Robust D-wave Pairing Correlations in a Hole-Doped Spin-Fermion Model for Cuprates

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(pairing correlations are studied numerically in the hole-doped spin-fermion model for cuprates. Simulations performed on up to 12 × 12 clusters provide robust indications of D-wave superconductivity away from half-filling. The pairing correlations are the strongest in the direction perpendicular to the dynamic stripe-like inhomogeneities that appear in the ground state at some densities. An optimal doping, where the correlations reach a maximum value, was observed at about 25\% doping, in qualitative agreement with high \(T_c\) cuprates' experiments. On the other hand, pairing correlations are suppressed by static stripe inhomogeneities.

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The nature of high temperature superconductors is an important open problem in the area of strongly correlated electrons. 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 few positive reports of ground-state SC in electronic models using truly unbiased many-body techniques. Recently, a simple spin-fermion (SF) model has been proposed for cuprates. The main advantage of the SF-model is its simplicity for numerical studies, while still keeping a realistic, unbiased, and non-trivial character. Previous studies have already shown that several of its properties, such as magnetic incommensurability, existence of a density-of-states pseudogap at the chemical potential, and the shape of the Fermi surface, resemble experimental data for high \(T_c\) cuprates. In addition, upon hole doping, the ground state exhibits charge incommensurability due to the formation of hole-rich vertical and horizontal stripes. The goal of this paper is to study for the first time the pairing correlations of this 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, correlated with the presence of dynamical stripes.

The SF-model is constructed as an interacting system of electrons and spins, mimicking phenomenologically the coexistence of charge and spin degrees of freedom in the cuprates. Its Hamiltonian is given by:

\[ H = -t \sum_{\langle ij \rangle \alpha} (c_{i \alpha}^\dagger c_{j \alpha} + \text{h.c.}) + J \sum_i s_i \cdot S_i + J' \sum_{\langle ij \rangle} S_i \cdot S_j, \]

where \(c_{i \alpha}^\dagger\) creates an electron at site \(i = (i_x, i_y)\) with spin projection \(\alpha\), \(s_i = \sum_{\alpha, \beta} c_{i \alpha}^\dagger \sigma_{\alpha \beta} c_{i \beta}\) is the spin of the mobile electron, the Pauli matrices are denoted by \(\sigma\), \(S_i\) is the localized spin at site \(i\), \(\langle ij \rangle\) 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 density \(\langle n \rangle = 1 - x\) of itinerant electrons is controlled by a chemical potential \(\mu\). Hereafter \(t = 1\) will be used as the unit of energy. \(J'\) and \(J\) are fixed to 0.05 and 2.0 respectively, values shown to be realistic in previous investigations. The temperature will be fixed to a low value: \(T=0.01\), which was shown before to lead to the correct high-\(T_c\) phenomenology.

To simplify the numerical calculations, avoiding the sign problem, the localized spins are assumed to be classical (with \(|S_i|=1\)). This approximation is not drastic, and it was already discussed in detail in Ref. [2]. The model will be analyzed using a Monte Carlo (MC) method, details of which can be found in Ref. [1]. To study the superconducting properties of the system, the pair correlation functions, \(C_w(r) = \langle \hat{\Delta}_w \hat{\Delta}_w^\dagger \rangle\), are measured. The index \(w\) indicates D- or extended S-wave pairing, and the pairing operator is given by \(\Delta_w^{ij} = \sum_{\alpha, \beta} \hat{c}_{i \alpha}^\dagger \sigma_{\alpha \beta} c_{j \beta} + \text{h.c.} = \Delta_w^{xy} + \Delta_w^{yx}\). To study the long distance behavior of the pairing correlations, results on \(N \times N\) (\(N = 8\) and 12), clusters are here presented. These results show that the D-wave correlations 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 \(\langle n \rangle = 0.75\) on a 12 × 12 cluster. The extended S-wave exhibits strong fluctuations, while the D-wave results are more robust and smoother. This shows that our SF-model captures the essence of hole pairing in AF backgrounds, where it is well known that \(d_{x^2-y^2}\) correlations dominate. Thus, from now on, we will concentrate only on the behavior of the D-wave pairing correlations (DPC).
FIG. 1. (a) D-wave (filled circles) and extended S-wave (open circles) 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) The long distance behavior of the correlations shown in (b), displayed in greater detail. (d) Correlations for $x=6$, as a function of density. (e) Same as (b) but with correlations measured parallel to the stripe-like charge inhomogeneities.

In Fig.1b we present the DPC versus distance (measured in the direction perpendicular to the stripe-like inhomogeneities) for several electronic 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 $\langle \Delta_i^x \rangle \sim 0.1$). At these densities expecting stronger pair correlations would be unrealistic, since the low carrier density as well as the previously extensively documented small quasiparticle weight $Z$ of holes in antiferromagnets suppresses the signal $\Delta_i^x$. 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, and they are even comparable to those reported in 2-leg ladders. The strongest correlations are observed at $\langle n \rangle \approx 0.75$, indicating the existence of an optimal doping as in real cuprates. This behavior can be observed in more detail in Fig.1c. In Fig.1d the DPC at distance $x=6$, is shown as a function of 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 that has nearly static stripes, can be qualitatively identified to the $x=1/8$ anomaly observed in the cuprates. The correlations in the direction parallel to the stripes are in Fig.1c and, surprisingly, they are about one order of magnitude smaller than those in Fig.1b. This is a remarkable general trend, and the reasons for this difference are discussed below.

Previous studies have shown that the system changes from an AF insulator to a metal upon doping 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.

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, while 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 the same parameters as in Fig.1b. Stripe-like inhomogeneities for all dopings are along the $x$ direction. (d) Magnetic structure factor along selected directions in momentum space for the same parameters as in part (c).

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 [1]. This inhomogeneous charge distribution produces a large peak at momentum \((0, \pi/3)\) in the charge structure factor \(N(q)\), shown in Fig.2c. It is also clear the nearly perfect AF order in the electron rich regions (white circles). The magnetic structure factor \(S(q)\), shown in Fig.2d, peaks at momentum \((\pi, 5\pi/6)\) in agreement with the AF order observed horizontally and the incommensurability induced vertically by the stripes, which carry a \(\pi\)-shift across them.

The results in Figs.1b,e are averages over MC time, and also over all the sites of the lattice. Measurements done directly on the individual snapshots were found to be similar to the averages, and indicate that the pair correlations are weaken along the AF regions. An intermediate value is obtained along the hole-rich stripes, but the largest correlation is observed along the direction perpendicular to the stripes (see 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 Fig.1b and 1e, the DPC functions are one order of magnitude larger in the direction perpendicular to the stripes than in the parallel direction. Note also that there is a substantial difference in the DPC perpendicular to the stripes corresponding to the densities 0.68 and 0.85 here analyzed. 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 regions parallel to the stripes, with an average local density of \(\sim 0.78\), are very weak. We believe that the AF order is 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 \(\sim 0.63\). However, the strongest correlations, indicated by triangles, occur, once again, along the direction perpendicular to the stripes. Along this direction the 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.

![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 \(\sim 0.97\). The filled squares are correlations along row 3, which has an average local charge \(\sim 0.67\). 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 \(\sim 0.78\). The filled squares are correlations along row 8, which has a local charge \(\sim 0.63\), and the triangles are correlations in the direction perpendicular to the stripes starting from row 6.](image)

![FIG. 4. (a) Representative snapshot of the spin and charge degrees of freedom on a 12 \times 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.](image)
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 \langle n \rangle (Fig.2c). The magnetic incommensurability, on the other hand, exhibits a very sharp peak at (\pi, 2\pi/3) (Fig.2d). As observed in Fig.1b, the 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 c. 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 \langle n \rangle (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 to be crucial for the development of robust DPC, at least within the SF-model. Although \langle n \rangle seems nearly featureless in the regime with the strongest pairing, the states are not homogeneous, as observed from the MC snapshots. In fact studies performed by us in the non-interacting system show that when the charge is uniformly distributed, the magnetic structure factor is featureless, and the DPC present strong fluctuations and are suppressed [12].

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, we present the DPC perpendicular to the charge inhomogeneities for \langle n \rangle = 0.75 on an 8 × 8 and a 12 × 12 cluster. 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 said above, are observed only in the larger cluster.

Summarizing, we have found evidence of robust D-wave pairing correlations in a doped SF-model, with a charge inhomogeneous ground state. Our results indicate that static AF order and D-wave pairing compete. The latter is enhanced when AF is replaced by magnetic incommensurability. Static, stripe-like charge inhomogeneities, only decrease 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" one. In addition, the hole attraction strength caused by antiferromagnetism should be maximized near half-filling, where two holes form a bound state in, e.g., the t-J model [4]. 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. [14], which provide evidence that SC can coexist with static stripe order in La_{1.6-x}Nd_{0.4}Sr_xCuO_4. However, when this coexistence is observed, T_c is at a minimum indicating 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 LSCO. In this situation, magnetic incommensurability manifest clearly as a peak in the magnetic structure factor, while \langle n \rangle is almost featureless. This is similar to the behavior observed with neutron scattering in high T_c cuprates [11].

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