FRUSTRATED SPIN (J-J') SYSTEMS DO NOT MODEL THE MAGNETIC PROPERTIES OF HIGH–TEMPERATURE SUPERCONDUCTORS.

Silvia Bacci*, Eduardo Gagliano*, and Franco Nori**

* Physics Department, Materials Research Laboratory, and
Science and Technology Center for Superconductivity
University of Illinois at Urbana-Champaign, Urbana, IL 61801

** Physics Department, University of Michigan, Ann Arbor, MI 48109–1120

ABSTRACT: We study the $t-J$ model with one hole and the frustrated Heisenberg $J-J'$ model in a square lattice. Specifically, we compute and compare for both, the doped and frustrated models, the dynamic spin-spin structure factor $S(\mathbf{q},\omega)$, and the B_{1g} Raman scattering spectrum $R(\omega)$ at zero temperature. The behavior of these quantities differs between the $t-J$ and the $J-J'$ models. We observe that both the B_{1g} Raman spectrum as well as the structure factor for the $t-J$ model are in qualitative agreement with experimental measurements while the corresponding results for the $J-J'$ model are not. These results indicate that the magnetic behavior of doped systems cannot be accurately modeled by a purely spin Hamiltonian. These results are of relevance to the claim that the effect of adding holes (doping) on the magnetic properties of the quantum Heisenberg antiferromagnet can be described by introducing second and sometimes third nearest-neighbor couplings, J' and J'' respectively, in the original (undoped) Hamiltonian.

1. INTRODUCTION

A central issue in high-temperature superconductivity is the relationship between doping and antiferromagnetism. When undoped, these materials display conventional Neél order which can be described by quantum Heisenberg models[1,2].

Strongly correlated electron systems II. Proceedings of the 1990 Adriatico Research Conference. G. Baskaran et.al., editors.

When doped, the long-range antiferromagnetic order is suppressed and superconductivity appears. These facts have been modeled by the $t-J$ Hamiltonian constrained to the subspace with no double occupancy which, in standard notation, is given by[3]

$$\mathcal{H} = -t \sum_{<i,j>,\sigma} (1 - n_{j-\sigma}) c^{\dagger}_{j\sigma} c_{i\sigma} (1 - n_{i-\sigma}) + J \sum_{<i,j>} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j) \quad (1)$$

This model has been derived in the large-U limit of a single band Hubbard model. In this case, J favors Neél order, while t tends to disrupt it. Describing the effect of the hole motion on the spin background has been a central issue in much recent work on models for high-temperature superconductors. Among the several descriptions proposed, we mention the spin bag[4], spiral[5] (see ref. [6] for the connection between the previous two), nematic[7], and dimer phases[8].

It has been proposed[9] that the effect of doping can be described by including further neighbor couplings, J' and J'', into the quantum Heisenberg model, the couplings being proportional to the doping δ. This proposal has provided a possible connection between purely spin systems[7,10] and doped ones[11]. A recent suggestion invokes an adiabatic continuation[12] between doped and frustrated models. This connection has been recently studied[13] in the context of the generalized flux phases.[14]

Here, we will address the question of whether the frustration can properly describe the magnetic properties of a doped quantum spin-1/2 Heisenberg model. The two-dimensional spin frustrated $(J-J')$ and the electronic $(t-J)$ models have been mostly studied *separately*. A link between them has been argued[9], while other works[15] have assumed it. The connection between these two models has been at the heart of much recent work on magnetic spin Hamiltonians as models for high-temperature superconductors. It is the purpose of this work to analyze this connection by computing several measurable quantities. More specifically, we compute and analyze the B_{1g} Raman spectrum and the dynamic spin-spin structure factor for the $t-J$ model with one hole, the $J-J'$ model, as well as the Heisenberg model, and qualitatively compare these results with the available experimental measurements. This comparison should indicate if, in the presence of a small density of carriers, integrating out the electronic degrees of freedom[9] leads to an effective $J-J'$ spin Hamiltonian. All our results are obtained through exact diagonalization on a 4×4 lattice with periodic boundary conditions.

2. FROM THE LARGE-U HUBBARD MODEL TO A PURELY SPIN HAMILTONIAN

First let us consider the one band Hubbard Hamiltonian

$$\mathcal{H}=-t\sum_{<i,j>,\sigma}(c^{\dagger}_{j\sigma}c_{i\sigma}+h.c.)+U\sum_{i}n_{i\uparrow}\,n_{i\downarrow} \tag{2}$$

We are interested in the large U limit. In this regime, the canonical transformation[16] that eliminates the mixing of doubly occupied and single occupied sites to order $O(t^2/U)$ gives the following transformed Hamiltonian

$$\mathcal{H}=-t\sum_{<i,j>,\sigma}b_i c^{\dagger}_{i\sigma}c_{j\sigma}b^{\dagger}_j+\frac{2t^2}{U}\sum_{<i,j>}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{n_in_j}{4}\right)$$
$$-\frac{t^2}{U}\sum_{<i,j,k,\sigma>}b_ic^{\dagger}_{i\sigma}c_{j\sigma}c^{\dagger}_{j-\sigma}c_{k-\sigma}b^{\dagger}_k-\frac{t^2}{U}\sum_{<i,j,k,\sigma>}b_ic^{\dagger}_{i\sigma}n_{j-\sigma}c_{k\sigma}b^{\dagger}_k+\ h.c. \tag{3}$$

where $\mathbf{S}_i=\frac{1}{2}c^{\dagger}_{i\alpha}\sigma_{\alpha\beta}c_{i\beta}$, and $n_i=n_{i\uparrow}+n_{j\downarrow}$, with $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$. Here b_i is a slave boson attached to the hole, which satisfies the condition $b^{\dagger}_ib_i+n_i=1$. The superexchange term favors antiferromagnetic order while the first and the third terms can reduce it. After many approximations[9], the above Hamiltonian can be written as

$$\mathcal{H}_{J-J'}=J\sum_{<i,j>}\mathbf{S}_i\cdot\mathbf{S}_j+J'\sum_{<ik>}{}'\mathbf{S}_i\cdot\mathbf{S}_k \tag{4}$$

where

$$J=\frac{2t^2}{U}\left(1-\left(\frac{U}{t}+5\right)x\right),\qquad J'=\frac{t^2}{U}x \tag{5}$$

and x is the doping parameter. The last term of eq.(4) has two equivalent terms if i and k are second-nearest neighbors, and one term if i and k are third nearest neighbors. The frustration term originates from the last explicit term of eq.(3). The above result, eqs.(4-5) assumes, among many other things, a small value of the doping.[17]

3. DESTRUCTION OF THE NEEL ORDER

The static magnetic structure factor $S(\mathrm{q})$[18] indicates that the effect of frustration and doping, on the *magnetic* properties, may be considered as being similar. The reason is that in relation to the pure antiferromagnetic Heisenberg, both of these models suppress the $S(\mathrm{q})$ peak at (π, π), broadening and shifting this peak to another $\vec{q}$-point. The meaning of these results is clear: when we add a large enough perturbation to the spin-1/2 Heisenberg Hamiltonian, the ground state is bound to change from the (unperturbed) Neél state to some other (distorted) state. This result is not surprising. Now, a more specific question is: how large must these perturbations be in order to destroy the Néel order? The critical values of the frustration parameter, $(J'/J)_c$, and of the doping parameter, x_c, are $(J'/J)_c \sim 0.5$ and $x_c \sim 0.05$. Therefore, $(J'/J)_c \sim 10\ x_c$. This *differs* from eq.(5) by a factor of 50. On the other hand, ab initio calculations[19] indicate that J' is around $2 - 10\%$ of J.

The magnetic excitations of the undoped insulating cuprates have been studied through Raman[20,21,22] and Neutron [23,24,25] measurements. Calculations based on the pure quantum Heisenberg model have been used to fit and to interpret the experimental data.[26] However, the situation for the doped materials is much less clear.

4. RAMAN SCATTERING FOR THE DOPED (t-J), HEISENBERG AND FRUSTRATED (J-J') MODELS

Let us first consider the Raman scattering.[20,21,22] The laser light incident on a magnetic insulator causes atomic motion and, therefore, a change in the distance between neighboring magnetic ions. This modulates the local exchange coupling and excites short-wavelength, high-energy spin excitations. The polarization-dependence of the scattered light allows the magnetic signal to be separated from other contributions. In La_2CuO_4 and $YBa_2Cu_3O_6$, the only excitations between ~ 0.1 eV and 1.5 eV are spin excitation because, (*i*) they are insulators with a large gap (~ 1.5 eV) to charge excitations, and (*ii*) phonon excitations have energies below $0.1eV$. In the insulating phase, the Raman intensity, as a function of energy transfer, has a clear peak for certain "allowed" polarizations . The first moments of the spectrum are in good agreement with calculations based on the antiferromagnetic Heisenberg model.[22,21] However, the observed broad line shape remains to be expained. In fact, the line asymmetry could be attributed to a resonant enhancement due to multiple-spin processes.[27] In the superconducting cuprates, the peak in the allowed polarizations *broadens* rapidly with doping.[22]

The scattering Hamiltonian which describes the interaction of light with the spin-pair is[28]

$$H_R = \sum_{<i,j>} (\mathbf{E}_{inc} \cdot \hat{\sigma}_{ij})(\mathbf{E}_{sc} \cdot \hat{\sigma}_{ij})\mathbf{S}_i \cdot \mathbf{S}_j \tag{6}$$

where $\mathbf{E}_{inc}$ and $\mathbf{E}_{sc}$ are the incident and scattered electric field vectors of the photons and $\hat{\sigma}_{ij}$ is a unit vector connecting the spin sites i and j. The Raman scattering intensity $R(\omega)$ at $T = 0$ is given by

$$R(\omega) = \int dt\ e^{i\omega t}\ \langle \psi_0 | H_R(t) H_R | \psi_0 \rangle \tag{7}$$

where $|\psi_0 >$ is the ground state. To study $R(\omega)$ numerically we used a Lanczos method adapted to the evaluation of dynamic properties.[29] Using this approach we can evaluate exactly any response function as well as the moments of this distribution.

Depending on the orientation of the incident and scattered electric fields with respect to the crystal directions, different scattering geometries can be analyzed. One of the most studied modes is the B_{1g}. Figure 1 shows the B_{1g} Raman spectrum for the two-dimensional spin-1/2 (a) pure Heisenberg Hamiltonian, (b) $t - J$ model with one hole, and (c) frustrated Heisenberg model. Here, we have selected some typical values of the parameters, however, other values of J'/J and t/J, not shown here, have also been considered. The dominant feature observed in the Raman spectra of figure 1 is the prominent two-magnon (2 nn spin flip) peak located at $\approx 3J$. The only effect of frustration (see fig.1c) is to continuously shift the spectra to lower energies (very rapidly) as a function of J' (approximately linearly for $J' \ll J$). This is in clear disagreement with the results for the doped

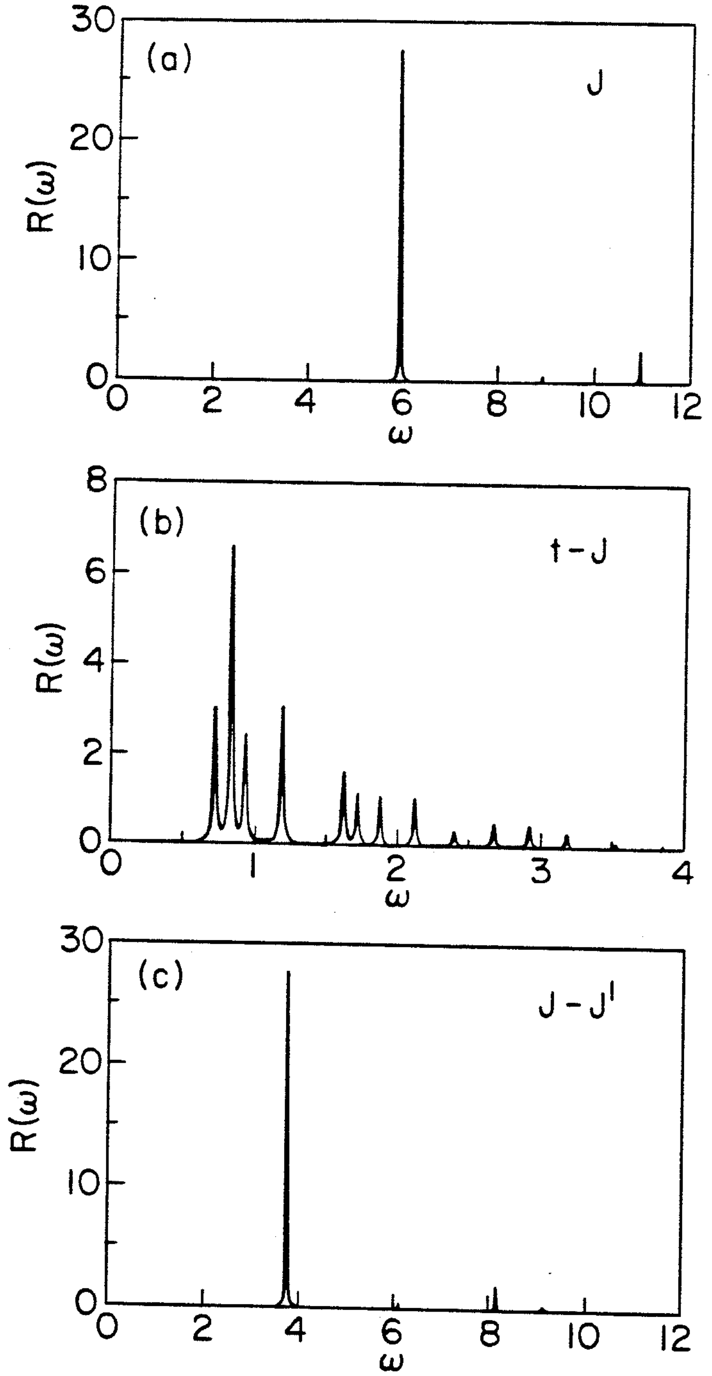

Figure 1. Raman spectrum for the B_{1g} geometry. (a) pure Heisenberg model, with $J=2$; (b) $t-J$ model with one hole, with $t=1$ and $J=0.4$; (c) frustrated Heisenberg model, with $J=2$ and $J'=0.4$. All these results are for a 4×4 lattice with periodic boundary conditions. Note that for the spin model the energy scale is $J=2$, while for the $t-J$ it is $t=1$.

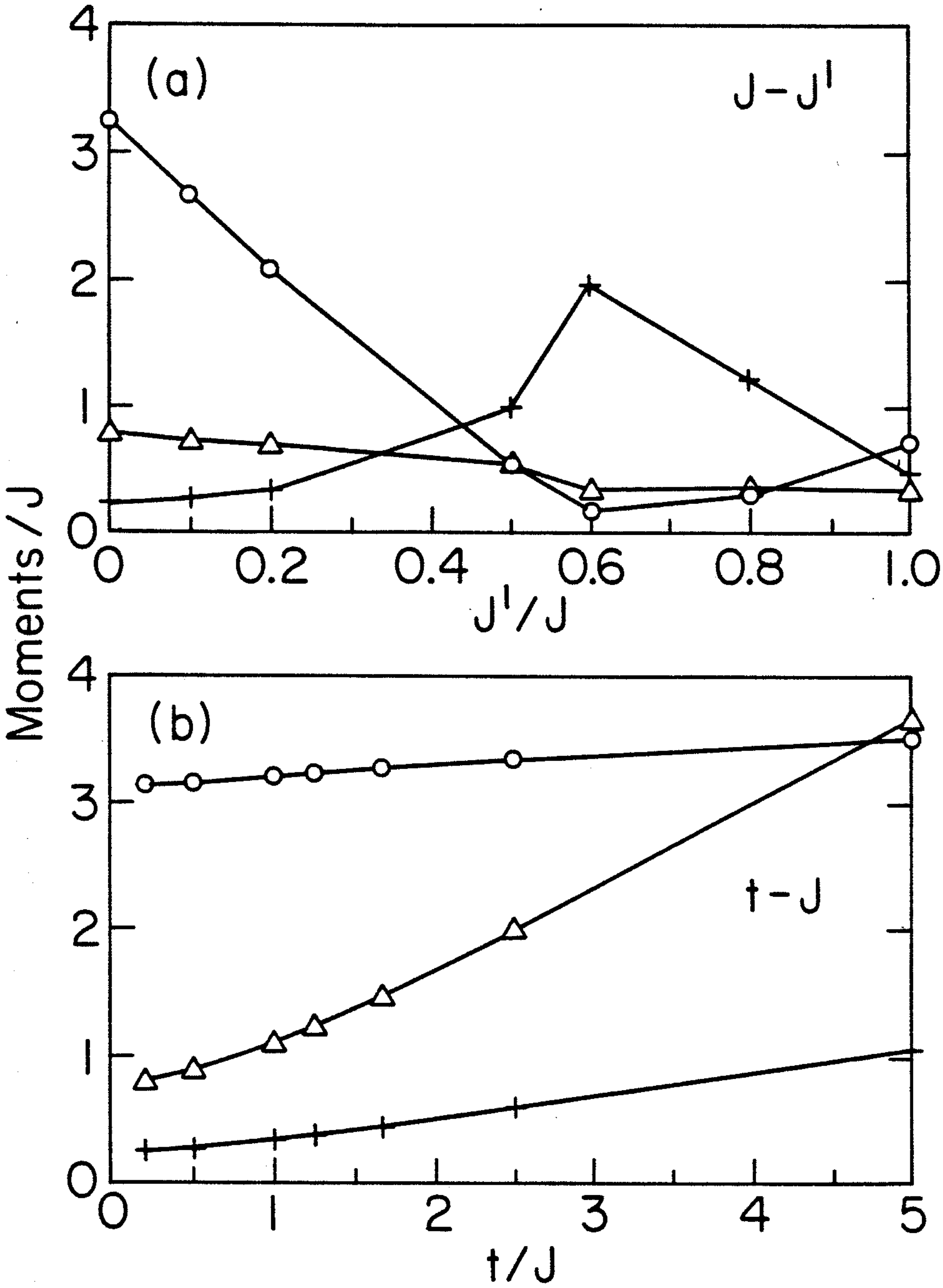

Figure 2. Moments of the B_{1g} Raman spectrum for (a) $J-J'$ model, and (b) $t-J$ model with one hole, as a function of the frustration parameter. The symbols refer to the center of gravity, M_1/J (∘), width of the spectrum M_2/J (△), and M_2/M_1 (+).

case (either the $t-J$ model or the experiments) since the frustrated case shows no low-frequency structure (below the prominent two-magnon peak), while the doped case exhibits a very rich structure at low energies. For the $t-J$ model, these excitations are the string states[5] as well as the two magnon processes in the neighborhood of the hole.[30] In this model, the hole motion is responsible for an entirely new type of states (string-type) located at the bottom of the spectrum. Furthermore, in the highly mobile limit, the intensity of the low frequency part of the spectrum becomes the dominant one, since the intensity of the two-magnon peak, which is the dominant one for $t < J$, decreases as t/J increases. So, we conclude that the behavior of the two-magnon peak located at $\approx 3J$ for $J' = x = 0$ is different in the two cases: doping rapidly *suppresses* this peak, while frustrating the system continuously *shifts* the peak to lower energies and increases its intensity up to $J'/J \approx 0.5$. Furthermore, the uniform shift as a function of frustration exhibited by the $J-J'$ model must be contrasted with the very complex structure that appears in the Raman spectrum as a function of doping and t/J. Similar results were also found to be valid for other values of the parameters.

The general features of these complex spectra can be better captured by studying their first moments.[21] In figure 2 we show the first two moments for the Raman spectrum of the (a) $J-J'$ model and (b) $t-J$ model with one hole, as a function of the parameters, J'/J and t/J, respectively. The first moment, M_1/J, corresponds to the center of gravity of the spectrum, while the second, M_2/J, measures its width. Let us start with the pure Heisenberg model. Increasing J'/J produces a *uniform* shift of the center of gravity towards zero frequency, for $J'/J \leq 0.6$. For $J'/J \geq 0.6$, the center of gravity slowly increases with increasing frustration. The corresponding behavior of M_1/J, as a function of t/J, is different, being in this case a straight line with positive slope. Increasing J'/J (t/J) produces a *decrease* (dramatic *increase*) in the width M_2/J of the Raman spectrum for the $J-J'$ ($t-J$) model. Clearly, the results between the frustrated and doped models differ substantially. It is important to note that the doped results qualitatively reproduce the experimental measurements in the B_{1g} geometry, while the frustrated Hamiltonian does not.

5. NEUTRON SCATTERING FOR THE DOPED (t-J), HEISENBERG AND FRUSTRATED (J-J') MODELS

Let us now consider the neutron scattering.[23,24,25] The quantum Heisenberg model has provided a qualitatively description of the undoped cuprates. However, the magnetic excitations in the superconducting cuprates have been more difficult to study not only because the magnetic scattering is weaker, in part due to the lack of long-range order, but also due to the scarcity of good samples. Currently, there is no detailed comparison between theory and experiments. Recent data[23] on the $S(\mathbf{q},\omega)$ of a $La_{1.85}Sr_{.15}CuO_4$ crystal with $\mathbf{q} = h(\pi/a, \pi/a)$, show a clear peak at $\mathbf{q} = (\pi/a, \pi/a)$, suggesting the presence of antiferromagnetic fluctuations, which appear to be inconmensurate with a maximum at $h \approx 0.85$. Neutron scattering data[24] for $YBa_2Cu_3O_{7-\delta}$ exhibit a broad peak in $S(\mathbf{q},\omega)$ near $\mathbf{q} = (\pi/a, \pi/a)$. Therefore, the main effect of doping is to broaden and shift the (π,π) peak.[25]

The $T = 0$ dynamic spin-spin structure factor, $S(\mathbf{q},\omega)$, is given by

$$S(\mathbf{q},\omega) = \frac{1}{N}\sum_{l}\sum_{m}\int dt\ e^{i\omega t - iq(l-m)}\langle\psi_0|S_l^z(t)S_m^z(0)|\psi_0\rangle \tag{8}$$

where the $S_l^z(t)$ is the z-component of the spin at site l, after time evolution in real time t, and $|\psi_0\rangle$ is the ground state wave function. In figure 3 we show $S(\mathbf{q},\omega)$ versus ω, for $\mathbf{q} = (\pi,\pi)$, of the spin-1/2 (a) pure Heisenberg antiferromagnet, (b) $t-J$ model, and (c) $J-J'$ model. Our goal now is to study the effects of frustration and doping on $S(\mathbf{q},\omega)$. We observe that the only effect of increasing J' is to shift all the peaks towards the low-energy region. This occurs for all peaks except the (π,π) which has a shift toward higher frequencies. This is precisely the peak shown in fig.(3c). A simple explanation of this behavior comes from the observation that the energy of the triplet state with momentum (π,π) and the ground state energy are almost parallel straight lines for $J'/J \leq 0.60$. The displacement of this peak appears to be a linear function of the frustration parameter, J'/J. On the other hand, the evolution of the structure as a function of (small) doping is very different, the spectrum now being broader and with a pseudoband. This behavior is shown in fig.3b for $J/t = 0.4$. For the $t = 0$ static-hole case, only two peaks are present, while the structure becomes much richer for the $t > 0$ case. In particular, there is

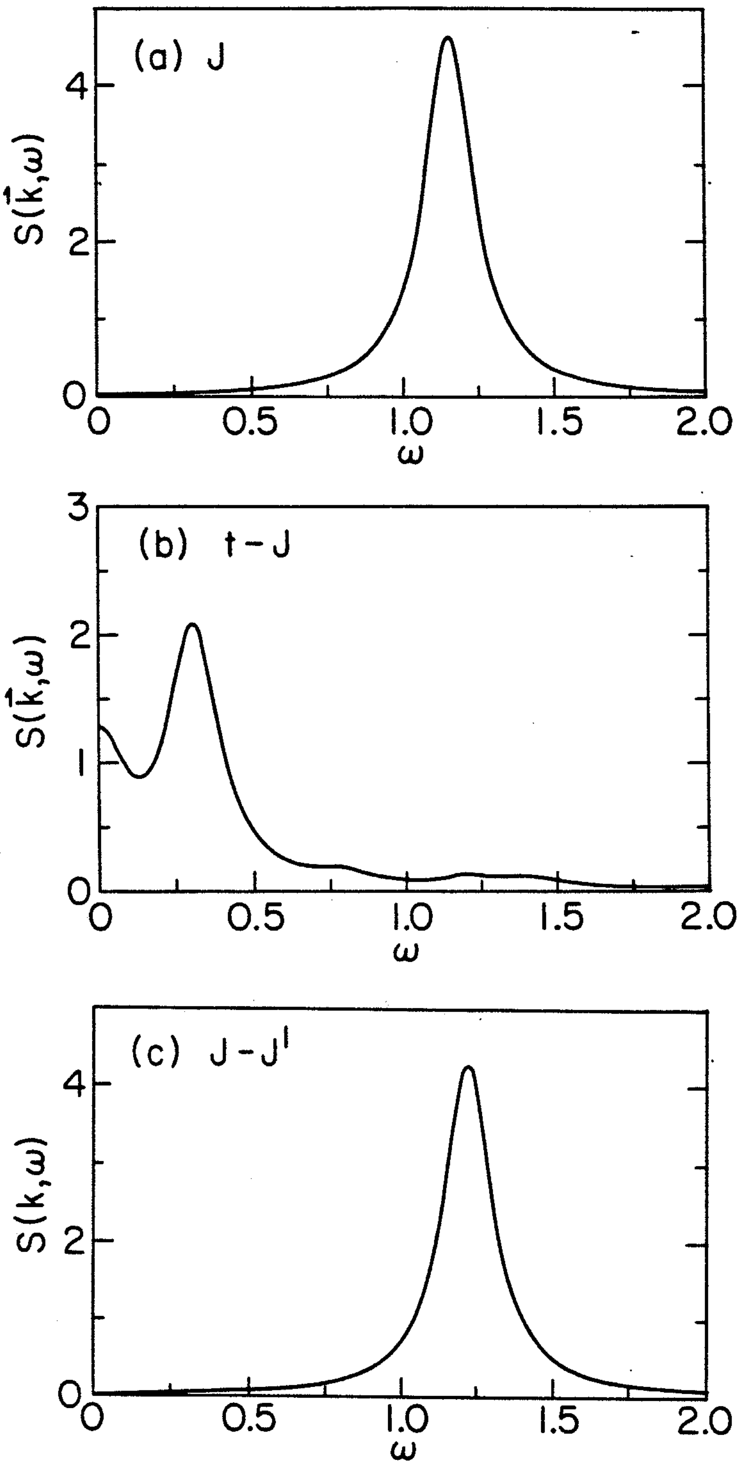

Figure 3. dynamic structure factor at $\mathbf{q} = (\pi, \pi)$ for the (a) pure Heisenberg model, with $J = 2$; (b) $t - J$ model with one hole, $t = 1$, $J = 0.4$; (c) frustrated Heisenberg model, with $J = 2$, $J' = 0.4$. All the results are for the 4×4 lattice with periodic boundary conditions.

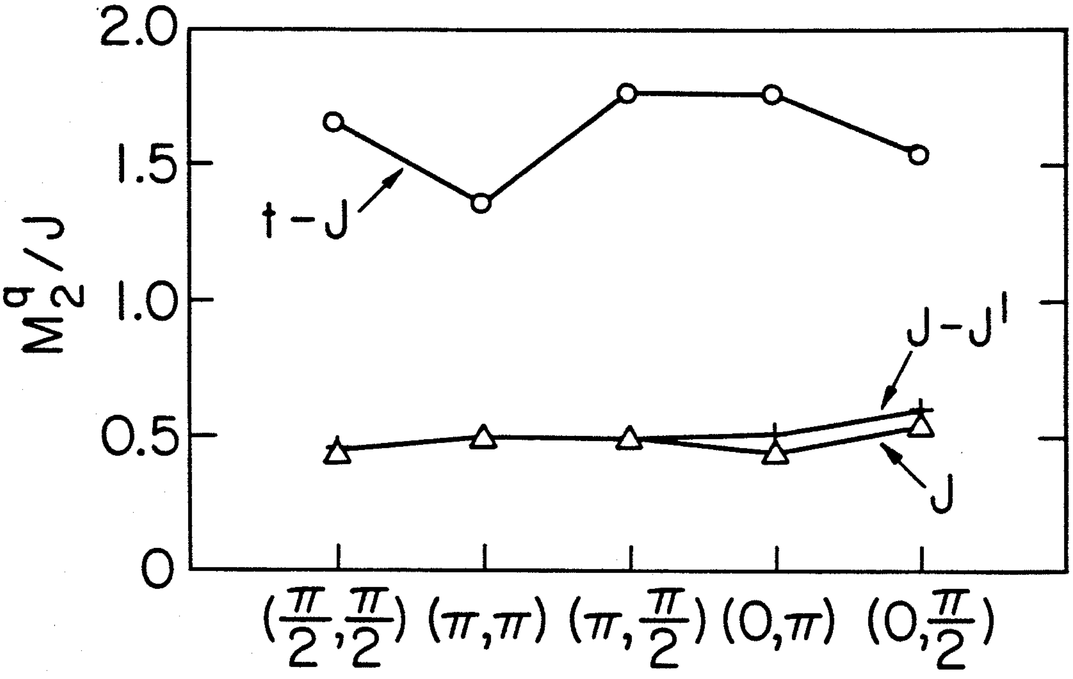

Figure 4. Width, M_2^{q}/J, of the $S(\mathrm{q},\omega)$ spectrum as a function of q. The parameter values are as in figure 3.

a broadening of the spectrum as one moves over the first brillouin zone. This is not the case for the pure Heisenberg and the frustrated Heisenberg antiferromagnets, since they show a monotonic behavior. The width M_2/J of the spectrum for the different models is shown in fig. 4. We think that the origin of these results is the fast destruction of the antiferromagnetism by the hole doping. In fact, the suppression of the antiferromagnetism[31] is local in the $t-J$ model, while it is global in the $J-J'$ model.

In an exact diagonalization study, the finite-size effects are unavoidable, however, we believe them to be small.[32] For instance, the neutron scattering results can be understood, in the insulating case, by the low-frequency, long-wavelength magnetic models.[2] However, since the hole motion reduces the AF order present at half-filling, we expect a suppression of spin excitations at long and intermediate wavelengths. On the other hand, the high-frequency *short*–wavelenght spin fluctuations probed by inelastic light scattering experiments (from energetic spin-pair two-magnon excitations) are much less dependent on finite-size effects. In fact, results for a 20-site lattice indicate that the same structure persists for the B_{1g} Raman spectrum.[32,33]

6. CONCLUSIONS

In summary, we have investigated the effects of doping and frustration on the 2D quantum Heisenberg model. We have analized the $T = 0$ dynamic structure factor of the spin-spin correlation function, $S(\mathrm{q}, \omega)$, and the Raman spectra, $R(\omega)$, by using an exact diagonalization technique on a 4×4 lattice . While the Heisenberg model quantitatively describes some characteristic features of the undoped materials, we believe the $t-J$ Hamiltonian to be the simplest available model that qualitatively describes the doped system. However, a more complicated model may be necessary for a quantitative description. Our results suggest that the predictions based on purely frustrated spin models are not appropiate, either quantitatively or qualitatively, for modeling the magnetic behavior of the doped systems. Furthermore, experimental observations in the superconducting cuprates can be qualitatively described by the $t-J$ model, but not with the $J-J'$ hamiltonian. Our observations and conclusions, obtained by looking at two different physical quantities in each model, are compelling because of their mutual consistency. Therefore, the charge and spin degrees of freedom might be so tightly coupled, in a doped system, that the magnetic properties cannot be properly modeled by a purely spin Hamiltonian.

This research has been supported by the Physics Department of the University of Michigan; DOE grant DE84-ER-45108; NSF grants DMR 86-12860, STC 88-09854, and PHY89-04035, supplemented by funds from NASA. The numerical calculations have been done in a Vax 6410. We acknowledge the Materials Research Laboratory for the use of its computational facilities.

REFERENCES

1. D.P. Arovas and A. Auerbach, *Phys. Rev. B* **38**, 316 (1988); *Phys. Rev. Lett.* **61**, 617 (1988); M. Takahashi, *Phys. Rev. B* **40**, 2494 (1989).
2. For recent reviews, see E. Manousakis, FSU-90 preprint; E. Dagotto, NSF-ITP-90 preprint.
3. F.C. Zhang and T.M. Rice, *Phys. Rev. B* **37**, 3759 (1988).
4. J.R. Schrieffer, X.G. Wen, and S.C. Zhang, *Phys. Rev. Lett.* **60**, 944 (1988); *Phys. Rev. B* **39**, 11663 (1989); A. Kampf and J.R. Schrieffer, *Phys. Rev. B* **41**, 6399 (1990).
5. W. Brinkman and T.M. Rice *Phys. Rev. B* **2**, 1324 (1970); B.I.Shraiman and E.Siggia, *Phys. Rev. Lett.* **60**, 740 (1988). See also, L. Bulaevskii and D. Khomskii *Sov. Phys. JETP* **25**, 1067 (1968); L. Bulaevskii, E. Nagaev, and D. Khomskii *Sov. Phys. JETP* **27**, 836 (1968).
6. D.M. Frenkel and W. Hanke, *Phys. Rev. B*, in press.
7. P. Chandra, P. Coleman and A. Larkin, *Phys. Rev. Lett.* **64**, 88 (1990).
8. D. Rokhsar and S.A. Kivelson, *Phys. Rev. Lett.* **61**, 2376 (1988); E. Fradkin and S. Kivelson, *Mod. Phys. Lett.* **4**, 225, 1990; N. Read and S. Sachdev, *Phys. Rev. Lett.* **62**, 1694 (1989).

9. M. Inui, S. Doniach and M. Gabay, *Phys. Rev. B* **38**, 6631 (1988).

10. P. Chandra and B. Doucot, *Phys. Rev. B* **38**, 9335 (1988). P. Locher *Phys. Rev. B* **41**, 2537 (1990); E. Dagotto and A. Moreo, *Phys. Rev. B* **39**, 4744 (1989); *Phys. Rev. Lett.* **63**, 2148 (1989); F. Figueirido et al, *Phys. Rev. B* **41**, 4619 (1989); M. Gelfand, R.R.P. Singh and D. Huse, *Phys. Rev. B* **40**, 10801 (1989); G. Mata and G.B. Arnold *Phys. Rev. B* **38**, 11582 (1988); L.B. Ioffe and A.I. Larkin *Int. J. Mod. Phys. B* **2**, 203 (1988); E. Gagliano, S. Bacci and E. Dagotto, UIUC preprint.

11. E. Dagotto, R. Joynt, A. Moreo, S. Bacci and E. Gagliano, *Phys. Rev. B* **41**, 2585 (1990); *ibid* **41**, 9049, (1990); C.-X. Chen, H.-B. Schuttler, and A.J. Fedro *Phys. Rev. B* **41**, 2581 (1990).

12. D. Rokhsar, UC-Berkeley-90 preprint.

13. F. Nori and G. Zimanyi, NSF-ITP-90 preprint

14. F. Nori, E. Abrahams, and G. Zimanyi, *Phys. Rev. B* **41**, 7277 (1990); F. Nori, B. Doucot and R. Rammal, NSF-ITP-90-138 preprint; I. Affleck and J.B. Marston, *Phys. Rev. B* **37**, 3774 (1988); **39**, 11538, (1989); G. Kotliar, *Phys. Rev. B* **37**, 3664 (1988). R. Rammal and J. Bellisard, preprints 1990; J.P. Rodriguez and B. Douçot, *Europhys. Lett.* **11**, 451 (1990); T.C. Hsu, *Phys. Rev. B* **41**, 11379 (1989).

15. X.G. Wen, F. Wilczek and A. Zee, *Phys. Rev. B* **39**, 11413 (1989).

16. A.B. Harris and R.V. Lange, *Phys. Rev.* **157**, 295, (1967); K.A. Chao, J. Spalek and A.M. Oles, *J. Phys. C*, **10**, L27, (1977); C. Gross, R. Joynt, and T.M. Rice, *Phys. Rev. B* , 36, 381 (1987); C. Gross, *Ann. Phys.* **189**, 53, 1989; H. Yokohama and H. Shiba, *J. Phys. Soc. Jpn.* **56**, 1490, 3570, (1987).

17. In this work we restrict ourselves to the one hole case. This is enough to show the discrepancies between the $t-J$ an the spin frustrated models.

18. A. Moreo, E. Dagotto, T. Jolicoeur, and J. Riera, *Phys. Rev. B*, to appear.

19. J.F. Annett, R.M. Martin, A.K. McMahan and S. Satpathy, *Phys. Rev. B* **40**, 2620 (1989); M. Hybertsen, E. Stechel, M. Schluter and D. Jennison,

preprint; H. Eskes, G. Sawatzky and L. Feiner, *Physica C*, to be published; T. Tohyama and S. Maekawa, *J. Phys. Soc. Japan*, **59**, 1760, (1990).

20. S.L. Cooper et. al *Phys. Rev. B* **37**, 5920 (1988); S.L. Cooper *et. al Phys. Rev. B* **38**, 11934 (1988); S. Sugai, S. Shamamoto, and M. Sato *Phys. Rev. B* **38**, 6436 (1988).
21. R.R.P. Singh, P.A. Fleury, K.B. Lyons and P.E. Sulewski *Phys. Rev. Lett.* **62**, 2736 (1989).
22. W.H. Weber and G.W. Ford, *Phys. Rev. B* **40**, 6890 (1989).
23. G. Shirane et al, *Phys. Rev. Lett.* **63**, 330 (1989).
24. J.M. Tranquada et al, preprint.
25. G. Aeppli et al *Phys. Rev. Lett.* **62**, 2052 (1989).
26. The fit consists in obtaining the exchange constant J from the experimental results. J is obtained from the spin wave velocity (Neutron scattering) and from the position of the two-magnons peak in the Raman spectrums using the Heisenberg model in the spin-wave approximation.
27. S. Sugai et al, *Phys. Rev. B* **42**, 1045 (1990).
28. J. Parkinson, *J.Phys. C* **2**, 2012, (1969).
29. E. Gagliano and C. Balseiro, *Phys. Rev. Lett.* **59**, 2999 (1987); *Phys. Rev. B* **38**, 11766 (1988).
30. E. Gagliano and S. Bacci, PRB in press; E. Dagotto and D. Poilblanc, PRB in press.
31. see, for example, N. Bulut et al *Phys. Rev. Lett.* **62**, 2192 (1989).
32. The two-magnon peak for the 20 sites cluster has a relative shift of $\approx 2\%$ (with respect to the 16 sites lattice) to higher frequencies. Its location is 3.045J (2.976J) for 20 (16) sites.
33. E. Stechel, in *High-T_c Superconductivity*, page 191, K.S. Bedell et al editors, (Addison-Wesley, 1990), reports results for the 18 sites cluster which also indicate that the same structure persists, i.e. no new peaks arise and a shift of the two magnons peak to higher frequencies. Also, the J' appears to have no special significance in the B_2 Raman geometry.