Detailed Lanczos study of one- and two-hole band structure and finite-size effects in the t-J model

T. Barnes
Physics Division and Center for Computationally Intensive Physics, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6373 and Department of Physics, University of Tennessee, Knoxville, Tennessee 37996-1200

A.E. Jacobs
Department of Physics, University of Toronto, Toronto, Ontario, Canada M5S 1A7

M.D. Kovarik
Physics Division and Center for Computationally Intensive Physics, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6373 and Department of Physics, University of Tennessee, Knoxville, Tennessee 37996-1200

W.G. Macready
Department of Physics, University of Toronto, Toronto, Ontario, Canada M5S 1A7
(Received 4 January 1991)

We present accurate numerical results for low-lying one- and two-hole states in the t-J model on a 4×4 lattice. We find six level crossings in the one-hole ground state for $0 < t/J < \infty$; accurate t/J values of these crossings and the associated ground-state quantum numbers are given. A degeneracy of $\mathbf{k} = (0,0)$ $S = 1/2$ and $S = 3/2$ one-hole levels at $t/J = 1/2$ is noted, which is consistent with a recent analytical result. For small t/J, the $S = 1/2$ one-hole and $S = 0$ two-hole bandwidths on the 4×4 lattice are $W_h = [1.190\,445\,7(1)]t$ and $W_{\rm hh} = [2.575(4)]t^2/J$, respectively. The origin of these qualitatively different behaviors is discussed, and a simple relation is found between the small-(t/J) one-hole bandwidth and a static-hole ground-state matrix element. The linear-t term in W_h is apparently a finite-lattice artifact. As a measure of finite-size effects we determined the rms hole-hole separation in the two-hole ground states; we find evidence of important finite-size effects for $t/J \gtrsim 1$, for which the rms hole-hole separation is clearly constrained by the 4×4 lattice. Intermediate-(t/J) hole separations and binding energies for $0.3 \lesssim t/J \lesssim 1$, however, scale approximately as powers of t/J, and can be used to give bulk-limit estimates for $t/J = 3$. In particular, we estimate that the bulk-limit ground-state rms hole-hole separation at $t/J = 3$ is $\approx 1.8a_0$, corresponding to 7 Å in the high-temperature superconductors. The similarity to the observed in-plane coherence length of $\xi_{ab} \approx 14$ Å supports the identification of t-J model hole pairs with the Cooper pairs of high-temperature superconductivity.

I. INTRODUCTION: THE t-J MODEL

The suggestion that two-dimensional Hubbard and Heisenberg spin systems[1,2] might provide useful models for the study of high-temperature superconductors[3] has motivated many recent investigations of the two-dimensional Heisenberg antiferromagnet with a hopping term. This t-J model[4–9] is described by the Hamiltonian

$$H = -t \sum_{<ij>,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}) + J \sum_{<ij>} (\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4} n_i n_j)\,, \tag{1}$$

with an implicit restriction to unoccupied or singly occupied sites. This Hamiltonian incorporates the large antiferromagnetic interaction observed between Cu^{2+} d electrons in the copper-oxygen planes (the J term) and allows hole hopping if vacancies are present (the t term). The t-J model was originally derived as a limit of the single-band Hubbard model for large Coulomb repulsion, $U/t >> 1$. Although its relevance to the Hubbard model is problematical for small t/J, it is nonetheless an interesting model of the interplay between hole dynamics and antiferromagnetism in itself.

Experiment finds that hole doping of antiferromagnetic insulators such as La_2CuO_4 and $YBa_2Cu_3O_{6.5}$ [which are modeled by (1) with one electron per site] leads to the disruption of antiferromagnetic order and results in a spin-glass phase followed by an insulator-to-metal transition; this metal has a superconducting phase characterized by a positive Hall coefficient and Cooper pairs with $|Q| = 2e$ (for a recent review see Birgeneau[10]). To compare the t-J model (1) with experiment one would like to determine whether this model predicts such a phase diagram. A more detailed question is whether (1) predicts the formation of hole-hole bound states which act as Cooper pairs, this being a candidate mechanism for high-temperature superconductivity.

Energies and other matrix elements of (1) have been studied extensively using Lanczos techniques (these applications have been reviewed by Dagotto[11]), and although it does appear that a bound two-hole system is energetically favored over two separate holes it is now widely believed that this pairing is actually the initial step of hole phase separation.[11–14] [Of course, phase separation has not been convincingly demonstrated for arbitrary t/J,[15,16] and has only been argued to occur for the large- and small-(t/J) limits.] Phase separation in the system (1) with finite hole doping will lead to a bulk-limit ground state with separate hole-rich and hole-free regions, and as this behavior is not observed in the superconductors it is an unphysical feature of the model.

It has been suggested that phase separation may be an artifact of the neglect of hole-hole Coulomb interactions,[11–13,17] and that the incorporation of this Coulomb repulsion may prevent hole clustering beyond the formation of two-hole bound states, due to the excessive Coulomb energy of larger hole clusters.[17] In a previous study[18] of the energies of static-hole clusters in the t-J model we presented numerical results which support this picture: In a generalized t-J-ϵ model with $e^2/\epsilon r$ hole Coulomb interactions we found that the range of dielectric constant ϵ for which hole clustering stops with hole pair formation in the insulating (dilute hole) phase is not far from the observed ϵ, given the experimental value of $J \approx 125$ meV.

Our previous numerical study of Coulomb effects in the t-J model considered the $t = 0$ limit only; one would obviously like to generalize this to $t > 0$ and study the effect of the hopping term on hole-pair formation and phase separation. In this paper we present detailed results for one-hole and two-hole properties in the t-J model for comparison with results incorporating the Coulomb interaction. In particular, we study the band structure and quantum numbers of low-lying one- and two-hole states in detail, and find evidence for simple scaling behavior in the intermediate-(t/J) regime, which allows extrapolation to the $t/J \approx 3$ of the high-temperature superconductors.

Before presenting these results we shall briefly summarize previous numerical studies of the t-J model. The first exact-diagonalization study of the t-J model on a periodic 4×4 lattice was due to Bonča, Prelovšek, and Sega,[8] who determined several one- and two-hole ground-state matrix elements, including one- and two-hole energies, bandwidths, magnetizations, spin-spin correlations, and hole-hole correlations, and concluded that two-hole bound states are energetically favored on 4×4 lattices for $t/J \lesssim 14$. Dagotto, Moreo and Barnes[9] later gave the one-hole ground-state energy for several values of t/J and ground-state hole energies in each $\mathbf{k}$ sector, and found that the one-hole ground state changes quantum numbers several times as t/J is increased from zero. Riera[19] studied one-, two-, and four-hole states on lattices up to 4×4 and noted the importance of testing for phase separation by measuring four-hole energies. Hasegawa and Poilblanc[20] gave the lowest-lying one-hole and two-hole energies at $t/J = 4.0$ on the 4×4 lattice in each momentum sector, and found that the two-hole ground-state level has d-wave symmetry (for $t/J \lesssim 10$) and a nontrivial degeneracy between momenta $(0,0)$ and $(\pi,0)$. They also quote results for one-hole states on the $\sqrt{18} \times \sqrt{18}$ lattice. Dagotto *et al.*[21] quote one-hole energies and bandwidths on the 4×4 lattice for several values of t/J; Chen and Schüttler[22] discuss low-lying one-hole states and bandwidths based on Lanczos studies on $\sqrt{8} \times \sqrt{8}$ and 4×4 lattices; Elser, Huse, Shraiman and Siggia[23] used Lanczos methods to study bandwidths and spin-spin correlations in one-holes states on the $\sqrt{18} \times \sqrt{18}$ lattice; and Itoh, Arai, and Fujiwara[24] have studied one- and two-hole states on $\sqrt{18} \times \sqrt{18}$ and $\sqrt{20} \times \sqrt{20}$ lattices. (These $\sqrt{18} \times \sqrt{18}$ and $\sqrt{20} \times \sqrt{20}$ results are of special interest in studies of finite-size effects and possible accidental degeneracies on the 4×4 lattice.) Finally, Dagotto, Riera, and Young[15] have tabulated s-, p-, and d-wave two-hole ground-state energies on the 4×4 lattice for several values of t/J.

We note in passing that two conventions for momenta of one-hole states are in common use, which differ by $\Delta\mathbf{k} = (\pi, \pi)$. In this paper we follow the more frequently used convention, which differs from that of Bonča, Prelovšek, and Sega[8] and Hasegawa and Poilblanc.[20] One should also note that some references have discarded the $-n_i n_j/4$ term in the spin-spin interaction in (1), which simply leads to an energy shift in no- and one-hole states but gives different wave functions for two and more holes.

Finally, many numerical studies of correlation functions and frequency-dependent response functions in one- and two-hole states in the t-J model have been reported. These include results for equal-time pairing correlations,[25] spin-spin correlation functions,[26] the optical conductivity,[27–29] pairing susceptibilities,[15] spectral functions,[21,30–32] and Raman spectra.[33,34]

Although the t-J model has been inaccessible to Monte Carlo studies due to the "minus-sign problem," there are no such difficulties in the static-hole limit ($t/J = 0$), which has been studied numerically by Barnes and Kovarik[18] on 4×4, 6×6, and 8×8 lattices. This study confirmed large finite-size effects in the ground-state energy of a single static hole in the t-J model, as predicted by spin-wave theory.[35,36] This result suggests that finite-size effects may also be important for $t/J > 0$, at least in single-hole states.

In addition to the numerical work there have been many approximate analytical studies of the t-J model, using small-cluster studies,[37,38] Green-function methods,[39,40] variational methods,[41–43] effective hole-magnetization Hamiltonians,[44,45] spin-wave calculations,[46] and string-basis calculations.[47,48] One conclusion of these approximate calculations which is of relevance here is that the one-hole ground state has $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$ in the bulk limit.

The remainder of this paper is organized as follows: In Sec. II A we present our results for one-hole energies and quantum numbers, and give accurate results for the t/J values of the various ground-state level crossings, including a degeneracy of one-hole levels with different total spin at $t/J = 1/2$. We also correct some minor numerical inaccuracies in previous work.[49] We then show that the small-(t/J) one-hole band structure on a finite lattice can be understood using degenerate perturbation theory in the hopping term, which leads to a simple relation between the small-(t/J) one-hole bandwidth and a static-hole matrix element; this allows a very accurate and independent bandwidth determination. In Sec. II B we present results for the lowest-lying two-hole states, in particular the energies and ground-state rms hole-hole separations. In Sec. II C we discuss approximate power-law behavior in hole energies and hole-hole separations at intermediate t/J, and extrapolate these results to give estimates for the bulk limit. Finally, Sec. III gives our conclusions.

II. RESULTS

A. One-hole states

1. Numerical results for one-hole energies

To generate our numerical results we used a Lanczos technique which is essentially identical to that described by Hasegawa and Poilblanc[20] for the t-J model, with the exception that we used only translational symmetries to construct our basis states rather than implementing parity and other discrete symmetries. The differences we find relative to other references, for example the complicated set of ground-state quantum number changes we show in Fig. 2, reflect our detailed scan in t/J and the large number of Lanczos iterations we have carried out, rather than any important improvement in technique.

On a 4×4 lattice the allowed values of k_x and k_y are $-\pi/2$, 0, $\pi/2$, and π. Parity and discrete rotation symmetry lead to degeneracies under the discrete transformations $(k_x, k_y) \leftrightarrow (\pm k_x, \pm k_y)$ and $(k_x, k_y) \leftrightarrow (k_y, k_x)$, which leave at most six nondegenerate momentum levels, which we take to be $(0,0)$, $(\pi/2, 0)$, $(\pi, 0)$, $(\pi/2, \pi/2)$, $(\pi, \pi/2)$, and (π, π). The one-hole ground-state levels with $(\pi, 0)$ and $(\pi/2, \pi/2)$ are degenerate; this finite-lattice artifact is due to a hypercubical symmetry of the 4×4 periodic lattice.[9,20,21]

In Table I and Figs. 1(a) and 1(b) we present the lowest-lying one-hole energies $e_h(\mathbf{k}) = E_h(\mathbf{k}) - E_0$ for the six independent momenta; we show the ranges $0 \le t/J \le 4.0$ in Fig. 1(a) and $0 \le t/J \le 0.6$ in Fig. 1(b). Here E_0 is the ground-state energy of the t-J model in the no-hole (Heisenberg) sector, which in our conventions is $16 \times (-1.201\,78\ldots)J$ on the 4×4 lattice. With a few exceptions we confirm the energies of Dagotto, Moreo, and Barnes[9] for $t/J = 0.5, 1.0$, and 2.0, Hasegawa and Poilblanc[20] for $t/J = 4.0$, Dagotto, Riera, and Young[15] for $t/J = 0.5, 1.0$, and 2.0, and Dagotto *et al.*[21] for $t/J = 0.1, 0.2, 0.5, 1.0$, and 5.0 (these are the t/J values that coincide with ours) to their quoted accuracies to within occasional discrepancies in the final digit. (Note that our momentum convention differs from that of Hasegawa and Poilblanc, as stated previously.) The minor discrepancies we have found with the literature are summarized in our references.

At small t/J on a finite lattice the one-hole energies are asymptotically linear in t as $t/J \to 0$ [see Fig. 1(b)], and a numerical fit to our results gives a bandwidth (for $S = 1/2$) of $W_h = 1.190\,446(1)t$, consistent with the $1.19t$ quoted by Dagotto *et al.*[21] The small-(t/J) band evidently has a symmetric linear-t dispersion about the degenerate $(\pi, 0)$ and $(\pi/2, \pi/2)$ levels, which them-

TABLE I. Lowest-lying one-hole energies $e_h(\mathbf{k}) = E_h(\mathbf{k}) - E_0$ for each independent momentum on a 4×4 lattice. The $(\pi, 0)$ and $(\pi/2, \pi/2)$ energies are degenerate.

t/J	$e_h(0,0)/J$	$e_h(\pi/2,0)/J$	$e_h(\pi,0)/J$	$e_h(\pi,\pi/2)/J$	$e_h(\pi,\pi)/J$
0.000	2.348 563 09	2.348 563 09	2.348 563 09	2.348 563 09	2.348 563 09
0.001	2.349 158 10	2.348 858 41	2.348 560 10	2.348 263 18	2.347 967 66
0.010	2.354 494 38	2.351 309 29	2.348 264 34	2.345 358 31	2.342 590 04
0.025	2.363 312 30	2.354 561 33	2.346 697 36	2.339 700 26	2.333 552 86
0.050	2.377 794 92	2.357 647 76	2.341 120 46	2.328 041 59	2.318 286 26
0.075	2.392 004 35	2.357 798 74	2.331 892 12	2.313 674 45	2.302 767 01
0.100	2.405 932 94	2.355 015 23	2.319 108 19	2.296 701 46	2.286 997 97
0.200	2.458 644 05	2.315 383 77	2.235 287 03	2.205 133 44	2.221 452 69
0.400	2.546 513 93	2.119 621 64	1.947 458 40	1.933 770 97	2.078 246 15
0.500	2.578 598 34	1.978 581 61	1.763 655 31	1.767 117 47	2.000 000 00
0.600	2.443 604 73	1.817 348 76	1.562 619 09	1.585 950 91	1.916 574 49
0.800	2.158 897 80	1.450 844 09	1.124 804 15	1.191 142 33	1.730 346 72
1.000	1.849 168 57	1.042 459 09	0.654 803 67	0.764 421 62	1.508 619 39
1.200	1.506 394 16	0.603 970 55	0.163 044 21	0.314 015 87	1.235 692 98
1.400	1.122 879 20	0.142 327 67	−0.344 641 27	−0.155 075 39	0.896 930 04
1.600	0.695 025 95	−0.337 835 07	−0.864 641 78	−0.639 490 76	0.489 854 14
1.800	0.225 585 86	−0.833 138 26	−1.394 532 37	−1.136 786 12	0.026 423 90
2.000	−0.278 189 74	−1.340 985 89	−1.932 580 59	−1.645 085 15	−0.476 985 31
3.000	−3.105 409 68	−4.009 320 04	−4.708 458 87	−4.307 894 53	−3.267 298 90
4.000	−6.135 716 81	−6.806 728 95	−7.574 029 14	−7.104 526 37	−6.228 771 82
5.000	−9.189 570 55	−9.743 648 33	−10.492 021 68	−9.985 165 63	−9.258 369 64
10.000	−24.927 475 60	−25.045 944 08	−25.450 107 50	−25.082 427 68	−24.901 265 32

selves depart from the static-hole energy quadratically ($\propto t^2/J$). This linear-t behavior is a consequence of degenerate perturbation theory on a finite lattice, as we shall subsequently demonstrate.

Two ground-state level crossings occur in the small- and intermediate-(t/J) regime, from (π,π) to $(\pi,\pi/2)$ at $t/J \approx 0.1526$ and from $(\pi,\pi/2)$ to $(\pi,0)$ at $t/J \approx 0.4814$ [see Fig. 1(b)]. These small-(t/J) level crossings are presumably finite-lattice artifacts which recede to $t/J = 0$ in the bulk limit; they follow from the linear-t one-hole bandwidth, which is itself a finite lattice effect in the $S = 1/2$ sector, as we shall discuss at the end of the next section. These crossings have previously been reported in the literature,[21,22] albeit with less accurate t/J values. For $t/J \gtrsim 0.4814$ the one-hole ground state remains a twelvefold-degenerate $S = 1/2$ multiplet comprising the momenta $(0,\pi), (\pi,0)$, and $(\pm\pi/2,\pm\pi/2)$ until $t/J \gtrsim 13$, where a complicated transition to the $S = 15/2$ Nagaoka state begins. With increasing t/J, the ground state changes from the $|S = 1/2\rangle$ state to $|S;\mathbf{k}\rangle = |3/2;(0,0)\rangle$ at $t/J \approx 12.8290$, to $|5/2;(\pi,\pi)\rangle$ at $t/J \approx 13.0582$, $|7/2;(0,0)\rangle$ at $t/J \approx 15.8469$, and finally becomes the $|15/2;(0,0)\rangle$ Nagaoka state with $e_h = -4t$ for $t/J \gtrsim 15.8972$. (This sequence of ground-state transitions is summarized in Fig. 2.) The final $S = (L^2-1)/2$ Nagaoka state is generated as a result of the global disordering effect of hole motion on the spin alignment of the entire lattice. Since this state requires disruption of the antiferromagnetic order throughout the entire lattice by a single hole, it appears at much larger t/J on larger lattices and recedes to $t/J = \infty$ in the bulk limit. (See Barnes, Dagotto, Moreo, and Swanson[50] for a clarification of why this random spin state is a member of the "ferromagnetic" Nagaoka multiplet.)

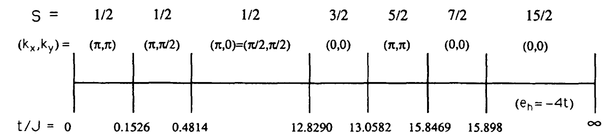

FIG. 2. One-hole ground-state level crossings and quantum numbers on the 4 × 4 lattice.

One can establish certain exact results for the t-J model at the special value $t/J = 1/2$; in particular we confirm Cappon's result[51] for the ground-state energy of a single hole with $\mathbf{k} = (\pi,\pi)$, which in our conventions is

$$e_h(\pi,\pi)\Big|_{t/J=1/2} = 4t \ . \qquad (2)$$

Note also that a level crossing in the $\mathbf{k} = (0,0)$ sector of the one-hole system takes place at $t/J = 1/2$ [see Fig. 1(b)], where $S = 1/2$ and $S = 3/2$ one-hole states are degenerate. Cappon[51] anticipates that such degeneracies at $t/J = 1/2$ will be accompanied by levels with one more and one less hole and with the average spin value (here $S = 1$), at energies separated by plus and minus $4t$, respectively; comparison of $e_h(0,0)/J \approx 2.578\,598\,34$ in Table I and the pure Heisenberg singlet-triplet gap[52] of $\approx 0.578\,598\,336J$ (in our conventions) shows that this relation is satisfied to high accuracy in the no- and one-hole sectors.

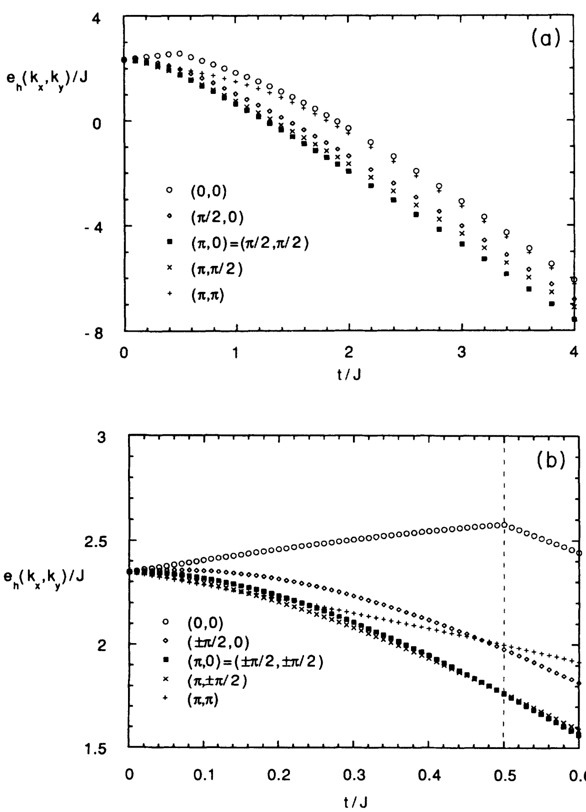

FIG. 1. (a) $e_h(k_x,k_y)/J$ vs t/J for $0 \le t/J \le 4$. (b) $e_h(k_x,k_y)/J$ for $0 < t/J < 0.6$.

2. Analytical one-hole band structure on a finite lattice for $t/J \ll 1$

The simple $\mathbf{k}$ dependence of the one-hole band at small t/J on a finite lattice can be understood using perturbation theory in the hopping parameter t. (For related discussions see Dagotto *et al.*[21] and Elser, Huse, Shraiman, and Siggia[23].) In a perturbative expansion in the hopping parameter, the states connected by $H_{\rm hop}$ are static-hole states in a Heisenberg spin background; as these unperturbed static-hole ground states all have the same zeroth-order (Heisenberg) energy, one must apply degenerate perturbation theory and construct a basis of linear combinations of these states which diagonalizes the hopping term. These linear combinations can be taken to be momentum eigenstates, and each has a hopping-term matrix element which is linear in t. Thus, the linear-t behavior of the one-hole bandwidth is a consequence of the degeneracy of static-hole states under hole translations. Note that the two-hole sector has different properties; application of the hopping term to a pair of nearest-neighbor static holes gives an inequivalent static hole configuration with a different unperturbed energy, so nondegenerate perturbation theory applies and the leading-order level shifts and bandwidth are proportional to $|\langle (hh)'|H_{\rm hop}|(hh)\rangle|^2/\Delta E_0(hh) \propto t^2/J$.

Degenerate perturbation theory as described above leads to a relation between the linear-t component of the small-(t/J) one-hole bandwidth and a static-hole matrix element. The **k**-diagonal superpositions of static-hole states, which are the unperturbed basis states in this approach, are given by

$$|\psi_h(\mathbf{k})\rangle = \sum_{\mathcal{S},\jmath} \Psi_0(\mathcal{S},\jmath\,) e^{i\mathbf{k}\cdot\jmath}\, |\mathcal{S},\jmath\,\rangle, \tag{3}$$

where $\jmath = (j_x, j_y)$ is the hole location, $\mathcal{S}$ is a generic $\hat{\mathbf{z}}$-diagonal spin configuration on the remaining $L^2 - 1$ occupied sites, and $\Psi_0(\mathcal{S},\jmath\,)$ is the amplitude to find the spin configuration $\mathcal{S}$ given a static hole at site $\jmath$, normalized to

$$\sum_{\mathcal{S}} |\Psi_0(\mathcal{S},\jmath\,)|^2 = 1\ . \tag{4}$$

The energy shift to leading order in the hopping term is

$$\delta E(k_x,k_y) = -t\left\langle \psi_h(\mathbf{k}) \left| \sum_{<ij>,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}) \right| \psi_h(\mathbf{k}) \right\rangle. \tag{5}$$

Application of a $c^\dagger_{\jmath\sigma} c_{\jmath\,'\sigma}$ hopping term to a static-hole ground state gives a new state with a new static-hole location $\jmath\,' = \jmath + \boldsymbol{\delta}$, where $\jmath\,'$ and $\jmath$ are nearest neighbors.

This new state has a nontrivial hopping-term matrix element with the initial state. The application of the hopping Hamiltonian to static-hole states with holes at each of the four nearest-neighbor sites to $\jmath$ thus leads to a nonzero matrix element with the state $|\mathcal{S},\jmath\,\rangle$, so that we find

$$H_{\rm hop}|\psi_h(\mathbf{k})\rangle = -t \sum_{\mathcal{S},\jmath,\boldsymbol{\delta}} \Psi_0(\mathcal{S},\jmath+\boldsymbol{\delta}) P(\boldsymbol{\delta}) e^{i\mathbf{k}\cdot(\jmath+\boldsymbol{\delta})} |\mathcal{S},\jmath\,\rangle\ . \tag{6}$$

The $\{P(\boldsymbol{\delta})\}$ are the phase factors introduced by hole hops in directions $\boldsymbol{\delta} = (1,0)$, $(-1,0)$, $(0,1)$, and $(0,-1)$, which depend on the ordering convention used to define the fermion basis states. Thus, to $O(t)$ we have

$$\begin{aligned}\langle \psi_h(\mathbf{k})|H_{\rm hop}|\psi_h(\mathbf{k})\rangle = -t \sum_{\mathcal{S},\jmath} \Psi_0(\mathcal{S},\jmath\,)[\ &\Psi_0(\mathcal{S},(j_x+1,j_y))P(1,0)e^{ik_x} + \Psi_0(\mathcal{S},(j_x-1,j_y))P(-1,0)e^{-ik_x} \\ &+\Psi_0(\mathcal{S},(j_x,j_y+1))P(0,1)e^{ik_y} + \Psi_0(\mathcal{S},(j_x,j_y-1))P(0,-1)e^{-ik_y}].\end{aligned} \tag{7}$$

The quantities $\sum_{\mathcal{S},\jmath} \Psi_0(\mathcal{S},\jmath\,)\Psi_0(\mathcal{S},\jmath+\boldsymbol{\delta}\,)P(\boldsymbol{\delta}\,)$ in (7) must be independent of $\boldsymbol{\delta}$ due to discrete rotational invariance, so we find

$$\begin{aligned}\langle \psi_h(\mathbf{k})|H_{\rm hop}|\psi_h(\mathbf{k})\rangle &= -t\ (e^{ik_x} + e^{-ik_x} \\ &\quad + e^{ik_y} + e^{-ik_y})\langle ||K||\rangle \\ &= -2t\ (\cos k_x + \cos k_y)\langle ||K||\rangle\ ,\end{aligned} \tag{8}$$

where $\langle ||K||\rangle$ is the reduced matrix element

$$\langle ||K||\rangle = \frac{1}{4}\left\langle \psi_h(0) \left| \sum_{<ij>,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}) \right| \psi_h(0) \right\rangle. \tag{9}$$

This quantity is simply an off-diagonal matrix element of the ground-state wave function of a static hole in the Heisenberg antiferromagnet; in terms of the static-hole ground state of a hole at site $\jmath$, $|\psi_{0h}(\jmath\,)\rangle = \sum_{\mathcal{S}} \Psi_0(\mathcal{S},\jmath\,)|\mathcal{S},\jmath\,\rangle$, this reduced matrix element is

$$\langle ||K||\rangle = \sum_{\mathcal{S}} \Psi_0(\mathcal{S}',\jmath\,'\,)\Psi_0(\mathcal{S},\jmath\,) \tag{10}$$

so the small-(t/J) bandwidth, defined here as $W_h = e_h(0,0) - e_h(\pi,\pi)$, is given by

$$\lim_{t/J\to 0} W_h = 8t \sum_{\mathcal{S}} \Psi_0(\mathcal{S}',\jmath\,'\,)\Psi_0(\mathcal{S},\jmath\,)\ . \tag{11}$$

In the above equations $\Psi_0(\mathcal{S}',\jmath\,'\,)$ is the amplitude to find a spin configuration $\mathcal{S}'$ in a static-hole ground state with a hole at $\jmath\,' = \jmath + \hat{x}$, where the pair $(\mathcal{S}', \jmath+\hat{x})$ is constructed from $(\mathcal{S},\jmath\,)$ by exchanging the hole at site $\jmath$ with the spin at site $\jmath + \hat{x}$. An independent Lanczos evaluation of the $S = 1/2$ static-hole matrix element (10) gives $\langle ||K||\rangle = 0.148\,805\,71(1)$ and hence a one-hole bandwidth of $W_h = [1.190\,445\,7(1)]t$ in the small-(t/J) limit, which is consistent with the $[1.190\,446(1)]t$ we previously estimated directly from our $t/J > 0$ Lanczos results for e_h. The theoretical small-(t/J) dispersion relation obtained from (8) and (10) is also consistent with the numerical results shown in Fig. 1(b) at the smaller values of t/J.

Note that our t-J basis used in the derivation of (11) does not employ the "checkerboard" minus-sign phase convention required to give negative off-diagonal terms in the spin-spin interaction Hamiltonian. In our basis the $\mathbf{S}_i \cdot \mathbf{S}_j$ Hamiltonian is positive off-diagonal, so that the $\{\Psi_0\}$, although real, are not of definite sign, and hence W_h is not positive definite. Negative W_h in (11) simply implies an inverted multiplet relative to $S = 1/2$, and hence a $\mathbf{k} = (0,0)$ level at the bottom of the band rather than (π,π).

There is an important caveat regarding this small-(t/J) dispersion relation. Elser, Huse, Siggia, and Shraiman[23] find that the conclusion that $W_h \propto t$ is invalid in the bulk limit, given a nonzero staggered magnetization. States of two nearest-neighbor static holes on an infinite lattice actually have zero overlap in (11) in the bulk limit, because the staggered magnetizations associated with static holes on different sublattices have opposite signatures. This leaves a bulk-limit one-hole bandwidth $W_h \propto t^2/J$. Alternatively, one can view the spontaneous selection of one Néel pattern as a dimerization of the system, which reduces the size of the Brillouin zone and results in a degeneracy of bulk-limit states which differ by $\Delta\mathbf{k} = (\pi,\pi)$. On a finite lattice there is a nonzero amplitude to find spin configurations similar to "wrong-signature" backgrounds associated with a static hole, so the wave-function overlap (11) does not vanish and one finds a bandwidth $W_h \propto t$ until one reaches the bulk limit.[23] Note however that static-hole states with zero staggered magnetization, such as states with sufficiently large total spin, will still have a linear-t bandwidth in the bulk limit at small t/J.

B. Two-hole states

1. *Numerical results for two-hole energies*

In Fig. 3(a) we show our results for $e_{2h}(\mathbf{k}) = E_{2h}(\mathbf{k}) - E_0$ for the lowest-lying two-hole levels (which have $S = 0$) for each independent momentum as functions of t/J for $0 \le t/J \le 4.0$. These two-hole energies are also given in Table II for representative values of t/J. For $t/J \le 4.1$ the lowest levels have momenta $(0,0)$ [degenerate with $(\pi,0)$], $(\pi/2,0)$ [degenerate with $(\pi,\pi/2)$], and $(\pi/2,\pi/2)$ [degenerate with (π,π)]. The degeneracy of the $(0,0)$ and $(\pi,0)$ ground states was first noted by Hasegawa and Poilblanc[20] and is an artifact of the 4×4 lattice; studies on $\sqrt{18} \times \sqrt{18}$ and $\sqrt{20} \times \sqrt{20}$ lattices[24] find the $(0,0)$ level below $(\pi,0)$, which is presumably true in the bulk limit as well. Beginning at $t/J \approx 4.1$ level crossings result in some lowest-lying levels that do not support these degeneracies in general. (The ground-state levels, however, apparently remain degenerate.) At $t/J = 5.0$ we find $e_{2h}(\pi,\pi)/J = -20.991\,425\,81$, and at $t/J = 10.0$, $e_{2h}(\pi,\pi/2) = -50.754\,43P\,31$ and $e_{2h}(\pi,\pi) = -51.018\,776\,08$; comparison with Table II shows that these are no longer degenerate with the $(\pi/2,\pi/2)$ and $(\pi/2,0)$ levels.

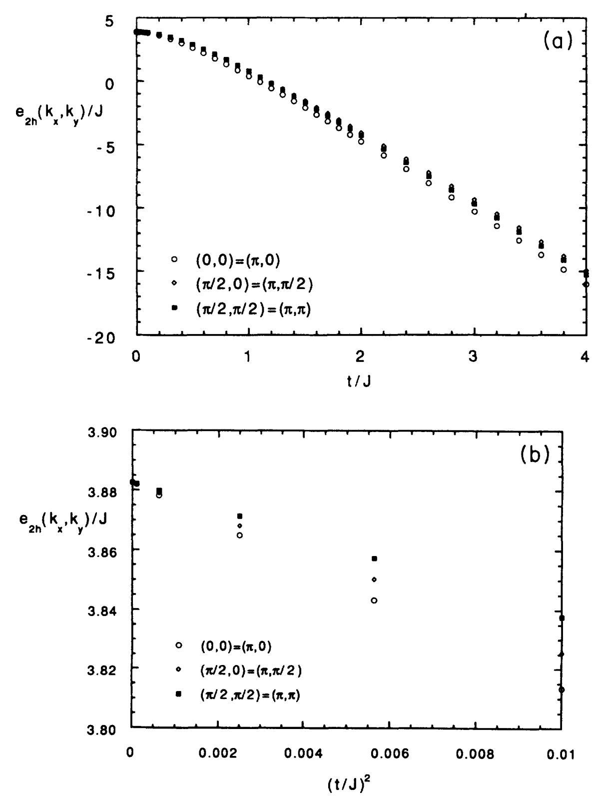

FIG. 3. (a) $e_{2h}(k_x,k_y)/J$ vs t/J for $0 \le t/J \le 4$. (b) $2_{2h}(k_x,k_y)/J$ vs $(t/J)^2$ for $0 \le t/J \le 0.1$.

Our results agree with the previous numerical studies of Hasegawa and Poilblanc[20] (for two d-wave levels at $t/J = 4.0$) and Dagotto, Riera, and Young[15] (for the d-wave two-hole ground-state energy at $t/J = 0.5, 1.0$, and 5.0) to the accuracy quoted by these references (after the trivial change in the Hasegawa and Poilblanc momentum convention noted previously). In Fig. 3(b) we show our results for small t/J, $0 \le t/J \le 0.1$, versus $(t/J)^2$. In the small-(t/J) limit the two-hole energies evidently depart from the static-hole energy as c_0t^2/J; this behavior can be understood perturbatively, as we noted in our discussion of the one-hole bandwidth. A numerical fit to c_0t^2/J gives a bandwidth estimate of $W_{\rm hh} = [2.575(4)]t^2/J$.

The hole-pair binding energy on a finite lattice may be defined by

$$\Delta_{2,1^2} = e_{2h}(\mathbf{k}) - 2e_h(\mathbf{k}') \ , \tag{12}$$

where $e_{2h}(\mathbf{k}) = E_{2h}(\mathbf{k}) - E_0$ and $e_h(\mathbf{k}') = E_h(\mathbf{k}') - E_0$. Here $E_h(\mathbf{k}')$ and $E_{2h}(\mathbf{k})$ are the energies of the ground states in the one- and two-hole sectors, and E_0 is the ground-state energy in the no-hole sector, as defined in Sec. II A. In Fig. 4 we show this two-hole binding energy $\Delta_{2,1^2}$ as a function of t/J for $0 \le t/J \le 4.0$. Although $\Delta_{2,1^2}/J$ does not change by more than 10% from the static-hole value of ≈ -0.8142 in this range, its detailed behavior for small t/J is rather complicated due to changes in the quantum numbers of the one-hole ground state. These imply changes in $\mathbf{k}'$ in the definition (12), which lead to cusps in $\Delta_{2,1^2}$. These cusps occur at $t/J \approx 0.1526$ and $t/J \approx 0.4814$ in Fig. 4, as noted in our discussion of one-hole quantum numbers. As the lowest $s = \frac{1}{2}$ one-hole level presumably has $\mathbf{k} = (\pi/2,\pi/2)$ in the bulk limit for all $t/J > 0$, a generalized two-hole binding energy $\tilde{\Delta}_{2,1^2}$ defined relative to this $(\pi/2,\pi/2)$

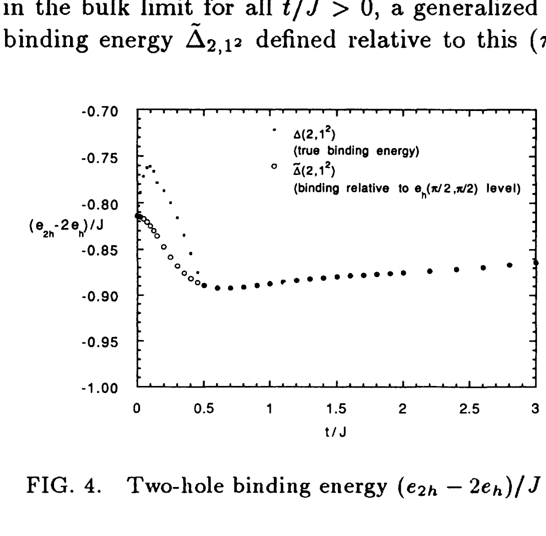

FIG. 4. Two-hole binding energy $(e_{2h} - 2e_h)/J$ vs t/J.

TABLE II. Lowest-lying two-hole energies $e_{2h}(\mathbf{k}) = E_{2h}(\mathbf{k}) - E_0$ for each independent momentum on the 4 × 4 lattice. Degeneracies are present in all these levels for $t/J \lesssim 4.1$; the $(\pi,0)$ level is degenerate with $(0,0)$, $(\pi/2,0)$ with $(\pi,\pi/2)$ and (π,π) with $(\pi/2,\pi/2)$. (See text for $t/J > 4$.)

t/J	$e_{2h}(0,0)/J$	$e_{2h}(\pi/2,0)/J$	$e_{2h}(\pi/2,\pi/2)/J$
0.000	3.882 735 19	3.882 735 19	3.882 735 19
0.010	3.882 023 53	3.882 152 66	3.882 281 80
0.025	3.878 293 79	3.879 098 14	3.879 902 75
0.050	3.865 060 70	3.868 240 07	3.871 423 10
0.075	3.843 298 76	3.850 315 95	3.857 348 56
0.100	3.813 413 58	3.825 570 78	3.837 764 29
0.200	3.623 478 43	3.665 391 29	3.706 993 30
0.400	3.013 294 86	3.131 568 86	3.231 213 89
0.500	2.638 366 72	2.796 827 88	2.909 122 82
0.600	2.233 417 81	2.432 604 53	2.543 828 20
0.800	1.358 672 98	1.639 867 23	1.717 175 45
1.000	0.422 346 48	0.784 133 54	0.806 354 90
1.200	−0.557 576 42	−0.118 762 78	−0.155 916 73
1.400	−1.570 078 74	−1.058 946 67	−1.152 297 61
1.600	−2.607 854 79	−2.029 427 66	−2.173 074 74
1.800	−3.665 790 10	−3.024 944 87	−3.212 302 36
2.000	−4.740 163 52	−4.041 443 66	−4.266 060 19
3.000	−10.280 770 95	−9.429 411 81	−9.678 805 84
4.000	−15.998 326 31	−15.100 204 45	−15.239 107 64
5.000	−21.830 562 94	−20.891 081 77	−20.929 349 28
10.000	−52.119 292 60	−51.388 173 90	−51.245 026 55

one-hole state is more relevant to bulk-limit results. This generalized binding energy is also shown in Fig. 4; note the increased binding with increasing t/J to a maximum binding of $\tilde{\Delta}_{2,1^2}/J \approx -0.892$ at $t/J \approx 0.66$, following which the binding slowly decreases. At $t/J = 3$, it is $\Delta_{2,1^2}/J = \tilde{\Delta}_{2,1^2}/J \approx -0.8639$.

2. Ground-state rms hole-hole separations and finite-size effects

A measure of the importance of finite-size effects is provided by the rms hole-hole separation in the two-hole ground states. [Recall that there are three degenerate two-hole ground states on the 4 × 4 lattice, with $\mathbf{k} = (0,\pi), (\pi,0)$, and $(0,0)$, and that only the first two have rotationally equivalent wave functions.] As t/J is increased to infinity, the rms hole-hole separation

$$r_{\rm rms} = \left\{ \langle \psi_0(hh;\mathbf{k})|\, r^2 \,|\psi_0(hh;\mathbf{k})\rangle \right\}^{1/2} \tag{13}$$

approaches a maximum value which is determined by the lattice size L. This maximum rms separation on the 4×4 lattice is $r_{\rm rms}(t/J = \infty) \approx 1.99 a_0$ (see Table III).

TABLE III. The rms hole-hole separation in the two independent two-hole ground states on the 4 × 4 lattice.

t/J	$r_{\rm rms}(0,0)/a_0$	$r_{\rm rms}(\pi,0)/a_0$
0.000	1.000 000 00	1.000 000 00
0.010	1.000 154 05	1.000 438 27
0.100	1.020 714 09	1.039 521 93
0.200	1.068 398 88	1.123 511 38
0.400	1.177 188 04	1.280 438 32
0.500	1.228 078 90	1.339 900 92
0.600	1.275 354 60	1.389 320 52
0.800	1.358 308 44	1.466 397 84
1.000	1.426 316 07	1.523 409 70
1.200	1.481 492 99	1.567 034 95
1.400	1.526 412 84	1.601 422 85
1.600	1.563 360 10	1.629 267 00
1.800	1.594 140 16	1.652 351 51
2.000	1.620 119 64	1.671 879 15
3.000	1.706 286 15	1.738 186 63
4.000	1.756 116 96	1.778 247 46
5.000	1.791 068 88	1.806 934 73
10.000	1.888 408 26	1.890 315 00

Figure 5 shows the rms separation versus t/J for the two independent ground states, and the asymptotic lattice maximum of $\approx 1.99 a_0$ is shown as a dashed line. We determined this maximum rms hole separation by iterating from a state with the two holes on nearest-neighbor sites as well as at the maximum allowed separation of $2\sqrt{2}$. The separation increases rapidly with increasing

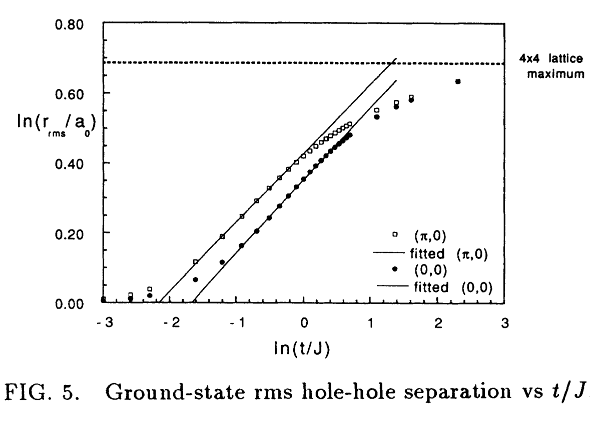

FIG. 5. Ground-state rms hole-hole separation vs t/J.

t/J, and has already traversed half the available range of $[1.0, 1.99]a_0$ on the 4×4 lattice at $t/J \approx 0.88$ for the $(\pi, 0)$ ground state and $t/J \approx 1.26$ for $(0,0)$. At larger values of t/J one sees a flattening of $r_{\rm rms}$ for $t/J \gtrsim 1$, which suggests the presence of important finite-size effects. In Sec. II C we shall discuss the t/J dependence of two-hole matrix elements for $t/J \lesssim 1$, and show that simple power-law behavior is suggested, and that this behavior can be extrapolated to give bulk-limit estimates at $t/J = 3$.

C. Power-law behavior in one- and two-hole states

One might expect energy levels and $r_{\rm rms}$ to scale approximately as powers of t/J for intermediate values of t/J. This behavior can be motivated by approximating the hole interaction by an effective linear potential, which arises from energetically unfavorable spin alignment in the wake of hole motion in an antiferromagnetic background. In the Ising case (the t-J_z model) this reasoning leads one to expect that hole motion produces a string of flipped spins of length $l \propto (t/J_z)^{1/3}$, so that the hole-hole separation of a pair of holes connected by a random string should scale as $r_{\rm rms}(\text{t-J}_z) \approx \sqrt{l} \propto (t/J_z)^{1/6}$. This effective linear potential description has been discussed by Bulaevskii, Nagaev, and Khomskii,[53] Shraiman and Siggia,[54] and Kane, Lee, and Read,[39] and the latter reference suggested the $r_{\rm rms}(\text{t-J}_z) \propto (t/J_z)^{1/6}$ behavior. This in turn suggests that the ground-state hole energy in the t-J_z model should scale approximately as $e_h/t \approx c_0 + c_1(t/J_z)^{-2/3}$, which was found to be a remarkably accurate parametrization over the range $0.02 < J_z/t < 1$ in recent Monte Carlo[50] and string-basis[47] studies.

In the t-J model we expect spin fluctuations to weaken the effective linear potential in a complicated dynamical manner; as a simple approximation we model this by a slower-than-linear potential, $V(l) \propto Jl^p$, where $0 < p < 1$. Simple dimensional arguments applied to the Schrödinger equation with this potential suggest that hole ground-state energies and the rms hole-hole separation should scale approximately as

$$e_h/t = c_0 + c_1(t/J)^{-2/(p+2)} , \tag{14}$$

(similarly for e_{2h}/t) and

$$l/a_0 \propto (t/J)^{1/(p+2)} \tag{15}$$

so that

$$r_{\rm rms}/a_0 \propto (t/J)^{1/(2p+4)} . \tag{16}$$

Hence for the physical range $0 < p < 1$ this potential model analogy leads us to expect that $r_{\rm rms}$ should behave as a power of t/J within the range

$$r_{\rm rms}/a_0 \propto (t/J)^{(0.17 \to 0.25)} . \tag{17}$$

Dagotto, Riera, and Young[15] previously found that the two-hole (d-wave) ground-state energy e_{2h}/t scales as $(t/J)^{-0.78(2)}$ over the range $2/3 \le t/J \le 5$, which through (16) implies $p = 0.56(6)$ and an $r_{\rm rms}$ scaling law of $r_{\rm rms}/a_0 \propto (t/J)^{0.195(5)}$.

If $r_{\rm rms}$ does scale as a power of t/J one should observe linear behavior in $\ln(r_{\rm rms}/a_0)$ versus $\ln(t/J)$. Our data for $r_{\rm rms}$ for the independent $\mathbf{k} = (\pi, 0)$ and $(0,0)$ ground states is displayed in this form in Fig. 5, and there is clear evidence for power-law behavior over the range $0.4 \lesssim t/J \lesssim 0.9$. [The linear region actually occurs somewhat lower in t/J for the $(\pi, 0)$, $(0, \pi)$ states, which have a larger rms radius for a given t/J and hence experience finite-size effects sooner as t/J is increased.] To estimate the power law we have fitted $r_{\rm rms}$ to the form

$$r_{\rm rms}/a_0 = \kappa_0 (t/J)^{\kappa_1} \tag{18}$$

over the ranges $0.3 \le t/J \le 0.8$ for $\mathbf{k} = (\pi, 0)$ and $0.4 \le t/J \le 0.9$ for $\mathbf{k} = (0,0)$. The result of this fit is

$$r_{\rm rms}(\pi, 0)/a_0 = [1.533(2)](t/J)^{0.198(4)} \tag{19}$$

and

$$r_{\rm rms}(0,0)/a_0 = [1.423(2)](t/J)^{0.210(4)}, \tag{20}$$

and these numerical fits are shown in Fig. 5. Evidently the observed power law is in good agreement with the 0.195(5) one expects from the e_{2h} power $-0.78(2)$ of Dagotto, Riera, and Young[15] combined with our Eqs. (14) and (16).

At the high-T_c value of $t/J = 3$ and given a CuO_2 site spacing of 3.79 Å, Eqs. (19) and (20) imply for the bulk limit

$$r_{\rm rms}(\pi, 0) = 7.2 \text{ Å} \tag{21}$$

and

$$r_{\rm rms}(0,0) = 6.8 \text{ Å}. \tag{22}$$

These numbers are similar to the coherence length $\xi_{ab} \approx 14$ Å observed in the high-temperature superconductors,[55] which provides a characteristic length scale of the Cooper pairs. We suggest that this result constitutes strong evidence in support of the identification of hole pairs as described by the t-J model with the Cooper pairs of high-temperature superconductivity.

III. CONCLUSIONS

We have presented accurate numerical results for one- and two-hole energies and rms hole-hole separations in the t/J model on a 4×4 lattice for a wide range of values of t/J. In the small-(t/J) limit we found an $S = 1/2$ one-hole bandwidth of $[1.190\,445\,7(1)]t$ and an $S = 0$ two-hole bandwidth of $[2.575(4)]t^2/J$, and have shown that these qualitatively different behaviors can be understood using simple perturbative arguments. An application of degenerate perturbation theory led to a relation between the one-hole bandwidth and a static-hole ground-state matrix element, which allowed an independent indirect bandwidth determination. We also determined the t/J values and quantum numbers associated with the six one-hole ground-state level crossings. Momentum degeneracies and several other level crossings were also noted, including a crossing of $\mathbf{k} = (0,0)$ $S = 1/2$ and $S = 3/2$ one-hole levels at $t/J = 1/2$, which has properties consistent with recent analytical results for $t/J = 1/2$.

Our results for the ground-state rms hole-hole separation on the 4×4 lattice indicate important finite-size effects for $t/J \gtrsim 1$. This suggests that previous studies of the two-hole system on a 4×4 lattice at $t/J \approx 3$ may incorporate large finite-size effects. As the characteristic length scale $r_{\rm rms}$ of the two-hole system actually grows as a relatively small power of t/J, we expect that 4×4 lattice results will at least be qualitatively similar to the bulk limit results, and should provide useful indications of bulk-limit physics. One may be able to avoid these finite-size effects by identifying power-law behavior in t/J and extrapolating to large t/J. In this paper we have identified such power-law behavior in the rms hole-hole separation for intermediate t/J ($0.3 \lesssim t/J \lesssim 1$) where finite-size effects are apparently small, so this matrix element can be extrapolated to give a bulk-limit estimate for $t/J = 3$. We find that the bulk-limit rms ground-state hole-hole separation at $t/J = 3$ is $r_{\rm rms} \approx 1.8a_0$, corresponding to ≈ 7 Å in the high-temperature superconductors. The similarity of this result to the observed high-T_c coherence length, $\xi_{ab} \approx 14$ Å, supports the identification of hole pairs in the t-J model with the Cooper pairs of the high-temperature superconductors.

We should emphasize that we do not interpret this to mean that the t-J model has a superconducting ground state at finite doping, but rather that an isolated hole pair in the t-J model has similarities to the observed Cooper pairs. A realistic generalization of the t-J model would need to address the problem of phase separation, presumably through the incorporation of hole-hole Coulomb repulsion.

ACKNOWLEDGMENTS

We are grateful to E. Dagotto for useful communications. This research was sponsored by the National Sciences and Engineering Research Council of Canada, the United States Department of Energy under Contract Nos. DE-AC05-840R21400 with Martin Marietta Energy Systems Inc. and DE-AS05-76ER03956 with the Physics Department of the University of Tennessee, and by the State of Tennessee Science Alliance Center under Contract No. R01-1061-68.

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