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Superconducting Instability in the Large-U Limit of the Two-Dimensional Hubbard Model

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We have investigated numerically the pairing instabilities of Gutzwiller wavefunctions. These are equivalent to a certain form of the resonant valence bond wavefunction. The case considered is a nearly half-filled two dimensional band with interactions given by a Hubbard model with large on-site Coulomb interactions. We find that the paramagnetic normal state is unstable to d-wave pairing but stable against s-wave pairing. The antiferromagnetic state is marginally stable against both types of pairing. These results can be explained as an interference effect resulting in enhanced antiferromagnetic spin correlation in the paired state.

I. Introduction

The unexpected discovery of high T_c superconductivity in the Cu-oxides by Bednorz and Müller [1] has aroused unprecedented interest. Right at the outset Anderson [2] proposed that the superconductivity originated in hole-like carriers introduced by doping in a Mott insulating state and developed out of a resonant valence bond (RVB) spin state. There are numerous other proposals; for a discussion of these see Refs. 3, 4. The RVB state was proposed previously by Anderson [5] as a description of the groundstate of a frustrated 2-dimensional Heisenberg lattice (e.g. a triangular lattice). In La_2CuO_4 and related materials the lattice is essentially a 2-dim square lattice so that the questions of the competition between the paramagnetic (PM) RVB and antiferromagnetic (AF) states as well as the instability of both states to superconductivity when holes are introduced needs to be investigated. In this paper we address the latter question.

Several approaches have been taken by others. All are based on transforming the original Hubbard Hamiltonian to an effective Hamiltonian which acts in the restricted Hilbert space with no doubly occupied sites. In one type of approach this effective Hamiltonian is treated by a mean field method involving a Gor'kov factorization of the Heisenberg spin-spin coupling term [6–8]. In particular Baskaran, Zou and Anderson and Ruckenstein, Hirschfeld and Appel show that in the mean field theory a RVB state can be obtained at 1/2-filling and a superconducting state in the presence of holes. Zhang [9] has shown that this theory predicts that the "extended s-wave" [10] and the d-wave state have the same critical temperature at 1/2 filling but the d-wave has a higher T_c at lower electron densities. However, these calculations can be questioned since the condition that the system must stay within the restricted Hilbert space without double occupancy is only approximately obeyed. The physics of the constrained and unconstrained systems can be expected to be quite different.

Recent work by Kivelson, Rokhsar and Sethna [11] and by Zou and Anderson [12] proposes that a Bose condensation of holes in the RVB state is to be identified with the superconducting transition.

Another approach is based on looking for a bound state of two holes in an AF ordered lattice. Such binding has been investigated by Takahashi for a Heisenberg lattice [13] using a moment method. Hirsch [14] has considered the related problem of holes in the oxygen states but strongly coupled to the Cu-spins. This latter model has been put forward by Emery [15].

It is, however, possible to investigate a number of these questions by using the variational Monte-Carlo (MC) method. This method allows accurate numerical evaluation of expectation values and matrix elements in wavefunctions with strong local correlations. For example, it has been used to evaluate Gutzwiller wavefunctions for the Hubbard Hamiltonian in 1-dim by Horsch and Kaplan [16], by Yokoyama and Shiba (YS) [17] in 2-dim and for the Anderson Hamiltonian by Shiba [18]. Previously we pointed out that it was better to work with the effective Hamiltonian when the onsite Coulomb interaction was large and examined many properties of the Gutzwiller wave-function in 1-dim [19]. In this approach the conditions on the Hilbert subspace are fully obeyed. Very recently YS have used this method to investigate the stability of the PM Gutzwiller wavefunction against long range AF ordering and indeed find it is only in the presence of a finite density of holes that the PM state is stable. These authors and Anderson et al. [20] point out that the Gutzwiller state has the form of an RVB state – a point we return to below. In this paper we examine the stability of both PM and AF wavefunctions to Cooper pairing in the s- and d-wave channels. Our key result is that a d-wave pairing is favored in the PM state but not in the AF state. s-wave pairing is not favored. Note a number of authors, Lee and Read [27], Ohkawa [22], and Cyrot [8] have proposed d-wave pairing in high-T_c superconductors, the first-named authors approaching the problem from smaller values of U, the onsite Coulomb interaction parameter. A scaling theory starting from weak coupling also finds d-wave superconductivity to be favorable, as shown by Schulz [23]. Miyake et al. [24], Scalapino et al. [25], Cyrot [26], and Lavagna et al. [27] have all proposed d-wave pairing in heavy-fermion systems.

II. Method

We consider a nearly-half-filled band of electrons described by a Hubbard model with $t/U \ll 1$, where t is the overlap integral between nearest neighbor sites. We make a canonical transformation to a representation where doubly occupied sites are eliminated, to first order. Details of this procedure can be found in Ref. 19.
The effective Hamiltonian is

$$H_{\text{eff}} = -t \sum_{\langle ij \rangle} (1-n_{i-\sigma}) C^{+}_{i\sigma} C_{j\sigma} (1-n_{j-\sigma}) + \text{h.c.} + 4(t^2/U) \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - n_i n_j/4) \quad (1)$$

in this representation, neglecting terms of higher order in the hole density and $t/U, n_i = \sum_\sigma n_{i\sigma}$. The kinetic energy comes from the hopping of the holes only and there is an AF coupling between the electron spins. The Gutzwiller wavefunction is defined as

$$|\psi_G\rangle = P_{D=0}|\psi_B\rangle = \prod_i (1-n_{i\uparrow} n_{i\downarrow})|\psi_B\rangle \quad (2)$$

where $|\psi_B\rangle = \prod_{|\mathbf{k}|<k_F,\sigma} C^{+}_{\mathbf{k}\sigma}|VAC\rangle$ is the band ground state and $P_{D=0}$ is a projection operator which eliminates all spatial configurations with doubly occupied sites. It has been shown [19] that this wavefunction has a very favourable spin correlation energy: for the half-filled case, e.g., $\langle\psi_G|\,\mathbf{S}_i \cdot \mathbf{S}_j|\psi_G\rangle = -0.442$ is within about 0.2% of the exact value in one-dimension, and in two dimensions the value of -0.275 is also lower than the value -0.25 in the Néel state. The kinetic energy in the less-than-half-filled case also compares very well with ground state estimates by other methods. We are therefore confident that the Gutzwiller wavefunction is an excellent variational candidate for the lowest energy state within the class of states lacking long-range magnetic order. It represents a Fermi liquid with a Fermi surface (at general values of the filling) which satisfies the Luttinger theorem. It has been pointed out by YS (also see Ref. 20) that it is also identical to a RVB state of Anderson [2]. We repeat the argument of YS here. A general unrenormalized RVB state may be written as

$$P_{D=0}\Big(\sum_{\mathbf{k}} a(\mathbf{k})\, C^{+}_{\mathbf{k}\uparrow}\, C^{+}_{-\mathbf{k}\downarrow}\Big)^{N/2}|VAC\rangle \quad (3)$$

with $\sum_k a(\mathbf{k}) = 0$. A particular choice [2] is $a(\mathbf{k}) = 1$, $k < k_F$ and $a(\mathbf{k}) = -1$, $k > k_F$. (We discuss a different RVB state, where $a(k)$ has a different form, in Sect. IV). The Gutzwiller state corresponds to $a(k) = 1$, $k < k_F$; $a(k) = 0$, $k > k_F$. However, adding a constant to $a(k)$ only changes the weight of a spatial configuration if it contains doubly occupied sites. Since these are projected out at the end anyway, the two forms for $a(k)$ lead to wavefunctions which differ only by a normalization factor. The same argument implies that the extended s-wave states, superconducting states in which $a(k)$ changes sign, are not distinct from ordinary s-wave states in projected wavefunction. YS have given a generalization of $|\psi_G\rangle$ which can have AF long range order. In Eq. (2), we substitute $c^{+}_{k\sigma}$ by $u_k c^{+}_{k\sigma} + \text{sgn}(\sigma) v_k c^{+}_{k+Q\sigma}$ where $\mathbf{Q} = (\pi, \pi)$. $2u_k^2 = 1 - \varepsilon_k/(\varepsilon_k^2 + \Delta^2)^{1/2}$ and $u_k^2 + v_k^2 = 1$, where ε_k is the band energy, $\varepsilon_k = -2t(\cos k_x + \cos k_y)$, and Δ is the gap energy. Only the lower band states are occupied. For

$\Delta=0$, this reduces to the PM Gutzwiller state given above. For the half filled band, in one dimension, $\Delta=0$ is the stable state, whereas on the square lattice in two dimensions $\Delta>0$ and there is AF long-range order. The relative stability of the AF ordered state with $\Delta>0$ and the PM state with $\Delta=0$ may be influenced by the dimerization of phonons. To take this effect into account would require us to enlarge the Hilbert space and we will not consider that. Other effects which can influence the normal-state stability are next-nearest neighbor coupling and the presence of holes. We will investigate the stability of both normal PM and normal AF states against Cooper pairing.

This is done by the MC method, which yields the relevant operator expectation values. Technical details are given in Refs. 16, 18, and 19. The electrons are placed on a lattice of L sites with periodic boundary conditions. L is chosen in the form (j^2+1) where j is an odd integer. This assures that the half-filled ground state is not degenerate, and further that the Fermi surface consists of $4k$-values. This situation is illustrated in Fig. 1 for $L=26$. We now ask the question: Is this Fermi sea unstable to Cooper pair formation? To find out, we take the number of electrons to be $L-2$, leaving two holes free to move the through the lattice. The ground state in the manifold with zero total z-component of magnetization is then sixteen fold degenerate in the non-interacting case. If it is possible to lower the energy by constructing a coherent combination of Gutzwiller states in this manifold which lowers the total energy including interactions, then an instability is indicated. It should be stressed, however, that the present calculation does not yield a good estimate for the binding energy, since no real attempt to optimize the wavefunction is made. Instead, a specific form for the $a(\mathbf{k})$ is chosen in which $a(\mathbf{k})$ differs from the ground state configuration only for the uppermost set of $\{\mathbf{k}\}$ at the Fermi surface. Further optimization would involve us with more Slater determinants and is hindered by calculational limitations. Therefore, the results in this paper should not be interpreted as relating to the actual superconducting state. Rather, they are to be interpreted in the spirit of Cooper's calculations of pair binding, indicating only whether or not the normal state is stable with respect to the formation of superconducting correlations. A poor estimate of the actual superconducting condensation energy is thereby obtained. (The Cooper binding energy and the BCS condensation energy differ by an exponential factor in the case of conventional superconductivity.)

The wavefunctions we choose are parametrized by $c(\mathbf{k}_i)$, $i=1, 2, 3, 4$, where $|\mathbf{k}_i|=k_F$, and $\mathbf{k}_1=(k_x, k_y)$, $k_2=(-k_y, k_x)$, $\mathbf{k}_3=(-k_x, -k_y)$, $\mathbf{k}_3=(k_y, -k_x)$. (See Fig. 1) We then write

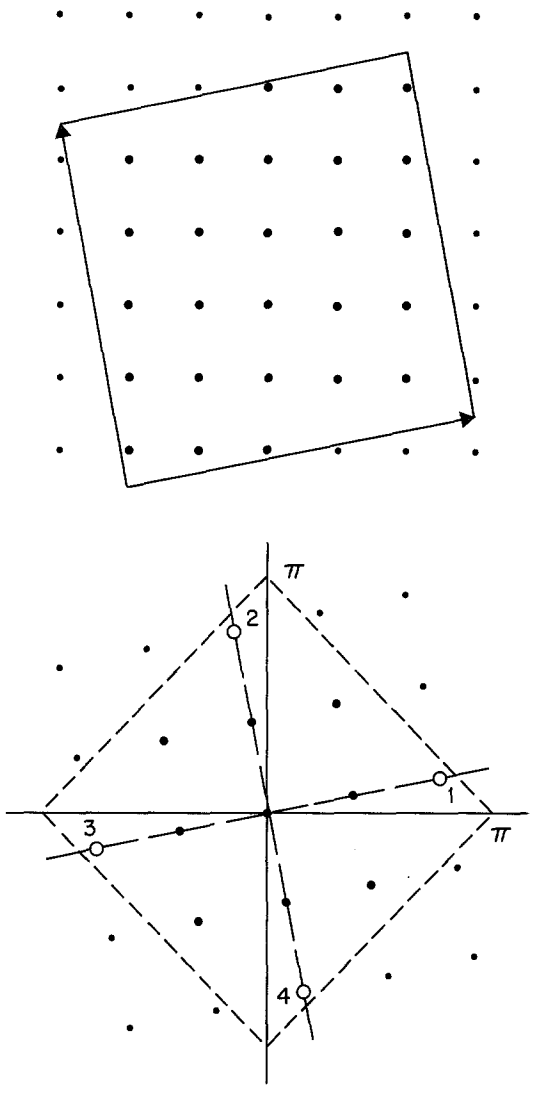

Fig. 1. The upper figure shows the sites in real space used in our calculation for total number of sites $L=26$ enclosed in the square. Periodic boundary conditions on the wavefunction are used, with periods shown by the arrows. When this lattice is half filled with electrons, the non-interacting ground state is non-degenerate with the Fermi surface shown in the lower figure as a dashed square in momentum space. To form the various wavefunctions described in the text, the $\mathbf{k}$ states 1 through 4 are taken to be empty

$$|\Psi\rangle=c_1|\Psi_G^1\rangle+c_2|\Psi_G^2\rangle+c_3|\Psi_G^3\rangle+c_4|\Psi_G^4\rangle, \tag{4}$$

where $|\Psi_G^1\rangle$ is the Gutzwiller state (PM or AF) with the wavevectors $\mathbf{k}_1\uparrow$ and $-\mathbf{k}_1\downarrow$ vacant, etc. The s-state is given by $c_1=c_2=c_3=c_4=1$, and we will consider the d-state given by $c_1=c_3=-c_2=-c_4=1$. Their energies are to be compared to those of an incoherent combination of the same $|\Psi_G\rangle$, which represents the normal state wavefunction. The energy difference is the binding energy of the two holes in the variational wavefunction.

To obtain reliable results in two dimension it is necessary to do calculations for several different lattice sizes and extrapolate to the infinite lattice limit. All our results are plotted in this way. It is also very important to minimize statistical errors. We are calculating energy differences so that it would appear to be necessary to subtract two numbers which are much larger than their difference. The only feasible way to accomplish this with acceptable error is to calculate both energies in a *single* MC run. One can take advantage of the freedom within the MC method of partitioning the summand into two factors one of which determines transition rates, and the other is then measured. A full explanation is given in the context of calculating off-diagonal operator expectation values in Ref. 19. This enables us to compute the difference between normal and superconducting states directly, without the need to subtract quantities which have individually a large uncertainty.

III. Results and Physical Interpretation

To set the stage for our results, we first review the underlying energetics of the PM and AF states. For the half-filled band, the Hamiltonian (1) reduces to a Heisenberg Hamiltonian

$$H_H = 4(t^2/U) \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - n_i n_j/4) \tag{5}$$

where $n_i n_j = 1$.

The energies calculated for the half-filled square lattice by YS are given in the table, and show that the AF state is the stable one. If we now inject a small number of holes into the system, the full Hamiltonian (1) must be used. If we keep in mind that the energy per bond is $4t^2/U$ times $(\mathbf{S}_i \cdot \mathbf{S}_j - 1/4) \approx 2t^2/U$, then we see from the table that the change in spin energy per hole is much larger than $8t^2/U$, which is the number one might naively expect from bond-breaking arguments. The kinetic energy, on the other hand, is not very different from that of a free hole. The holes are completely delocalized and therefore very efficient at disturbing the bonds between the spins. We aim to show that this tendency can be reduced by pairing the holes in d-wave configurations.

We compute first the spin correlation energy gain from the Cooper pairing:

$$\Delta E_s = \langle \psi_S | H_H | \psi_S \rangle - \langle \psi_N | H_H | \psi_N \rangle \tag{6}$$

for a series of lattices having up to 122 sites, with H_H given by Eq. (5). Note that in the thermodynamic limit we can ignore the change in the expectation value of the $n_i n_j$ term. The change in kinetic energy has also been calculated. We have found in every case that this change was very small: zero to within the accuracy of the calculation ($\sim 1\%$). This is partly due to the fact that the four **k**'s we allow for the Cooper pair are all degenerate, but this choice does not preclude kinetic energy airising from the relative motion in the pair. That this energy is very small indicates stability of the d-wave state for a wide range of values of the parameters t and U. For the wavefunction used here, the change in spin energy may be taken as the total energy change.

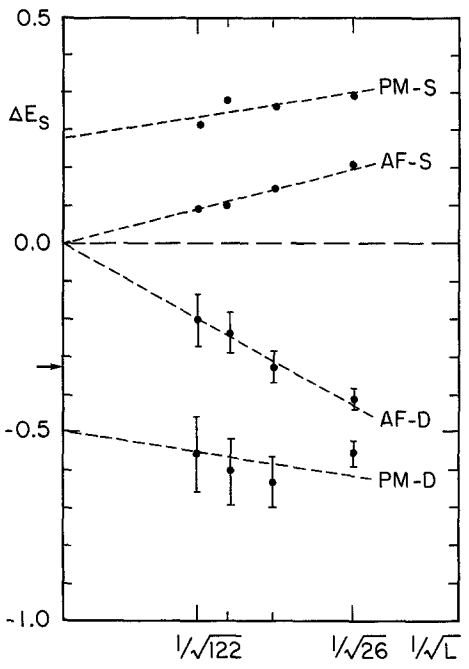

Fig. 2. Binding energies in units of $4t^2/U$ for various superconducting wavefunctions. PM$-S$ and AF$-S$ denote the s-wave states formed from paramagnetic and antiferromagnetic normal states, respectively. PM$-D$ and AF$-D$ are the corresponding d-wave states. The binding energy is the difference between the spin correlation energies in the superconducting and normal states. A negative result implies that the normal state is unstable. See Eq. (6) for a definition of ΔE_s

Let us discuss first the paramagnetic normal state. Figure 2, together with the extrapolated numbers in the table, Rows 4 and 5, shows that there is a strong tendency toward binding in the d-wave channel. To understand the magnitude of the binding, again take a naive localized picture for the holes. The effect of putting two holes at random in a half-filled PM lattice (see Table 1, Row 2) is to break eight bonds, costing an energy $(32t^2/U)(\mathbf{S}_i \cdot \mathbf{S}_j - 1/4) \approx 17t^2/U$ relative to the half-filled state. The energy saved by putting the two holes in the d-wave paired state relative to the normal state thus corresponds to about 1.5 bonds. This is a large number. The pairing energy gained in this way is larger than one could get by localizing

Table 1. Summary of data and results. PM and AF denote paramagnetic and antiferromagnetic wavefunctions. Row 1 is the kinetic energy of a single hole introduced into a half-filled lattice. Row 2 is the spin correlation energy per bond in the half-filled lattice. Row 3 is the change in this quantity summed over all bonds when a hole is introduced into the half-filled state. Row 4, 5 are the change in spin energy when pairing correlations are introduced into the normal state wavefunctions, taking a Heisenberg interaction. Rows 6, 7 are the same change if the x and y components of the interaction are omitted. Rows 8, 9, and 10 are the nearest neighbor hole-hole correlation functions. The numbers in Rows 2 and 3 are taken from Ref. 17. In rows 2 through 7, to convert to energy units, multiply by $4t^2/U$, the energy per bond

	PM	AF
1. Kinetic energy/hole	$-2.72\,t$	$-2.52\,t$
2. $\sum_{\langle ij\rangle} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$/bond	-0.27	-0.32
3. $\sum_{\langle ij\rangle} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$/hole	$+19.2$	–
4. ΔE_s for d-wave	-0.5 ± 0.2	0.0 ± 0.05
5. ΔE_s for s-wave	$+0.3 \pm 0.1$	0.0 ± 0.05
6. ΔE_s^z for d-wave	-0.17 ± 0.07	-0.22 ± 0.1
7. ΔE_s^z for s-wave	-0.1 ± 0.03	$+0.08 \pm 0.02$
8. g in normal state	1.1 ± 0.1	1.6 ± 0.2
9. g in d-wave state	1.1 ± 0.1	6.9 ± 0.2
10. g in s-wave state	1.1 ± 0.1	0.0 ± 0.2

the holes on adjacent sites in the pair, ignoring phase relationships, and arguing that the number of broken bonds is thereby reduced. This only saves one bond and of course would cost considerable kinetic energy in the relative hole motion, far more than is present in our wavefunction.

The conclusion is inescapable that there is quantum-mechanical interference associated with the phases of the hole wavefunctions which gives rise to a surprisingly extensive rearrangement of the spins. Any picture, such as the fewer broken bonds picture, which ignores these phases, will not lead to the large energy actually involved. Further evidence for this point of view is offered by the data for the s-wave state, for which the effective interaction is positive. We discuss the interference question and the difference between s- and d-wave states in more detail at the end of this section.

The AF normal state, in contrast to the PM-state, is marginally stable to both s- and d-wave superconductivity. Figure 2 shows that there is no energy associated with the change due to Cooper pairing in the infinite-lattice limit. This is in agreement with the work of Takahashi [13] who studied the problem of two holes in an AF background by a variational method, and found no binding energy. In Fig. 3 we plot the correlation of only the z-components of spin ΔE_s^z and the extrapolations are given in the table, Rows 6 and 7. This would be proportional to the

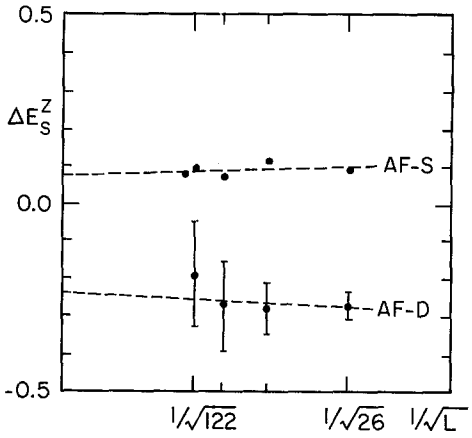

Fig. 3. Binding energies for the AF superconducting states for an Ising interaction in units of the Ising coupling constant. Error bars for the s-wave state have been omitted for clarity. For each lattice size they are the same as those for the d-wave state

total energy if the interactions were Ising-like. (This is only possible if there is very strong spin orbit coupling in the two-dimensional layer. For copper and oxygen that is very unlikely.) It is interesting that binding can take place for this case but only for the d-wave pairing. This indicate that arguments for binding [8, 14] based on the ability of the AF lattice to heal itself after two holes pass through, but not one, are valid for the Ising case. The Heisenberg interaction, on the other hand, gives the lattice without holes the ability to heal itself because of spin flip terms and apparently this is enough to unbind the pairs. This effect shows up in the nearest neighbor hole-hole correlation function:

$$g = L \sum_{\langle ij\rangle} \langle \psi | (1-n_i)(1-n_{j'}) | \psi \rangle. \tag{7}$$

This measures the probability that the two holes are adjacent and is normalized to unity for random positioning of the holes. For the three AF cases it is plotted in Fig. 4, and results given in the table, Rows 8–10. There is already an enhancement from randomness in the normal state, as was found previously in the one-dimensional normal PM state [19]. There is a very large enhancement in the d-wave case, which is the right superconducting wavefunction for Ising interaction. Some of the condensation energy must clearly come from the fewer broken bonds effect for this case, as well as from the absence of a healing effect. The s-wave wavefunction has *less* chance for adjacent holes even than the normal state; it seems likely that this accounts for at least part of the negative binding energy of this state.

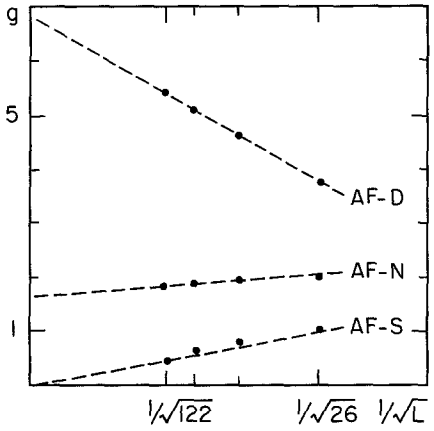

Fig. 4. The nearest-neighbor hole-hole correlation function is plotted as a function of the lattice size L for the AF states. A value of 1 corresponds to random placement of the holes

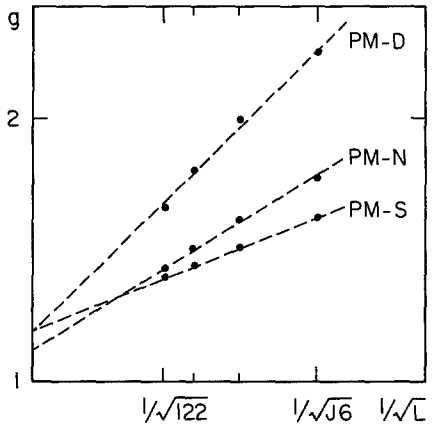

Fig. 5. Hole-hole correlation function for different lattice sizes for the PM states

The PM hole-hole correlation functions are plotted in Fig. 5. Here there are no indications that the spatial correlations are enhanced in the superconducting phase, either in the stable d-wave state, or in the unstable s-wave state. The phasing of the hole wavefunctions is clearly the crucial mechanism at work. This is a far more subtle physical phenomenon than the fewer broken bonds effect, but our results show clearly that this completely quantum-mechanical mechanism is the dominant factor at work in producing the d-wave instability for the PM system. Strong spatial correlations are not expected since we have paired holes in the outermost shell of $\mathbf{k}$ states, which corresponds to a long correlation length. However, we have demonstrated that such correlations are not crucial for having a large spin correlation energy. This fact also means that the pairing mechanisms is likely to remain effective even when the long-range Coulomb interaction is added to the problem. This would change the Hamiltonian of Eq. (5), e.g., the coefficient of the final term would become positive. It is necessary to consider this effect, since the usual downward renormalization of the long-range Coulomb pseudopotential in electron-phonon superconductors due to mismatch of time scales will not take place in the present system. If the pairs are not tightly bound in space, as indicated by our results, then the long range repulsion may not greatly suppress the pairing instability.

The interference effect arises as follows. Consider a spin configuration which is AF ordered. Let the up (down) spins belong to the set $\mathbf{R}_i$ ($\mathbf{R}'_i$), where $R_{ix}+R_{iy}=$even, $R'_{ix}+R'_{iy}=$odd. The lattice constant is taken equal to one. The weight of such a configuration in the PM superconducting Gutzwiller wavefunction is proportional to

$$|c_1 \Gamma_1^{\uparrow}\Gamma_1^{\downarrow}+c_2\Gamma_2^{\uparrow}\Gamma_2^{\downarrow}+c_3\Gamma_3^{\uparrow}\Gamma_3^{\downarrow}+c_4\Gamma_4^{\uparrow}\Gamma_4^{\downarrow}|^2 \tag{8}$$

where $\Gamma_1^{\uparrow}$ is defined as the Slater determinant whose elements are of the form $\exp(\mathrm{i}\mathbf{k}_j\cdot\mathbf{R}_i)$ with $\mathbf{k}_j$ the set of all $\mathbf{k}$'s in the Fermi sea *except* $\mathbf{k}_1\cdot\Gamma_1^{\downarrow}$ is similar; it contains instead the R'_i and excludes $-\mathbf{k}_1$ instead of $\mathbf{k}_1$. Now, with the spin configuration fixed, compare $\Gamma_1^{\uparrow}$ and $\Gamma_2^{\uparrow}$. They differ only in one column, namely $\Gamma_1^{\uparrow}$ includes a column $\exp(\mathrm{i}\mathbf{k}_2\cdot\mathbf{R}_i)$, while $\Gamma_2^{\uparrow}$ includes a column $\exp(\mathrm{i}\mathbf{k}_1\cdot\mathbf{R}_i)$. The two matrices are otherwise the same. However

$$\mathbf{k}_2=\mathbf{k}_1+\mathbf{Q}, \qquad \mathbf{Q}\xrightarrow[L\to\infty]{}(\pi,\pi).$$

Hence

$$\exp(\mathrm{i}\mathbf{k}_2\cdot\mathbf{R}_i)=\exp(\mathrm{i}\mathbf{k}_1\cdot\mathbf{R}_i)\cdot\exp[\mathrm{i}\pi(R_{ix}+R_{iy})]$$
$$=\exp(i\mathbf{k}_1\cdot\mathbf{R}_i)$$

and $\Gamma_1^{\uparrow}=\Gamma_2^{\uparrow}$. Similarly, $\Gamma_1^{\downarrow}=-\Gamma_2^{\downarrow}$. Therefore, to maximize the amplitude (8), we need $c_1=-c_2$. It is clear that this argument can be extended to c_3 and c_4 and leads directly to the d-wave state. The s-wave $c_1=c_2=c_3=c_4$, on the other hand, gives destructive interference for the AF configuration and is therefore very unfavorable. The normal state wavefunction by definition has no interference; it therefore lies between the s- and d-wave states in energy. The relative amplitudes are in fact 4:2:0 for d-wave:normal:s-wave. In the PM case the configuration $R_{ix}+R_{iy}=$odd, $R'_{ix}+R'_{iy}=$even has the same weight as the above configuration and then $\Gamma_1^{\uparrow}=-\Gamma_2^{\uparrow}$, $\Gamma_1^{\downarrow}=\Gamma_2^{\downarrow}$, etc., the d-wave interference is also constructive. The d-wave state is still a spin singlet and thus this argument, which in itself ensures only that there will be a large gain for the $\langle S_i^z S_j^z\rangle$ energy, applies also to the x and y parts of the spin-spin interaction. When we apply the argument to the AF wavefunctions there is a crucial differ-

ence. These are not spin singlets. Even though the d-wave gains energy in the z-component of the interaction, it is permitted to, and does, lose energy in the x- and y-(spin flip) components. The net gain turns out to be zero.

It is evident that a global change in amplitudes is involved in the comparison of the various states. This is not surprising since, in the wavefunctions considered, the holes are delocalized. This is probably a good approximation in spite of the fact that, in the AF lattice with a single hole, formation of a spin polaron is favored.

IV. Discussion

We would now like to compare our results in some detail to previous work. Hirsch [14] has proposed a binding mechanism within a model of Cu – O layers with holes on the 0 sites. His arguments apply also to a simple Hubbard model on a square lattice, and an AF ground state for the half-filled case. In the regime where $J_z > J_x, J_y$, the J's denoting the effective AF couplings he derives a linear attractive potential between holes for short separations based on the observation that the number of broken bonds in the AF lattice is proportional to the separation. This is consistent with our results: we also find binding in the $J_z > J_x, J_y$ system, and a concomitant enhancement of the hole-hole correlation. Contrary to Hirsch, [14] however, we find pairing only for d-wave, not s-wave, states. Our results also indicate that the binding energy becomes zero rather than remaining finite for the isotropic $J_x = J_y = J_z$ AF coupling. This is also found by Takahashi [13].

Our results may also be compared to the RVB picture, because, as noted above, the Gutzwiller state is a form of RVB state. We should point out, however, that we found in previous work [19] that the insulating half-filled state did not have a linear dispersion relation in one dimension. If we make the identification of a "spinon" with a change in the $\mathbf{k}$-distribution in (2) by a shift of one $\mathbf{k}$ from below to above the pseudo Fermi surface by an amount $\Delta\mathbf{k}$, then this excitation was found to have an energy proportional to $(\Delta\mathbf{k})^2$. This is in contradiction to the mean-field result of Zou and Anderson [22]. It is important also to keep in mind that excitations greated in this way are not orthogonal to one another or to the ground state.

In the less-than-half-filled case, the normal state considered in this paper is a Fermi liquid with a Fermi surface enclosing $N/2$ $\mathbf{k}$ values, where N is the number of electrons. It is this state which is unstable to d-wave superconductivity. If, on the other hand, one takes the view that the introduction of holes into the insulating state creates topological solitons but leaves the $\mathbf{k}$-distribution fixed, then the number of $\mathbf{k}$'s involved in the wavefunction exceeds $N/2$. This is perfectly possible within the expression (3) for the variational wavefunction. It has not yet proved possible to investigate such a function with our numerical technique. With regard to Bose condensation in general, we have concentrated on pairing instabilities, but nothing in our results rules out other (perhaps more exotic) instabilities of the Fermi liquid normal state.

It would be premature to compare our results in a serious way with experiment, since they relate to a model which may well be oversimplified. We only wish to point out that La_2CuO_4 has been found to be antiferromagnetic under some circumstances [28]. Antiferromagnetism and superconductivity never seem to occur in the same sample. This agrees with our finding that the PM, but not the AF, wavefunction has a superconducting instability in the presence of the physically realistic isotropic spin-spin interaction.

The calculations presented here can be extended in several directions. d-wave states of different symmetry should be investigated, as well as more general superconducting wavefunctions in which the momentum distribution is more strongly modified. Particularly interesting would be to discover what effect doping (N/L ratio, in our notation) has on the superconducting instability.

In summary, we have investigated the properties of variational Gutzwiller-type wavefunctions for the Hubbard model on a square lattice, concentrating on the non-degenerate nearly half-filled band. For wavefunctions which have AF long range order no energy is gained by condensation into a superconducting state. If an Ising-like AF coupling is added to the effective Hamiltonian, then d-wave superconductivity is obtained. Paramagnetic wavefunctions are unstable to d-wave superconductive pairing. s-wave superconductivity is unfavorable for all possible normal states. The main physical effect at work is constructive interference between different hole wavefunctions in the d-wave state.

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