

# Dynamical properties of the single-hole $t$ - $J$ model on a 32-site square lattice

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We present results of an exact diagonalization calculation of the spectral function  $A(\mathbf{k}, \omega)$  for a single hole described by the  $t$ - $J$  model propagating on a 32-site square cluster. The minimum energy state is found at a crystal momentum  $\mathbf{k}=(\pi/2, \pi/2)$ , consistent with theory, and our measured dispersion relation agrees well with that determined using the self-consistent Born approximation. In contrast to smaller cluster studies, our spectra show no evidence of string resonances. We also make a qualitative comparison of the variation of the spectral weight in various regions of the first Brillouin zone with recent angle-resolved-photoemission data.

The  $t$ - $J$  model has received a lot of attention in recent years. It is believed to be the simplest strong-coupling model of the low-energy physics of the anomalous metallic state of high-temperature superconductors.<sup>1,2</sup> The Hamiltonian of the model is

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} (\tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \text{H.c.}) + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j), \quad (1)$$

where  $\langle ij \rangle$  denotes nearest-neighbor sites, and  $\tilde{c}_{i\sigma}^\dagger$ ,  $\tilde{c}_{i\sigma}$  are the constrained operators,  $\tilde{c}_{i\sigma} = c_{i\sigma}(1 - c_{i,-\sigma}^\dagger c_{i,-\sigma})$ .

Although understanding the  $t$ - $J$  model doped with many holes is an important issue in the (potential) resolution of the high- $T_c$  mystery, the single-hole state is by itself an interesting and important problem. For example, it leads to the many-body wave functions which are the starting point of any rigid-band filling analysis.<sup>3</sup> Further, the single-hole model has been studied in great detail by various analytical and numerical theoretical techniques,<sup>4</sup> and recently angle-resolved photoemission (ARPES) data for the insulating, antiferromagnetically-ordered  $\text{CuO}_2$  planes in  $\text{Sr}_2\text{CuO}_2\text{Cl}_2$  have become available,<sup>5</sup> thus allowing for detailed comparisons between theory and experiment. To be specific, these results on the properties of a single hole in the  $\text{CuO}_2$  plane provide a direct test of how well the  $t$ - $J$  model (or any other microscopic Hamiltonian) describes the low-energy physics of the  $\text{CuO}_2$  plane.<sup>6</sup>

In this paper we report exact diagonalization results, found using the Lanczos algorithm, for a single hole described by the  $t$ - $J$  model on a 32-site square lattice. We use  $t$  as the unit of energy, i.e.,  $t = 1$ . Figure 1 shows the distinct  $\mathbf{k}$  points in the reciprocal space of the 32-site square lattice. Previous calculations for this model were mostly done on the 16-site ( $4 \times 4$ ) square lattice, where the  $\mathbf{k}$  points along the antiferromagnetic Brillouin zone (ABZ) edge [from  $(0, \pi)$  to  $(\pi, 0)$ ] are degenerate. Other square lattices that have been studied (18-, 20-, and 26-site) do not have the important  $\mathbf{k}$  points along the ABZ edge, viz., the single-hole ground-state wave vector  $(\pi/2, \pi/2)$  nor many points along the  $(1, 1)$  di-

rection [from  $(0, 0)$  to  $(\pi, \pi)$ ]. The 32-site square lattice is the smallest one which has these high symmetry points, and does not have the spurious degeneracy of the  $4 \times 4$  square lattice. Thus, this paper represents a major advance in the exact, unbiased, numerical treatment of an important strong-coupling Hamiltonian.

In order for us to complete the exact diagonalization on such a large lattice, we use translation and one reflection symmetry to reduce the total number of basis states to about 150 million. At  $\mathbf{k}=(3\pi/4, \pi/4)$ , no reflection symmetry can be used and the total number of basis states is about 300 million. To study the effect of finite system sizes, we will supplement our results with data obtained from smaller systems: the  $N=16$  ( $4 \times 4$ ) cluster, as well as a 24-site ( $\sqrt{18} \times \sqrt{32}$ ) cluster that includes many of the important wave vectors.<sup>7</sup>

The electron spectral function is defined by

$$A(\mathbf{k}, \omega) = \sum_n |\langle \psi_n^{N-1} | \tilde{c}_{\mathbf{k}, \sigma} | \psi_0^N \rangle|^2 \delta(\omega - E_0^N + E_n^{N-1}), \quad (2)$$

where  $E_0^N$  and  $\psi_0^N$  are the ground-state energy and wave function of the model at half filling, respectively, and  $E_n^{N-1}$  and  $\psi_n^{N-1}$  are the energy and wave function of the  $n$ th

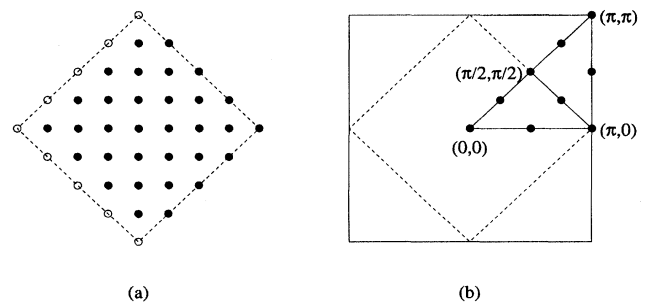


FIG. 1. (a) The 32-site square lattice employed in this study. (b) The distinct  $\mathbf{k}$  points in the reciprocal space of this lattice.

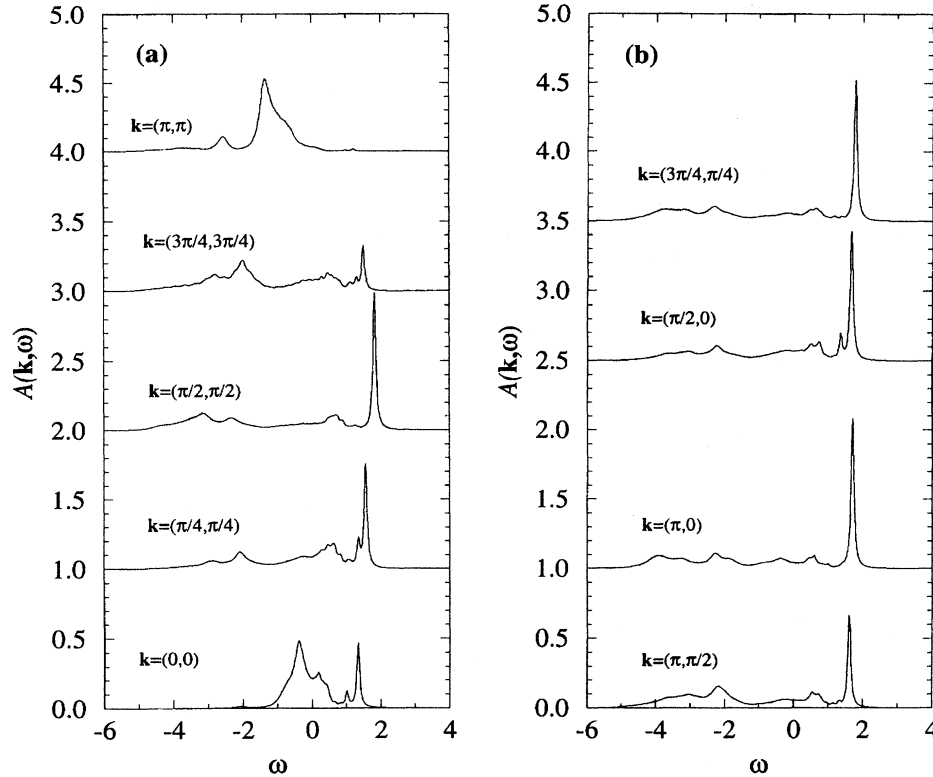


FIG. 2. The electron spectral function  $A(\mathbf{k}, \omega)$  for  $J=0.3$ .

eigenstate of the single-hole state, respectively.  $A(\mathbf{k}, \omega)$  is calculated using a continued fraction expansion<sup>8</sup> with 300 iterations and an artificial broadening factor  $\epsilon=0.05$ . We obtain  $A(\mathbf{k}, \omega)$  that are well converged using these quantities.

Figure 2(a) shows  $A(\mathbf{k}, \omega)$  at  $J=0.3$  from  $(0,0)$  to  $(\pi, \pi)$ . At  $(0,0)$ , the spectrum has a quasiparticle peak at  $\omega \sim 1.34$  and a broad feature at lower energies. As  $\mathbf{k}$  moves away from  $(0,0)$  along the  $(1,1)$  direction towards  $(\pi, \pi)$ , spectral weight shifts from the broad feature to both a higher-energy quasiparticle peak and the low-energy tail of the spectrum. The quasiparticle peak increases in intensity and shifts to higher energies, reaching the valence band maximum at  $(\pi/2, \pi/2)$ . When  $\mathbf{k}$  goes further towards  $(\pi, \pi)$ , the quasiparticle peak moves to lower energies and its intensity drops significantly. Spectral weight moves towards the central part of the spectrum again, eventually leaving only a very small quasiparticle peak at  $\omega = 1.2313$ , and a broad low-energy structure. Figure 2(b) shows  $A(\mathbf{k}, \omega)$  at other distinct  $\mathbf{k}$ .

From Fig. 2 one sees that along the ABZ edge  $A(\mathbf{k}, \omega)$  are qualitatively similar.<sup>9</sup> They have strong quasiparticle peaks which do not disperse much. The intensity of the quasiparticle peak is the largest at  $(\pi, 0)$ . As  $\mathbf{k}$  moves from  $(\pi, 0)$  to  $(\pi/2, \pi/2)$ , the intensity of the quasiparticle peak decreases and is the smallest at  $(\pi/2, \pi/2)$  along the ABZ edge. This can be made quantitative by calculating the quasiparticle weight, which is defined by

$$Z_{\mathbf{k}} = \frac{|\langle \psi_m^{N-1} | \tilde{c}_{\mathbf{k}\sigma} | \psi_0^N \rangle|^2}{\langle \psi_0^N | \tilde{c}_{\mathbf{k}\sigma}^\dagger \tilde{c}_{\mathbf{k}\sigma} | \psi_0^N \rangle}, \quad (3)$$

and is proportional to the area under the quasiparticle peak. Table I shows the values of  $Z_{\mathbf{k}}$ .  $Z_{\mathbf{k}}$  is the largest at  $(\pi, 0)$ ,

and remains large along the edge of the ABZ. Outside the ABZ,  $Z_{\mathbf{k}}$  decreases very fast, especially along the  $(1,1)$  direction.  $(\pi/2, \pi/2)$  is a saddle point:  $Z_{\mathbf{k}}$  is a maximum along the  $(1,1)$  direction, but a minimum along the direction from  $(0, \pi)$  to  $(\pi, 0)$ .

From our spectral function results we have extracted a quasiparticle dispersion relation, and in Fig. 3 we display the resulting  $E(\mathbf{k})$ , which is the location of the quasiparticle peak of  $A(\mathbf{k}, \omega)$ . The numerical values of  $E(\mathbf{k})$  are tabulated in Table I. In agreement with earlier (and smaller system size) results, we find that the band maximum and minimum are at  $(\pi/2, \pi/2)$  and  $(\pi, \pi)$ , respectively.<sup>10</sup> Further, the valence band maximum is located at  $\mathbf{k} = (\pi/2, \pi/2)$ , consistent with the large theoretical effort that was applied to the single-hole problem.<sup>4</sup> The solid line in Fig. 3 is the self-consistent Born approximation (SCBA) result on a  $16 \times 16$

TABLE I. Quasiparticle weight  $Z_{\mathbf{k}}$  and energy  $E(\mathbf{k})$  of the 32-site  $t$ - $J$  model at  $J=0.3$ . The half-fill ground-state energy  $E_0^N$  is  $-11.329\,720$ .

| $\mathbf{k}$                       | $Z_{\mathbf{k}}$ | $E(\mathbf{k})$ |
|------------------------------------|------------------|-----------------|
| $(0,0)$                            | 0.145 200        | 1.339 454       |
| $(\frac{\pi}{4}, \frac{\pi}{4})$   | 0.234 239        | 1.563 812       |
| $(\frac{\pi}{2}, \frac{\pi}{2})$   | 0.311 065        | 1.832 213       |
| $(\frac{3\pi}{4}, \frac{3\pi}{4})$ | 0.098 759        | 1.509 999       |
| $(\pi, \pi)$                       | 0.005 499        | 1.231 307       |
| $(\pi, \frac{\pi}{2})$             | 0.211 046        | 1.672 890       |
| $(\pi, 0)$                         | 0.341 747        | 1.710 318       |
| $(\frac{\pi}{2}, 0)$               | 0.295 290        | 1.619 414       |
| $(\frac{3\pi}{4}, \frac{\pi}{4})$  | 0.320 631        | 1.777 018       |

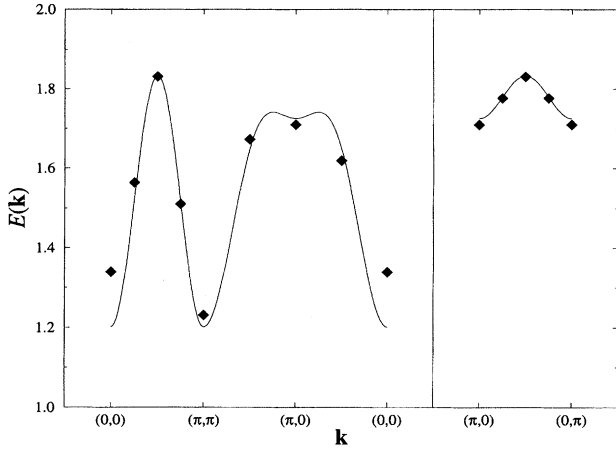


FIG. 3. The quasiparticle dispersion relation of the 32-site  $t$ - $J$  model at  $J=0.3$ . The solid line is from the SCBA calculation of Ref. 11, but with a vertical offset to make  $E(\pi/2, \pi/2)$  agree with ours.

square lattice.<sup>11</sup> The agreement between our 32-site dispersion relation and that of the SCBA calculation is encouraging.

To study the finite-size effects in our results, we can compare our cluster to smaller system size results. Unfortunately, a comparison of the spectral function is limited by the availability of the particular  $\mathbf{k}$  points in smaller lattices. When comparing  $A(\mathbf{k}, \omega)$  of the 16-,<sup>12,13</sup> 18-, 20-, 26-,<sup>13</sup> and 32-site lattices at  $(0,0)$  and  $(\pi, \pi)$ ,<sup>14</sup> we find that the high-energy features (including the quasiparticle peak) are not very sensitive to the system size. However, the low-energy features are smeared out and broadened in larger systems — this point was also made in Ref. 13. We also calculated the spectral function for the 24-site lattice.<sup>7</sup> Although it is not square, this cluster has the same five  $\mathbf{k}$  points along the  $(1,1)$  direction as the 32-site lattice.  $A(\mathbf{k}, \omega)$  at these points are qualitatively similar to those of the 32-site results, except for detailed values of the intensity. We conclude that the 24-site lattice is large enough to capture the essential shape of the spectral function along the  $(1,1)$  direction, while the 16-site lattice is too small, especially where the lower-energy features are concerned. In particular, the well-defined secondary peaks found at  $(\pi/2, \pi/2)$  on the 16-site lattice, which were interpreted to be related to the “string picture,”<sup>12</sup> are not found in our 32-site system. Hence we find no evidence supporting the string picture (at least for this value of  $J$ ). Further, the single-hole energy, defined as  $E_h = E_0^{N-1} - E_0^N = -E(\pi/2, \pi/2)$ , is calculated at  $0.1 \leq J \leq 0.8$  for the 32-site system. Fitting to the form  $E_h - J = a + bJ^\nu$  gives  $a = -3.24$ ,  $b = 2.65$ , and  $\nu = 0.72$ . This is consistent with the 16-site results,<sup>12</sup>  $a = -3.17$ ,  $b = 2.83$ , and  $\nu = 0.73$ , and also with the large cluster estimate of the SCBA calculations.<sup>11</sup> However,  $\nu$  is not  $\frac{2}{3}$  as suggested in the string picture.<sup>15</sup>

Figures 4 and 5 show the bandwidth  $W = E(\pi/2, \pi/2) - E(\pi, \pi)$  and the quasiparticle weight  $Z_{(\pi/2, \pi/2)}$  at different  $J$  for  $N=16, 24$ , and 32. Fitting to the functional forms  $a + bJ^\nu$  is more difficult. The best estimates of the coefficients are shown in the graphs. (The negative  $y$

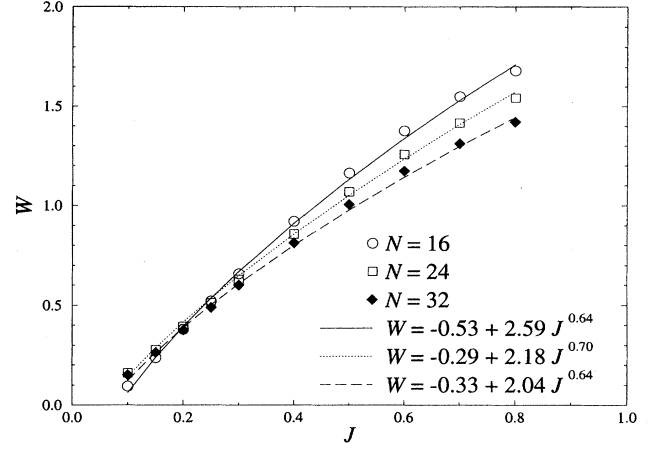


FIG. 4. The bandwidth of the  $t$ - $J$  model at various  $J$  for  $N=16, 24$ , and 32. The lines represent the best fits with the indicated functional form.

intercept of  $W$  versus  $J$  is nonphysical and has been accounted for by higher-order processes in  $t$ .<sup>16</sup>) For  $J \leq 0.4$ ,  $W$  can be fitted reasonably well by a linear relation in  $J$ . Also, we find that  $Z_{(\pi/2, \pi/2)}$  does not scale monotonically with  $N$  in this range of  $J$ . Consequently, we feel that a precise extrapolation to large  $N$  based on available numerics is not justified. However, our results support the hypothesis that at the  $J$  value of physical interest ( $J \sim 0.3$ )  $Z_{(\pi/2, \pi/2)}$  remains nonzero for macroscopic  $N$ .

Finally, our results also allow for a comparison to the experimental dispersion relation data of Wells *et al.*<sup>5</sup> It is clear that the flat dispersion relation that we find along the ABZ does not agree with the measured  $E(\mathbf{k})$ , in direct contradiction to a recent theory of the ARPES spectra based on the  $t$ - $J$  model.<sup>17</sup> The behavior of  $Z_{\mathbf{k}}$  along the ABZ edge also differs from experimental results:  $Z_{\mathbf{k}}$  is a minimum at  $\mathbf{k} = (\pi/2, \pi/2)$  along this direction, while the intensity of the ARPES peak is a maximum. Our exact, unbiased numerical results clearly demonstrate that the  $t$ - $J$  model cannot explain the data. However, as was shown in previous work,<sup>6,7</sup> it is

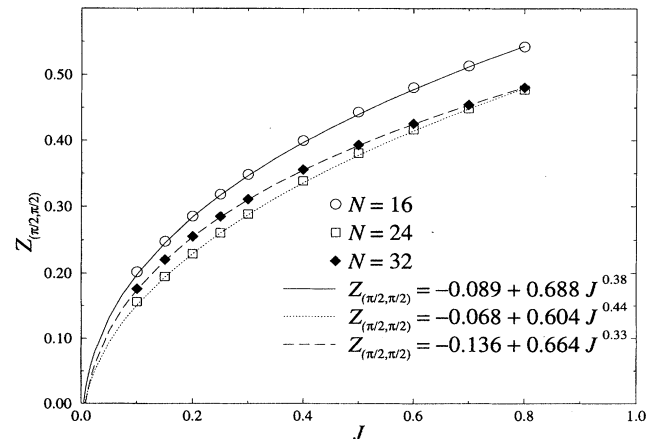


FIG. 5. The same as in Fig. 4 but for the quasiparticle weight  $Z_{(\pi/2, \pi/2)}$ .

now known that a  $t'$  is required to describe hole motion via a single-band model in a  $\text{CuO}_2$  plane. Thus, we defer a more quantitative comparison of theory and the dispersion relation obtained by experiment until a future publication wherein the effect of  $t'$  will be presented. A qualitative comparison to the variation of spectral weight as a function of  $\mathbf{k}$  found numerically to that found in the ARPES data shows one surprising agreement. To be specific, note that the  $t$ - $J$  model is a strong-coupling model which when undoped displays long-ranged antiferromagnetic broken symmetry. Thus one expects that for only one hole, there should be an equivalence of  $A(\mathbf{k}, \omega)$  under a shift of a reciprocal lattice vector of the magnetic lattice. As seen in Fig. 2 our results clearly do not display this feature. However, neither do the ARPES

experiments,<sup>5</sup> and thus, unlike the original conjecture of Ref. 5, the strength of the on-site correlations cannot necessarily be resolved via photoemission.

Summarizing, we have presented the spectral function of a single hole propagating on a 32-site square lattice described by the  $t$ - $J$  model.<sup>18</sup> These exact, unbiased, numerical data now serve as an acid test of analytical theories of this important strong-coupling Hamiltonian.

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<sup>10</sup>Note that at  $(0,0)$  and  $(\pi, \pi)$ ,  $E(\mathbf{k})$  are not the lowest-energy states in their respective symmetry sectors. The lowest-energy states with these momenta are not  $S=\frac{1}{2}$  states, and hence do not

appear in the spectral function. Also, although the quasiparticle peak that we find at  $(\pi, \pi)$  is extremely small,  $E(\pi, \pi)$  is given very accurately by the Lanczos iterations.

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