Phase separation and pairing in coupled chains and planes

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Abstract

A generalization of the $t-J$ model in a system of two coupled chains or planes is studied by numerical diagonalization of small clusters. In particular, the effect of density fluctuations between these one- or two-dimensional coupled layers on intralayer phase separation and pairing is analyzed. The most robust signals of superconductivity are found at quarter filling for couplings just before the fully interlayer phase separated regime. The possibility of an enhancement of the intralayer superconducting pairing correlations by the interlayer couplings is investigated.
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High-T$_c$ superconductors$^1$ have a layered structure consisting of Cu-O layers and some other intermediate layers. While it is widely believed that the pairing takes place within Cu-O layers, it is also well known that the critical temperature depends also on the number of these layers per unit cell and on the distance between them.$^2$ Consequently, since the early days of high-T$_c$ superconductivity, there have been attempts to include these two features in a consistent theoretical framework.$^3$

One of the simplest models proposed to describe Cu-O planes in high-T$_c$ superconductors is the two-dimensional $t$–$J$ model.$^4$ This model gives results in reasonable agreement with experiments for many of the magnetic and electronic properties of these materials.$^5$ Numerical studies have also given indications of pairing in the $d_{x^2−y^2}$ mode in some regions of the parameter space,$^6,^7$ although in general, and especially for the physically relevant region of parameters, these indications are not the strong signals we would expect that correspond to high-T$_c$ superconductivity. This somewhat negative behavior has led some authors to think that there is an important feature which is missing in this model. Since there is a relation between the number of planes and the value of the critical temperature, it is natural to ask if the $t$–$J$ model could be generalized to include the coupling between Cu-O layers.

Another important property that characterizes the phase diagram of the $t$–$J$ model is the property of phase separation (PS).$^8$ For sufficiently large values of $J/t$ the system undergoes a separation of two phases: a hole-rich phase and an electron-rich phase. This phase separation is driven by the same force that also gives rise to
pairing, which is a necessary condition for superconductivity. It is possible that just before phase separation, density fluctuations could enhance pairing leading to superconductivity. This scenario has been confirmed in at least two situations: the $t - J - V$ model, where $V$ is a repulsive interaction between holes in nearest-neighbor sites,$^9,10$ and the two-dimensional (2d) $t - J$ model close to quarter filling.$^6$ Another case we could add to this list is the one-dimensional (1d) $t - J$ model for $J/t$ larger than 2 (the “supersymmetric” point).$^{11}$ In a more general study, Emery and Kivelson$^{12}$ suggested that the property of phase separation could account for some of the “anomalous” properties that characterize the normal state of high-$T_c$ superconductors.

In this sense, the first motivation for this work is to study how interlayer coupling affects pairing correlations and phase separation in the $t - J$ model in a system of two coupled layers. In general, we refer to chains or planes as one- or two-dimensional “layers”, respectively.

However, if the number of particles and total magnetization is kept fixed for the whole system of coupled layers, a new important feature appears. It is natural to assume that by symmetry there is an equal number of holes on each chain or plane. However, this is only true on average. As it is shown below, in many cases it is energetically possible that there are fluctuations in the density of holes between the two parts of the system. In this case, snapshots of the system would show that there are different numbers of holes on each of the layers. We call this situation “interlayer phase-separated regime”. This regime first appears in the absence of transversal
couplings, and in this case it is quite easy to understand its origin.

The main purpose of this work then is to study how the interlayer PS evolves when transversal couplings are switched on, and to study the interplay between this type of phase separation with the intralayer PS and with intralayer pairing of holes. In particular, we are interested in investigating previous ideas about the relation of phase separation and superconductivity\(^{12}\) taking into account this new source of density fluctuations.

For that purpose, we have used Lanczos techniques to calculate the ground state in finite clusters. Most of the results reported in this work refer to coupled chains because in this case we can study correlations at larger distances than in the case of coupled planes, and then we expect to reduce finite size effects. Moreover, as can be seen below, most of the properties studied show a very similar behavior for coupled one- and two-dimensional layers.

The \(t - J\) model for the two-layer system is defined by the Hamiltonian:

\[
H = -t_\parallel \sum_{<ij>,\alpha,\sigma} \left( \tilde{c}_{\alpha,i,\sigma}^\dagger \tilde{c}_{\alpha,j,\sigma} + \tilde{c}_{\alpha,j,\sigma}^\dagger \tilde{c}_{\alpha,i,\sigma} \right) + J_\parallel \sum_{<ij>} (\mathbf{S}_{\alpha,i} \cdot \mathbf{S}_{\alpha,j} - \frac{1}{4} n_{\alpha,i} n_{\alpha,j}) \]

\[
- t_\perp \sum_{i,\sigma} \left( \tilde{c}_{1,i,\sigma}^\dagger \tilde{c}_{2,i,\sigma} + \tilde{c}_{2,i,\sigma}^\dagger \tilde{c}_{1,i,\sigma} \right) + J_\perp \sum_{i} (\mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i} - \frac{1}{4} n_{1,i} n_{2,i}),
\]

where the notation is standard. The label \(\alpha = 1, 2\) indicates the two layers of the system. The couplings \((t_\parallel, J_\parallel)\) refer to the intralayer interactions, while \((t_\perp, J_\perp)\) are the interlayer coupling constants. In the case of two coupled chains, most of our results
are for the 8 sites chain with periodic boundary conditions. In the case of coupled planes, we have considered for each plane the tilted cluster denoted as $\sqrt{8} \times \sqrt{8}$. The total number of sites in both lattices is $N_s = 16$. For each hole density, $x = N_h/N_s$ ($N_h$ : number of holes), we have considered $t_\perp = 0.0, 0.2, 0.4, 0.6, 0.8, \text{ and } 1.0$. As usual, we adopt $t_\parallel = 1$. For each $t_\perp$, we have taken $J_\perp = J_\parallel \times t_\perp^2/t_\parallel^2$, and $J_\parallel$ remains as a free parameter.

This relation between $J_\perp, J_\parallel, t_\perp$, and $t_\parallel$ is the one that would appear from the reduction of the one- or three-band Hubbard model to an effective $t - J$ model, in the limit of strong Coulomb repulsion in the copper sites. However, we are going to consider values of $J_\perp, J_\parallel >> t_\parallel, t_\perp$, i.e. beyond the range of validity of such construction. The main reason to adopt that relation is to recover the isotropic situation when $t_\perp = 1$. Presumably a value of $J_\perp$ constant and eventually equal to zero should be considered.

This model has been numerically examined before for the case $J_\perp = 0$ although for rather smaller lattices. In that study, it was found that intralayer superconducting correlations are enhanced by $t_\perp$. In the present study we obtain different results, as discussed below.

The fluctuations of hole density between layers or interlayer phase separation are easy to understand in the case of the uncoupled $t_\perp = 0$ limit. In this case we can study larger clusters in order to avoid possible finite size effects. Let us consider the case of two $4 \times 4$ planes with a total number of 16 holes (quarter filling).
For $J_{\parallel} = 0$, the ground state of the total system consists of the product of the ground state of each plane with 8 holes each, i.e. the total energy is $E(J_{\parallel} = 0) = E_1^{(8)} + E_2^{(8)} = 2 \times (-14.3475)$. In this case there are no density fluctuations and we call this regime an interlayer homogeneous regime. Now, for $E(J_{\parallel} = 2)$, the ground state consists of two parts: one which is a product of the ground state in one plane with 6 holes and the ground state on the other plane with 10 holes, and the other in which the number of holes in the two planes are interchanged. In this case, $E(J_{\parallel} = 2) = E_1^{(6)} + E_2^{(10)} = -26.0627 + (-17.4066) < 2 \times E_1^{(8)} = 2 \times (-21.6386)$. In the same way, at $J_{\parallel} \geq 3$, the system jumps back and forth between the state in which one layer is empty and the other is at half-filling and the state where these occupancies are interchanged. It is worth noting that for $J \approx 3.5$, at quarter filling, a previous study\textsuperscript{6} found the peak of the pairing susceptibility with long-range pairing correlations in the $4 \times 4$ cluster. We see now that for two coupled $4 \times 4$ planes, this density is not stable at this value of $J$. Similar behavior is also found for two chains of 16 sites each in the $t_{\perp} = 0$ case, and for various fillings.\textsuperscript{18}

To study these interlayer density fluctuations, the natural order parameter is then

$$f_d(J_{\parallel}, t_{\perp}, x) = < N_1^2 > - < N_1 >^2,$$

where $N_1$ is the hole number operator for one of the layers, and $< N_1 >= N_h/2$ by symmetry. This order parameter varies between zero, which corresponds to the interlayer homogeneous state, and a number which depends on the number of sites and on the number of holes, which corresponds to the fully phase-separated interlayer regime. The same information is given by the sum of
the hole-hole correlations over the sites of one layer.

The second property we are interested in measuring is the intralayer PS. There are several ways to measure this property. For the case of coupled chains, we have computed a very direct measure of the clustering of holes defined as \( X = S(2\pi/L) \), where \( S \) is the Fourier transform of the hole-hole correlations along one chain and \( L \) is the chain length. This quantity varies between zero (even number of holes) for the homogeneous phase, and a positive number which can be calculated analytically when the holes are clustered together. This definition of \( X \) can be extended to 2d.

To study superconductivity, we compute the pairing correlations:

\[
C(j) = \frac{1}{L} \sum_i < \Delta_{i+j} \Delta_i >
\]

(2)

where the pairing operator \( \Delta_i = \sum_{\mu} g_{\mu} c_{1,i+\mu,\downarrow}^\dagger c_{1,i,\uparrow} \), \( i + \mu \) are the nearest-neighbors sites of site \( i \). For chains \( g_{\mu} = 1 \) for \( \mu = 1, 2 \). For planes, \( g_{\mu} \) defines the extended \( s \) or the \( d_{x^2-y^2} \) symmetries in the usual way. The pairing susceptibility is defined as \( \chi_p = (1/L) \sum_j C(j) \), where the sum extends over the sites of one layer.

We start by discussing the results for coupled chains of 8 sites each with 4 holes. Figure 1a shows the interlayer density fluctuations as a function of \( J_\parallel \). For \( t_\perp \leq 0.6 \) there is a sharp crossover from the homogeneous to the phase-separated regime at \( J_\parallel \approx 4.25 \). In the PS regime the number of holes in each plane is 0 or 4. For \( t_\perp \geq 0.8 \) this crossover disappears and the system is homogeneous for all \( J_\parallel \). Figure 1b shows the intralayer order parameter \( X \) as a function of \( J_\parallel \) for the same values of \( t_\perp \). In this
case, $X$ approaches its maximum value for 4 holes, equal to its maximum value for 2 holes, $X_{\text{lim}} = 1.707$. For small values of $t_\perp$ there is a sharp increase for the value of $J_\parallel$ at which the interlayer PS occurs. The pairing susceptibility as a function of $J_\parallel$ is shown in Fig. 1c. For $t_\perp \leq 0.4$ the peak of $\chi_p$ is located just before the interlayer PS border, and the decrease of $\chi_p$ is very sharp as it enters in this region. By contrast, for $t_\perp \geq 0.6$, the peak of $\chi_p$ starts to shift to lower values of $J_\parallel$ and its intensity decreases. Figure 1d shows the pairing correlations as a function of the distance for the values of $J_\parallel$ at which $\chi_p$ has its peak for each value of $t_\perp$. At these values of $J_\parallel$ the pairing correlations at the largest distance, $C(L/2)$, has its largest value for all $J_\parallel$ at a given $t_\perp$. It is seen that the decrease in the peak of $\chi_p$ as $t_\perp$ is increased corresponds essentially to a reduction of $C(r)$ at short distances. In fact, for $t_\perp = 1.0$ we actually see a tiny enhancement of $C(L/2)$ with respect to $t_\perp = 0$, but in any case $C(L/2)$ is too small to indicate the presence of superconductivity.

The same properties were computed for the same system but with $J_\perp = 0.0$ for all $t_\perp$. In general their behavior is quite similar to those shown in Fig. 1a. The main difference found was that, for the interlayer density fluctuations, as $t_\perp$ increases, the crossover from interlayer homogenous to PS regimes takes place for smaller values of $J_\parallel$ as $t_\perp$ increases, and that even for the largest value of $t_\perp$ studied, this crossover is still present although somewhat rounded off. At the filling considered (4 holes), the pairing correlations decay also very rapidly as a function of the distance.

Some of these patterns are also found for the case of quarter filling for the same
lattice. However, at this filling the processes are more interesting. In the absence of coupling between chains, $t_\perp = 0$, the system undergoes two successive interlayer crossovers (Fig. 2a), first from the homogeneous state to the state where there are 2 or 6 holes on each chain indicating a partial PS, and the second to a state in which there are 0 or 8 holes on each chain, or fully interlayer PS. As $t_\perp$ is increased, the first crossover becomes smoother, while the second is still sharp up to $t_\perp \simeq 0.4$. Finally, for $t_\perp \geq 0.6$, the second crossover is also washed out. For $t_\perp \geq 0.8$, the system stays in the interlayer homogeneous state for all $J_\parallel$. For large $t_\perp$, the behavior of the intralayer PS order parameter (Fig. 2b) is very similar to that of Fig. 1b, where for large $J_\parallel$, $X$ approaches its maximum value $\simeq 1.707$. However, for small $t_\perp$, it can be seen that $X$ increases with $J_\parallel$ but has a decrease each time the system has a crossover to an interlayer PS state. This behavior in $X$ can be understood by computing the maximum values it can take for the system with (4,4) holes quoted above, the system with (2,6) holes equal to 0.854, and for the fully PS regime (0,8), where $X = 0$. Figure 2c shows the intralayer pairing susceptibility $\chi_p$, which, as in the case of 4 holes, presents its maximum in the region of partial interlayer PS close to the crossover to the fully phase-separated interlayer regime for $t_\perp \leq 0.4$. Also, as in the case of 4 holes for large $t_\perp$, the peak is shifted to smaller values of $J_\parallel$ and its intensity decreases. The pairing correlations as a function of distance, computed at the peak of $\chi_p$, are displayed in Fig. 2d. First, it must be emphasized that in this case the correlations show a much more robust behavior at large distance than
in the case of 4 holes. This behavior is reminiscent of similar results in one and two dimensions for the $t - J$ model,\textsuperscript{6,10} indicating the presence of superconductivity. Secondly, it is clearly seen that the pairing correlations are \textit{suppressed} by the interlayer coupling. Another possibility of examining these results consists in varying $t_{\perp}$ keeping $J_{\parallel}$ fixed. For example, the pairing correlations computed at $J_{\parallel} = 2.25$ show the most robust pairing at large distances at $t_{\perp} \simeq 0.8$. A similar enhancement of the pairing correlations for nonzero interlayer coupling occurs at $J_{\parallel} = 5.0$. A detailed analysis of this behavior is given in Ref. 17.

Finally, in Fig. 3 we show some results for two coupled $\sqrt{8} \times \sqrt{8}$ planes. We consider periodic boundary conditions along both directions in the plane. As in the case of two coupled chains, we found the strongest signal of superconductivity at quarter filling. Fig. 3a shows the interlayer density fluctuations as a function of $J_{\parallel}$ for various values of $t_{\perp}$. The two crossovers found are equivalent to those found in the coupled chains case at the same filling. However, even for $t_{\perp} = 1.0$ there is in this cluster a crossover to the interlayer phase-separated regime. The intralayer order parameter $X$ also shows the typical vanishing as $J_{\parallel}$ increases beyond the region of fully PS. The most important feature, which generalizes to coupled 2d systems what was already found for coupled 1d systems, is the presence of the peak of the pairing susceptibility in the region of partial interlayer PS just before the crossover to the fully PS regime. At these values of $J_{\parallel}$, the s-wave pairing correlations have a true long-distance behavior, as can be seen for $t_{\perp} = 0.0, 0.6, \text{ and } 1.0$ in Fig. 3d. In
this figure we have included for comparison the pairing correlations for the 4 holes case, computed also at the maximum of the pairing susceptibility. The fact that s-pairing dominates over d-pairing, contrary to what was found for the $4 \times 4$ lattice, is presumably a finite size effect.

Summarizing, the idea of enhancement of pairing close to phase separation, as exposed in previous studies, is verified in a new scenario. The new feature of the present study with respect to previous work on the $t - J$ model is the presence of a different source of density fluctuations: the interlayer phase separation phenomena. For a fixed value of $t_\perp$, the strongest pairing occurs, as $J_\parallel$ is varied, just before the crossover to the fully interlayer PS regime. In general, the pairing is suppressed by interlayer coupling. However, in some cases, if $J_\parallel$ is kept fixed, pairing correlations are enhanced by increasing the interlayer coupling, according to previous results for the $t - J^{15}$ and Hubbard models.

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**FIGURE CAPTIONS**

**Figure 1** a) Interlayer density fluctuations, b) intralayer PS order parameter, and c) pairing susceptibility, as a function of $J_{∥}$ for the coupled 8 sites chain with four holes. The symbols corresponding to various values of $t_{⊥}$ are defined in a). In d), the pairing correlations computed at the peak of the susceptibility as a function of the distance are shown.

**Figure 2** a) Interlayer density fluctuations, b) intralayer PS order parameter, and c) pairing susceptibility, as a function of $J_{∥}$ for the coupled 8 sites chain with 8 holes. d) Pairing correlations computed at the peak of the susceptibility as a function of the distance. The symbols for different $t_{⊥}$ are defined as in Fig. 1.

**Figure 3** a) Interlayer density fluctuations, b) intralayer PS order parameter, and c) pairing susceptibility, as a function of $J_{∥}$ for the coupled $\sqrt{8} \times \sqrt{8}$ planes with 8 holes. d) Pairing correlations computed at the peak of the susceptibility as a function of the distance for 8 holes, $t_{⊥} = 0.0$ (circles), 0.6 (squares), 1.0 (diamonds), and 4 holes, $t_{⊥} = 0.0$ (filled circles), 0.4 (filled squares).