_w(\mathbf{r}) = \langle \hat{\Delta}^{w}_{\mathbf{i+r}} \hat{\Delta}^{w\dagger}_{\mathbf{i}} \rangle$, are measured. The index w indicates D- or extended S-wave pairing, and the pairing operator $\hat{\Delta}^{w}_{\mathbf{i}}$ is standard.

To study the long distance behavior of the pairing correlations, results on $N \times N$ ($N = 8$ and 12) clusters are presented. These results show that the D-wave pairing correlations (DPC) are stronger than S wave for all the values of the parameters studied. A typical comparison between the two correlations is shown in Fig. 1a for $\langle n \rangle = 0.75$. The extended S wave exhibits strong oscillations, while the D-wave results are more robust and smoother. This shows that our SFM captures the essence of hole pairing in AF backgrounds, where it is well known that $d_{x^2-y^2}$

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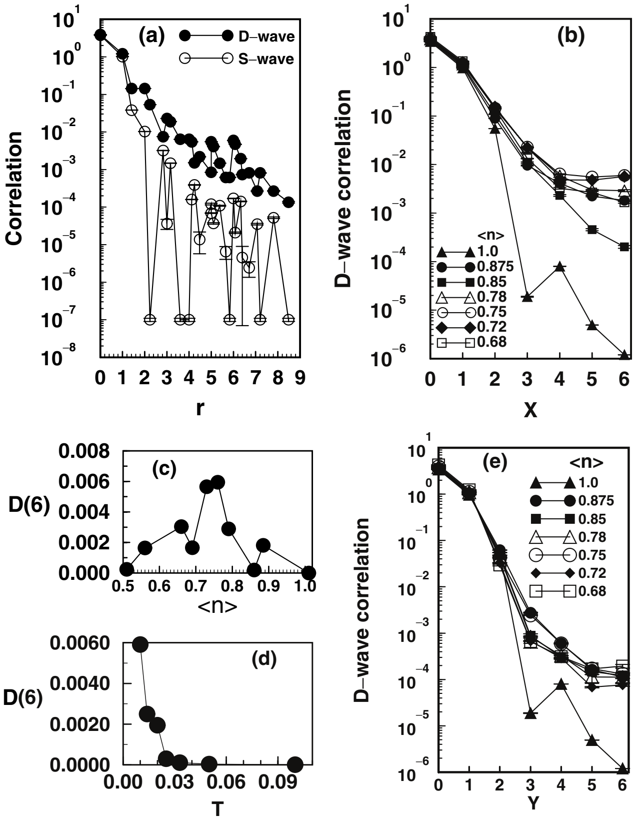

FIG. 1. (a) D-wave and extended S-wave pairing correlation versus distance r, on a 12×12 lattice at $\langle n\rangle = 0.75$. (b) D-wave pairing correlations along the direction perpendicular to the charge inhomogeneities at the densities indicated. (c) Correlations for $x = 6$, $D(6)$, as a function of density. (d) $D(6)$ for $\langle n\rangle = 0.75$ as a function of temperature. (e) Same as (b) but with correlations parallel to the stripelike charge inhomogeneities.

tendencies dominate [1]. Thus, below we will concentrate only on the behavior of the DPC.

In Fig. 1b, the DPC vs distance (measured in the direction *perpendicular* to the stripe) are presented for several densities. At half-filling the correlations are very small, i.e., $\sim 10^{-6}$, at the largest distance, but they develop a fairly robust tail of order 10^{-2} at small hole doping (corresponding to an order parameter $\langle \hat{\Delta}^{w}_{\mathbf{i}} \rangle \sim 0.1$). At these densities, expecting stronger pair correlations would be unrealistic, since the low carrier density as well as the small quasiparticle weight Z of holes in antiferromagnets suppresses the signal [7]. In addition, the pairing operator, being nearest neighbors, is not optimized to fit the actual pair size. Ours is among the strongest signals for D-wave SC found in unbiased studies of realistic high T_c models, even comparable to those reported in two-leg ladders and the 2D t-J model [8]. The strongest correlations are observed at $\langle n\rangle \approx 0.75$, indicating the existence of an optimal doping as in real cuprates [9]. In Fig. 1c the DPC at distance $x = 6$ is shown versus electronic density, and the existence of an optimal doping is again clear. The dip at $\langle n\rangle \sim 0.85$, which corresponds to a state with nearly static stripes, can be qualitatively identified to the $x = 1/8$ anomaly of the cuprates [10]. The pairing correlations at the longest distance as a function of temperature, displayed in Fig. 1d for $\langle n\rangle \approx 0.75$, allow us to estimate a $T_c \approx 0.02$–0.04 in units of t. If $t = 0.5$ eV ≈ 5000 K, then $T_c \approx 150$ K, a very reasonable value.

Correlations in the direction parallel to the stripes (Fig. 1e) are, surprisingly, about 1 order of magnitude smaller than those in Fig. 1b. This is a remarkable general trend, and the reasons are discussed below.

Previous studies have shown that the system changes from an AF insulator to a metal upon doping [2]. The large suppression of the pairing correlations at half-filling is expected due to the absence of holes. However, as observed in Fig. 1b, an increase of about 4 orders of magnitude occurs when the system is doped and becomes metallic. To understand this phenomenon, we will analyze the properties of the charge and spin configurations (MC "snapshots") that contribute the most to the enhancement of the DPC, starting at densities for which fairly static stripes are stabilized.

The spin and charge distribution for a typical MC snapshot at $\langle n\rangle = 0.85$ is shown in Fig. 2a. When the local density is smaller than the average density the circles proportional to the local charge density are shown in gray. As observed, the gray circles determine two fairly static horizontal stripes [11]. This inhomogeneous charge distribution produces a large peak at momentum $(0, \pi/3)$ in $N(q)$ (Fig. 2c). The nearly perfect AF order in the electron rich regions (white circles) is also clear. $S(q)$ (Fig. 2d) peaks at $(\pi, 5\pi/6)$ in agreement with the AF order observed horizontally and the incommensurability induced vertically by the π shift carrying stripes.

The results in Figs. 1b and 1e are averages over MC time, and over all the lattice sites. Measurements on the individual snapshots were found to be similar to the averages, and indicate that the pair correlations are weaker along the AF regions. An intermediate value is obtained along hole-rich stripes, but the largest correlation is observed along the direction perpendicular to the stripes (Fig. 3a).

An analogous effect, but more enhanced, is observed for $\langle n\rangle = 0.68$, Fig. 2b, where four nearly static horizontal stripes are stabilized. $N(q)$ (Fig. 2c) peaks at momentum $(0, 2\pi/3)$, while $S(q)$ (Fig. 2d) at $(\pi, 2\pi/3)$. In this case, according to Figs. 1b and 1e, the DPC functions are 1 order of magnitude larger perpendicular to the stripes than in the parallel direction. To shed some light on these issues, in Fig. 3b correlations for the snapshot shown in Fig. 2b are presented. The correlations (circles) along the AF domains parallel to the stripes, with an average local density of ~ 0.78, are very weak. The AF order appears responsible for this depletion. The DPC are stronger along the hole-richer stripes, as indicated by the squares in Fig. 3b. In this case, the local density is ~ 0.63. However, the strongest correlations, indicated by triangles, occur, once again, perpendicular to the stripes. Along this direction the

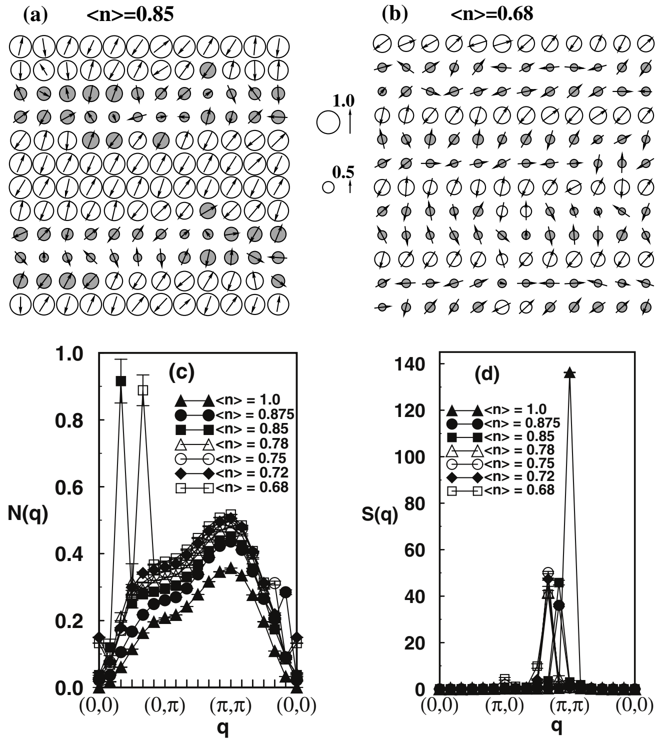

FIG. 2. (a) Representative snapshot of the spin and charge degrees of freedom on a 12×12 cluster at $\langle n \rangle = 0.85$, in the regime of nearly *static* stripes. The area of the circles is proportional to the electronic charge, the length of the arrows is proportional to the projection of the localized spins on the X-Y plane. When $n(i) < \langle n \rangle$ the circles are gray. (b) Same as (a) but for $\langle n \rangle = 0.68$. (c) Charge structure factor along selected directions in momentum space for parameters as in Fig. 1b. Stripelike inhomogeneities for all dopings are along the x direction. (d) Magnetic structure factor along selected directions for the same parameters as in (c).

local charge is very inhomogeneous and magnetic incommensurability occurs. These observations lead us to believe that local charge homogeneity and AF order do not favor D-wave pairing, while local charge inhomogeneity and its associated magnetic incommensurability promote it. Thus, the difference in the perpendicular correlations for $\langle n \rangle = 0.85$ and 0.68 mentioned above may be related to the AF reduction in electron-rich regions, as the system is doped away from half-filling.

The largest DPC are obtained for densities where charge fluctuations appear to be *dynamical*, according to the snapshots, and their time evolutions, during several MC runs. This is in agreement with expectations based on experimental results [12]. To further confirm this picture, in Fig. 4a a typical MC snapshot for $\langle n \rangle = 0.78$ is shown. Although the charge distribution is clearly inhomogeneous, the electron-rich AF domains are not separated by static stripes. We have observed that the shape of these domains changes substantially during the MC simulation, confirming that the charge structures are dynamical. As a result, only a small peak at $(0, \pi/2)$ is observed in $N(q)$ (Fig. 2c). The magnetic incommensurability, on the other hand,

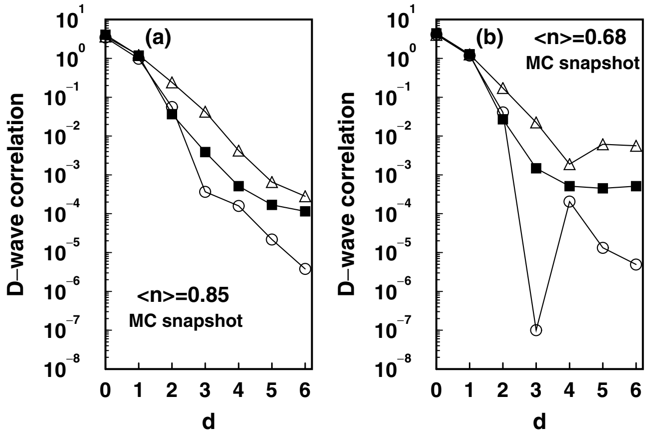

FIG. 3. (a) D-wave correlations for the representative snapshot shown in Fig. 2a. The circles indicate correlations along row 6 (counting from the bottom of Fig. 2a), which corresponds to an AF array with local charge ~ 0.97. The filled squares are correlations along row 3, which has an average local charge ~ 0.67. The triangles are correlations in the direction perpendicular to the stripes starting from row 2 and averaged over all the columns. (b) D-wave correlations for the snapshot shown in Fig. 2b. The circles indicate correlations along row 3 (counting from the bottom of Fig. 2b), which corresponds to an AF array with local charge ~ 0.78. The filled squares are correlations along row 8, which has a local charge ~ 0.63, and the triangles are correlations in the direction perpendicular to the stripes starting from row 6.

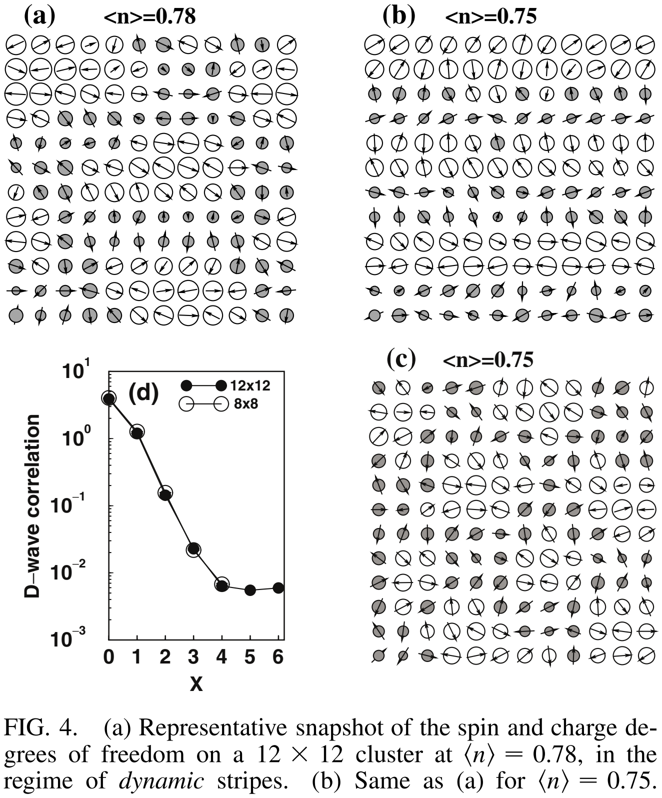

FIG. 4. (a) Representative snapshot of the spin and charge degrees of freedom on a 12×12 cluster at $\langle n \rangle = 0.78$, in the regime of *dynamic* stripes. (b) Same as (a) for $\langle n \rangle = 0.75$. (c) Snapshot for the same parameters as in (b) obtained at a later time during the simulation. (d) DPC in the direction perpendicular to the stripes using two lattice sizes.

exhibits a sharp peak at $(\pi, 2\pi/3)$ (Fig. 2d). As observed in Fig. 1b, pairing correlations are enhanced in the direction parallel to the spin incommensurability, which is mainly vertical based on $S(q)$. Also in Fig. 1b it can be seen that the pairing correlations are the strongest for $\langle n\rangle = 0.75$. The corresponding snapshots are in Figs. 4b and 4c. As in the previous case, a dynamical inhomogeneous charge distribution is observed. Rigid stripes appear at times during the simulation (Fig. 4b), but they become distorted after a few subsequent MC iterations (Fig. 4c). A very weak peak at $(\pi/3, \pi/3)$ exists in $N(q)$ (Fig. 2c), while a sharp peak at $(\pi, 2\pi/3)$ (Fig. 2d) is found in its magnetic counterpart. Similar behavior was observed at $\langle n\rangle = 0.72$ and 0.875.

Our conclusion is that weak charge inhomogeneity and magnetic incommensurability appear crucial for a robust DPC, within the SFM. Although $N(q)$ is nearly featureless in the regime with the strongest pairing, the states are *not* homogeneous, as observed from the MC snapshots. Studies performed by us in the noninteracting system show that for charge truly uniformly distributed, the magnetic structure factor is featureless, and the DPC present strong oscillations and are suppressed [13].

A comparison of results on 8×8 and 12×12 clusters indicates that charge inhomogeneities become more dynamical as the system size increases. For example, at $\langle n\rangle = 0.75$ the stripes appear static on 8×8 clusters but, as shown, are more dynamical on 12×12 ones. In Fig. 4d, the DPC perpendicular to the charge inhomogeneities is presented for $\langle n\rangle = 0.75$ on 8×8 and 12×12 clusters. The figure shows that, on one hand, finite size effects are small but, on the other hand, a long range tail starts developing on the 12×12 cluster, and it is not apparent in the 8×8 one; its origin appears to be related to the development of fluctuations in the charge distribution that, as expressed above, are observed only in the larger cluster.

The SFM studied here has also been widely analyzed in the HF context, but focusing on $J' = 0$ and small J regime in which SC has been elusive. Our results show that a small but nonzero J' and intermediate J may lead to profound changes in the ground-state properties, inducing DPC. Our study also suggests that stripe formation could potentially occur in HF systems as well.

To summarize, we have found indications of robust D-wave pairing correlations in a doped SFM, with a charge inhomogeneous ground state [15]. Our results indicate that static AF order and D-wave pairing compete. The latter is enhanced when AF is replaced by magnetic incommensurability. Static, stripelike charge inhomogeneities, decrease only the strength of the pairing correlations, as compared with the effect of dynamic charge inhomogeneities. This is reasonable since a "liquid" charge distribution should be more favorable to pairing than a "crystal" order. In addition, the hole attraction strength caused by antiferromagnetism should be maximized near half-filling, where two holes bind in the t-J model [1]. As a consequence, an optimal doping emerges where AF pairing is still robust, while static stripes do not compete with superconductivity. A similar behavior was observed in Ref. [16], which seems to provide evidence that SC coexists with static stripes in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$. However, in this case T_c is at a minimum suggesting that static stripe order competes with SC. According to our results, D-wave SC is expected to be maximized when the charge inhomogeneities are the most dynamic, a situation that appears to occur in doped $La_{2-x}Sr_xCuO_2$. In this situation, magnetic incommensurability manifests clearly as a peak in $S(q)$, while $N(q)$ is almost featureless (as reported using neutron scattering in high T_c cuprates [12]).

A. M. is supported by NSF under Grant No. DMR-9814350, the NHMFL, and MARTECH.

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