# Derivation of a one-band Hubbard model for CuO planar materials

Silvia B. Bacci, Eduardo R. Gagliano, and Richard M. Martin
*Physics Department, Material Research Laboratory, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801*

James F. Annett
*Physics Department, The Pennsylvania State University, 104 Davey Laboratory, University Park, Pennsylvania 16802*
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We have performed numerical studies of multiband Hubbard models for the Cu-O planes of the high-$T_c$ materials. For the range of realistic parameters, all low-energy ( $\leq 2$ eV) charge and spin excitations are described by the single-band (possibly extended) Hubbard model with $U \simeq W$, where $W$ is the bandwidth.

A key impediment to progress in the theory of high-$T_c$ superconductivity has been the absence of any clear picture of the nature of the electronic Hamiltonian. Attempts to explain the unusual properties and superconductivity have led to many different models in which strong electron-electron interactions play a crucial role. Anderson has argued that the essential physics is contained in the one-band Hubbard model, which is proposed to form a *Luttinger-liquid* state qualitatively different from a usual Fermi liquid.[1] Laughlin has proposed that the system is a *spin liquid* with elementary excitations having fractional statistics.[2] On the other hand, others have proposed that the properties can be understood in a *weak-interacting* regime[3] and as an *antiferromagnetic* Fermi liquid[4] or by an almost localized Fermi-liquid description.[5] Also, it has been claimed that *multiband models* with more degrees of freedom are essential to describe the low-energy properties.[6] Such models have often been analyzed in certain limiting approximations which lead to the effective strong-coupling one-band Hubbard model or its simplified version, the widely studied $t$-$J$ model.[7]

In this work we present results of exact calculations of ground states and excitation spectra of small periodic cells. We considered two cell sizes, $2\times 2$, $Cu_4O_8$ and (for the simpler models) $\sqrt{8}\times\sqrt{8}$, $Cu_8O_{16}$. Our purpose is to establish which models are applicable and what are the regimes of parameters appropriate for the CuO planes.[8] To this end we compare the excitations of multiband models with those of the one-band Hubbard and $t$-$J$-like models considering the *quantum numbers* as well as the *overall behavior* of the low-energy levels with the parameters. The essential point of our work is that by considering the evolution of the properties as a function of the parameters we establish the qualitative regime of the models, although there is not a perfect fit at all energies of the full multiband spectra by the simpler ones.

From our study we conclude that all low-energy ( $\leq 2$-eV ) charge and spin excitations of the CuO planes in high-$T_c$ materials, *both* the stoichiometric and doped, are described by a one-band Hubbard model with $U \simeq W$, where $W$ is the bandwidth. At half-filing the one-band Hubbard model is an insulator with a gap and spin excitations in reasonable agreement with experiments, and a fitting of the energy levels using a Heisenberg model gives $J \simeq 0.1$ eV. However, this fit is not good, even for the lowest states, which indicates the presence of extra terms not included in a pure Heisenberg antiferromagnet. In the doped case, the $t$-$J$ approximation becomes better as the doping concentration is increased.

In comparison, a previous calculation[9] found a reduction to a one-band Hubbard model with $U \simeq 1.5W$. This difference may be crucial since qualitative changes in the properties of the charge excitations arise in this range, indicating a possible change from weak- to strong-coupling regimes. The differences with the present work presumably result from the type of clusters considered and the emphasis in Ref. 9 on only the low-energy spin excitations. The authors of Ref. 9 have also found[10] that $U$ close to our result is needed to fit charge excitations, and this value of $U$ is supported by recent x-ray-absorption experiments by Chen *et al.*[10]

Our starting point is the three-band Hubbard model (3BHM) (Refs. 6 and 8) (Cu $3d_{x^2-y^2}$ and the two O $2p_\sigma$), defined by the Hamiltonian $H = H_d + H_p + H_{pd}$,

$$H_d = \varepsilon_d \sum_{i,\sigma} d^\dagger_{i\sigma} d_{i\sigma} + U_d \sum_i n_{di\uparrow} n_{di\downarrow} , \tag{1a}$$

$$H_p = \varepsilon_p \sum_{l,\sigma} p^\dagger_{l\sigma} p_{l\sigma} + \sum_{\langle l,l'\rangle,\sigma} t^{ll'}_{pp} (p^\dagger_{l\sigma} p_{l'\sigma} + \text{H.c.}) , \tag{1b}$$

$$H_{pd} = \sum_{\langle i,l\rangle,\sigma} t^{il}_{pd} (d^\dagger_{i\sigma} p_{l\sigma} + \text{H.c.}) . \tag{1c}$$

Here $i$ denotes a Cu site and $l$ denotes O sites; each link is considered only once. The operator $d^\dagger_{i\sigma}$ ($p^\dagger_{l\sigma}$) creates a $Cu_{3d}$ ( $O_{2p}$ ) hole at site $i$ ($l$). Here $t_{pp}$ is the O-O hopping matrix elements and $t_{pd}$ is the Cu-O hybridization. The matrix elements $t^{ll'}_{pp} = \pm t_{pp}$ take into account the sign due to the symmetry of the O($2p$) states, and $t^{il}_{pd} = \pm t_{pd}$ of the Cu($3d$). We considered the values of the parameters as obtained from constrained density functional theory, $t_{pp} \simeq 0.65$ eV, $t_{pd} \simeq 1.6$ eV, $U_d = 8.5$ eV, and $\Delta \simeq 3$–$5$ eV.[8] The on-site Coulomb repulsion $U_p \simeq 4$–$6$ eV at an O site has not been taken into account explicitly, since, because

 

of the large O bandwidth ($\simeq 5$ eV), these holes will be delocalized and so their effective repulsion is reduced.

Because of the complexity of this model, its low-energy excitations have been analyzed under different limiting approximations. For example, an effective $t$-$J$ Hamiltonian has been derived for $t_{pp}=0$ by applying perturbation theory on $t_{pd}$ (i.e., assuming $t_{pd} \ll U_d, \Delta$ and $U_d - \Delta$, where $\Delta = \varepsilon_p - \varepsilon_d$ is the charge-transfer energy).[7] On the other hand, for large O-O hopping, the three-band Hubbard model has been reduced to a two-band effective Hamiltonian, which is equivalent to an Anderson lattice model with long-range hopping terms.[11] We also have considered this model, for which calculations can be done on larger cells, $\sqrt{8}\times\sqrt{8}$. The obtained results are very similar to those for the 3BHM, thus supporting the conclusions of our finite-cell study.

Because the charge-transfer energy $\Delta$ is the least well-established parameter in the three-band model, we first consider the overall trends as a function of $\Delta$. In Fig. 1(a) we present the energy spectrum for the undoped (one hole per Cu) 3BHM in the $2\times2$ lattice, as a function of $1/\Delta$, changing $\varepsilon_p$, and taking $\varepsilon_d=0$. In all cases the ground state has the same symmetry and is insulating. For large values of $\Delta$, the upper bands correspond to double occupied sites and the excitations in the low-energy band are spin waves well described by the antiferromagnetic Heisenberg model. On the other hand, for intermediate values of $\Delta$, the low-energy band contains both spin and charge excitations. We will focus upon $\Delta \simeq 4-5$ eV, since this range best fits the observed energy gap in the insulator, as discussed below.

A similar calculation for the single-band Hubbard model is shown in Fig. 1(b), where we present the energy spectra for the undoped compound in the $2\times2$ lattice. Comparing Figs. 1(a) and 1(b) we note an impressive similarity. States with energies up to 3 eV are in reasonable quantitative agreement for the entire range of the parameters, with $U$ varying, but always of order $\Delta$ or $U_d$, whichever is smaller. In Table I we summarize the values of the single-band Hubbard parameters which fit the spectra of the three-band model for several values of $\Delta$ and $t_{pd}$ considered for the undoped system. As $U/t$ increases, the double occupancy decreases; this in turn is reflected in a reduction of the hopping and, as a total result, a narrowing of the band. The value of $U/t$ is determined primarily by the magnitude of the gap in the addition and removal spectra discussed below, and the value of $t$ is adjusted to fit the dispersion of the band. We calculated also the energy spectra of the undoped Hubbard model in an eight-site lattice, which is shown in Fig. 1(c). The features of the spectra are not very sensitive to the lattice size, confirming the general validity of the mapping. Note, however, that as the system size is increased, slightly higher values of the $U/t$ parameter will be obtained. This result, together with the calculated gaps, leads us to conclude that $U \simeq W$ gives a better description of the thermodynamic limit of the CuO planes.

In Fig. 2(a) we summarize the fitting of the low-energy spectra of the multiband and single-band Hubbard models for the undoped $2\times2/4$ cluster and $\Delta=4$ and 5 eV, showing the space-group quantum numbers of each state. Here all states, except one, correspond to spin excitations. Although the lower spin waves excitations in the strong or intermediate $U/t$ regimens are similar, states at

TABLE I. Effective parameters obtained from the fitting to the single-band Hubbard model for different sets of the three-band Hubbard parameters. All energies are in units of eV.

| $t_{pd}$ | $\Delta=3$ | $\Delta=4$ | $\Delta=5$ |
|---|---|---|---|
| 1.6 | $U=2.4$, $t=0.57$ | $U=3.0$, $t=0.54$ | $U=3.4$, $t=0.48$ |
| 1.3 | $U=2.3$, $t=0.50$ | $U=2.7$, $t=0.43$ | $U=2.9$, $t=0.37$ |

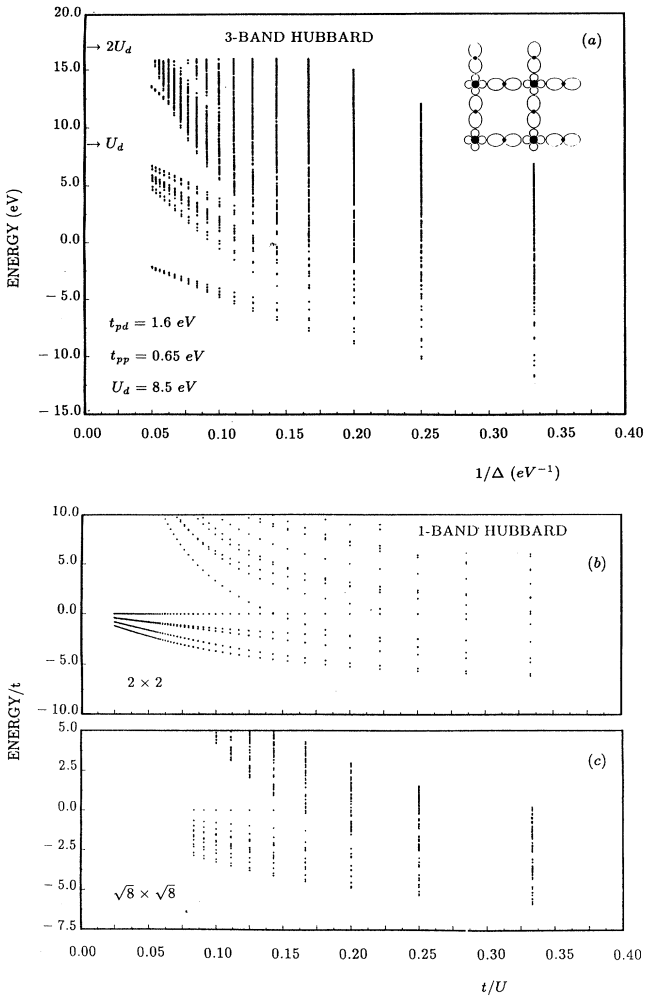


FIG. 1. Energy spectrum of (a) three-band Hubbard model as a function of $1/\Delta$ for the undoped $2\times2/4$ system. The parameters are $t_{pd}=1.6$ eV, $t_{pp}=0.65$ eV, and $U_d=8.5$ eV. One-band Hubbard model as a function of $t/U$ for the undoped (b) $2\times2/4$ and (c) $\sqrt{8}\times\sqrt{8}/8$ clusters.

somewhat higher energy are qualitatively different since charge excitations are mixed into the low-energy band in the small intermediate $\Delta, U$ regime, but not in the strong-coupling limit. The lowest charge excitation shown in Fig. 2 (a), which has developed from the *upper* Hubbard band, has quantum numbers $(\pi,\pi), B_2$.

In order to compare with the strong-coupling limit of the Hubbard model, i.e., the Heisenberg Hamiltonian, it is essential to consider the larger-size cells. This is because in the $2\times2$ cell, with periodic boundary conditions, two neighboring O sites around each Cu are required to be equivalent. This leads to overcounting of the hopping terms and errors in the value of $J$ deduced. (No such error occurs in mapping the three- to the one-band Hubbard model because in that case the overcounting is the same in both cases.) Therefore, we consider mapping the 1BHM onto the Heisenberg model using the $\sqrt{8}\times\sqrt{8}$ cell. In Fig. 2(b) we show the comparison for the cases $U/t=8$ and 12, which represent the ranges considered here and in Hybersten *et al.*[9] We see that for the case $U/t=12$ the fit is rather good for the lowest five to six states, but is much poorer for higher states. For the case $U/t=8$, only the lowest three states are even approximately described. Interestingly, we find that in this range the value of $J$ that results from fitting these lowest states is rather insensitive to the value of $U$. In fact, the range of $J$ that we obtain by fitting the lowest excited states, on intermediate scale (shown in the figure with an arrow) or the highest state of the band, are $J=0.08-0.13$ and $0.08-0.18$ eV for $U/t=12$ and 8, respectively. Since the fitting is not perfect in any case, we conclude that for all reasonable values of $U/t$ the lowest spin excitations are described approximately by a Heisenberg model with $J\simeq0.1$ eV; considering the range of uncertainties in all the parameters, this is in as good agreement as should be expected with values of $J\simeq0.13-0.16$ eV quoted from analysis of neutron[12] and Raman experiments.[13] We emphasize that the fit is not good for higher excitations, which indicates the presence of other terms; these include four-spin exchange terms, which have been found previously in perturbation treatments of the Hubbard model[14] and which have been proposed to explain aspects of Raman spectroscopy.[15] In fact, it has been proposed[15] that the Raman data at energies of order $4J$ require terms other than the Heisenberg model, such as four-spin cyclic interactions. The observed deviations from the Heisenberg model support this idea.[16] Our findings vis-à-vis the Heisenberg model are in some disagreement with those found by Hybertsen *et al.*,[9] where a clear fitting to a one-band Hubbard with $U/t\simeq12$ and to a Heisenberg model was obtained, and from this mapping a value of $J=0.128\pm0.005$ eV was determined. We believe the precise value of $J$ is not so accurately given by any calculations to date.

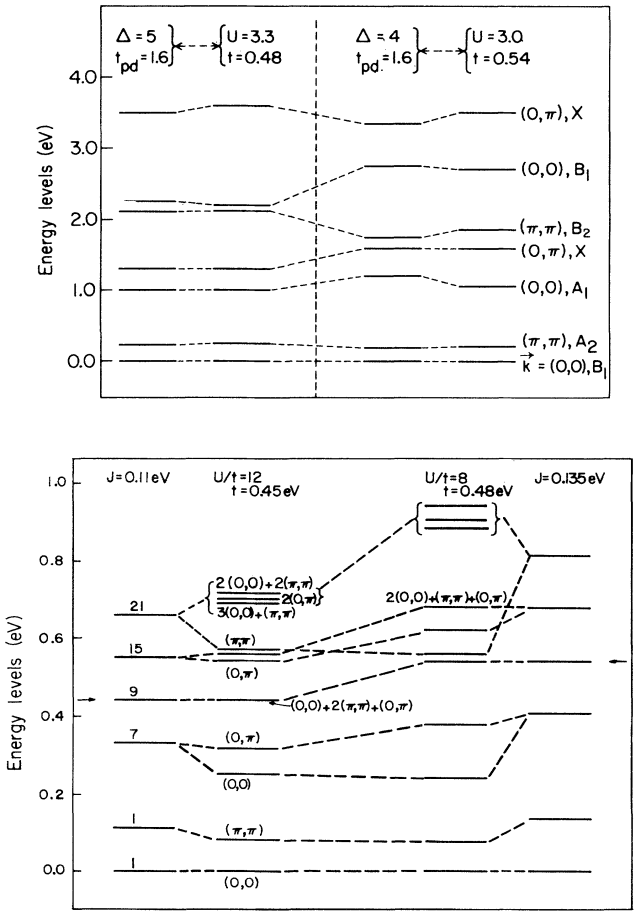


FIG. 2. (a) Mapping of the low-energy levels of the stoichiometric compound for different values of the multiband parameters. (b) Comparison of the low-energy levels of the one-band Hubbard and Heisenberg models for $U/t=8$ and 12 for the $\sqrt{8}\times\sqrt{8}$ cluster with periodic boundary conditions. Each state with $\mathbf{k}=(0,\pi)$ has a degeneracy of 6.

Calculations on doped cases show that the excitations are well described by the *same* Hubbard model. In Fig. 3 we show the results for the one-hole-doped, $2\times2$ cluster, comparing three-band, one-band Hubbard, and $t$-$J$ models, in parts (a), (b), and (c), respectively. As in the stoichiometric case, for large charge-transfer energy $\Delta$, the spin and charge excitations are well separated and the system remains in an insulating state with moderate doping. On the other hand for $\Delta\simeq3-5$ eV, the spin and charge excitation spectra overlap and moderate doping leads to a metallic state.

What happens when the hole concentration is increased? Using available results[17] for the Hubbard model in a $4\times4$ cluster, we compare in Fig. 4 the ground-state energy of the Hubbard and $t$-$J$ models for moderate doping as a function of $t/U$. In the obtained range $U\leq W$, the $t$-$J$ model becomes progressively more appropriate as the doping is increased. At high doping concentrations, the double occupancy is very small $\sim10^{-2}$, and so a very good agreement can be expected between both models.[18] This feature is also in agreement with recent Monte Carlo calculations for the three-band Hubbard model.[19]

In Fig. 5 we present, for the three-band Hubbard model in the $Cu_4O_8$ cluster and $\Delta=5$ eV, the total addition

and removal of one-particle spectra (PES and IPES) for an initial undoped and doped state.[20] Several general features can be extracted from this calculation. Whereas the $d$ spectral weight near the Fermi energy decreases in the doped system, the $p$ weight increases, indicating that the doped holes are mainly of $O_{2p}$ in nature. Similar results are found for other parameter sets. For the stoichiometric compound (upper figure), the insulating gap obtained from the combination of the PES and IPES spectra is $E_{gap} \simeq 2.2$ eV. The holes in the insulating system are mainly Cu states in character (60–70%), although there exists a strong $Cu_{3d}$-$O_{2p}$ hybridization. The lower part of the figure corresponds to the one-hole-doped case in the same cell. The zero gap indicates that the system has already undergone the *metal-insulator* transition.

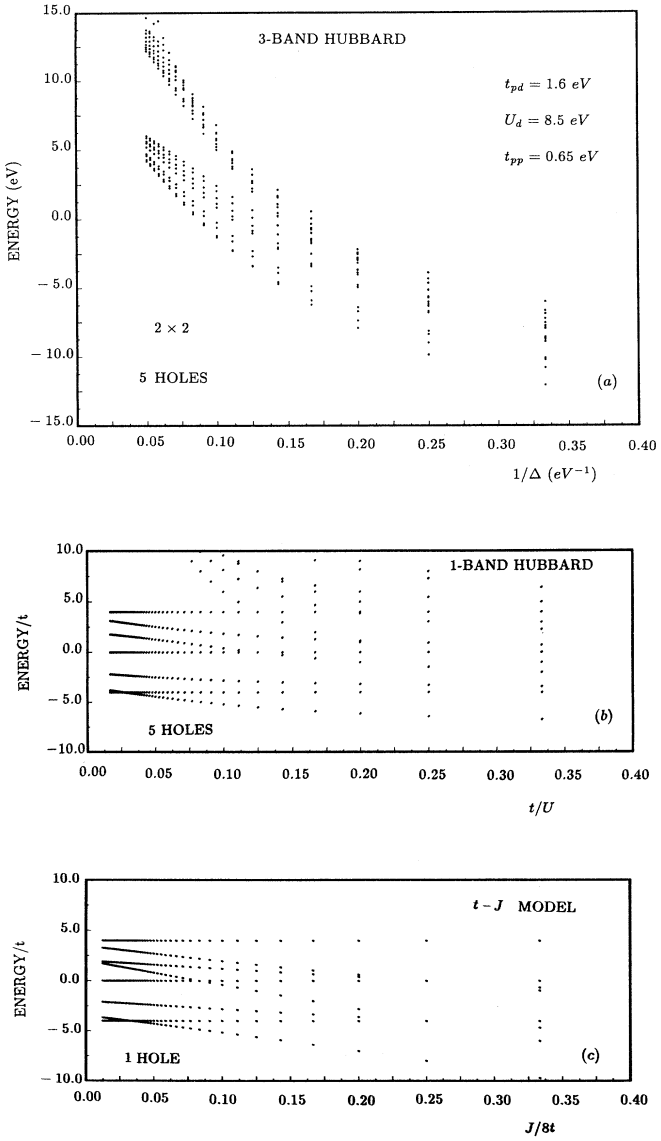


FIG. 3. Energy spectrum for the one-hole-doped, 2×2 cluster for (a) three-band Hubbard model as a function of $1/\Delta$, where the parameters are as in Fig. 1(a) (only the six lowest states of each **k** subspace are included here); (b) the one-band Hubbard model as a function of $t/U$; and (c) the $t$-$J$ model vs $J/8t$. Note that, for this cluster size, the strong-coupling limit of the Hubbard model gives $J = 8t^2/U$.

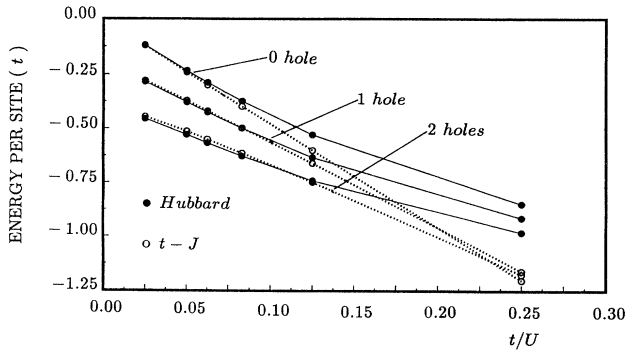


FIG. 4. Comparison of the ground-state energy of the one-band Hubbard and $t$-$J$ models vs $t/U$ for zero, one, and two holes in the 4×4 cluster with periodic boundary conditions and $J = 4t^2/U$.

In Fig. 6 we show the one-particle spectral function for the $\sqrt{8} \times \sqrt{8}$ cell of the one-band Hubbard model with $U = W$ for the half-filled (eight holes) and doped (nine holes) cases. The metal-insulator transition is also apparent here and in all the cases studied for $U/t \leq 8$. Nevertheless, for higher values ($U/t \geq 12$), where the spin and charge excitations are separated, the system behaves differently, being an insulator even in the one-particle-doped case, although with a much smaller gap compared with the one of the stoichiometric compound, which is $\sim U$.[21]

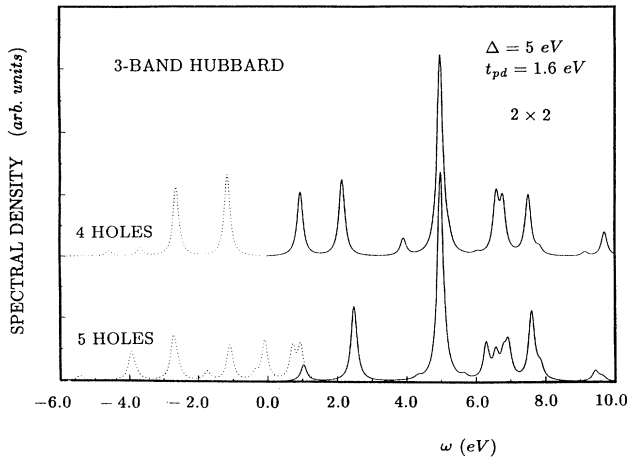


FIG. 5. One-particle spectral function of the 3BHM for the $Cu_4O_8$ cluster. The parameters are as in Fig. 1(a).

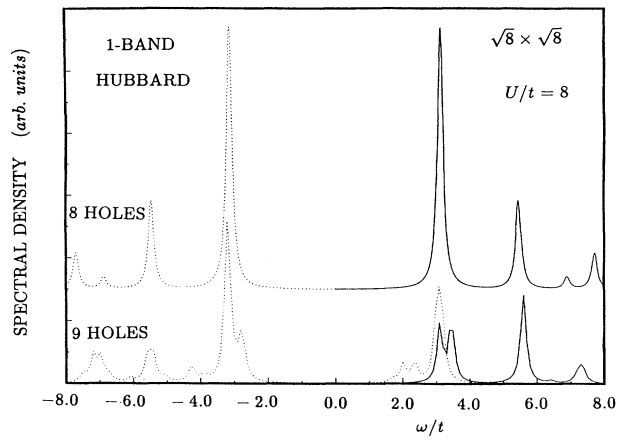


FIG. 6. One-particle spectral function of the one-band Hubbard model for the $\sqrt{8}\times\sqrt{8}$ cluster at $U/t=8$. The upper figure corresponds to the insulating state, while the other to the one-hole-doped system ($S=\frac{1}{2}$ subspace).

In order to give support for the proposed intermediate regime, let us now see if the predicted behaviors are in agreement with the experimental magnetic properties of $La_2CuO_4$. First, we note that, for $\Delta\simeq 4-5$ eV, the insulating gap in the half-filled case, $E_g=1.75-2.2$ eV, respectively, is close to the experimental value for $La_2CuO_4$, $E_g\simeq 1.65-2.0$ eV.[22] Note that, since the value of the gap should decrease with the system size, we consider $\Delta=3$ eV and its one-band mapping $U/t=4$ to give a too small gap $\sim 1.5$ eV, as compared with the experimental result. The value of $U$ in the one-band model which we find to fit the gaps is similar to that deduced recently by Chen *et al.*[10] The regime with $U$ less than or of order $W$ has been studied by Monte Carlo calculations, which have shown that the undoped system at *all* nonzero values of $U/t$ exhibits strong antiferromagnetic correlations.[23,24] Let us remark also that both the spin-wave spectrum and sublattice magnetization as calculated in the weak-coupling regime extrapolate correctly to the strong-coupling limit, recovering the Heisenberg results.[25] Finally, at zero doping, experiments indicate that the spin dynamics can be described in the *long-wavelength* limit by the nonlinear $\sigma$ model. Note, however, that the *same* effective action can be obtained from the one-band Hubbard model and any value of $U/t$, since the magnitude of $U/t$ affects only the renormalization of the nonlinear $\sigma$-model parameters.[26,27]

There is a simple argument supporting the parameters which we find. Our bare bandwidth $W=8t\sim 4$ eV is essentially the same as found in local-density-approximation calculations. The $U$ which we find in this small-cluster study, $2.4\le U\le 3.4$ eV, is also simply rationalized. For the lower limit $\Delta=3$ eV, since the Wannier functions that describe this $d_{x^2-y^2}$ band have charge $\gamma\simeq 60\%$ on a Cu site and $\beta\simeq 10\%$ on each of the four O neighbors, the interaction between two electrons in this state is $U_{\rm eff}\simeq(\gamma^2U_{dd}+4\beta^2U_{pp}+8\gamma\beta U_{pd})\simeq 3.5$ eV. A similar calculation for $\Delta=5$ eV gives $U_{\rm eff}\simeq 4.6$ eV. In each case these results are an upper limit for $U_{\rm eff}$ since correlations such as those found by McMahan *et al.*[8] will reduce the repulsion.

In conclusion, we believe our calculations have established that the appropriate model for electrons in CuO planes of the high-$T_c$ materials is a one-band Hubbard model in the regime $U\simeq W$, where $W=8t$ is the bandwidth. This has been shown to follow from more complex multiband models with parameters which have previously been derived and compared with electron spectra. We expect there must be other terms such as $t'$, and of course, in a complete model it may be essential to also include other effects, such as interplanar interactions, electron-phonon coupling, etc. For the insulating case we have shown that the magnetic excitations are described reasonably well by the Hubbard model with $U\simeq W$, which leads to $J\simeq 0.1$ eV. The half-filled Hubbard model with $U\le W$ has been extensively studied by quantum Monte Carlo with results which are in reasonable agreement with experiment for many low-energy properties. Our results for the metallic nature of the doped system are also in agreement with earlier work on the Hubbard model, which found a small binding of holes in similar range $U/t\le 10$,[28] a range in which the $t$-$J$ model leads to phase separation. Together with the tendency for $d$-wave pairing at small $U/t$,[29] this may indicate a connection between the one-band Hubbard model and the existence of superconductivity at high temperatures in these materials.

## ACKNOWLEDGMENTS

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[1] P. W. Anderson, Science **235**, 1196 (1987).
[2] R. Laughlin, Science **243**, 525 (1988).
[3] J. R. Schrieffer, X.-G. Wen, and S.-C. Zhang, Phys. Rev. Lett. **60**, 944 (1988); A. Kampf and J. R. Schrieffer, Phys. Rev. B **41**, 6399 (1990).
[4] A. Millis, H. Monien, and D. Pines, Phys. Rev. B **42**, 167 (1990).
[5] K. Levin *et al.*, Rev. Mod. Phys. (to be published).
[6] V. J. Emery, Phys. Rev. Lett **58**, 2794 (1987).
[7] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).
[8] A. K. McMahan, R. M. Martin, and S. Satpathy, Phys. Rev. B **38**, 6650 (1988); **42**, 6268 (1990); M. S. Hybertsen, M.

Schluter, and N. E. Christensen, *ibid.* **39**, 9028 (1989); J. F. Annett, R. M. Martin, A. K. McMahan, and S. Satpathy, *ibid.* **40**, 2620 (1989); Y. Ohta, T. Tohyama, and S. Maekawa, Phys. Rev. Lett. **66**, 1228 (1991).

[9]M. Hybertsen, E. Stechel, M. Schluter, and D. Jennison, Phys. Rev. B **41**, 11 068 (1990).

[10]A value of $U=4.1$ eV has been derived [E. Stechel and M. Hybertsen (private communication)] and shown to be consistent with x-ray absorption in $La_{2-x}Sr_xCuO_{4+\delta}$; C. T. Chen *et al.*, Phys. Rev. Lett. **66**, 104 (1991).

[11]J. F. Annett and R. M. Martin, Phys. Rev. B **42**, 3929 (1990).

[12]G. Shirane *et al.*, Phys. Rev. Lett. **59**, 1613 (1987); J. M. Tranquada *et al.*, Phys. Rev. B **40**, 4503 (1989); G. Shirane *et al.*, Phys. Rev. Lett. **63**, 330 (1989); G. Aeppli *et al.*, *ibid.* **62**, 2052 (1989).

[13]K. B. Lyons *et al.*, Phys. Rev. Lett. **60**, 732 (1988); S. L. Cooper *et al.*, Phys. Rev. B **37**, 5920 (1988); **38**, 11 934 (1988); S. Sugai *et al.*, *ibid.* **38**, 6436 (1988); W. H. Weber and G. W. Ford, *ibid.* **40**, 6890 (1989); R. R. P. Singh *et al.*, Phys. Rev. Lett. **62**, 2736 (1989).

[14]A. H. MacDonald *et al.*, Phys. Rev. B **41**, 2565 (1990).

[15]S. Sugai *et al.*, Phys. Rev. B **42**, 1045 (1990); E. Gagliano *et al.*, Europhys. Lett. **12**, 259 (1990); H. J. Schmidt and Y. Kuramoto, Physica C **167**, 263 (1990).

[16]For $U/t=4$ (12) the ground-state energy of the Hubbard model differs from the corresponding to the Heisenberg model with multiple-spin interactions by 6% (0.06%) ($4\times4$ cluster).

[17]G. Fano, F. Ortolani, and A. Parola, Phys. Rev. B **42**, 6877 (1990).

[18]A. Moreo, D. Scalapino, and E. Dagotto (unpublished).

[19]G. Dopf, A. Muramatsu, and W. Hanke, Phys. Rev. B **41**, 9264 (1990).

[20]To calculate spectral functions, we use the method described in E. R. Gagliano and C. A. Balseiro, Phys. Rev. Lett. **59**, 2999 (1987); Phys. Rev. B **38**, 11 766 (1988).

[21]We have performed similar calculation for the undoped 2BHM in both cluster sizes. In the periodic cell $Cu_8O_{16}$, the IPES spectra shows that the main features of the low-energy part of the spectrum remain the same for both lattice sizes, supporting in this way the predictions of the finite-cluster calculation. The splitting of the states with momentum $\mathbf{k}=(0,\pi)$, $\mathbf{k}=(\pi,0)$, and $(\pm\pi/2,\pm\pi/2)$ is directly related to the oxygen $t_{pp}$ interaction, and it can also be described by a one-band Hubbard model, with second-nearest-neighbor $t'$ interaction. Note that, because of the particle-hole symmetry of the Hubbard model, the one-particle spectra obey $(n\rightarrow n\pm1,t')=(n\rightarrow n\mp1,-t')$. Then, for the electron-doped case, the sign of $t'$ is reversed with respect to the hole-doped compound, as was pointed out in Ref. 9. The electron-doped case has a first excited state with momentum $\mathbf{k}=(0,\pi)$. The splitting between this state and $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$ is $\sim0.4$ eV, to be compared with $\sim0.35$ eV obtained with the one-band Hubbard and $t'/t\simeq-0.2$. This ratio is consistent with the value $\sim-0.17$ obtained in Ref. 9.

[22]S. L. Cooper *et al.*, Phys. Rev. B **42**, 10 785 (1990); T. Thio *et al.*, *ibid.* **42**, 10 800 (1990).

[23]J. Hirsch, Phys. Rev. B **31**, 4403 (1985); M. Imada, J. Phys. Soc. Jpn. **57**, 42 (1988); J. Hirsch and S. Tang, Phys. Rev. Lett. **62**, 591 (1989).

[24]S. R. White *et al.*, Phys. Rev. B **40**, 506 (1989).

[25]J. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. B **39**, 11 663 (1989).

[26]E. Fradkin, in *Field Theories of Condensed Matter Systems,* edited by D. Pines (Addison-Wesley, Reading, MA, 1991), Chap. 3.

[27]S. John and P. Voruganti (unpublished).

[28]J. Riera and A. Young, Phys. Rev. B **39**, 9697 (1988); E. Dagotto *et al.*, *ibid.* **41**, 811 (1990); E. Dagotto *et al.*, *ibid.* **41**, 9049 (1990).

[29]J. E. Hirsch and H. Q. Lin, Phys. Rev. B **37**, 5070 (1988).