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Indications of spin-charge separation in the two-dimensional extended *t-J* model

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The two-dimensional extended t-J model is studied computationally in a broad region of parameter space, motivated by recent photoemission experiments for the undoped cuprate $Ca_2CuO_2Cl_2$ [F. Ronning *et al.*, Science **282**, 2067 (1998)]. The one-hole ground state is shown to develop robust antiferromagnetic (AF) correlations between spins separated by the mobile hole (i.e., across the hole). This effect tends to decouple charge from spin, and the quasiparticle weight becomes negligible, particularly at momenta $(0,\pi)-(\pi,0)$. Studies with more holes show precursors of metallic stripe formation, with holes sharing their individual spin arrangements, and AF correlations generated across the stripe. [S0163-1829(99)51230-7]

Electronic strong correlations are widely believed to be crucial for the explanation of the anomalous properties of high-temperature superconductors. Several aspects of the cuprate phenomenology are indeed contained in the two-dimensional (2D) t-J model, including tendencies towards d-wave pairing upon hole doping. However, angle-resolved photoemission (ARPES) studies by Wells *et al.*[1] on the insulating compound $Sr_2CuO_2Cl_2$ revealed important discrepancies between experimental data and t-J model predictions[2] near momenta $\mathbf{k}=(\pi,0)-(0,\pi)$, of relevance for the doped cuprates. Moreover, recent ARPES experiments by Ronning *et al.*[3] for $Ca_2CuO_2Cl_2$ reported indications of a hole dispersion with $d_{x^2-y^2}$ characteristics even in such an undoped compound, a remarkable and unexpected result. Clearly the one-hole case must be better understood before addressing a finite hole density.

In addition, 2D t-J model studies have not been able to stabilize the metallic stripes proposed as an explanation of neutron-scattering experiments, with individual stripes affecting only one CuO chain with hole density $n=0.5$.[4] Instead, a pattern with stripes involving two adjacent chains has emerged using the density matrix renormalization group method with suitable boundary conditions.[5] Since the study of stripes in the 2D t-J model seems a subtle problem, it is important to develop new scenarios to generate metallic stripes upon doping to guide the interpretation of experimental results. With a similar motivation, Laughlin[6] recently argued for the possible existence of a new, but still unknown, fixed point in an extended parameter space that could influence the behavior of holes in antiferromagnets. Observing a new fixed point is potentially important for a proper analysis of the cuprates.

To search for theories beyond those currently available, a systematic analysis of the ''extended'' t-J model should be carried out. In this model, next-nearest-neighbor (NNN) hopping terms at distances $\sqrt{2}a$ (t') and $2a$ (t'') are added to the standard t-J model, which only contains a nearest neighbor amplitude t (a is the lattice spacing). The importance of NNN hoppings to reproduce ARPES results was discussed by Nazarenko *et al.*,[7] Belinicher *et al.*,[8] Eder *et al.*,[9] and Kim *et al.*,[10] and addressed by other groups.[11] Tohyama *et al.* also remarked on the importance of NNN amplitudes.[12] The optimal values of t'/t, and t''/t (-0.35 and 0.25, respectively[9]) are compatible with band structure calculations.[13] It is currently accepted that the extended t-J model produces a quasiparticle dispersion in excellent agreement with ARPES data. However, intuition is still lacking on the effect of t' and t'' on the behavior of holes.

The main motivation of this paper is to contribute to the clarification of the physics contained in the 2D extended t-J model at low hole density. Pursuing such a goal, several surprises have been found. The most interesting is the stabilization by NNN hoppings of a dynamically generated complex structure around mobile holes containing robust antiferromagnetic (AF) correlations ''across the hole'' (AH) [Fig. 1(a)]. Similar correlations were noticed in the standard t-J model on ladders[14] and using small clusters with NNN hoppings.[15] However, the physical origin of the AH correlations, the full spin arrangement around the hole, and especially its consequences, remain to be identified. In particular, due to the AH structure here it is argued that the vicinity of the hole carries a small spin, correlated with a tiny quasiparticle (q.p.) weight Z in the one-particle spectral function, particularly at $\mathbf{k}=(\pi,0)-(0,\pi)$. This is suggestive of spin-charge separation in two dimensions, at least at short distances, a phenomenon searched for since the early proposals of high-T_c theories. The present results suggest that this effect may be relevant at the couplings currently believed to be realistic for the cuprates.

Our analysis starts with the observation that the one-hole ground-state q.p. weight Z in the t-J model vanishes only in the limit when $J/t\rightarrow 0$ since the size of the spin-1/2 spin-polaron around the hole, regulated by string excitations, diverges as $J\rightarrow 0$.[2] However, even at $J/t=0$ a state with vanishing Z is not obtained since in this limit the one-hole

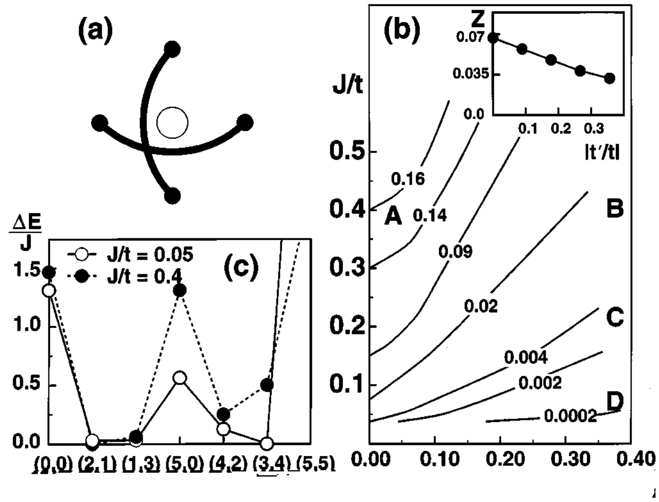

FIG. 1. (a) Schematic representation of the AF bonds across the hole (solid lines) of the extended t-J model. Shown are five sites, with the hole at the center; (b) lines of constant Z corresponding to momentum $(\pi,0)$, obtained using a 20-sites cluster with one hole, a grid of 16 points in parameter space, and smooth interpolations among them, providing sufficient accuracy for our qualitative discussion. t'/t'' is fixed to -1.4. Points A, B, C, and D are mentioned in the text (B corresponds to the currently accepted coupling for the cuprates). In the inset, Z for an 18-site cluster and $\mathbf{k}=(\pi/3,\pi/3)$ is shown vs $|t'/t|$, at $J/t=0.125$; (c) energy of a hole on a 20-sites cluster for the available momenta, relative to the one-hole ground-state energy. $t'/t=-0.35$, $t''/t=+0.25$ and J/t's are indicated. The momenta are in units of $\pi/5$.

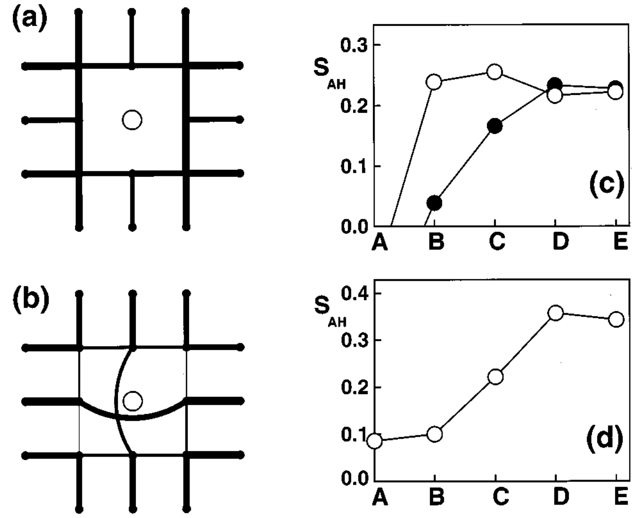

FIG. 2. Spin correlations in the mobile hole reference frame obtained using a 20-sites cluster with one hole, and $\mathbf{k}=(\pi,0)$. (a) corresponds to $J/t=0.4$ and $t'=t''=0$, while (b) is for $J/t=0.2$, $t'/t=-0.35$, and $t''/t=+0.25$. The width of the lines is proportional to the strength of the AF bonds. Only AF correlations at distances a and $2a$ are shown; (c) the strength of the AF correlation across-the-hole $S_{\rm AH}$ for the ground state of one hole on a 20-sites cluster with $\mathbf{k}=(\pi,0)$. A positive (negative) result represents an AF (FM) correlation. Shown are data in the x direction (open) and y direction (full). The points A,B,C,D [Fig. 1(b)] and E correspond to ($J/t=0.4, t'/t=0.0, t''/t=0.0$), $(0.4,-0.35,+0.25)$, $(0.2,-0.35,+0.25)$, $(0.05,-0.35,+0.25)$, and $(0.05,-1,+1)$, respectively; (d) same as (c) but on an 18-sites cluster with $\mathbf{k}=(\pi/3,\pi/3)$. Here x and y directions are equivalent.

ground-state becomes ferromagnetic (FM) due to the Nagaoka mechanism. However, additional hole-hopping terms may stabilize a more exotic ground state since the extra hole mobility can scramble severely the spin background near the hole, avoiding the localizing tendencies of the string excitations.

To analyze such a possibility, Z has been calculated in the extended t-J model. Results are shown in Fig. 1(b), using exact diagonalization (ED) techniques on 18- and 20-sites clusters.[2] The ratio t'/t'' was fixed to -1.4 in most of our study, as suggested by fits of ARPES dispersions for $Sr_2CuO_2Cl_2$.[9] From Fig. 1(b) it is clear that adding amplitudes $t'/t<0$ and $t''/t>0$ drastically reduces Z at $\mathbf{k}=(\pi,0)$, making it virtually negligible in large regions of parameter space. The inset of Fig. 1(b) shows that similar results are obtained close to $\mathbf{k}=(\pi/2,\pi/2)$, although the reduction of Z with increasing NNN hoppings is much stronger at $(\pi,0)$. The shape of the constant-Z lines seems mainly regulated by the strength of t' and t'' relative to J, reasonable since t is renormalized to J by AF fluctuations,[2] while t' and t'' are only partially renormalized since they connect same sublattice sites. Note that the region of very small J/t of the t-J model, hidden by the FM instability, is substantially expanded by the addition of NNN hoppings.

The remarkable isotropy around $(\pi/2,\pi/2)$ found in ARPES experiments[1,3] for $Sr_2CuO_2Cl_2$ is reproduced in the extended t-J model,[7–11] and Fig. 1(c) for a 20-sites lattice confirms that the four available momenta near $(\pi/2,\pi/2)$ indeed have lower energy than $(\pi,0)$, once the proper set of NNN hoppings[9] is used. However, Fig. 1(c) also shows that similar results are found at smaller couplings $J/t=0.05$, keeping the NNN hoppings the same.[16] This suggests that a quasi-isotropic dispersion around $(\pi/2,\pi/2)$ may exist in the broad parameter region with small Z. In this respect, points B, C, and D of Fig. 1(b) share similar properties, different from the traditionally studied regime of point A. This will be a recurrent conclusion of the results analyzed below.

To understand the drastic reduction of Z after adding NNN hoppings, consider in Figs. 2(a) and 2(b) the spin correlations in the hole reference frame. Shown are results for a 20-sites cluster exactly solved and momentum $(\pi,0)$, of importance for the cuprates. Results are presented for points A and C of Fig. 1(b). Similar results have been obtained using the optimized reduced basis approximation technique[17] on clusters of size 4×8 with 1.5×10^6 states, and also with ED on 16-sites clusters, suggesting that finite-size effects are small. Figure 2(a) shows that in the absence of NNN hoppings the spin correlations present simple AF tendencies.[18] The hole carries a spin cloud and Z is finite.[2] However, including extra hoppings the spin correlations are qualitatively different [Fig. 2(b)]. Note the presence of AF correlations across the hole, in both directions. The hole motion induces a coupling between sites of the same sublattice. It is important to note that the across-the-hole AF bond is not isolated but it is supplemented in both directions by other robust AF bonds resembling dynamically generated 1D Heisenberg segments along each axis [Fig. 2(b)], individually weakly coupled to the rest of the spins. Figures 2(c) and 2(d) show the strength of the AH bond at several points in parameter space. Comparing with Fig. 1(b), it is apparent that the stronger those correlations are, the weaker Z is.

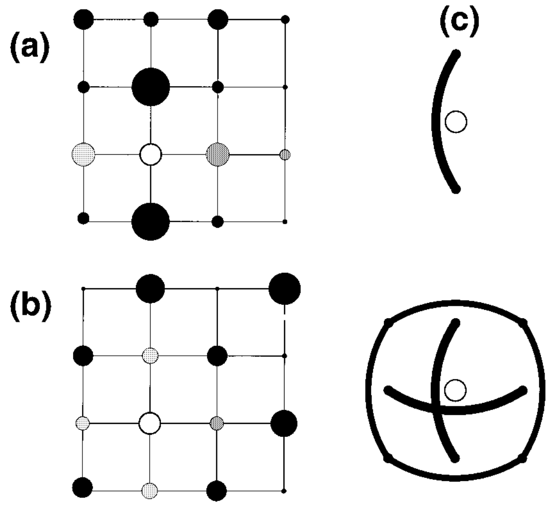

FIG. 3. (a) $\langle S_i^z \rangle$ around a mobile hole (open circle) on a 4×4 cluster with one hole, total spin z projection $+1/2$, $J/t=0.4$, $t'=t''=0$, and $\mathbf{k}=(\pi,0)$. The area of the circles is proportional to $\langle S_i^z \rangle$. The gray circles denote a negative $\langle S_i^z \rangle$; (b) Same as (a) but for $J/t=0.1$, $t'=-t''=-t$; (c) schematic representation of the 3- and 9-site clusters mentioned in the text, the latter at $J/t=0.1$, $t'/t=-0.35$ and $t''/t=0.25$. The hole is at the center and the solid lines represent the ground-state dominant AF bonds, which are stable in a broad region of parameter space.

The robust AF correlations among pairs of spins near the hole suggest that the total spin 1/2 of the one-hole problem, defined on an even number of sites cluster, may not be located near the hole. This can be analyzed by calculating the local spin $\langle S_i^z \rangle$ at site i in the mobile hole reference frame, with the overall constraint $\Sigma_i \langle S_i^z \rangle = 1/2$. At $J/t=0.4$ and $t'=t''=0$, Fig. 3(a) shows $\langle S_i^z \rangle$ around the mobile hole for $\mathbf{k}=(\pi,0)$. Here the spin distribution is nontrivial and some results are even negative along the direction of movement of the hole. However, the large spin next to the hole along the y axis suggests that spin and charge are bounded. On the other hand, at $J/t=0.1$ and $t'=-t''=-t$ [Fig. 3(b)], here shown as an extreme but illustrative example, $\langle S_i^z \rangle$ is considerably more spread than in Fig. 3(a). A robust AH-spin arrangement near the hole appears correlated with local spin-charge separation tendencies, which is intuitively reasonable.

To gain insight into the AH state, consider first just three sites in an open chain, containing one hole, one spin up and one down (six states). Since J is not crucial in this analysis simply use $J=0$, and allow for the hole to move at distance a $(2a)$ with amplitude t (t''). Two eigenstates are in competition for the ground state. One has FM correlations (Nagaoka state) and the lowest energy for $t''<0$. However, if $t''>0$ a spin-singlet state with energy $E=\frac{1}{2}[-t''-\sqrt{(t'')^2+8t^2}]$ is stabilized [Fig. 3(c)]. The spin-singlet nature of this state leads in a natural way to AH bonds. Then, the extra $t'<0$ and $t''>0$ hoppings have the important role of favoring the singlet state over the competing FM state.[19,20]

Further semiquantitative insight can be gained from the analysis of a 9-sites cluster with open boundary conditions [Fig. 3(c)]. Here there are 630 states in the zero total-S^z subspace, and characteristics already similar to those found in the numerical analysis of Figs. 2(a) and 2(b) were observed in its solution. The ground state of this small cluster is dominated by a hole at the center, in a large region of parameter space. The similarities of the ground-state correlations on 9-sites and larger clusters suggest, once again, that the effects discussed here are mainly local in space and they can be observed in simple toy models.

Qualitative understanding of the AH-state formation can be obtained from the 1D-Hubbard model at $U/t=\infty$.[21] In this limit holes and spins fully decouple and the wave function in the spin sector corresponds to that of a 1D Heisenberg chain involving all spins, as if the holes were absent from the problem. In other words, a state such as $|\cdots+-+-0+-+0-+\cdots\rangle$, with AF bonds across the holes, has an important weight in the ground state. Explicit calculations performed as part of this effort have indeed shown that the 1D t-J-t'-t'' model presents AH bonds quite similar to those in Fig. 2(b). However, if a similar procedure is attempted in 2D, i.e., the effective removal of the hole from the system by linking the two vertical and horizontal neighboring spins with a Heisenberg coupling J, frustration cannot be avoided. Then, a straightforward generalization to 2D of the 1D results is expected to fail. However, the numerical results shown here lead us to suggest that a compromise can be found between the tendencies to produce a charge-spin decoupling and the frustration that prevents it. This can be achieved by creating 1D-like spin arrangements in both directions, as shown in Fig. 2(b). Each of these dynamically generated ''chains'' individually resemble the results found in the 1D $U/t=\infty$ Hubbard model.[21] By this procedure, spin and charge can locally decouple in 2D, as suggested by the computational results.

The spin arrangement around the 2D hole at $\mathbf{k}=(\pi,0)$ reported here is different from previous alternatives discussed in the literature. Although averaging spin correlations around the hole would only indicate a reduction of antiferromagnetism in favor of a ''spin-liquid'' state, the spin arrangement in this region has more structure than a mere bubble of weakly interacting spins would have. In addition, while naively it may appear that the AH bond could be described as a spin-singlet formation in a short-range resonant-valence-bond (RVB) state, Fig. 2(b) shows that it is better to represent it as an AF-bond part of a 1D Heisenberg segment, an unexpected result in a 2D system. Note also that moving holes using NNN hoppings in a RVB state would tend to leave the ''length'' of the short spin singlets at just a, an effect opposite to what was reported here, namely, NNN hoppings were found to enhance the AH bonds. Then, the AH state represents a new paradigm for the visualization of the spin distortion around a hole in an AF background.

In Figs. 4(a)–4(c) results are shown for two holes at point B of Fig. 1(b), the realistic couplings for the cuprates. Figure 4(a) contains the spin arrangement for two holes on a 4×4 cluster with periodic boundary conditions (PBC) and at distance $2a$, obtained from the zero-momentum ground state using a suitable projector operator. With one hole at the origin, the most likely position for the second hole is precisely at distance $2a$, unlike for $t',t''=0$ which is dominated by distance a. The row where the holes are located is clearly different from the rest, resembling a 4×1 cluster with two holes. This suggests that holes tend to move in a 1D path with density 0.5. These 1D paths resemble metallic stripes, conceptually different from the insulating stripes with one

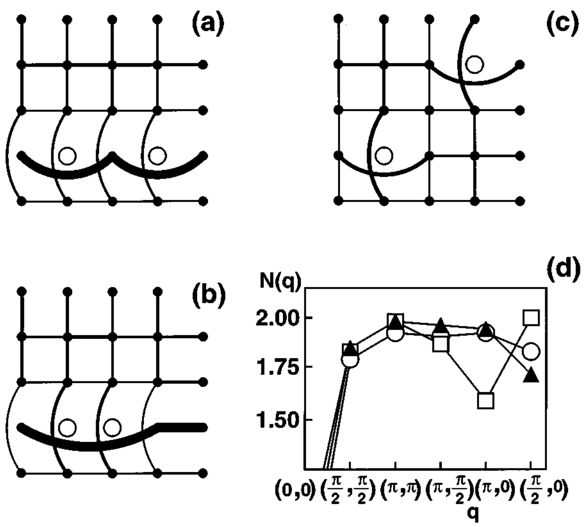

FIG. 4. (a) AF correlations corresponding to the 4×4 two-hole ground state with PBC and $J/t=0.4$, $t'/t=-0.35$, $t''/t=+0.25$, for the case when the mobile holes (open circles) are projected to be at distance $2a$ along the x axis. The bond width is proportional to the strength of the AF correlation. The horizontal AH-bond strength is close to a perfect singlet, but this is due to the boundary conditions on the 16-sites cluster. In the bulk, its strength is expected to be reduced roughly by a factor of 2; (b) same as (a) but with the holes at distance a; (c) same as (a) but with the holes at distance $2\sqrt{2}a$; (d) $N(q)$ for a two-holes 4×4 cluster. Squares, circles, and triangles are results for ($J/t=0.4$, $t'/t=0$, $t''/t=0$), (0.4,−0.35,0.25), and (0.1,−0.35,0.25), respectively.

hole per site found near the large J/t phase separated region of the standard t-J model when $1/r$ Coulomb interactions are added.[22] Figure 4(b) is a natural consequence of Fig. 4(a), when holes move using the hopping t. An interesting property of Figs. 4(a) and 4(b) is the arrangement of the spins not on the 4×1 stripe. They form robust AF bonds across the path of the two holes, as observed experimentally.[4] This effect is not present for holes with low mobility near phase separation, but in the context discussed here it is natural since it evolves from the AH bonds of individual holes. Figure 4(c) corresponds to holes not along a 1D path, carrying the surrounding environments of isolated holes. Figure 4(d) contains the Fourier transform of the charge correlations $N(q)$, enhanced at $(\pi,0)$ due to configurations Figs. 4(a) and 4(b). Calculations for four holes on 16 sites show patterns similar to those in Fig. 4. In particular, the configuration with holes forming a square of side $2a$ has a substantial weight in the ground state and contains two of the 1D-like paths of Fig. 4(a), running in each direction.

It is important to remark that for the standard t-J model with J/t between 0.1 and 0.5 and $t'=t''=0$ the correlations across the stripe are actually FM on the 16-sites cluster, although the spin correlation among the two spins of the two-holes 4×1 row is still AF and robust. The NNN hoppings are needed to stabilize a structure with characteristics similar to those observed in experiments.[4] Actually, results quantitatively similar to Figs. 4(a)–4(c) were obtained also at point C of Fig. 1(b), and even in an extreme case such as $J/t=0.1$, $t'=-t$, and $t''=t$.

Summarizing, here it has been reported that a mobile hole in the extended t-J model generates a complex spin arrangement in its vicinity containing AF bonds across the hole. This is correlated with a small Z and indications of spin-charge separation at $\mathbf{k}=(\pi,0)$. Further work will clarify the relevance of the one-hole AH bonds at finite hole density. However, studies of two and four holes on small clusters have already provided a glimpse of a possible new mechanism for metallic stripe formation, which does not rely on phase separation tendencies and it is operative at small J/t.

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