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Numerical Study of the Wheatley-Hsu-Anderson Interlayer Tunneling mechanism of High T_c Superconductivity

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We present results obtained (by exact diagonalization) for the problem of two $t-J$ planes with an interlayer coupling $t_\perp$. Our results for small hole concentrations show that in-plane superconducting correlations are enhanced by $t_\perp$. When the constraint on double occupancy in the $t-J$model is relaxed, the enhancement disappears. These results illustrate the inter–layer tunneling mechanism for superconductivity.

Ever since Anderson's proposal [1] that the physics of the high T_c superconductors is contained in the one band Hubbard Hamiltonian

$$H = -t \sum_{i,j} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{1}$$

in the limit of large U, the Hubbard model and its derivative, the $t - J$ model

$$H = -t \sum_{<i,j>} c^{\dagger}_{i\sigma}(1 - n_{i-\sigma}) c_{j\sigma}(1 - n_{j-\sigma}) + J \sum_{<i,j>} (\vec{S}_i.\vec{S}_j - \frac{1}{4} n_i n_j) \tag{2}$$

where $J = \frac{4t^2}{U}$

have been the subject of several analytical studies. Despite these attempts, a complete quantitative understanding of the ground state of these Hamiltonians is still lacking. Finite size clusters of these models have also been analyzed extensively [2] by exact diagonalization and Variational Monte Carlo techniques. These studies indicate that several of the anomalous normal state properties of the CuO superconductors could be accounted for by the $t - J$ Hamiltonian. However in these numerical studies, there are no robust signals of a superconducting phase in either the Hubbard or the $t - J$ model [4]. In our view this is hardly surprising since superconductivity in the CuO compounds is governed by a scale that is neither t nor J, but the interlayer coupling $t_{\perp}$. This was first proposed by Wheatley, Hsu and Anderson [5](WHA).

We now describe the basic physics behind the WHA mechanism . There is now increasing evidence that the normal state of the high T_c superconductors is a non-Fermi liquid [3]. The low energy excitations are spin–charge decoupled (the spinons and holons) i.e. real electron like quasi-particles having both spin and charge are absent asymptotically at the Fermi energy. This phenomenon is called "confinement" of real electrons close to the Fermi surface. These features are known to be present in the 1–d Hubbard model as has been discussed, for example, by Anderson and Ren [6]. It is believed that the 2–d Hubbard model or the $t - J$ Hamiltonian would reproduce these features. Because of spin–charge decoupling or the confinement of electron like excitations, single electron motion between two CuO planes (which necessitates real scattering processes between the spin and charge degrees of freedom) gets suppressed i.e., the first order process in $t_\perp$, which transfers a real electron from a plane to a neighboring plane, becomes ineffective asymptotically at the fermi level [7]. However, the second order processes generated by $t_\perp$ are not suppressed. This is because the $t_\perp$ term to second order gives rise to processes that do not leave an unpaired spin in a layer but creates/annihilates a spinon pair comprising an "up" and a "down" spinon in a singlet state. Since in the RVB ground state such spinon pair fluctuations are present, these processes are not suppressed. These can be seen within the framework of second order perturbation theory [8] which generates a term of the form $c^{l\dagger}_{i\uparrow}c^{l\dagger}_{j\downarrow}c^{m}_{j\downarrow}c^{m}_{i\uparrow} + h.c.$, which can be rewritten as $b^{l\dagger}_{ij}b^{m}_{ij}$ where b_{ij} are the usual singlet operators (here l and m label different layers).

It therefore follows that the processes that are not suppressed are those that transport a pair of electrons in a singlet state between the CuO planes. Since these are precisely the superconducting fluctuations, we conclude that the effect of the $t_\perp$ is to cause electron pair tunneling between the layers which in turn causes superconductivity. In the language of spinons and holons, this implies that the CuO plane already supports spinon pair excitations as the spinons form a paired condensate. The inter plane coupling causes pairs of holons to hop between layers by creating or annihilating spinon pairs. i.e. there is a "leakage" of ODLRO to the holons from the spinons caused by the inter plane coupling $t_\perp$ [8]. Insofar as *spin quantum numbers* are concerned, a pair of electrons (holes) in a singlet state is the same as a pair of antiholons (holons). Thus electron (hole) tunneling to second order causes antiholon (holon) pair tunneling.

From these arguments it is clear that the occurence of superconductivity is crucially related to two factors:

(i). a large U (or irrelevance of double occupancy) which causes spin-charge decoupling and

(ii). the effect of $t_\perp$ on the the $2-d$ planes having spin-charge decoupling.

Since our main results concern (ii), let us briefly consider relaxing the requirement (i). Then the problem reduces to that of two coupled $t - J$ planes with no constraint on double occupancy. The problem is also similar to that of two conventional BCS-superconducting planes coupled by $t_\perp$. Since $U = 0$, there is no suppression of single electron motion between the planes. This causes $t_\perp$ to act as a "pair breaker" i.e. the pairing energy can be lost at the expense of kinetic energy gained by hopping between the planes. This is the reason that mean field studies (where the single–occupancy constraint is not imposed exactly) on coupled $t - J$ planes show a decrease in T_c with $t_\perp$ [9]. In our numerical study, we find that $t_\perp$ causes superconducting correlations to decrease marginally. On the contrary, in the case of $t - J$ planes with no double occupancy, we see that the inter–plane coupling *enhances* in–plane superconducting correlations. We therefore conclude that $t_\perp$ can enhance superconducting correlations only when the condition $n_i = 0$ or 1 is imposed exactly.

We have performed exact diagonalization [10] studies on $4 + 4$, $5 + 5$ and $6 + 6$ site clusters. These clusters consist of two planes coupled by the $t_\perp$ term. We use periodic boundary conditions. In addition we use two different geometries for the $6+6$ case :(a) for a closed chain and (b) a grid. We have presented results only for the grid geometry since the results for the closed chain are qualitatively similar. We have chosen, on a scale of $|t| = 1$, $J = 0.31$, and varied $|t_\perp|$ from 0 to 0.9. Our results are therefore of direct relevance to the CuO compounds in the region of small $t_\perp$. To illustrate the effect of $t_\perp$ in the absence of U, we have also diagonalized a $4 + 4$ cluster with two holes after relaxing the constraint on double occupancy. We give below a short description of the numerical aspects of the computations.

We have used a basis for the Hamiltonian matrix in which S_z is diagonal, so that the only diagonal matrix elements are those of the $\sum_{<i,j>} S_i^z S_j^z$ term. The off-diagonal elements come from the $\sum_{<i,j>} S_i^+ S_j^- + S_i^- S_j^+$ and the t and $t_\perp$ terms. Note that the off–diagonal elements are mutually exclusive in the sense that a given pair of distinct basis states can at best be connected by one of these three off–diagonal terms. In addition, this basis also excludes all states with double occupancies. We compute the lowest eigenvector if the ground state is non-degenerate and all the degenerate ones if the ground state is degenerate (which it typically is for $t_\perp = 0$)using the conjugate gradient method [11]. We use a simulated annealing based algorithm [12] to get an improved starting guess for the conjugate gradient.

To look for superconductivity we compute the extended–singlet correlation function as defined by Hirsch [4] which we explain below.

Let

$$b_{ij} = \frac{1}{\sqrt{2}}[c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow}],$$

where (i, j) are nearest neighbor sites in a plane. Then the extended–singlet pairing correlation (SPX) is defined as

$$\chi = \frac{1}{N} \sum_{<i,j><k,l>} \langle b_{ij} b_{kl}^\dagger \rangle \tag{3}$$

where $\langle \cdots \rangle$ represents expectation value in the ground state. Here N is the number of in–plane sites. If χ scales as N, then the result suggests a superconducting instability in the thermodynamic limit. (We look only for s-wave pairing).

The results of the above computations show several interesting features that are size–independent (see Fig. 1,2 and 3). First, we note that for the case of two holes, the SPX always increases with $t_\perp$. For cluster sizes $4+4$, $5+5$ and $6+6$, this corresponds to a doping of $\simeq 25\%$, 20% and 16% respectively. As soon as we add two more holes, we enter a region of large doping. The results with four holes therefore show a qualitatively different behavior. The SPX in this case is not affected much by $t_\perp$. The results resemble those of the unconstrained $t - J$ model. The same behavior persists for larger hole concentrations. In this sense, we suggest that we have crossed over from a non–Fermi liquid phase (which is sensitive to $t_\perp$) to a phase which is less of a non–Fermi liquid.

Next we consider the limit $t_\perp \to 0$. In this limit with two holes in the system, the ground state has one hole in each layer on an average. Therefore the contribution to SPX is dominated by terms of the form $< O_{12} O_{12}^\dagger >$, $< O_{12} O_{23}^\dagger >$. Such essentially on–site correlations are not related to superconducting order in the thermodynamic limit. In previous studies [2] of the $t - J$ model, it was noticed that only such terms contributed to the SPX. This led to the conclusion there are no incipient long–range (superconducting) correlations in the

$t-J$ model. Our results for $t_\perp = 0$ also reflect this. (Also note that for the case of $4+4$ with 2 holes and with no constraint on double occupancy, the SPX is maximum for $t_\perp = 0$. As discussed earlier, this shows the "pair breaking" nature of $t_\perp$.)

However as $t_\perp$ increases, the long–range correlations increase rapidly. In fact, it is this behavior of the long–range correlations that causes the enhancement of the total SPX with $t_\perp$. To show this, we have subtracted in the expression for SPX, those terms with none of the indices $< i, j >, < k, l >$ in eq.(3) equal i.e. terms wherein bonds $< i, j >$ and $< k, l >$ neither overlap nor touch, and examined the resulting behavior of SPX with $t_\perp$ for $6+6$ with two holes. The results are shown in Fig. 4. The figure demonstrates the dramatic increase of the "long range" part of the pair susceptibility by a factor of 30. A similar increase is noticed for the $4+4$ and $5+5$ cases. We observe similar results for a large U Hubbard model where the enhancement of pair susceptibility due to interlayer tunneling is clearly visible.

Finally we address the question of finite size scaling. Comparison of our data for the $4+4$ and $6+6$ cases shows a scaling which is slightly smaller than N. From our results it is also clear that $5+5$ is quantitatively different. This we believe to be an even–odd feature.

Since we have not diagonalized larger clusters, we are aware that these results are not conclusive with regard to scaling. However we believe that these preliminary results are very encouraging and point in the right direction towards further numerical studies. For it is clear from the definition of the SPX and our criterion for superconductivity that any instability in the thermodynamic limit has to come from these long range correlations. In our study, we find that the contribution to the SPX (for a given $t_\perp \neq 0$) from the long range correlations increases with size. This suggests the presence of a superconducting phase in the thermodynamic limit. Another limitation we have faced is in varying the number of holes. The crossover from small doping to the overdoped case needs more careful scrutiny. But again our results suggest that the feature indeed exists.

One can also question whether the small systems we have investigated can exhibit the physics of spin–charge decoupling. It is difficult to answer this question quantitatively. However the recent numerical work by Jagla and co–workers [13] clearly demonstrates the phenomenon of spin–charge decoupling in a finite size system.

To summarize, we have addressed the question of the effect of the interlayer coupling $t_\perp$ on in–plane superconducting correlations (SPX) in the context of the $t-J$ model with the constraint on double occupancy imposed exactly. Our results for two holes in 4+4, 5+5 and 6+6 sites show that these correlations are increased by $t_\perp$. This happens because of the rapid increase of the long–range correlations with $t_\perp$. This feature disappears as we increase the number of holes or when the constraint on double occupancy is relaxed. The former suggests the existence of a crossover point between small and heavy doping regimes based on this contrasting behavior of SPX as a function of $t_\perp$. Work is currently in progress in evaluating dynamic correlation functions and the effect of a magnetic field on these correlations.

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Figure Captions

1. SPX for the $4+4$ cluster. The dashed line represents the behavior of SPX when the constraint on double occupancy in the $t-J$ model is relaxed.

2. SPX for the $5+5$ cluster.

3. SPX for the $6+6$ cluster.

4. Long range correlations in $6+6$ cluster with two holes (see text for explanations).