

Binding of holes and the pair spectral function in the t - J model

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Clusters of the two-dimensional t - J model with two holes and up to 26 sites are diagonalized using a Lanczos algorithm. The behavior of the binding energy with system size suggests the existence of a finite critical value of J above which binding occurs in the bulk. Only the d -wave pair-field operator acting on the Heisenberg ground state has a finite overlap with the two-hole ground state for all the clusters considered. The related spectral function associated with the propagation of a d -wave (singlet) pair of holes in the antiferromagnetic background is calculated. The quasiparticle peak at the bottom of the spectrum as well as some structure appearing above the peak survive with increasing cluster size. Although no simple scaling law was found for the quasiparticle weight the data strongly suggest that this weight is finite in the bulk limit and is roughly proportional to the antiferromagnetic coupling J (for $J < 1$).

I. INTRODUCTION

The possibility that high-temperature superconductivity in the quasi-two-dimensional cuprates would be a new phenomenon based on purely electronic interactions¹ has motivated a huge theoretical effort to better understand the physics of two-dimensional strongly correlated electrons. The Hubbard model and its large coupling version, the t - J model, are two of the simplest theoretical models used to describe the low-energy excitations of the copper oxide planes. Although it is difficult to develop a satisfactory perturbative analysis in the case of strongly repulsive interactions, numerical methods can often provide useful information on both static and dynamical properties of these systems. Exact diagonalization (ED) studies do not suffer from random noise problems like stochastic Monte Carlo methods, in particular in the vicinity of the antiferromagnetic Mott insulator phase. ED studies are therefore well adapted to the calculations of dynamical correlation functions at small doping density. However, so far ED studies have been restricted to fairly small clusters (typically 4×4). Recently, an attempt was made to handle larger sizes (up to 26 sites) in order to perform a finite-size analysis of the data²⁻⁴ in the close vicinity of the insulator magnetic phase. Although this analysis was restricted to the special limit of a single hole in the antiferromagnet (AF) it gives some hints about the hole propagation at small but finite doping fractions^{2,3} in the region where the antiferromagnetic correlation length is still larger than the spatial extension of the hole wave function. This work strongly suggested that the quasiparticle (QP) peak seen at the bottom of the spectral function survives in the thermodynamic limit.³ However, this analysis neglects the role of a possible hole-hole effective attraction that might occur for more than a single hole in the AF. The purpose of the present work is to study the case of two holes, i.e., the simplest case that, nevertheless, includes the effect of the effective attraction between the holes. The issue of binding is of great importance in the search for superconductivity in models of

strongly correlated fermions. By a similar finite-size analysis, I shall attempt to give an estimate of the binding energy and of the pair spectral function in the thermodynamic limit. Partial results for the binding energy and QP weight have been reported elsewhere.⁵ The emphasis here is put on the energy dependence of the complete spectral function $A_{2h}(\omega)$ and on its behavior with system size.

In standard notations the t - J Hamiltonian reads

$$\mathcal{H} = J \sum_{i,\epsilon} [(S_i^z S_{i+\epsilon}^z - \frac{1}{4} n_i n_{i+\epsilon}) + \frac{1}{2} (S_i^+ S_{i+\epsilon}^- + S_i^- S_{i+\epsilon}^+)] - t \sum_{i,\epsilon,\sigma} (\tilde{c}_{i,\sigma}^\dagger \tilde{c}_{i+\epsilon,\sigma} + \text{H.c.}) \quad (1.1)$$

The first term is the usual antiferromagnetic coupling between spins which splits into a diagonal part and a spin-flip part. The second term describes the hopping of the holes (i.e., where spins are missing). The sum over i, ϵ is restricted to nearest-neighbor bonds along x and y on a 2D square lattice, $\tilde{c}_{i,\sigma}^\dagger = (1 - n_{i,-\sigma}) c_{i,\sigma}$ is the hole creation operator and $n_i = \sum_{\sigma} c_{i,\sigma}^\dagger c_{i,\sigma}$. So far, t will set the energy scale.

The Hamiltonian (1.1) with zero, one, and two holes is diagonalized on clusters of increasing sizes by a standard Lanczos procedure. It is important in this analysis that all the clusters have the same shape, namely, a square. One should expect in this case a smoother extrapolation to the thermodynamic limit. If the (integer) coordinates of the cluster periods are (n, m) and $(-m, n)$, the cluster contains $N = n^2 + m^2$ sites. The following analysis is based on clusters of sizes 4×4 , $\sqrt{18} \times \sqrt{18}$, $\sqrt{20} \times \sqrt{20}$, and $\sqrt{26} \times \sqrt{26}$. In order to be able to handle the largest size (26 sites), use of complete translation and rotation symmetries (for zero and two holes) as well as time reversal (for an even number of fermions) is necessary and the Hamiltonian is diagonalized in each symmetry sector. The size of the Hilbert space increases exponentially with the cluster size. In the relevant symmetry sector [for discussion about ground-state (GS) symmetry, see Sec. II]

TABLE I. Symmetry properties of the half-filled (top half) and two-hole (bottom half) GS. The fermion convention is used.

	4	8	10	16	18	20	26
$S_z \rightarrow -S_z$	+1	+1	-1	+1	-1	+1	-1
\mathbf{K}	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)	(0,0)
\mathcal{R}_{90°	d	s	s	s	s	d	s
$S_z \rightarrow -S_z$			+1	-1	+1	-1	+1
\mathbf{K}			(0,0)	(0,0)	(0,0)	(0,0)	(0,0)
\mathcal{R}_{90°			d	d	d	s	d

the Hilbert space for two holes contains, after symmetry reduction, 3332, 13 858, 58 274 and 4 229 236 states for $N=16, 18, 20$, and 26 sites, respectively.

II. GROUND-STATE ENERGY AND BINDING

Symmetry properties of the Heisenberg GS $|\Psi_0^N\rangle$ and of the two-hole (singlet) GS $|\Psi_0^{N-2}\rangle$ are summarized for various cluster sizes in Table I. The symmetries of the half-filled GS are known exactly⁶ but depend on convention to represent the spins. In the following, I use the fermion representation at half filling. $|\Psi_0^N\rangle$ and $|\Psi_0^{N-2}\rangle$ are both invariant under lattice translations (total momentum $\mathbf{K}=0$) and even (odd) under spin reversal for $4p$ ($4p+2$) fermions. This last feature is a simple consequence of the singlet nature of these states. Although at half filling, in the spin language, the GS is always invariant under a 90° rotation around any lattice site (s wave),⁶ fermion reordering can lead to an extra minus sign, e.g., for $N=4$ (Ref. 7) or $N=20$, the half-filled GS becomes d wave in the fermion convention [see Table I (top half)]. It is worth noticing that in such a case the two-hole GS is s wave [see Table I (bottom half)]. However in most cases the half-filled GS is s wave and the two-hole GS is d wave.

The physical idea of an effective attraction between the holes can be simply understood in the Ising limit of Hamiltonian (1.1), i.e., when the spin-flip term is neglected. In this case the half-filled GS is the simple classical Néel state and obviously two holes added in this background can minimize the magnetic energy cost by sitting on nearest-neighbor sites. Although this crude explanation neglects the delocalization energy of the holes (t term) this picture was indeed shown numerically to be correct provided that $J>0.18$ (Ref. 8). The situation is not so clear in the fully quantum case (1.1) where spin fluctuations are included. Numerical calculations of the binding energy on the 4×4 (Refs. 9–12), $\sqrt{18}\times\sqrt{18}$ (Ref. 13),

and $\sqrt{20}\times\sqrt{20}$ (Ref. 14) clusters suggested that binding still occurs but above a slightly larger critical value of J , as expected. From a recent calculation of the hole density correlation functions in a restricted Hilbert space on clusters with up to 26 sites, Prelovšek and Zotos¹⁵ quote a critical value of J of order 0.2. However this technique gives poor accuracy for the GS energy and cannot be applied to calculate directly the binding energy (see below). On the other hand, Boninsegni and Manousakis,¹⁶ using Green's function Monte Carlo simulations which were carried out on large clusters at $J\geq 0.4$, and extrapolated to the bulk limit, and on smaller J/t ratios, reported a critical value of J of order 0.28.

The GS energies of a single-hole $E_0^{N-1} - E_0^N$, as well as the corresponding GS quantum numbers have been reported elsewhere.² The two-hole GS energies $E_0^{N-2} - E_0^N$ are listed in Table II for various cluster sizes and J values. Note that the size dependence is weak. The data of the 26 site cluster confirm the J^v dependence ($v\sim 0.9$) reported earlier for the 4×4 cluster.¹¹

The binding energy is defined quantitatively by

$$\Delta_{2h} = E_0^{N-2} + E_0^N - 2E_0^{N-1}. \quad (2.1)$$

Binding occurs when $\Delta_{2h} < 0$ in the bulk. In this case $|\Delta_{2h}|$ gives the magnitude of the attractive potential between the two holes. The simple (crude) arguments stated above would give an attraction of the order of a fraction of J . On the contrary, if binding does not take place, one would expect $\Delta_{2h} \rightarrow 0$ when $N \rightarrow \infty$.

Δ_{2h} vs J is shown in Fig. 1(a) and the corresponding data are listed in Table III. For $N=26$, Fig. 1(a) shows a significant increase of the critical value of J above which binding occurs, $J_c \sim 0.125$ for $N=26$. In Fig. 2(a) the same data are plotted vs $1/N$. Although Δ_{2h} is a small number corresponding to the difference between two quantities of the same magnitude, its behavior with system size is rather smooth (although not monotonic). Note that the jump of the single-hole GS momentum^{2,17}

TABLE II. Two-hole ground-state energies of the t - J model $E_0^{N-2} - E_0^N$ on clusters 4×4 , $\sqrt{18}\times\sqrt{18}$, $\sqrt{20}\times\sqrt{20}$, and $\sqrt{26}\times\sqrt{26}$ for several values of J (0.1 to 1).

	0.1	0.15	0.2	0.3	0.5	0.75	1
16	-5.211 929	-4.761 848	-4.366 113	-3.651 412	-2.370 082	-0.922 098	0.422 346
18	-5.372 725	-4.989 488	-4.622 850	-3.925 908	-2.635 292	-1.154 138	0.227 037
20	-5.391 175	-5.002 799	-4.632 916	-3.932 952	-2.644 911	-1.174 090	0.195 934
26	-5.293 633	-4.873 587	-4.489 433	-3.786 540	-2.527 792	-1.099 776	0.235 903

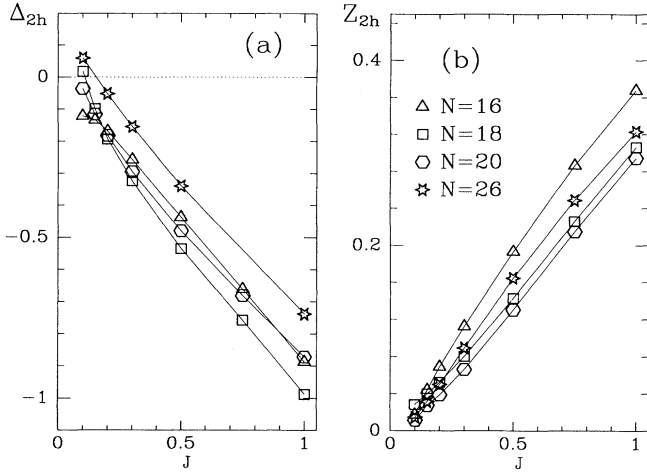


FIG. 1. (a) Binding energy Δ_{2h} and (b) spectral weight Z_{2h} vs J . The symbols corresponding to the different clusters are shown on the plot.

between the different clusters may be responsible for a small systematic error. Figure 2(a) shows unambiguously that binding occurs for, let us say, $J > 0.5$. However the strong size dependence at smaller J does not enable us to give any accurate estimation of the critical value of J for the bulk. I simply note that even for the largest size considered here, $\Delta_{2h} \sim -J$, one would expect a somewhat smaller (absolute) value in the bulk. This means that these numbers might still be far from the expected ones in the thermodynamic limit and it is then difficult to perform any extrapolations. On the basis of these data, I can, nevertheless, speculate that the critical value of J lies in the range 0.3–0.5. This is of central importance since the binding of holes is a necessary condition, but not sufficient, for the appearance of superconductivity.

In this work I have not studied the transition (with increasing J) towards phase separation,¹⁸ i.e., when the holes tend to cluster in a separate region of space and separate from the spins rather than bind by pairs (if long-range Coulomb repulsion is neglected). In fact, according to previous work,^{10,15} the hole delocalization energy prevents the transition toward phase separation occurring at the same critical value of J at which binding first appears, but rather leads to phase separation at a larger value of J . Therefore, in this scenario, there exists a finite range of J where holes do form pairs but do not phase separate from the spins. Further work is clearly needed and diagonalization of four holes on 26 sites

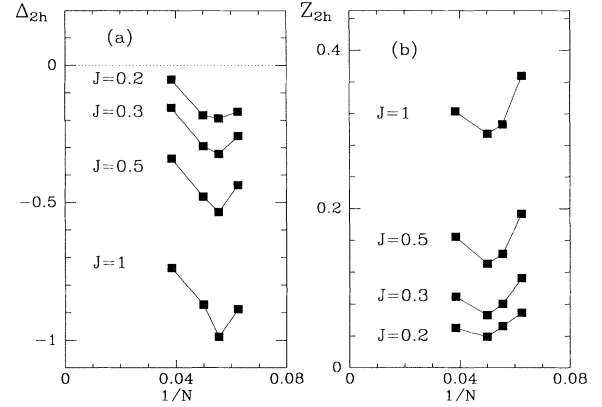


FIG. 2. (a) Binding energy Δ_{2h} and (b) spectral weight Z_{2h} plotted (arbitrarily) vs inverse system size $1/N$. The value of J corresponding to each set of points is indicated on the plot on the left side of the corresponding data.

would certainly help to clarify this issue. This is left for future work.

III. QUASIPARTICLE WEIGHT AND SPECTRAL FUNCTION

Let us now consider dynamical correlations. To study the propagation of a pair of holes in the underlying AF background, it is useful to define the pair spectral function,

$$A_{2h}(\omega) = \sum_m |\langle \Psi_m^{N-2} | \Delta^\dagger | \Psi_0^N \rangle|^2 \delta(\omega + E_0^N - E_m^{N-2}). \quad (3.1)$$

As defined above, $|\Psi_0^N\rangle$ is the antiferromagnetic GS at half filling (N spins on N sites). The sum is performed over a complete set of eigenstates (Ψ_m^{N-2}) of the two-hole sector ($N-2$ spins), with corresponding energies E_m^{N-2} . In the numerical results below, for plotting purposes, the δ functions are replaced by sharp Lorentzians of small width $\epsilon \approx 0.02$. Δ^\dagger is the usual pair creation operator,

$$\Delta^\dagger = \frac{1}{\sqrt{N}} \sum_{i,\epsilon} \mathcal{F}(\epsilon) \tilde{c}_{i,\uparrow}^\dagger \tilde{c}_{i+\epsilon,\downarrow}^\dagger, \quad (3.2)$$

where the form factor $\mathcal{F}(\epsilon) (= \pm 1)$ can have s - or d -wave symmetry. As seen previously, it is remarkable that the

TABLE III. Binding energies in the t - J model on clusters 4×4 , $\sqrt{18} \times \sqrt{18}$, $\sqrt{20} \times \sqrt{20}$, and $\sqrt{26} \times \sqrt{26}$ for several values of J (0.1 to 1). Note that for 18 sites a level crossing appears in the one-hole sector (indicated by an asterisk).

	0.1	0.15	0.2	0.3	0.5	0.75	1
16	-0.121 909	-0.133 874	-0.169 305	-0.257 734	-0.437 502	-0.661 252	-0.887 262
18	0.016 983*	-0.098 624*	-0.194 140	-0.323 806	-0.535 906	-0.757 922	-0.988 101
20	-0.036 409	-0.115 937	-0.182 936	-0.295 488	-0.479 8095	-0.681 616	-0.871 744
26	0.059 531		-0.051 799	-0.154 960	-0.340 200		-0.738 611

half-filled and two-hole GS have systematically opposite quantum numbers (i.e., ± 1) under a 90° rotation (around a lattice site). Therefore, it is clear that only the d -wave pair operator [i.e., $\mathcal{F}(\pm\mathbf{x})=1$ and $\mathcal{F}(\pm\mathbf{y})=-1$] has a nonzero matrix element between the two GS. For this reason, I shall restrict myself to this choice so far. Note that the pair operator (3.2) is odd under spin reversal and is invariant under lattice translations so that, in addition to its d -wave nature, it has precisely the right translation and spin symmetries (it is a singlet) to connect the two GS. In the right-hand side of Eq. (3.1) the sum is then restricted to the states of the same symmetry class as the two-hole GS.

The calculation of the spectral function (3.1) is done in three steps. First the Heisenberg GS is calculated. In practice, the number of Lanczos iterations required to obtain a good accuracy of the GS increases slowly with the system size (crudely, it is proportional to the system size). Typically, for the Heisenberg GS I have reached a high accuracy after 60, 150, 400, and 600 iterations for $N=16, 18, 20$, and 26 , respectively. Note that the GS energy converges in much fewer iterations than the corresponding wave function, in any case, less than 50 iterations. In the second step, the pair operator is applied on the Heisenberg GS. Lastly the vector generated in the second step is used as the initial vector of a second Lanczos run in the two-hole subspace. The spectral function can be generated by a continued fraction expansion that can be truncated after N_{it} iterations.¹⁹ I have carefully studied the convergence of the spectral function as a function of N_{it} . Figure 3 shows the behavior of A_{2h} for

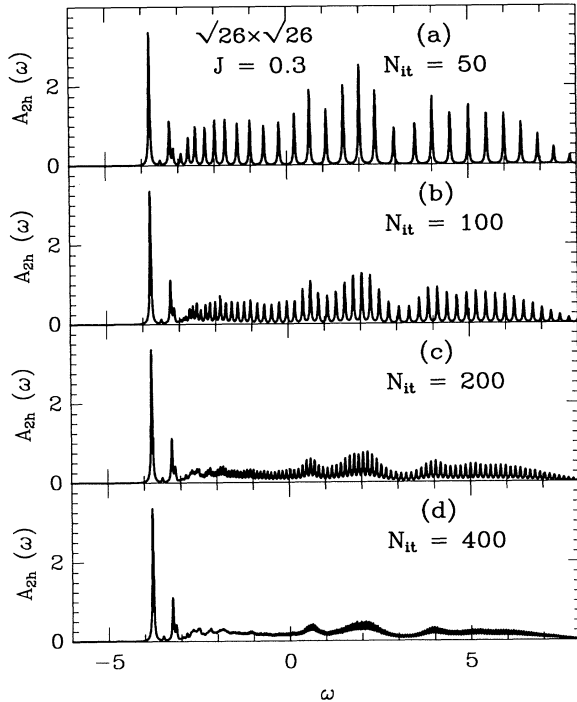


FIG. 3. Spectral function of the d -wave pair operator vs frequency (in units of t) for $N=26$ and $J=0.3$. The Lanczos iteration number N_{it} used to calculate the continued fraction of the spectral function is shown on the plots.

increasing N_{it} in the case of the 26 site cluster. At small N_{it} the spectral weight is distributed on a small number of δ functions. It is important to note that the low-energy part of the spectrum is the first to converge when N_{it} is increased. Figure 3 shows that a complete convergence on the whole physically relevant energy range can be obtained after a rather small number of iterations, much smaller than the size of the Hilbert space. Empirically, I have noticed that the value of N_{it} required to obtain a good convergence does not grow much faster than, let us say, the system size N . For example, $N_{it}=200, 400, 500$, and 450 iterations are needed for 16, 18, 20, and 26 sites.

The spectral function is plotted in Fig. 4 for increasing cluster size and for $J=0.1, 0.3$, and 1 . Observe that most of the features of the 4×4 cluster²⁰ survive when the cluster size is increased; (i) a QP peak lies at the bottom of the band and (ii) a significant amount of spectral weight is spread at higher energy over a range of a few t (for details see discussion below). This is very similar to the single-hole spectral function.^{2,3} Note that the few peaks seen in the case of the smallest size (16 sites) are smeared out when N is increased and eventually merge into an almost perfect continuous background for $N=26$, except for $J=1$. It is also remarkable that the various local maxima in the background [at $\omega \sim 0.8$ in Fig 4(d) or $\omega \sim 0.5, 2$, and 4 in Fig. 4(h)] are located at almost the same frequencies for the various sizes N considered. However it is not clear whether the secondary peaks (of finite width) observed immediately above the QP peak in Figs. 4(h) and 4(i) are still finite-size effects or whether they are related to any physical low-energy resonances (see below for discussion). It should be noted that, similar to the single-hole case,⁴ Figs. 4 suggest that no real gap separates the QP peak from the rest of the spectrum at higher energy.

Let us now study more quantitatively the behavior of the weight of the QP peak. Similar to the one-hole case, I can define the Z factor as the square of the overlap,²¹

$$Z_{2h} = \frac{|\langle \Psi_0^{N-2} | \Delta^\dagger | \Psi_0^N \rangle|^2}{\langle \Psi_0^N | \Delta \Delta^\dagger | \Psi_0^N \rangle}. \quad (3.3)$$

The denominator is a simple normalization factor,²² so that Z_{2h} represents the *relative* spectral weight (between 0 and 1) located in the QP peak.

One of the key issues of the problem of strongly correlated fermions is the possibility that spin and charge decoupling which take place in one dimension²³ would also occur in two dimensions as proposed by Anderson²⁴ and Varma *et al.*²⁵ If such a scenario is valid then, as a simple consequence of the spin-charge separation, one would expect the absence of a sharp QP. It is then crucial to test this hypothesis. Previous calculations^{2,3} suggested that the single-hole Green's function in the AF background does exhibit an undamped QP pole. However, since this approach neglected any possible hole-hole interaction, it is necessary to reexamine the same problem when more than a single hole is present. The case of two holes considered here is the first step towards the finite-hole density.

Z_{2h} is plotted in Fig. 1(b) as a function of J . Figure 1(b) shows that Z_{2h} varies almost linearly with J in the range $0.1 < J < 1$. It is also interesting to compare these data with the single-hole QP weight Z_{1h} obtained recently on the same clusters,³

$$Z_{1h} = \sum_{\sigma} |\langle \Psi_{0,\sigma}^{N-1} | c_{\mathbf{K},\sigma}^{\dagger} | \Psi_0^N \rangle|^2, \quad (3.4)$$

where \mathbf{K} stands for the finite momentum of the one-hole GS.¹⁷ Table IV shows the data for Z_{2h} for the various clusters as well as $(Z_{1h})^2$ on 26 sites. We note that, to a

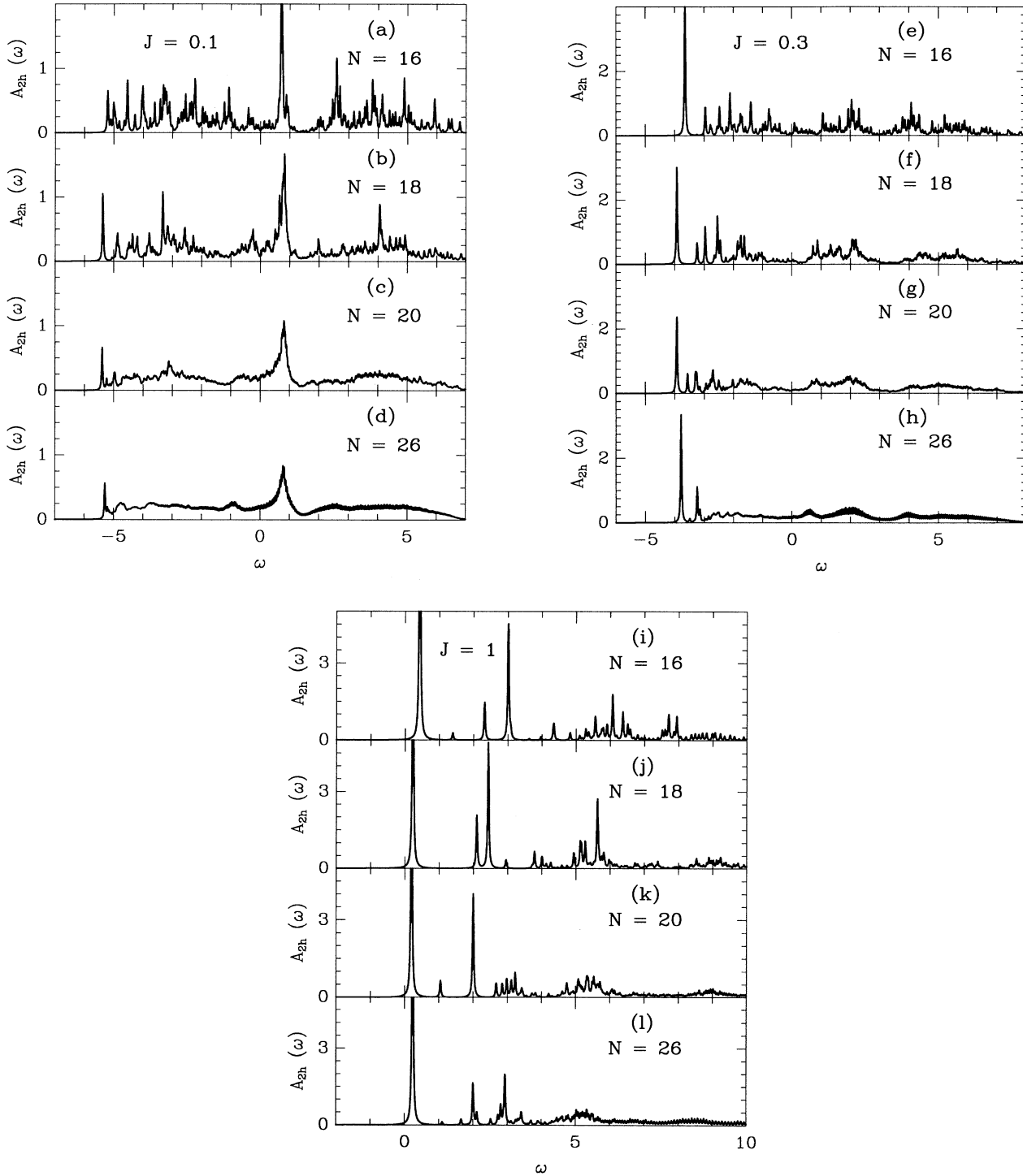


FIG. 4. Spectral function of the d -wave pair operator vs frequency for increasing cluster sizes. (a)–(d) $J=0.1$, (e)–(h) 0.3 , and (i)–(l) 1 . The frequency ω is measured in units of t .

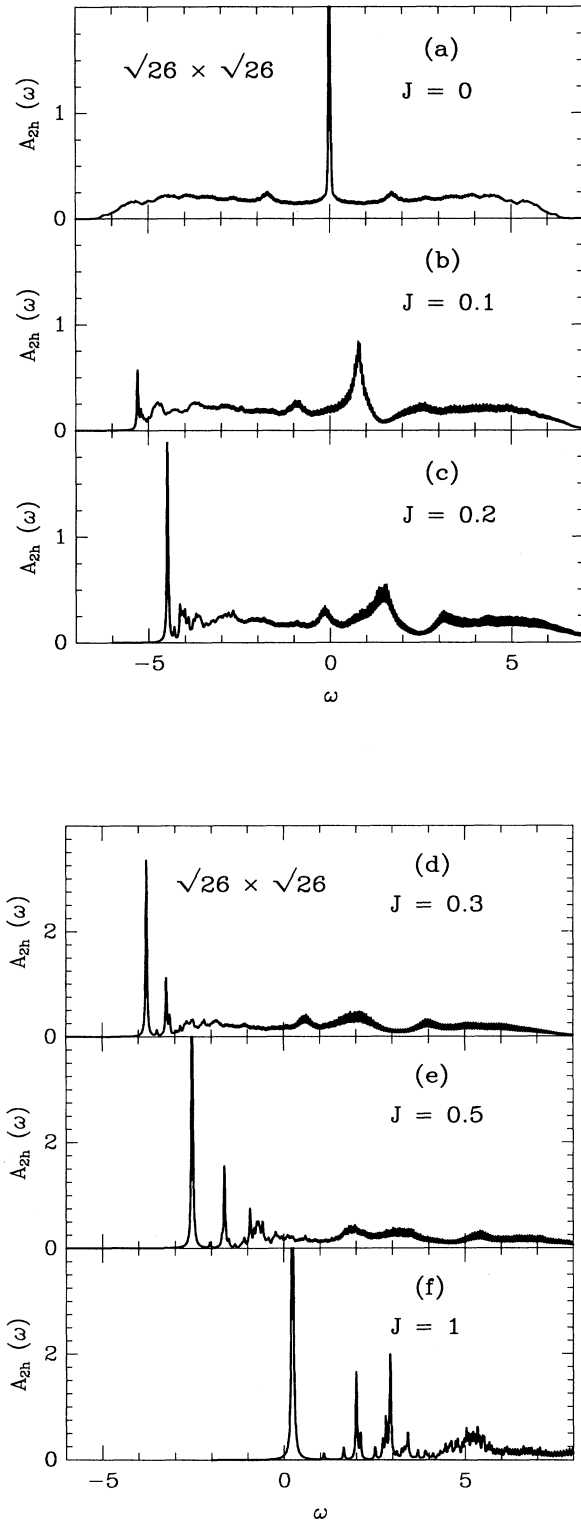


FIG. 5. Spectral function of the d -wave pair operator vs frequency on the $\sqrt{26} \times \sqrt{26}$ cluster for various J values. ω is measured in units of t . The continued fraction expansion was truncated after $N_{it}=450$ iterations (except for $J=0$, where $N_{it}=550$).

good approximation, $Z_{2h} \simeq (Z_{1h})^2$.

Although Z_{2h} is quite small in the physically interesting range $0.1 < J < 0.5$ only a finite-size analysis can tell whether or not it vanishes in the bulk. The data for Z_{2h} are plotted in Fig. 2(b) as a function of $1/N$. It should be noted that, contrary to the one-hole case^{3,17} the GS momentum is identical for all the clusters and equal to 0. No simple scaling law can be deduced from these plots. However, the numbers at $N=26$ seem to indicate a convergence toward a finite number in the bulk.

Last, let me consider the behavior of the spectral function versus the coupling constant J as shown in Figs. 5(a)–5(f). There are many similarities with the behavior of the single-hole spectral function calculated on the 4×4 (Ref. 26) and larger clusters.⁴ In the limit $J=0$, the spectrum in Fig. 5(a) is symmetric around $\omega=0$. This is in fact easy to understand. The change $\omega \rightarrow -\omega$ is equivalent to $t \rightarrow -t$, i.e., $\tilde{c}_{i,\sigma} \rightarrow -\tilde{c}_{i,\sigma}$ for, let us say, the even sites. Under such a transformation one can easily check that $\Delta^\dagger \rightarrow -\Delta^\dagger$ so that eventually $A_{2h}(\omega) = A_{2h}(-\omega)$ for $J=0$. The spectral density is almost constant over an energy range of $\sim 13t$. A sharp peak (actually a δ function) can be seen at $\omega=0$. When J is turned on [Figs. 5(b) and 5(c)] the spectrum is no longer symmetric with respect to ω and no longer (rigorously) bounded from above (strictly speaking, in the bulk) since there now exist states with excitation up to a magnetic energy $\propto NJ$, N being the system size. However, in practice, the matrix elements in (3.1) decrease exponentially with increasing energy outside an energy range of a few t (~ 10 – $12t$). As seen above, a QP peak of weight $\propto J$ appears at the bottom of the band. However for small J most of the spectral weight lies above. The sharp $\omega=0$ peak of the $J \rightarrow 0$ limit is rapidly broadened by J . Reminiscence of this peak can still be clearly seen up to $J=0.2$. If J is increased further [Figs. 5(d)–5(f)] most of the features of the $J=0$ limit vanish. On the other hand, sharp peaks (nevertheless, of finite width) appear right above the QP peak. These structures are characteristic of the $J \simeq t$ region and might be related to the internal structure of the pair. Indeed, the two holes (for sufficiently large J) are confined on neighboring sites by some effective potential which increases linearly with the hole separation if spin fluctuations are not considered. It is interesting to note that the appearance of these resonances coincide with the approximate J value at which binding sets up (see Sec. II).

IV. CONCLUSION

In this paper, calculations of the binding energy as well as of the pair-field spectral function (of d -wave symmetry) have been reported for the t - J model. By diagonalizing clusters with up to 26 sites and two holes, it has been definitely established that binding between holes occurs only above a critical threshold of J , in agreement with previous work. I estimate this critical value to be in the range 0.3–0.5. The spectral function of the pair operator shows unambiguously a QP peak at the bottom of the

TABLE IV. Spectral weight Z_{2h} of the QP peak in the pair spectral function of the t - J model on clusters 4×4 , $\sqrt{18} \times \sqrt{18}$, $\sqrt{20} \times \sqrt{20}$, and $\sqrt{26} \times \sqrt{26}$ for several values of J (0.1 to 1). For comparison, Z_{1h}^2 corresponding to the one-hole GS on 26 sites is also listed on the last line (marked by an asterisk).

	0.1	0.15	0.2	0.3	0.5	0.75	1
16	0.017 334	0.043 994	0.069 076	0.112 460	0.193 285	0.286 379	0.376 510
18	0.028 308	0.039 858	0.052 372	0.080 068	0.142 729	0.225 824	0.306 358
20	0.011 259	0.027 350	0.038 865	0.066 018	0.130 332	0.214 760	0.294 387
26	0.014 675	0.031 535	0.050 113	0.089 192	0.164 575	0.248 636	0.322 983
26*				0.081 419	0.155 884		0.318 740

band which does not seem to broaden or disappear when the system size is increased. Its weight grows almost like J for $J < 1$. In the physical region $0.1 < J < 0.5$ most of the spectral weight is spread above the peak on a wide energy range of the order of a few t . Two qualitatively different regimes are found: (i) for $J \leq 0.25$, the spectral function exhibits a pronounced bump around the band center which eventually merges into a sharp $\omega=0$ peak when $J=0$; (ii) for $J > 0.25$, especially $J \sim 1$, sharp (small) resonances are seen above the QP peak. These structures might be related to the internal nature of the pair bound by some effective potential.

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¹⁷For most clusters (except 4×4) the one-hole momentum $(\pi/2, \pi/2)$ does not belong to the reciprocal space of the cluster so that the actual GS momentum is the allowed wave vector in the closest vicinity of $(\pi/2, \pi/2)$.

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