Dynamical pair susceptibilities in the t-J and Hubbard models

Elbio Dagotto
Institute for Theoretical Physics, University of California at Santa Barbara, Santa Barbara, California 93106

Jose Riera and A. P. Young
Physics Department, University of California at Santa Cruz, Santa Cruz, California 95064
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We study dynamical properties of two holes in the t-J, t-J_z, and Hubbard models using exact diagonalization techniques on small clusters. For the three models we found that the ground state of two holes has d-wave symmetry. Studying the dynamical d-wave pairing susceptibility at zero momentum, we observed a quasiparticle-like peak at the bottom of the spectrum in a broad region of parameter space. The lowest-energy p-wave state is close in energy to the d-wave ground state, and they both behave qualitatively similarly, while the lowest-energy states of the s-wave and extended-s-wave subspaces have higher energies and present no quasiparticle peak. The ground-state energy of two holes in the t-J model scales with J as a power law. Binding energies for different symmetries as well as dynamical properties for nonzero momentum are also discussed.

There is considerable interest in the analysis of strongly correlated electronic systems since it is believed that variations on the Hubbard or Heisenberg models in two dimensions may contain the basic ingredients for understanding the mechanism leading to a superconducting phase in the recently discovered high-T_c materials.[1] Since the appropriate region of parameter space seems to be the strong-coupling regime, then standard mean-field or weak-coupling expansions are not reliable and numerical methods (or more sophisticated analytic approaches) are necessary to study static and dynamic properties of the Hubbard model. In this paper we concentrate on the dynamics of two holes in these strongly correlated systems.

The numerical study of dynamical properties of the t-J model was initiated[2,3] recently in the one-hole subspace. It was found that there is a quasiparticle-like peak at the bottom of the spectrum in a wide range of values of $J/t \geq 0.2$ and that its energy scales like $J^{\sim 0.7}$ for small J. This is compatible with the "string picture" prediction ($J^{0.66}$) in the Ising limit[4] where the movement of the hole creates a string of overturned spins whose energy grows proportional to J and the length of the path of the hole. For large paths the problem is well approximated by a Schrödinger equation with a linear potential from where the J dependence of the results can be obtained exactly by a change of variables. The numerical results[2,3] suggest that even for a Heisenberg model where quantum fluctuation can in principle destroy the string of overturned spins, this scenario is still valid at least at low energies (the effective potential may be linear at short distance but flat at large distance). Other states have been identified in the spectrum corresponding to excited levels of the hole in a linear confining-like potential. This result would have been very difficult to obtain without numerically analyzing the spectral function of the hole.

The static ground-state properties of the two-hole subspace of the t-J model have been studied numerically by several groups.[5-7] On a 4×4 lattice it was found that holes attract in the t-J model forming bound states in a finite region of J/t, while for large J/t phase separation takes place.[5,8] This is reasonable, since for static holes the number of broken bonds should be minimized to reduce the antiferromagnetic energy of the spins favoring the clustering of holes. In the context of the one-band Hubbard model the binding energy E_B has been also evaluated using a new Monte Carlo technique[9] on a 4×4 lattice and exact diagonalization techniques on an eight-site lattice.[5] There it was found that E_B is negative near $U \sim 4-5t$ but small in absolute value, and it is not clear if that result will survive the bulk limit. The symmetry of the two-hole bound state was found in these models using different methods. Diagrammatic,[10] variational,[11] and exact diagonalization techniques for the t-J model,[5,6] and Monte Carlo[12] and spin-bag[13] studies for the Hubbard model all suggest that the symmetry of the state is d wave.

The purpose of this paper is to study the dynamical properties of the two-hole subspace of the t-J and Hubbard models. In particular, we want to analyze if there is a quasiparticle in the spectrum, how close in energy are the other states with different symmetries under rotation, and if the above mentioned string picture valid for one hole can be extended to two holes. Another motivation for our analysis is that spectral functions are being measured experimentally and thus we can in principle compare our predictions with the behavior of the new superconducting materials. The pairing susceptibilities that we present below *may* be relevant in the superconducting regime while the one-hole spectral functions presented in Refs. 2 and 3 are important at low doping of holes before superconductivity occurs.

The t-J model is defined by the Hamiltonian[14]

$$H = J \sum_{\mathbf{i},\hat{\delta}} (\mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{i}+\hat{\delta}} - \tfrac{1}{4} n_{\mathbf{i}} n_{\mathbf{i}+\hat{\delta}}) - t \sum_{\mathbf{i},\hat{\delta},\sigma} (\bar{c}^{\dagger}_{\mathbf{i},\sigma} \bar{c}_{\mathbf{i}+\hat{\delta},\sigma} + \mathrm{H.c.}) , \quad (1)$$

where the notation is standard and $\bar{c}^{\dagger}_{\mathbf{i},\sigma}$ is a hole operator acting in the space where there is no double occupancy. We work on a two-dimensional lattice with periodic boundary conditions. Note that in Eq. (1) we included a term $\frac{1}{4} n_{\mathbf{i}} n_{\mathbf{i}+\hat{\delta}}$ which appears in the derivation of the t-J model from the Hubbard model.[5] For zero and one holes this term is a constant, but not for more holes. In the strong-coupling expansion of the Hubbard model there are other hopping terms that for simplicity we do not include in Eq. (1), but they will be discussed below. The t-J_z model is defined from Eq. (1) simply by replacing $\mathbf{S}$ by S^z in the spin-spin interaction. The other model we studied was the one-band Hubbard model defined as

$$H = -t \sum_{\mathbf{i},\hat{\delta},\sigma} (c^{\dagger}_{\mathbf{i},\sigma} c_{\mathbf{i}+\hat{\delta},\sigma} + \mathrm{H.c.}) + U \sum_{\mathbf{i}} (n_{\mathbf{i},\uparrow} - \tfrac{1}{2})(n_{\mathbf{i},\downarrow} - \tfrac{1}{2}) , \quad (2)$$

where again the notation is standard. For the t-J and t-J_z models we worked on 4×4 lattices, while for the Hubbard model the size of the Hilbert space restricted our work to a $\sqrt{10}\times\sqrt{10}$ lattice, the same as that used in Ref. 3 for one hole. The dynamical properties of the two-hole subspace can be obtained by studying the pairing correlation functions

$$P(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle \Delta^{\dagger}(t) \Delta(0) \rangle , \quad (3)$$

where the expectation value is taken in the ground state with no holes. Here the pairing operator for the t-J model is defined as

$$\Delta^{\dagger} = \sum_{\mathbf{k}} f(\mathbf{k}) \bar{c}^{\dagger}_{\mathbf{k},\uparrow} \bar{c}^{\dagger}_{\mathbf{Q}-\mathbf{k},\downarrow} , \quad (4)$$

where the sum is over all momenta $\mathbf{k}$ of the lattice weighted by the function $f(\mathbf{k})$ which defines the symmetries under rotation of the operator while $\mathbf{Q}$ is the total momentum of the two-hole system. In what follows we will mainly discuss the special case $\mathbf{Q}=(0,0)$, where we have considered four possibilities: if $f(\mathbf{k})=\cos(k_x) - \cos(k_y)$ then we study a d wave, $f(\mathbf{k})=\cos(k_x)+\cos(k_y)$ corresponds to an extended s wave, and $f(\mathbf{k})=\sin(k_\nu)$ corresponds to a p_ν wave ($\nu=x,y$). The d- and s-wave states are singlets, while the p wave is a triplet. For the Hubbard model we have considered also the possibility of an on-site s wave defined by $f(\mathbf{k})=1$ [of course for this model the hole operators in Eq. (4) are replaced by electron operators]. If higher harmonics are introduced in the definition of $f(\mathbf{k})$, then the two holes can be located at distances larger than only one lattice spacing, but we have not considered that possibility in this paper.

As numerical technique we used a Lanczos method adapted to the evaluation of dynamical properties. According to standard linear response theory $P(\omega)$ can be written as

$$P(\omega) = -\mathrm{Im} \left\{ \langle \psi_0 | \Delta \frac{1}{\omega + E_0 + i\epsilon - H} \Delta^{\dagger} | \psi_0 \rangle \right\} , \quad (5)$$

where $|\psi_0\rangle$ is the ground state of the Heisenberg model with zero holes and energy E_0, which we obtain with the Lanczos method. ϵ is a small parameter that gives a finite width to the δ functions appearing in Eq. (5). $P(\omega)$ can now be evaluated by a continued fraction expansion using the Lanczos method. For a finite system $P(\omega)$ consists of δ functions corresponding to those states $|n\rangle$ of the two-hole subspace having a projection on $\Delta^{\dagger}|\psi_0\rangle$ with an intensity proportional to $|\langle n|\Delta^{\dagger}|\psi_0\rangle|^2$. As a test of our method we checked that the lowest-energy peak has the same energy as that provided by an independent Lanczos calculation of the two-hole ground state. For more details see Refs. 2, 3, and 15.

In Tables I and II we present the ground-state energies of the t-J and t-J_z models in different subspaces for a 4×4 lattice. In Fig. 1(a) we show our results for $P(\omega)$ at $J=0.4$ and $t=1$ in the t-J model using the d-wave pairing operator (here and below $\epsilon=0.05$ and we used 100 iterations of the continued fraction expansion). There is a large quasiparticle-like peak at the bottom of the spectrum showing that the state $\Delta^{\dagger}|\psi_0\rangle$ is a good approximation to the ground state of the system. Beyond the first peak there are many other lower-intensity peaks presenting some structure as happened for one hole.[2] Increasing the value of J, the first peak accumulates more spectral weight (note that the intensity of the peaks in absolute value depends on the particular normalizations we use; thus, only relative intensities are physically interesting). For $J=2.0$ [Fig. 2(a)], only a few peaks can be easily observed beyond the dominant one, although there are many more of negligible spectral weight. In analogy to what happened in the one-hole subspace,[3] we believe that

TABLE I. Ground-state energy of two holes in the t-J model [Eq. (1)] on a 4×4 lattice at different values of J. The total momentum is zero.

J	d wave	p wave	s wave
0.2	−4.366	−4.173	−4.192
0.4	−2.993	−2.624	−2.366
0.6	−1.775	−1.234	−0.641
0.8	−0.646	0.066	0.863
1.0	0.422	1.292	2.131
2.0	5.277	6.716	7.257

TABLE II. Same as Table I but for the t-J_z model. The s-wave energy is given exactly by $E=3.5J_z$.

J_z	d wave	p wave
0.2	−4.832	−4.771
0.4	−3.381	−3.337
0.6	−2.131	−2.119
0.8	−0.999	−1.000
1.0	0.057	0.054
2.0	4.721	4.726

these excitations can be explained as follows: At large J the ground state approximately corresponds to the two holes located at a distance of one lattice spacing forming a d-wave state. Excited states can be obtained by moving a hole one additional lattice spacing creating a (length one) string of overturned spins or, equivalently, a spin flip in the vicinity of a hole (like a trapped spin wave).

For values of J/t between 0.4 and 2.0 we found a smooth interpolation between the results of Figs. 1(a) and 2(a). However, for $J=0.2$ although the quasiparticle can still be distinguished in the spectrum, its spectral weight is now approximately equal to that of another state that appears at higher energies (while many other states have comparable spectral weights). For $J=0$, $P(\omega)$ is symmetric under $\omega \rightarrow -\omega$ and has a large peak at $\omega=0$ plus a mostly incoherent spectrum on both sides (see Fig. 3). The total width of the spectrum is reduced from the naive values $16t$ corresponding to that of a free particle to $\sim 13.3t$ due to strongly correlated properties of the fermions in this limit. This result is actually very close to the obvious generalization of the self-retracing ray approximation of Brinkman and Rice[16] to two holes, i.e.,

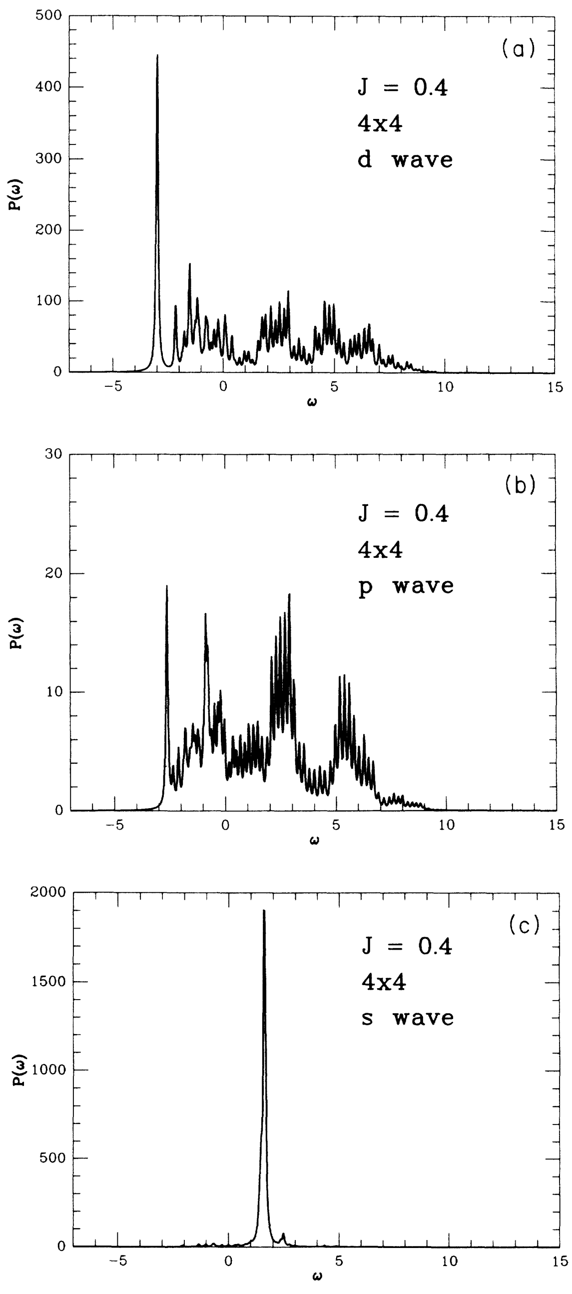

FIG. 1. $P(\omega)$ for the t-J model on a 4×4 lattice at $J=0.4$, $t=1$ for (a) d-wave symmetry, (b) p-wave symmetry, and (c) s-wave (extended) symmetry.

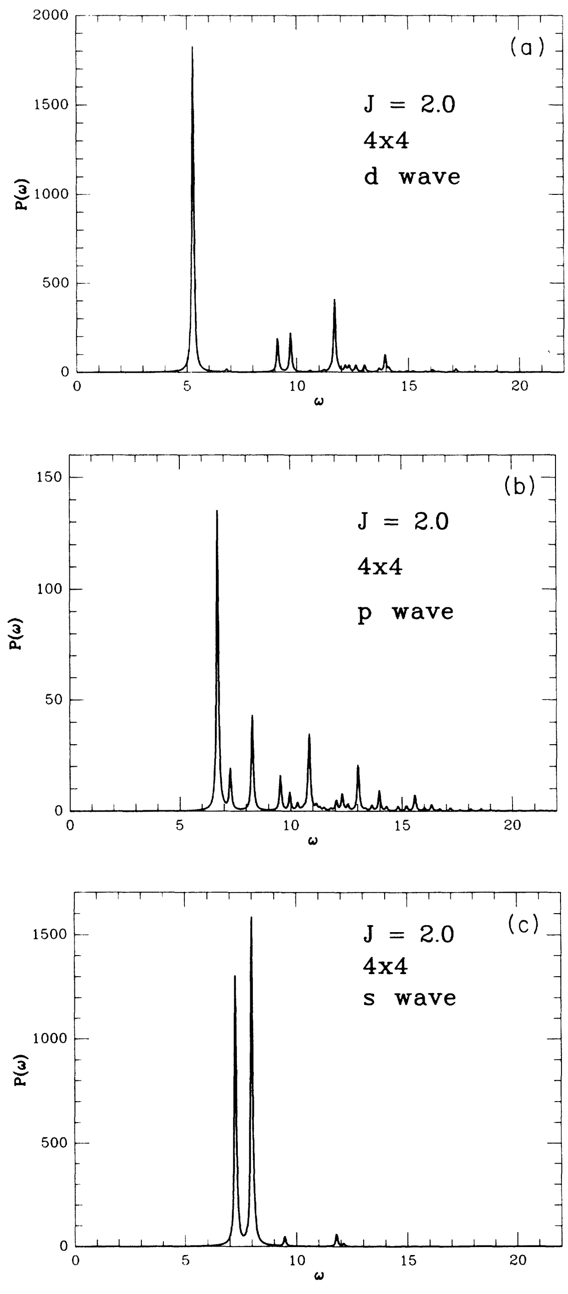

FIG. 2. $P(\omega)$ for the t-J model on a 4×4 lattice at $J=2.0$, $t=1$ for (a) d-wave symmetry, (b) p-wave symmetry, and (c) s-wave (extended) symmetry.

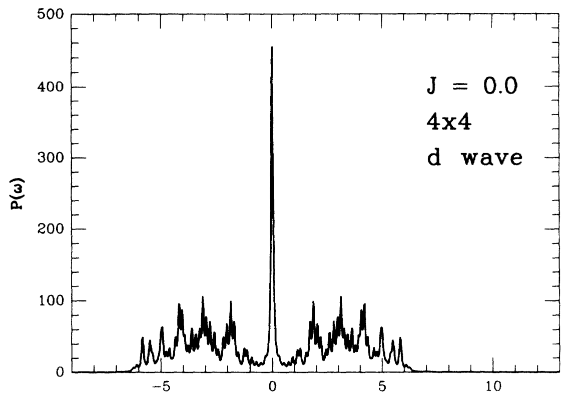

FIG. 3. $P(\omega)$ for the t-J model on a 4×4 lattice at $J=0.0$, $t=1$ for d-wave symmetry.

width $=8\sqrt{3}t\sim13.9t$. For finite J, the *total* width of the spectrum does not change much. For the t-J_z model we obtained very similar results. We also analyzed the J-t-t' model where t' ($\sim J$) corresponds to a second-neighbor hopping term as it appears from the strong-coupling expansion of the Hubbard model. The results for the d-wave pairing susceptibility are qualitatively very similar to those found for the t-J model.

In Figs. 1(b), 1(c), 2(b) and 2(c) we show the p- and extended-s-wave pairing susceptibilities for $J=0.4$ and 2.0, respectively. For the p wave the general trend is that qualitatively the spectral function is similar to that of the d wave, although, of course, they differ in details, especially regarding the intensity of the peaks, which is much smaller for the p wave. For the s wave the situation is drastically different. In this case there is no large peak at the bottom of the spectrum, and thus we conclude that there is no quasiparticle-like excitation in this subspace. Note, however, that at intermediate energies a very large peak appears in the spectrum having most of the spectral weight. This is a general trend that is present for all the interesting values of J. Only at very large J (>2) does the first peak in the spectrum accumulate enough spectral weight to become the dominant peak. This peculiar behavior of the s-wave susceptibility can be understood from the Ising limit (the t-J_z model) where the situation is similar. In that case there is only *one* peak in the spectral function of the s-wave susceptibility at energies very close to those where we found the large peak in the t-J model. It can be shown that this is due to the fact that the state $\Delta^\dagger|\psi_0\rangle$ for an s wave is an *eigenstate* of the t-J_z model. For the d wave the minus sign used in the definition of $f(\mathbf{k})$ avoids the problem and the state is not an eigenstate. To prove these results care must be taken with signs appearing from fermionic permutations. Actually, we remark that if the spins would have had bosonic statistics then the d wave would have had this pathological behavior rather than the s wave. This is also in agreement with recent exact results on the half-filled Hubbard model,[17] where it was shown that d and s symmetries usually interchange places by changing the statistics.

We fitted the ground-state energy of the t-J model of two holes as a function of J for different symmetries. For the d-wave (p-wave) subspace we found that the data can be approximated very well by a power-law behavior $J^{0.78\pm0.02}$ ($J^{0.79\pm0.02}$) in the region $0.2\le J\le1.5$. On the other hand, the energy of the extended s-wave ground state cannot be fitted reliably with a power law. Are these results compatible with the string picture found to be a good approximation for the one-hole subspace?[2] For that comparison it is important to note that the influence of the term $\frac{1}{4}n_i n_{i+\delta}$ should be taken into account in the fitting procedure since it is not present in the original formulation of the t-J model.[4,3] We proceeded in two ways: First we removed that term from the Hamiltonian and repeated the calculation for the d-wave subspace. Now the energy of the first peak can be approximated very well by a power law $J^{0.69\pm0.02}$ whose exponent is in excellent agreement with the string picture which predicts a value of $\frac{2}{3}$. We have also simply subtracted from the energy obtained with the full Hamiltonian Eq. (1) the value that would correspond to that term in the Ising limit, i.e., $-7J/4$. In such a way we also found $J^{0.69\pm0.01}$ (in the same interval of J) in excellent correspondence with the previous result. Then, we conclude that once the term $\frac{1}{4}n_i n_{i+\delta}$ is properly taken into account then the results for the ground-state energy are in good agreement with the string picture as for one hole. We have not attempted to fit the energies of higher excited states as we did for the one-hole subspace.[2,3]

We also analyzed the binding energy of two holes[5] defined as

$$E_B=(E_{2h}-E_{0h})-2(E_{1h}-E_{0h})\ , \tag{6}$$

where E_{nh} denotes the ground-state energy of the subspace with n holes. E_{1h}, E_{0h} can be obtained from previous work.[18] For two holes and d-wave symmetry we found that the binding energy is negative and behaves as $|E_B|\sim J^{1.00\pm0.05}$ for $0.2\le J\le1.0$. For the p-wave subspace pairing begins at $J=0.8$ and is weaker than for the d-wave case. For the s-wave subspace there is no pairing for realistic values of J. A similar situation occurs for the t-J_z model.

Finally, for the t-J model we present results for nonzero total momentum. Due to the particular geometry of the 4×4 lattice the t-J model with two holes has a degenerate ground state since the subspaces with total momentum $\mathbf{Q}=(0,0)$ and $\mathbf{Q}=(0,\pi),(\pi,0)$ have the same ground-state energy. This spurious symmetry is also responsible for the degeneracy between $\mathbf{Q}=(\pi/2,\pi/2)$ and $\mathbf{Q}=(0,\pi),(\pi,0)$ in the one-hole subspace.[3] To study the dynamics of $\mathbf{Q}=(\pi,0)$ and in order to include the ground state of this subspace as part of the spectrum, it is necessary to take $f(\mathbf{k})=\sin(k_x)$. The reason is that Lanczos studies have shown[6] that the ground state with $\mathbf{Q}=(\pi,0)$ changes sign under a rotation in π around a site, but under a reflection with respect to the x axis it is invariant. We found numerically that the pairing susceptibility of this state behaves qualitatively in a similar way to the d- and p-wave spectrum for $\mathbf{Q}=(0,0)$, i.e., there is a quasiparticle-like peak at the bottom of the band. It would be very interesting to find numerically which state [$\mathbf{Q}=(0,0)$ or $\mathbf{Q}=(0,\pi),(\pi,0)$] becomes the ground state for a large lattice. The Monte Carlo simulations performed so far have not analyzed the possibility of a nonzero momentum in the pairing operator, although work is in progress.[19]

Now we present results for the Hubbard model. In Fig. 4(a) we show $P(\omega)$ for the *d*- and *p*-wave pairing operators on a ten-site lattice at $U=10$, $t=1$ (the strong-coupling region) which corresponds to $J=0.4$ in the *t-J* model. The ground state presents a large peak at the bottom of the spectrum, but others are of comparable spectral weight. There is a large difference in intensity between the *p*- and *d*-wave susceptibilities, but there is a good correspondence in the position and intensity of the peaks between the two as happens in the *t-J* model. For the *s*- and extended-*s*-wave susceptibilities [Fig. 4(b)] we found that most of the spectral weight is concentrated at high energies, again in agreement with the *t-J* model. In Figs. 5(a) and 5(b) we present results at $U=4$ as a representative of the weak-coupling region. For the *d*- and *p*-wave states the quasiparticle peak now has most of the spectral weight. This is not surprising since at $U=0$ the pairing susceptibilities for these symmetries have only one peak at $\omega\sim 2$ (for a ten-site lattice), i.e., $\Delta^{\dagger}|\psi_0\rangle$ is an eigenstate of the model in that limit. By continuity we expect a similar result to survive in the weak-coupling region. On the other hand, it can be easily checked that for the *s*- and extended-*s*-wave state $\Delta^{\dagger}|\psi_0\rangle$ is not an eigenstate at $U=0$ and, for a ten-site lattice, it presents two peaks, one at $\omega=2$ and the other at $\omega=8$, the latter with the largest spectral weight. It is the smooth continuation of this peak to higher values of U that produces the anomalous concentration of spectral weight at large energies that we found in the *s*-wave subspace.

Due to the similarities found between the spectral functions of one and two holes in the *t-J* model, we remark that the conductivity $\sigma(\omega)$ of the two-hole subspace may present a shape similar to that recently calculated in the one-hole subspace,[20] i.e., due to the movement of the hole (low-*J* picture) or to spin waves (large-*J* picture) a broad low-energy structure appears similarly to that observed experimentally at intermediate energies. At very high energies charge excitations will be observed if the Hubbard model is used.

Recently, we received a paper by Hasegawa and Poilblanc[21] where the dynamics of two holes in the *t-J* model is studied. However, the conclusion of that paper is that *no* quasiparticle-like state was found with zero total momentum, in contradiction to our results. The reason for the disagreement is that in Ref. 21 a state with a hole creation operator acting over the exact ground state of the one-hole subspace was used to study the dynamics of two holes, rather than our pairing operators. For the particular choice of quantum numbers made in Ref. 21

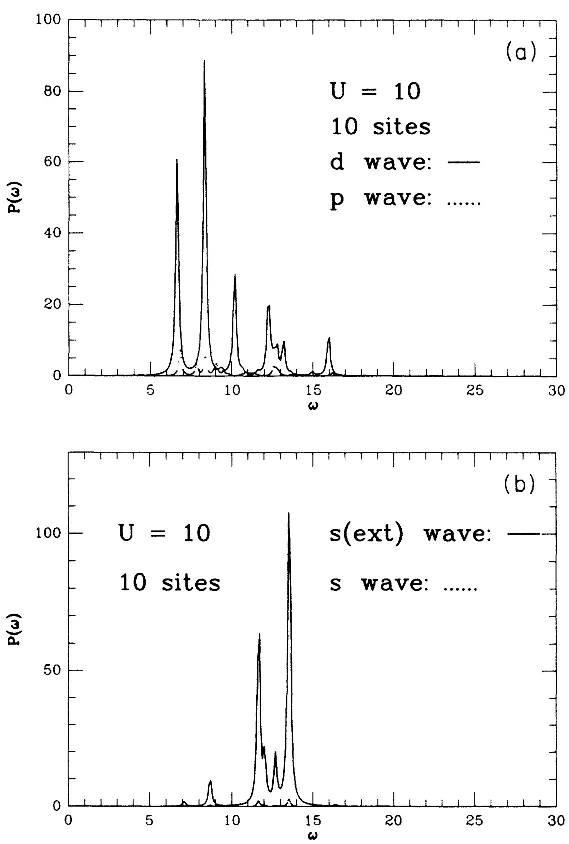

FIG. 4. $P(\omega)$ for the Hubbard model on a 10 site lattice at $U=10$, $t=1$ for (a) *d*- and *p*-wave symmetries, (b) *s* and extended *s* symmetries.

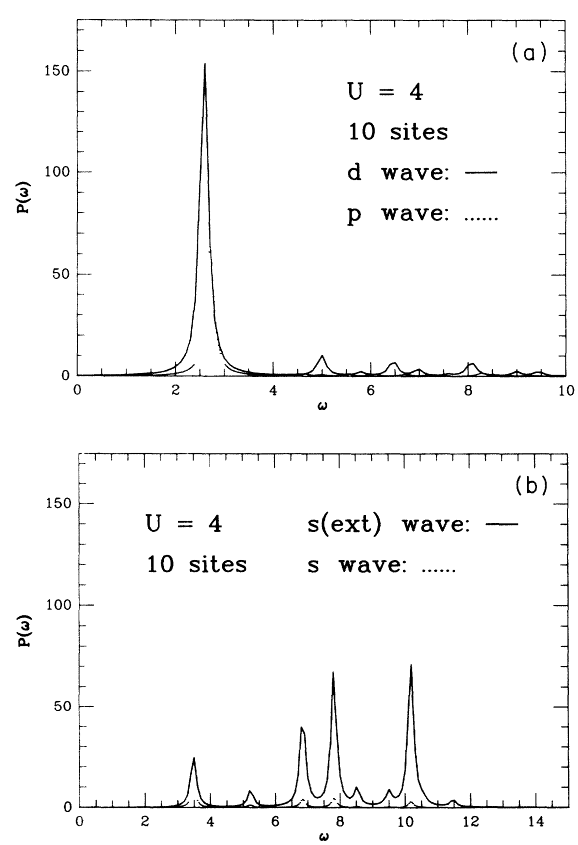

FIG. 5. $P(\omega)$ for the Hubbard model on a 10 site lattice at $U=4$, $t=1$ for (a) *d*- and *p*-wave symmetries, (b) *s* and extended *s* symmetries.

this state can be shown to have very small overlap with the actual ground state of two holes, and this is why the absence of a quasiparticle peak was concluded in that reference. To show this result simply replace the exact one-hole ground state by a hole operator with $\mathbf{k}=(\pi/2,\pi/2)$ acting over a Néel state ($|N\rangle$). We know that this approximation works very well.[3] Then, the two-hole state used in Ref. 21 can be approximated by $\bar{c}^{\dagger}_{-(\pi/2,\pi/2)}\bar{c}^{\dagger}_{(\pi/2,\pi/2)}|N\rangle$, which is explicitly *orthogonal* to the state created by the d-wave pairing operator acting over a Néel state [$f(\mathbf{k})=0$ if $k_x=k_y$].

After completing this work, we received a paper by White[22] with Monte Carlo results for the pairing susceptibilities of the Hubbard model at $U=4$. For the d-wave susceptibilities his results for the quasiparticle peak are in qualitative agreement with ours. However, the results for the s and extended-s susceptibilities are not, as can be easily seen comparing our Fig. 5(b) with Ref. 22. The gap between the d- and s-wave subspaces reported in that reference is $\sim 4-5t$ while our result is much smaller ($<1t$). We believe that the continuation from imaginary to real time done by Monte Carlo (MC) calculations only reproduced the *high* intensity peaks of our Fig. 5(b) at ω between 7 and 10, missing the low-energy one at $\omega \sim 3.5$, which is the actual ground state in the s-wave subspace and should be used to study gaps. Note that this result is also obvious from Fig. 2 of Ref. 22 since the s and extended-s waves *cannot* have peaks at different positions, since they have exactly the same lattice symmetries. Only the intensity of the peaks can change. We believe, therefore, that the recently developed MC methods to obtain real-frequency information, although promising, should still be applied in combination with Lanczos

Summarizing, we have studied the dynamical properties of pairing operators. We found good qualitative agreement between the t-J, t-J_z, and one-band Hubbard models. The general pattern is that the ground state of these models in the zero total momentum subspace is a d wave for physically interesting values of the parameters. Their pairing susceptibilities present a quasiparticle peak in a broad region of parameter space. The p wave is close in energy and has a similar qualitative behavior although with lower intensity peaks and weaker binding energy. Then, p-wave pairing in slightly modified variations of the Hubbard model is *not* completely excluded. On the other hand, the s- and extended-s-wave states have a different behavior, having most of the spectral weight concentrated at high energies and without a quasiparticle peak. At least at low doping our numerical evidence shows that the s-wave pairing is strongly suppressed. We are currently evaluating the bandwidth (W) of the two-hole quasiparticle. Preliminary results suggest that W is small (at small J) as in the one-hole case, and thus the effective mass of the two-holes bound state is large.

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