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Phase diagram of the two-dimensional t-J model at low doping

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The phase diagram of the planar t-J model at small hole doping is investigated by finite-size scaling of exact diagonalization data of $\sqrt{N}\times\sqrt{N}$ clusters ($N\leq 26$). Hole-droplet binding energies, compressibility, and static spin and charge correlations are calculated. Short-range antiferromagnetic correlations can produce attractive forces between holes leading to a very rich phase diagram including a liquid of d-wave hole pairs (for $J/t \gtrsim 0.2$), a liquid of hole droplets (quartets) for larger J/t ratios ($J/t \gtrsim 0.5$), and, at even larger coupling J/t, an instability towards phase separation.

Studying the behavior of holes in two-dimensionnal (2D) antiferromagnets is crucial to understand the origin of pairing in the high-T_c cuprate superconductors. In these materials chemical substitutions in the parent stoichiometric compound lead to injecting mobile holes in the CuO_2 antiferromagnetic planes. Besides transport properties these holes will also drastically affect the antiferromagnetic (AF) correlations in the planes. On the theoretical side, motion of holes in antiferromagnets can be simply described by the so-called t-J model,[1,2] a strong coupling version of the well-known Hubbard model. Previous numerical studies[3] have given reliable information, especially in the limit of a single hole. It is believed that holes behave like quasiparticles, at least at the bottom of the coherent band, although spin fluctuations strongly enhance their effective masses and reduce their quasiparticle weights.[4]

Finite-size scaling analysis becomes easier at commensurate densities such as $n = 1/2$ (quarter filling). In this case, exact diagonalizations (ED) studies of the t-J model[5] have suggested the existence of superconducting correlations in the vicinity of the phase separation phase.[6] This regime is however quite far from the experimental situation.

At small but finite doping (e.g., electron density $n \sim 0.8$–0.9) fewer theoretical results are known. However it is believed that this class of models reproduces successfully[7] the large Fermi surface observed in angular resolved photoemission studies in the metallic phase of doped high-T_c materials. In addition, possible observation of shadow bands due to strong short-range antiferromagnetic correlations has been suggested in both experimental[8] or theoretical studies.[9]

The magnetic coupling J can generate an effective coupling between holes. This is particularly clear in the (unphysical) large J/t regime where the magnetic energy cost is minimized by having holes sitting on nearest neighbor sites. In this regime, the uniform state becomes in fact unstable towards a phase separated state.[6] High temperature expansions[10] also predict phase separation for $J/t \gtrsim 1$. However, small cluster calculations have shown that for smaller and more realistic J/t ratios individual pairs could be stable.[11,12] Preliminary results[13] state that larger clusters of holes could also form in the intermediate parameter range. Other possible candidates in this parameter regime are nonuniform striped phases.[14,15]

In this work, more insights into the nature of the phase diagram at *small doping* are obtained from a detailed numerical study. Indeed, since analytic perturbation treatments are poorly controlled in the relevant physical regime, exact diagonalizations of small 2D square clusters by the Lanczos algorithm[16] were performed.[17] Studies in the regime of small finite hole densities are delicate since only different discrete values of the densities can be achieved on different clusters and interpolations between them then become necessary. First, finite-size scaling of binding energies of n-hole clusters provides an indication of the stability of liquids of pairs or droplets in the *vanishing* hole concentration regime. Hole-hole correlations obtained for $n \sim 0.85$ also confirm the stability of pairs at finite density even at small J/t ratios. The compressibility for arbitrary hole densities ($n \lesssim 0.8$) and various system sizes is calculated to perform an extrapolation to the thermodynamic limit. The domain of the phase separated region is then estimated. We also discuss the behavior of the static spin and charge structure factors at intermediate density $n \sim 0.85$.

The t-J model defined on a square lattice reads

$$H = t \sum_{\mathbf{x},\mathbf{y}\ N.N.} c^{\dagger}_{\mathbf{x},\sigma} c_{\mathbf{y},\sigma} + \frac{J}{2} \sum_{\mathbf{x},\mathbf{y}\ N.N.} \left(\mathbf{S_x}\cdot\mathbf{S_y} - \frac{n_{\mathbf{x}} n_{\mathbf{y}}}{4} \right),$$

where $c^{\dagger}_{\mathbf{x},\sigma}$ and $\mathbf{S_x}$ are creation and spin operators at site $\mathbf{x}$. Ground state (GS) energies and equal-time correlation functions in the GS are obtained on small $\sqrt{N}\times\sqrt{N}$ N-site clusters at low hole densities by the Lanczos method. Typically $N = 18$, 20, and 26.

Let us first consider a fixed finite number of holes $N_h = n$ ($N_h = 2$, 4) on various clusters of increasing sizes. These holes will form an n-particle bound state if the binding energy $\Delta_n = E_{h,n} + E_{h,0} - 2E_{h,n/2}$, where $E_{h,n}$ is the GS total energy for a system with $N_h = n$, converges towards a negative value in the limit of infinite system size. Strictly speaking such quantities give indications about the stability of n-particle bound states only in the limit of *vanishing* hole density.

A simple broken-bond counting argument shows that, at large J/t, two holes injected in the AF can minimize the local magnetic energy by forming a bound state. Finite-size scaling has shown[11] that this picture is actually correct even down to $J = J_{B,2} \simeq 0.2$. Δ_2 calculated for $N = 26$ is shown in Fig. 1 and becomes negative when the paired state is stable. The hole-hole pair has a $d_{x^2-y^2}$ orbital symmetry. Figure 2(a) shows the hole-hole density correlations of the pair $C_h(\mathbf{r}) = \frac{N}{N_h(N_h-1)}\langle n_h(\mathbf{r})n_h(0)\rangle$ for all possible distances ($\mathbf{r} \neq 0$) between the holes compatible with the cluster shape. Note that the normalization factor is chosen so that $\sum_{\mathbf{r}\neq 0} C_h(\mathbf{r}) = 1$. Correlations at the intermediate distance of $\sqrt{2}$, i.e., when the holes stay across the diagonal of a plaquette on the *same sublattice*, are dominant.[12] This singlet hole pair can in fact be viewed as a combination of a triplet pair with a nearby spin triplet excitation.[12] The two-hole GS exhibits flux quantization in a ring in units of $hc/2e$,[18] also a signature of a paired state. Last, pair formation is also consistent with the observation that the dynamical response of the d-wave pair creation operator exhibits on small clusters a sharp δ peak of weight $Z_{2h} \propto J/t$ down to small values of J/t.[11]

We now consider the possibility of larger droplets of holes. Indeed, above $J_{B,2}$ residual interactions between pairs might be sufficiently attractive to stabilize, e.g., hole quartets. GS energies of four-holes can be calculated for the three possible orbital symmetries (s, p, or d wave) of the wave function (with zero total momentum). The lowest energy is obtained in the s-wave channel. In order to estimate the onset of clustering Δ_4 has been evaluated on various lattices of size up to $N = 26$ and the data are displayed in Fig. 1. Note that the critical value $J_{B,4}$ at which Δ_4 changes sign depends weakly on the system size while the slope $|\partial\Delta_4/\partial J|$ at this point decreases for increasing size. Existence of droplets was also suggested from the study of four-point hole density correlations on smaller systems.[19]

Figure 1 then strongly suggests that when $J/t \in [J/t|_{B,2}, J/t|_{B,4}]$ with $J/t|_{B,2} \sim 0.2$ and $J/t|_{B,4} \sim 0.5$ individual hole pairs exist without forming larger clusters. This result based on a scaling of Δ_n is, strictly speaking, only valid in the limit of vanishing hole density. In order to investigate the stability of the pairs at finite doping we have calculated the hole-hole correlations $C_h(\mathbf{r})$ in a 26-site cluster at density $n \sim 0.85$ (i.e., with four holes). The results shown in Fig. 2(b) for various separations $|\mathbf{r}|$ reveal dominant correlations at distance $\sqrt{2}$ as in the case of a single pair [see Fig. 2(a)]. Note also that the density correlations at the largest distances available in the cluster always remain significant in this parameter regime which is consistent with the existence of separate

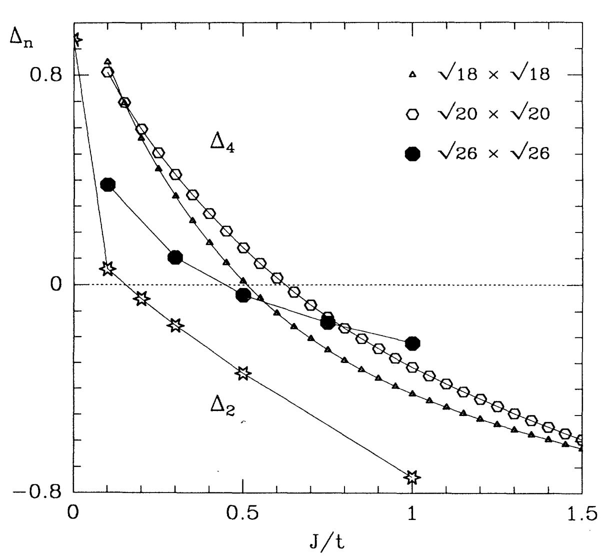

FIG. 1. Binding energy Δ_4 vs J for clusters of 18, 20, and 26 sites. The 26-site cluster hole-hole binding energy Δ_2 is also indicated by open stars.

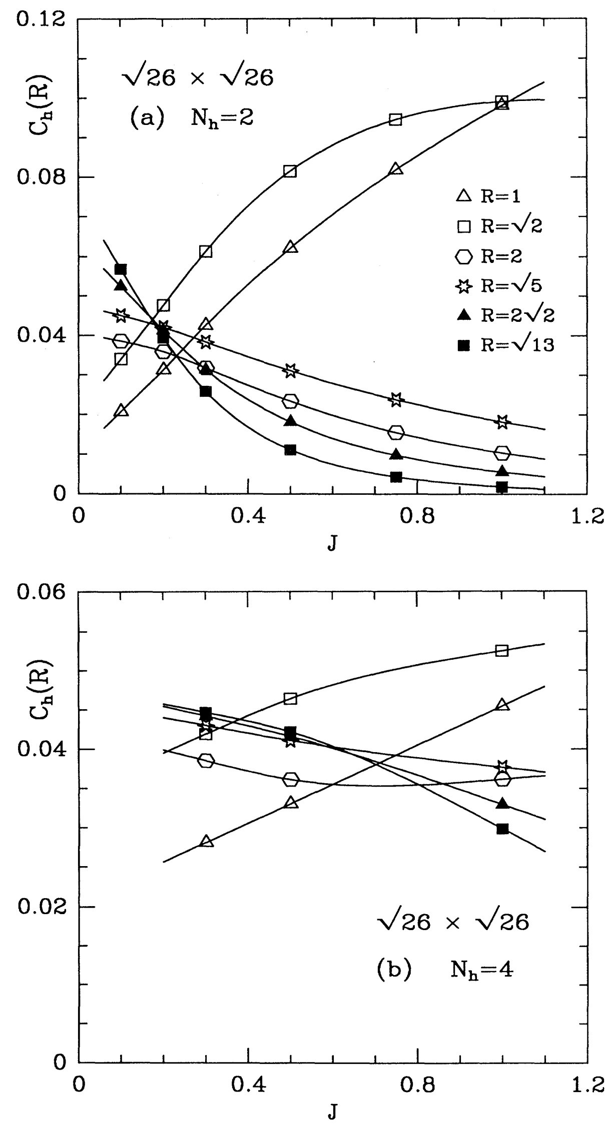

FIG. 2. Hole-hole correlation function for various hole separation vs J/t obtained on a 26-site cluster with two (a) and four (b) holes. The various symbols associated to the allowed distances are indicated on the figure.

pairs in the cluster. The data shown in Fig. 2 are in qualitative agreement with previous data obtained on smaller systems[20] giving credibility to small cluster calculations.

Formation of droplets should not be confused with phase separation (PS) between hole-free and hole-rich phases even though both phenomena have the same microscopic origin. The issue of phase separation can be addressed by studying the inverse compressibility κ^{-1} defined by $\kappa^{-1} = \partial^2(E_{h,n}/N)/\partial n_h^2$. In a uniform system κ^{-1} is finite and positive. On finite clusters $\kappa^{-1} < 0$ signals the instability of the homogeneous phase. However, we stress that a rigorous determination of the PS region can only be achieved by a finite-size scaling at *constant hole density*. Such a study is attempted in Figs. 3(a) and 3(b) showing the GS energy per site vs hole density n_h for two different system sizes. The thermodynamic limit is obtained in two steps: (i) an interpolation between data points at constant cluster size and (ii) an extrapolation at constant hole density assuming $N^{-3/2}$ finite-size corrections. We have checked by considering other system sizes (data not shown for clarity) that such an $N^{-3/2}$ behavior is actually very well satisfied provided that $J \gtrsim n_h t$. For $J \gtrsim 1$ it is clear that the PS region extends from $n_h = 0$ to $n_h \simeq 0.12$. For smaller values of J $|\kappa^{-1}|$ quickly becomes very small and we can assume that there is no sign of PS for $J/t < 0.75$ (Ref. 21) consistently with the results obtained by high temperature expansions.[10] Our results then suggest that a liquid of hole quartets is sta-

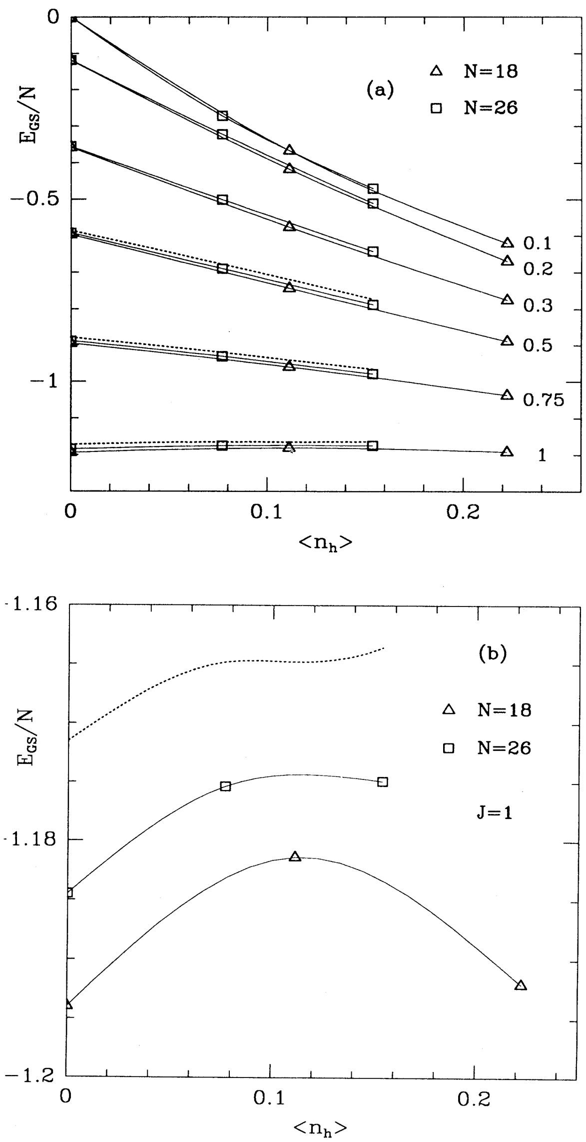

FIG. 3. (a) Energy per site vs hole density for 18 and 26 site clusters and various J/t values (indicated on the plot). Continuous lines are interpolations between data points corresponding to the same system sizes. Extrapolation to the thermodynamic limit are indicated by dotted lines. (b) Data for $J/t = 1$ only shown on an enlarged scale.

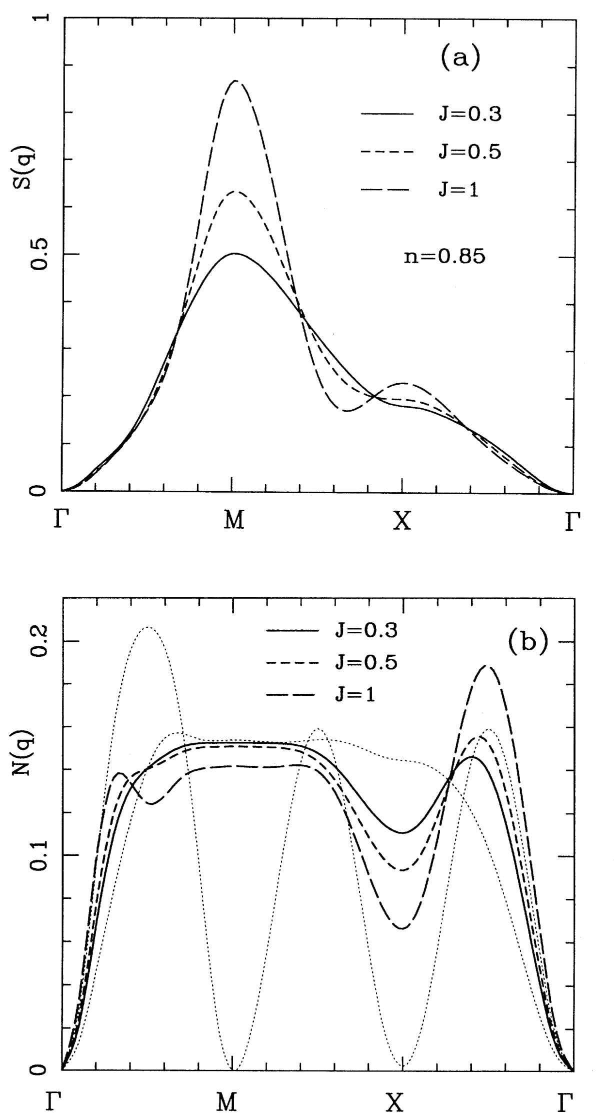

FIG. 4. Static spin (a) and charge (b) structure factors $S(\mathbf{q})$ and $N(\mathbf{q})$ along symmetry lines of the Brillouin zone for various J/t ratios as indicated on the plot. Γ, M, and X correspond to $(0,0)$, (π,π), and $(\pi,0)$, respectively. In (b) the dotted thin lines are obtained assuming the N_h holes behave as noninteracting spinless fermions with various dispersion relations (see text).

ble in a small region of the phase diagram, as a precursor of the PS instability line. This should be contrasted to the small *electron* density case where the gas of electron quartets is never stable.[22]

We finish this study by the investigation of the static spin and charge structure factors defined by $S(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{r}} \langle S_z(\mathbf{r})S_z(0)\rangle e^{i\mathbf{q}\cdot\mathbf{r}}$ and $N(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{r}} \left[\langle n_h(\mathbf{r})n_h(0)\rangle - n_h^2\right] e^{i\mathbf{q}\cdot\mathbf{r}}$, respectively. Our data are complementary to the data obtained in the thermodynamic limit but at finite temperature by Puttika *et al.*[23] The data obtained for $N = 26$ with a density of $n \sim 0.85$ (four holes) are shown in Figs. 4(a) and 4(b). A smooth interpolation between the discrete $\mathbf{q}$ points of the reciprocal lattice of the 26-site cluster has been performed assuming that the correlations in real space remain small at distances larger than the cluster size. $S(\mathbf{q})$ in Fig. 4(a) shows a pronounced peak at (π,π) even for small values of J. This indicates that large commensurate antiferromagnetic spin correlations ($\xi_{\rm AF} \sim 3$) still survive for hole doping as large as 15%. $N(\mathbf{q})$ shown in Fig. 4(b) exhibits along the Γ-M line a behavior very similar to noninteracting spinless fermions with nearest neighbor hopping (dotted line). However, a clear dip is observed at X. This behavior cannot be explained by a simple Fermi surface effect. For example, a different tight-binding spinless model whose dispersion has a minimum at Σ [momentum $(\pi/2,\pi/2)$] would give much more structure than observed (other dotted line). We interpret the dip at X as the signature of strong short-range correlations between holes characteristic of the paired state.

We conclude this paper by suggesting a possible phase diagram in Fig. 5 based on the results discussed above. When J exceeds some critical values $J_{B,2}$ and $J_{B,4}$ holes injected into the antiferromagnetic phase form a liquid of d-wave pairs and a liquid of quartets (D), respectively. At larger J/t ratios the t-J model phase separates (PS). Also note the existence of a ferromagnetic region (F) at very small J as predicted by high temperature expansions[24] or ED.[25] Two crucial issues still remain to be addressed, namely the exact nature of the normal paramagnetic phase (P) and possible pair-pair correlations (superconductivity) in the pair liquid phase.

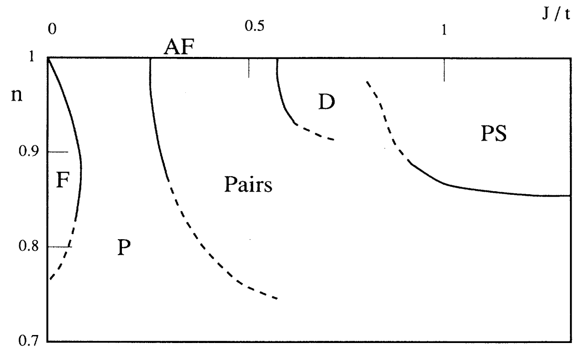

FIG. 5. Schematic picture of the J/t-n phase diagram.

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