Ground state properties and dynamics of the bilayer $t - J$ model

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We present an exact diagonalization study of bilayer clusters of $t - J$ model. Our results indicate a crossover between two markedly different regimes which occurs when the ratio $J_{\perp}/J$ between inter-layer and intra-layer exchange constants increases: for small $J_{\perp}/J$ the data suggest the development of 3D antiferromagnetic correlations without appreciable degradation of the intra-layer spin order and the $d_{x^2-y^2}$ hole pairs within the planes persist. For larger values of $J_{\perp}/J$ local singlets along the inter-layer bonds dominate, leading to an almost complete suppression of the intra-layer spin correlation and the breaking of the intra-layer hole pairs. The ground state with two holes in this regime has $s$-like symmetry. The data suggest that the crossover may occur for values of $J_{\perp}/J$ as small as 0.2. We present data for static spin correlation function, magnetic structure factor and spin gap. We calculate the momentum distribution and electronic spectral function of the "local singlet state" realized for large $J_{\perp}/J$, and show that it deviates markedly from that of a single layer, making it an implausible candidate for modelling high-temperature superconductors.

I. INTRODUCTION

In connection with the so-called spin-gap phenomenon observed in high-temperature superconductors the properties of coupled layers of 2D $t - J$ model have recently attracted considerable attention. In this work we present results obtained by exact diagonalization of small clusters, which may provide a rough guideline for this problem. Our data were obtained by diagonalization of clusters of size $2 \times 8$ and $2 \times 10$, essentially the limit that can be reached by the exact diagonalization technique. Clearly these are still very small systems, and subtle low-energy effects certainly will escape our study. However, one may expect that even small clusters can mimic the short range correlation functions (which solely determine the total energy) roughly correct, and when interpreted with care our calculations thus may provide a crude phase diagram of the bilayer. Our key result is that already for fairly moderate values of the inter-layer exchange a qualitatively new type of ground state is realized, which deviates significantly from that of a single layer.

The model under consideration reads

$$H = - \sum_{<i,j>,\sigma} t_{i,j}(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + H.c.) + \sum_{<i,j>} J_{i,j} | S_i S_j - \frac{\sigma_i \sigma_j}{4} |.$$  

Here the $S_i$ are the electronic spin operators, $\hat{c}_{i,\sigma}^\dagger = \hat{c}_{i,\sigma}(1 - n_{i,-\sigma})$ and the sum over $<i,j>$ stands for a summation over all pairs of nearest neighbors. Our system consists of two planes, labelled $A$ and $B$ for later reference, the $z$-axis of the coordinate system is taken to be perpendicular to the planes. We distinguish between the hopping integral and exchange constant between nearest neighbors in the same plane, which we denote by $t$ and $J_z$, and between nearest neighbors in different planes, which we denote by $t_{\perp}$ and $J_{\perp}$. There is presently an unclear situation as to the correct choice of parameter values, experimental estimates for the ratio $J_{\perp}/J$ vary from 0.085 to over 0.3, up to 0.55. As for the inter-layer hopping integral $t_{\perp}$, the situation is even more unclear. Let us note that inter-layer hopping integrals derived from band structure calculations for cuprate superconductors are meaningless on the level of the $t - J$ model, because the "hole" in the $t - J$ model stands for an extended object, the Zhang-Rice singlet, which has very different hybridization matrix elements with orbitals outside the plane than a "bare" electron. We will therefore consider different ratios of the various parameters and study their impact on e.g. the nature of the ground state.

II. UNDOPED BILAYER

To begin with, we briefly discuss the spin correlations of an undoped bilayer. Figure shows the nearest-neighbor static spin correlation function in plane and
out-of-plane as well as the spin structure factor for momentum transfer \((\pi,\pi,0)\) and \((\pi,\pi,\pi)\). As \(J_\perp/J\) increases, there is initially a fairly symmetric splitting between \(S(\pi,\pi,0)\) and \(S(\pi,\pi,\pi)\), their average \(\bar{S}(\pi,\pi) = \frac{1}{2}(S(\pi,\pi,0)+S(\pi,\pi,\pi))\) remaining almost constant. The latter quantity measures the antiferromagnetic correlations within a single plane. In this range of \(J_\perp/J\), there is virtually no degradation of the antiferromagnetic order within the planes. The maximum of \(S(\pi,\pi,\pi)\) is reached rather precisely for \(J_\perp/J = 1\), and for this value the nearest neighbor spin correlation function within and between the planes are equal. Quite obviously, for this parameter value the bilayer is closest to a 3D Heisenberg antiferromagnet. When \(J_\perp/J\) is increased further, \(S(\pi,\pi)\) decreases and so does the intra-layer nearest neighbor spin correlation function. The spin correlations within the plane now decrease and local singlets along the inter-layer spin correlations and dominant interlayer spin correlations has also been found by Liechtenstein et al. [9] within a weak coupling framework, as well as by Normand et al. [10] within slave-boson mean field theory. This seems to be a very general property of bilayer systems.

At this point, the possibility of fairly strongly finite-size effects on the critical value of \(J_\perp/J\) becomes obvious: since the transition to the state with pronounced \(z\)-axis spin correlations implies the breaking of the in-plane pair, it follows that an overestimation of the in-plane hole binding energy will lead to an artificial stabilization of the "conventional" \(B_1\) ground state. To see this, we first define the binding energy as \(\Delta_B = (E_0^{(1h)} - E_0^{(0h)}) - 2 \cdot (E_0^{(1h)} - E_0^{(0h)}) = (E_0^{(1h)} + E_0^{(0h)}) - 2 \cdot E_0^{(0h)}\) where \(E_0^{(0h)}\) denotes the ground state energy with \(\nu\) holes. In small clusters of \(t - J\) model this quantity is negative [9], so that in the limit \(J_\perp,t_\perp \to 0\) the 2 hole ground state of the bilayer will approach a product of an undoped layer and a layer with two bound holes. The binding energy \(\Delta_B\) then represents a kind of charge transfer energy, i.e. it gives the cost in energy upon transferring one of the two holes to the other layer. Hole binding within the planes thus opposes the formation of the \(A_1\) state, and since it is known that finite-size calculations for the 2D \(t - J\) model tend to substantially overestimate \(\Delta_B\) [2], this may have an impact on the crossover between the two different ground states. In order to further investigate this issue, we add to the Hamiltonian a repulsive interaction between holes in the same plane:

\[
H_V = V(\sum_{i,j \in A} n_i n_j + \sum_{i,j \in B} n_i n_j).
\]

Such a term does not affect the intra-plane dynamics; it only reduces the loss of energy which occurs when a hole is transferred between the two layers. In particular, if we adjust \(V = \Delta_B\) this term precisely cancels the effects of the in-plane binding energy which may contain large finite-size effects. Figure 3 then shows (for the value \(J/t = 0.4\)) the change of the crossover value of \(\langle 1 - \bar{S}_1 \rangle^{\text{crit}}\) when the in-plane repulsion is increased. There is an obvious linear dependence and for completely "balanced" intra-layer binding energy (i.e. for vanishing hole transfer energy) we find \(\langle 1 - \bar{S}_1 \rangle^{\text{crit}} = 0.17\). For \(J/t = 0.2\) the same procedure gives \(\langle 1 - \bar{S}_1 \rangle^{\text{crit}} = 0.15\) (for completely balanced binding energy), so that in the parameter region of possible relevance for cuprate superconductors the crossover to the unpaired state may occur for fairly small values of \(J_\perp/J\).

For completeness we have to address possible ground state degeneracies. For the single 10-site cluster with

III. DOPED CASE

We next consider the doped bilayer, more precisely the ground states with two holes of the \(2 \times 8\) and \(2 \times 10\) bilayer. These show the same overall trends as the undoped bilayer, however within a much smaller range of \(J_\perp/J\). Figure 2 shows the nearest neighbor spin correlation functions as functions of \(J_\perp/J\) and demonstrates that the crossover to a state with almost vanishing in-plane spin correlations and dominant \(z\)-axis spin correlations is much more abrupt than for the undoped system. Hole doping obviously makes it easier for the inter-plane terms to dominate over the in-plane exchange. The strong difference as compared to the undoped case moreover shows that results for undoped bilayer systems may have limited significance for the doped bilayer.

The second major difference as compared to the undoped bilayer is, that the crossover from the small to large \(J_\perp/J\) regime is now accompanied by a ground state level crossing. For small values of \(J_\perp/J\) the 2 hole ground state of the \(2 \times 10\) bilayer belongs to the \(B_1\) (or \(d_{x^2-y^2}\)) representation of the \(C_{4v}\) point group, reflecting the well-known fact [10] that two holes in the \(t - J\) model always form a bound state with this symmetry. In this state, the two holes can be found in the same plane with high probability i.e. the in-plane bound state obviously persists to some degree. This changes completely when \(J_\perp/J\) is increased beyond a certain critical value: the ground state now has the \(A_1\) (or \(s\)) symmetry and the two holes are in different planes almost with probability 1. A rough "phase diagram" of the \(2 \times 10\) bilayer is given in Figure 3. Table 1 shows the hole density correlation function \(g(R) = \sum_i(1 - n_i)(1 - n_{i+R})\) for both \(B_1\) and \(A_1\) state near the crossover. An analogous level crossing also can be found in the \(2 \times 8\) cluster, for comparable values of \(J_\perp/J\), so that it does not seem to originate from some spurious effect due to the special geometry of one of these two clusters. Strong inter-layer spin correlations thus are incompatible with \(d\)-wave pairing of holes within the planes, and change the symmetry properties of the ground state. It is interesting to note that the incompatibility of \(d\)-wave pairing within the planes and strong interlayer spin correlations has also been found by Liechtenstein et al. [9] within a weak coupling framework, as well as by Normand et al. [10] within slave-boson mean field theory. This seems to be a very general property of bilayer systems.

When \(J_\perp/J\) is increased further, \(\bar{S}(\pi,\pi)\) decreases and so does the intra-layer nearest neighbor spin correlation function...
periodic boundary conditions there exists a special permutation of the sites which leaves all nearest neighbor relations invariant; this is analogous to the well-known $2^4$ hypercube symmetry of the $4 \times 4$ cluster with periodic boundary conditions. This artificial symmetry operation therefore commutes with any Hamiltonian involving only nearest neighbor terms and introduces artificial degeneracies. Clearly, for the $2 \times 10$ bilayer there exists an analogous permutation of $z$-axis bonds, leading to artificial degeneracies as well. We have always neglected the degenerate ground states with finite momentum, because we believe that the ground state with vanishing momentum is the most natural representative of the infinite system. In the single layer case, this is confirmed by the fact that the $\vec{k} = 0$ ground states of different clusters all have very analogous properties, whereas the degenerate finite momentum ground states disappear for larger clusters. It is moreover straightforward to see, that these degenerate states cannot add much new information: for example the average nearest neighbor spin correlation functions can be expressed as derivatives of the total energy with respect to the exchange constants $J$ and $J_{\perp}$, the probability to find the two holes in different planes is related to the derivative with respect to the parameter $V$ in $[\mathcal{H}]$, so that these quantities must be rigorously the same for all symmetry-degenerate ground states.

We now turn to the spin correlations, shown in Figures 2 and 3. The $B_1$ state shows the same symmetric splitting of $S(\pi, \pi, 0)$ and $S(\pi, \pi, \pi)$ which was seen already in the undoped spin-bilayer; the inter-plane spin correlations increase only moderately. Quite obviously, in this state the development of inter-layer spin correlations is accomplished by the "lock in" of the directions of the local staggered magnetization $M_S$ in the two planes, with essentially unchanged intra-plane correlations. By contrast, the $A_1$ state shows dominant inter-plane correlations and, as shown in Figure 2, already for values of $J_{\perp}/J \sim 1$ it rapidly approaches the limit of a product state of $z$-axis singlets.

In order to further clarify the mechanism by which inter-layer spin correlations are built up, we now study the probability distribution of the staggered magnetization in the ground state. More precisely, we denote by $M_{\mu, \nu}$ the set of basis states which have staggered magnetization $\mu$ in the A-plane and staggered magnetization $\nu$ in the B-plane. Then, we can define the operator

$$P_{\mu, \nu} = \sum_{\alpha \in M_{\mu, \nu}} |\Phi_{\alpha}\rangle\langle\Phi_{\alpha}|,$$

and its ground state expectation value $S(\mu, \nu) = \langle P_{\mu, \nu} \rangle$. It may be interpreted as the total weight of states with single-layer staggered magnetizations $\mu$ and $\nu$. Figure 4 shows this quantity for two values of $J_{\perp}/J$. For vanishing inter-layer coupling the ground state is simply the product of two single-layer ground states, and if one chooses fixed $z$-component of the momentum, $S(\mu, \nu)$ must be completely symmetric, i.e. $S(\mu, \nu) = S(\mu, -\nu) = S(-\mu, \nu) = S(-\mu, -\nu)$. The data then show, that for increasing $J_{\perp}/J$ there is first a slight shift of weight from the $(+, +)$ and $(-, -)$ quadrants to the $(+, -)$ and $(-, +)$ quadrants: the staggered magnetization of the two layers "locks in". However, states with large staggered magnetization still do have appreciable weight, and the correlation between the values of $M_S$ in the two planes is not yet strong. This changes completely when we increase $J_{\perp}/J$ beyond the crossover to the $A_1$ ground state: $S(\mu, \nu)$ is now concentrated near the line $\mu = -\nu$, and along this line it drops sharply towards large values of $M_S$. The values of $M_S$ in the two layers are now strongly correlated: when there is e.g. a fluctuation towards a large positive value of $M_S$ in the $A$-plane, it must be accompanied by a fluctuation to a large negative value in the $B$-plane. These results are precisely what one would expect if the spins were distributed randomly within the planes, but under the constraint that nearest neighbor spins in $z$-direction always are antiparallel. Analysis of the probability distribution $S_{\mu, \nu}$ thus confirms the scenario inferred from the spin correlation function: there is a regime of small $J_{\perp}/J$, where the system responds to the inter-layer coupling by a weak "lock-in" of the staggered magnetization in the two planes, while no appreciable change of the intra-layer correlations takes place. For large $J_{\perp}/J$, on the other hand, we have the clear signatures of the $z$-axis singlet state.

We next consider the "spin gap", defined as

$$\Delta_{\text{spin}} = E_{0, \Gamma_0}(\pi, \pi, \pi) - E_0$$

Here $E_0$ denotes the energy of the ground state (which has momentum $0$) and $E_{\Gamma_0}(\pi, \pi, \pi)$ denotes the lowest energy in the subspace of states with momentum $(\pi, \pi, \pi)$ and the same point group symmetry $\Gamma_0$ as the ground state. Inspection shows that the $\vec{k} = 0$ ground state is always a singlet, the $(\pi, \pi, \pi)$ state always a triplet, so that $\Delta_{\text{spin}}$ indeed represents the gap which would be observed in the dynamical spin correlation function with momentum transfer $(\pi, \pi, \pi)$. We note that $\Delta_{\text{spin}}$ is prone to massive finite-size effects, as can be seen e.g. from the fact that even an undoped 2D cluster has a "spin gap" of $\approx 0.4J$ [3]. The values of $\Delta_{\text{spin}}$ determined from the small clusters thus may at best indicate a rough qualitative trend, but clearly have no quantitative significance. Then, Figure 8 shows the spin gap over a wide range of $J_{\perp}/J$. It is remarkable that the gap initially decreases with increasing $J_{\perp}$ and in fact shrinks appreciably at the level crossing to the strong $z$-axis correlation ($A_1$) state. It is only for values of $J_{\perp}/J > 1$ that the spin gap becomes large and grows linearly with $J_{\perp}$, reflecting the saturation of the $z$-axis spin correlation function (see Figure 5). For an undoped system and in the limit $J_{\perp}/J \rightarrow \infty$ it is easy to see that a single $z$-axis triplet bond can propagate in a "background" of $z$-axis singlets with a nearest neighbor hoppibg element of $J/2$, so that the spin gap should be $J_{\perp} - z(3J/2)$, with $z$ the number of nearest neighbor $z$-axis bonds. The resulting asymptotic expressions $\Delta_{\text{spin}} = J_{\perp} - J$ for the ladder ($z = 2$) and
\( \Delta_{\text{spin}} = J_\perp - 2J \) for the bilayer (\( z = 4 \)) indeed provide excellent estimates for the undoped systems (compare Figure 2 in Ref. [3]): for the doped system, however, the numerical result rather suggests the asymptotic expression \( \Delta_{\text{spin}} = J_\perp - (J/2) \), which would imply a reduction of the effective hopping element for the triplet-bond by a factor of 4. This indicates, that the propagation of the \( z \)-axis triplet is inhibited by the presence of mobile holes, so that there must be a strong interplay between the local singlets/triplets and the holes.

Figure 9 shows the spin gap for other parameter values in the range \( J_\perp / J < 1 \) and demonstrate that increasing values of \( J_\perp / J \) initially tend to reduce \( \Delta_{\text{spin}} \), as would be expected from an enhancement of antiferromagnetic correlations. It is interesting to note that the crossover \( B_1 \to A_1 \) never leads to an increase of \( \Delta_{\text{spin}} \). While the significance of these data should not be overestimated, we may state that in the small clusters there is no indication of any widening of the spin gap due to interlayer coupling, at least not for "reasonable" values of \( J_\perp / J \).

### IV. LOCAL SINGLET STATE

We now proceed to a study of the "\( z \)-axis singlet state" which is realized for larger \( J_\perp / J \). As has been shown above, this state may appear already for quite moderate values of \( J_\perp / J \approx 0.2 \), which in fact been postulated to be realized in actual high-temperature superconductors. In fact, this state may be considered a qualitatively new feature of the bilayer system, as compared to the single-layer ground states studied extensively before. We first consider the limiting case of vanishing in-plane parameters \( J \) and \( t \) [4]. Depending on the relative magnitude of \( t_\perp \) and \( J_\perp \), the ground state of the \( 2 \times N \) bilayer with an even number of holes \( n_h \) can take two quite different forms (see Figure 6): it is either the product of \( N-n_h/2 \) \( z \)-axis singlets and \( n_h/2 \) empty \( z \)-axis bonds with energy \( (N-n_h/2) \cdot J_\perp \) or it is a product of \( N-n_h \) \( z \)-axis singlets and \( n_h \) singly occupied \( z \)-axis bonds with energy \( (N-n_h) \cdot J_\perp - n_h \cdot t_\perp \). The degeneracy of this ground state is lifted by the intra-plane terms of the Hamiltonian.

We assume that the most important intra-plane term in the Hamiltonian is the hopping integral \( t \). Then, a singly occupied bond can propagate to a nearest neighbor in a single-step process with the effective hopping integral \( t/2 \), whereas an empty bond propagates to a nearest neighbor via a two step process where the intermediate state has a broken \( z \)-axis singlet; in the regime of large \( J_\perp / t \) perturbation theory would give an effective hopping integral \( \sim t^2 / J_\perp \). We thus have the interesting situation that, depending on the relative strength of parameters, two very different "fixed points" may be appropriate to describe the bilayer system: if the arrangement of holes in empty bonds is preferred, the system should correspond to a gas of \( n_h/2 \) hard core bosons, propagating via nearest neighbor hopping of strength \( \sim t^2 / J_\perp \). On the other hand, if the arrangement of holes along singly occupied bonds is preferred, the bilayer should correspond to a system of \( n_h \) spin-1/2 fermions, propagating via nearest neighbor hopping of strength \( t/2 \). In both cases, however, there is a positive nearest neighbor hopping matrix element for either hole-like "Fermions" or "Bosons", so that the holes may be expected to accumulate at the in-plane momentum \( (\pi, \pi) \).

The calculated values of the electron momentum distribution function \( n(\vec{k}) = \langle \hat{c}_{\vec{k} \sigma} \hat{c}_{\vec{k} \sigma}^\dagger \rangle \), given in Tables I and II, then indeed show an enhanced hole-occupancy of \( (\pi, \pi) \) in the \( A_1 \) state even for moderate values of \( J_\perp \) and \( t_\perp \); this is very pronounced in the \( 2 \times 8 \) system, but also in the \( 2 \times 10 \) bilayer one can realize an enhanced depression at \( (\pi, \pi) \) and a tendency towards the "flattening" of \( n(\vec{k}) \) in the remainder of the Brillouin zone. This indicates that the momentum distribution with "hole pockets" at \( (\pi, \pi) \), which would be expected in the limit of large inter-layer coupling indeed seems to persist in the \( A_1 \) state also for moderate values of the inter-layer coupling. This picture is confirmed by the single particle spectral function \( A(k, \omega) \), shown in Figure 11. Due to restrictions in computer memory, we have evaluated this quantity only for the \( 2 \times 8 \) bilayer. The topmost peaks in the photoemission spectra are located at \( (\pi/2, \pi/2) \) and \( (\pi, 0) \) (due to the special symmetry of the \( 2D \) 8-site cluster these momenta are in fact identical for the \( A_1 \) state, but there is no appreciable low energy weight in the inverse photemission spectrum at either of these momenta: quite obviously these \( k \)-points are "occupied". This is in clear contrast to the spectral function for the \( B_1 \) state [4] which showed a rather obvious Fermi level crossing at \( (\pi, 0) \). Another notable feature is the strong contrast between the relatively sharp peaks in the bonding channel (i.e. \( k_z = 0 \)) and the more diffuse spectra in the antibonding one, which have markedly enhanced incoherent continua. This indicates that electrons in the bonding channel are the "more well-defined" excitations of the system, as one would expect it for a product state of doubly and singly occupied bonds. The strong difference between the \( k_z = 0 \) and \( k_z = \pi \) spectra is again in contrast to their almost identical shape in the \( B_1 \) ground state [4]. The available data thus rather consistently suggest that even for moderate values of \( J_\perp \) and \( t_\perp \) the "\( z \)-axis singlet state" bears a strong resemblance to the \( J_\perp, t_\perp \to \infty \) limit, which in particular implies the accumulation of holes at \( (\pi, \pi) \).

### V. SUMMARY AND DISCUSSION

In summary, we have studied the effects of interlayer exchange in a bilayer \( t - J \) model. The data rather consistently suggest a crossover between two very different regimes: for small and moderate values of the inter-plane exchange coupling there is no qualitative change of the
spin correlations, the in-plane hole pairing with \(d_{x^2-y^2}\) symmetry persists and the inter-plane exchange induces 3D antiferromagnetic correlations. For increasing values of \(J_z/J\) there is a crossover to a state with dominant inter-layer spin correlations, where the intra-layer hole pairing is completely suppressed. We note that this feature may well persist in the infinite system if the pairing state remains short ranged; in this case, it would be the short range correlations which dominate the physics, and these may be expected to be described properly even for the short range correlations which dominate the physics, ing state remains short ranged; in this case, it would be interpreted as a narrowing of the spin gap at the crossover. The result that strong inter-layer coupling suppresses the in-plane \(d_{x^2-y^2}\) pairing clearly would be hard to reconcile with the ever growing experimental evidence for d-type symmetry of the superconducting order parameter in the cuprate superconductors [13] and the experimental fact that \(T_c\) seems to increase with the number of closely coupled layers in these compounds. In addition, our data indicate that the "z-axis singlet state" realized for large \(J_z/J\) has fairly unusual properties such as a tendency towards "hole pockets" at the in-plane momentum \((\pi, \pi)\), so that it does not seem to be a very promising candidate for modelling real high-temperature superconductors. Moreover, the relatively strong difference between the z-axis singlet state and the "conventional" single layer ground state would make it hard to understand why many properties of single and double layer cuprates are relatively similar.

Clearly, the simplest way to resolve these problems is to assume that the values of \(J_z/J\) in the actual materials are too small to ever induce the z-axis singlet state. Unfortunately strong finite size effects do not allow us to give a very accurate estimate of the critical value where the crossover occurs. Then, a possible enhancement of antiferromagnetic spin correlations due to the onset of 3D correlations in the more conventional ground states realized for lower \(J_z/J\) may be more easy to reconcile with experiment: it seems plausible that pairing theories which rely on antiferromagnetism, such as the antiferromagnetic spin fluctuation theory [14], or the antiferromagnetic van-Hove scenario [15] would profit from the onset of 3D correlations, so that the exchange coupling of several CuO\(_2\) planes could be favourable for achieving higher \(T_c\)’s.

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**TABLE I.** Comparison of the hole density correlation function \(g(R)\) in the lowest state with \(B_1\) symmetry and the lowest state with \(A_1\) symmetry of the \(2 \times 10\) bilayer \(t-J\) model. Parameter values are like in Table 1.

| \(R_{\text{in-plane}}\) | \(B_1\) | \(A_1\) |
|-----------------|--------|--------|
| \(R_z = 0\) | (0, 0) | (0, 0) |
| \(R_x = 1\) | 0.000 | 0.0189 |
| \(A_1\) | (0, 0) | (0, 0) |
| \(R_z = 0\) | 0.000 | 0.0115 |
| \(R_x = 1\) | 0.2217 | 0.1038 |

**TABLE II.** Comparison of the momentum distribution function \(n(\vec{k})\) for the lowest state with \(A_1\) symmetry and the lowest state with \(B_1\) symmetry of the \(2 \times 10\) bilayer \(t-J\) model. Parameter values are like in Table 1.

| \(k_{\text{in-plane}}\) | \(A_1\) | \(B_1\) |
|-----------------|--------|--------|
| \(k_x = 0\) | 0.5357 | 0.5399 |
| \(k_x = \pi\) | 0.5214 | 0.5416 |
| \(k_y = 0\) | 0.5321 | 0.5278 |
| \(k_y = \pi\) | 0.4367 | 0.4730 |

**TABLE III.** Comparison of the momentum distribution function \(n(\vec{k})\) for the lowest state with \(A_1\) symmetry and the lowest state with \(B_1\) symmetry of the \(2 \times 8\) bilayer \(t-J\) model. Parameter values are like in Table 1.

| \(k_{\text{in-plane}}\) | \(A_1\) | \(B_1\) |
|-----------------|--------|--------|
| \(k_x = 0\) | 0.5466 | 0.5469 |
| \(k_x = \pi\) | 0.5014 | 0.5014 |

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FIG. 1. (a) Static nearest neighbor spin correlation function $\langle \vec{S}_i \cdot \vec{S}_j \rangle$ for the ground state of the undoped $2 \times 10$ bilayer. (b) Static spin structure factors $S(\pi, \pi, 0)$ (diamonds) and $S(\pi, \pi, \pi)$ (crosses) and average $\bar{S}(\pi, \pi)$ (squares) for the same state.

FIG. 2. Static nearest neighbor spin correlation function $\langle \vec{S}_i \cdot \vec{S}_j \rangle$ for the ground state of the $2 \times 10$ bilayer with two holes. Parameter values are $t = 1$, $J = 0.2$, $t_\perp = 0.1$.

FIG. 3. "Phase diagram" for the $2 \times 10$ bilayer with two holes for two values of $t_\perp/t$. The figure indicates the regions of stability of the $A_1$ and $B_1$ ground state for different parameter values. The respective critical values of $J_\perp/J$ have been obtained by interpolating ground state energies and are accurate only to $\sim \pm 0.05$.

FIG. 4. Critical value of $(J_\perp/J)_{\text{crit}}$ for the crossing $B_1 \rightarrow A_1$ as a function of the intra-plane repulsion parameter $V$.

FIG. 5. Nearest neighbor spin correlation function $\langle \vec{S}_i \cdot \vec{S}_j \rangle$ for the $2 \times 10$ bilayer with two holes. (b) Static spin structure factors $S(\pi, \pi, 0)$ (diamonds) and $S(\pi, \pi, \pi)$ (crosses) and average $\bar{S}(\pi, \pi)$ (squares) for the same system. Parameter values are $t = 1$, $J = 0.4$, $t_\perp = 0.5$.

FIG. 6. Same as Figure 4 for $J = 0.2$.

FIG. 7. Probability distribution $S_{\mu, \nu}$ for the ground state of the $2 \times 8$ bilayer with two holes and different $J_\perp/J$. The distribution has been averaged over the areas indicated in the figure. Parameter values are $J_\perp/J = 0.4$ (a) and $J_\perp/J = 1$ (b), the other parameters are $t = 1$, $J = 0.4$, $t_\perp = 0.5$ for both figures.

FIG. 8. (a) Spin gap $\Delta_{\text{spin}}$ as a function of $J_\perp/J$ for $J = 0.2$, $t_\perp = 0.1$, $2 \times 10$ bilayer. (b) $\Delta_{\text{spin}}$ for different parameter values in the $2 \times 10$ bilayer, $t = 1$.

FIG. 9. Possible ground states of the bilayer model in the limit $t, J \rightarrow 0$: the holes are on "singly occupied bonds" (a) or on "empty bonds" (b).

FIG. 10. Single particle spectral function $A(k, \omega)$ for the $2 \times 8$ bilayer. The vertical line marks the Fermi energy, the frequency range $\omega > E_F$ ($\omega < E_F$) corresponds to electron creation (annihilation). The full (dashed) line refers to the bonding (antibonding) channel. Parameter values are like in Table 11.

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Figure 1

In-plane $\leftrightarrow$
Out-of-plane $\rightarrow$

$\langle \vec{S_i} \cdot \vec{S_j} \rangle$

(a)

$J_{\perp}/J$

(b)

$S(\vec{q})$

$J_{\perp}/J$
Figure 5

(a) 

\[
\langle \vec{S}_i \cdot \vec{S}_j \rangle
\]

In-plane ◇

Out-of-plane —

\[
J_{\perp} / J
\]

(b) 

\[
S(\vec{q})
\]

\[
J_{\perp} / J
\]
Figure 6

(a) $\langle \vec{S}_i \cdot \vec{S}_j \rangle$

(b) $S(\vec{q})$

$J_{\perp}/J$

In-plane

Out-of-plane

$J_{\perp}/J$
Figure 8

(a) $\Delta_{\text{spin}}/J$ vs $J_\perp/J$

(b) $\Delta_{\text{spin}}/J$ vs $J_\perp/J$

- $J = 0.4$, $t_\perp = 0.1$
- $J = 0.4$, $t_\perp = 0.5$
- $J = 0.2$, $t_\perp = 0.1$
- $J = 0.2$, $t_\perp = 0.5$
Fig. 7a
Fig. 7b

$S(\mu, \nu)$
Figure 9
