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Spin Excitations of the Extended *t-J* Model: Neutron Scattering

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Dynamical spin susceptibility, $\chi(\boldsymbol{q}, \omega)$, of the *t-J* model with transfer integrals of the extended spatial range has been evaluated based on the slave-boson mean-field theory for both LSCO- and YBCO-type Fermi surfaces. In the former, the width and height of the incommensurate (IC) peaks are seen to have strong dependences on ω and the temperature, T. Interestingly, and in agreement with experiments, the IC peaks at low energy become sharper in the singlet RVB state which, in our classification, corresponds to the superconducting state in the region of optimal doping. In the case of YBCO, the dependences on ω and T at $\boldsymbol{q}=\boldsymbol{Q}\equiv(\pi, \pi)$, the antiferromagnetic wave vector, have particular features which share common qualitative characteristics with the experimental findings.

Various experiments on spin excitations probed typically by neutron scattering and nuclear magnetic relaxation have revealed exotic features of high-T_c cuprates.[1] There have been several theoretical attempts to understand these either phenomenologically,[2,3] or microscopically based on the Hubbard model[4] and the *d-p* model.[5] On the other hand, the *t-J* model, which is considered to be relevant for high-T_c cuprates after the pioneering work by Anderson,[6] and Zhang and Rice,[7] and by subsequent studies,[8–13] has been studied by use of the slave-boson mean-field theory.[14–17] This theory predicts solid and quantitative results to be critically checked with experiments, thereby enabling us to search eventually for the essential cause of this fascinating phenomenon. So far we have clarified its static properties, which include the following.

1) The difference in the spin fluctuations, i.e., incommensurate (IC) one in $La_{2-x}Sr_xCuO_4$ (LSCO) and commensurate (C) one in $YBa_2Cu_3O_{6+x}$ (YBCO), is due to the difference of the Fermi surfaces.

2) The apparent possible classification of high- and low-doping regions separated by the optimal doping, which was clearly noted first by Rice[18] in the YBCO family and later found to be universal,[19] can be at least qualitatively understood by the mean-field phase diagram of the *t-J* model, whose schematic structure is shown in Fig. 1. In this phase diagram not only the uniform RVB (U-RVB) of spinons but also their singlet RVB (S-RVB) originally introduced by Anderson[6,20] have been taken into account together with the bose condensa-

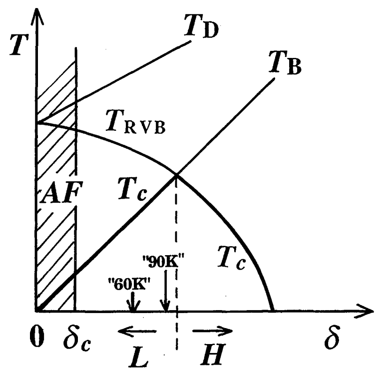

Fig. 1. A schematic representation of the mean-field phase diagram of the (extended) *t-J* model in the plane of the doping rate, δ, and the temperature, T. T_D, T_{RVB} and T_B are onset temperatures of the uniform RVB (coherent motions of spinons and holons), the singlet RVB pairing and the Bose condensation of holons, respectively. The calculated T_{RVB} is given in ref. 17, Fig. 13. The arrows with "60 K" and "90 K" are the locations in our classification of T_c=60 K and T_c=90 K YBCO systems.

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tion of holons.[21)]

In this letter we will further explore the implications of this theoretical framework, especially their dynamical aspects to be compared with experiments of neutron scattering. We focus on samples with doping rate near optimal T_c by the reason stated below.

Our model is given by

$$H=-\sum_{i,j;s} t_{ij}\tilde{c}_{is}^{\dagger}\tilde{c}_{js}+\sum_{\langle i,j\rangle} J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j, \tag{1}$$

where $\tilde{c}_{is}=c_{is}(1-n_{i,-s})$ excludes the double occupancy and J is assumed only for the neighboring sites, while t_{ij} has a finite spatial extent with values, t (nearest neighbor), t' (next-nearest neighbor) and t'' (third-nearest neighbor). As in refs. 15 and 17, we assume $t/J=4$, $t'/t=-1/6$, $t''/t=0$ for LSCO and $t/J=4$, $t'/t=-1/6$, $t''/t=1/5$ for YBCO.

In the slave-boson technique we write $\tilde{c}_{is}=b_i^{\dagger}f_{is}$ with holon (b_i) and spinon (f_{is}) operators. In the mean-field approximation we take into account both order parameters, $\langle f_{is}^{\dagger}f_{js}\rangle$ and $\langle f_{i\uparrow}^{\dagger}f_{j\downarrow}^{\dagger}\rangle$, for the uniform and singlet RVB with the d-symmetry, respectively. The dynamical spin susceptibility, $\chi(\boldsymbol{q},\omega)$, is given by[14)]

$$\chi(\boldsymbol{q},\omega)=\chi_0(\boldsymbol{q},\omega)/[1+J_q\chi_0(\boldsymbol{q},\omega)], \tag{2}$$

based on the random phase approximation of the J-term in eq. (1), where $J_q=J(\cos q_x+\cos q_y)$, (lattice spacing is assumed to be unity) and $\chi_0(\boldsymbol{q},\omega)$ is that of free spinons in the uniform or singlet RVB states, as the case may be. In the present numerical calculation, χ_0 has been calculated by introducing a small but finite imaginary part, $\Gamma=0.008J$, in the denominator of its integrand, thereby smearing its singularities.

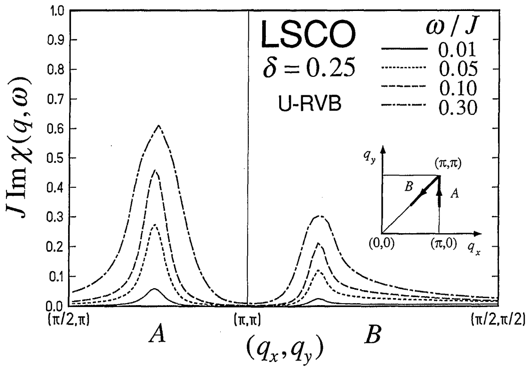
We will first show the results of the numerical calculations of $\mathrm{Im}\,\chi(\boldsymbol{q},\omega)$.

I. LSCO

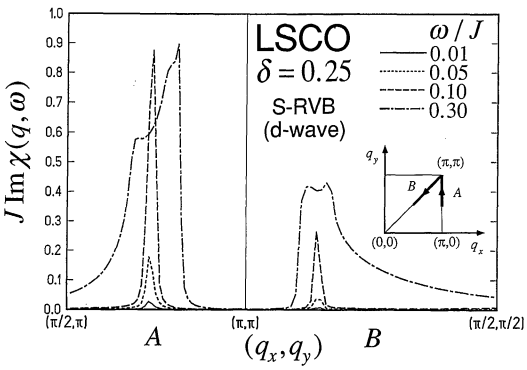
1) The $\boldsymbol{q}$-dependences in the uniform RVB state ($T=T_{\mathrm{RVB}}$, where $T_{\mathrm{RVB}}=0.046J$ in the present case of $\delta=0.25$) for several choices of $\omega/J=0.01$, 0.05, 0.10 and 0.30, are shown in Fig. 2(a).

2) The $\boldsymbol{q}$-dependences in the singlet RVB state ($T=0.3\ T_{\mathrm{RVB}}$) for the same choice of parameters are shown in Fig. 2(b).

II. YBCO



(a)



(b)

Fig. 2. The $\boldsymbol{q}$-dependences of $J\,\mathrm{Im}\,\chi(\boldsymbol{q},\omega)$ for $\omega/J=0.01$, 0.05, 0.10 and 0.30 in the case of $t'/t=-1/6$, $t''/t=0$ (LSCO type) and $\delta=0.25$. (a) In the uniform RVB state (U-RVB) at $T=T_{\mathrm{RVB}}=0.046J$. (b) In the singlet RVB state (S-RVB) with d-symmetry at $T=0.3\ T_{\mathrm{RVB}}=0.014J$.

1) The ω-dependences at $\boldsymbol{q}=\boldsymbol{Q}\equiv(\pi,\pi)$ for several choices of temperature both at and below T_{RVB} are shown in Fig. 3 for $\delta=0.20$.

2) The T-dependences at $\boldsymbol{q}=\boldsymbol{Q}\equiv(\pi,\pi)$ for several choices of ω are shown in Fig. 4.

3) The $\boldsymbol{q}$-dependences near $\boldsymbol{q}=\boldsymbol{Q}$ for $\omega=0.1\ J$ in both the uniform ($T=T_{\mathrm{RVB}}$) and the singlet RVB states ($T=0.3\ T_{\mathrm{RVB}}$) for $\delta=0.20$ are shown in Fig. 5.

In the above calculations the values of the doping rate, δ, are rather of qualitative nature in the present mean-field calculation and should not be taken so seriously.

In the following, the discussions on these numerical results will be given for LSCO and YBCO, respectively.

I. LSCO

The peak height and the width of IC peaks

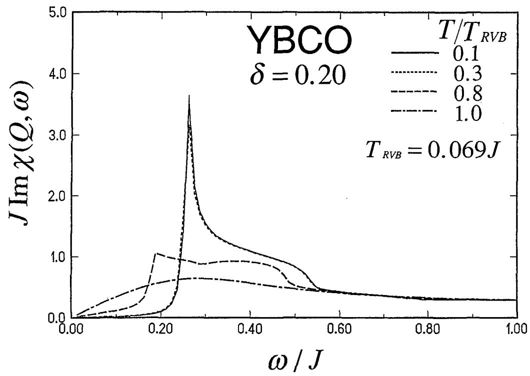


Fig. 3. The ω-dependences of $J\,\mathrm{Im}\,\chi(\boldsymbol{q}, \omega)$ at $\boldsymbol{q}=\boldsymbol{Q}\equiv(\pi, \pi)$ for several choices of temperature, both at and below T_{RVB} in the case of $t'/t=-1/6$, $t''/t=1/5$ (YBCO type) and $\delta=0.20$ with $T_{\mathrm{RVB}}=0.069J$.

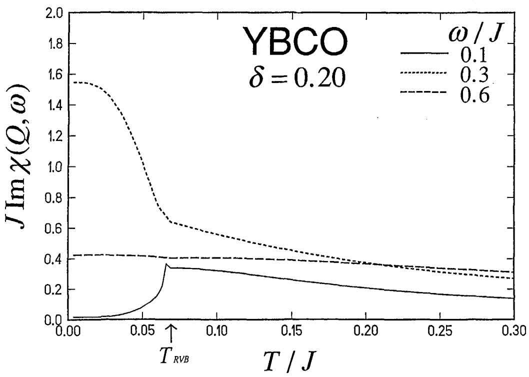


Fig. 4. The T-dependences at $\boldsymbol{q}=\boldsymbol{Q}\equiv(\pi, \pi)$ for $\omega/J=0.1$, 0.3 and 0.6 for YBCO, $\delta=0.20$. The arrow indicates $T=T_{\mathrm{RVB}}=0.069J$.

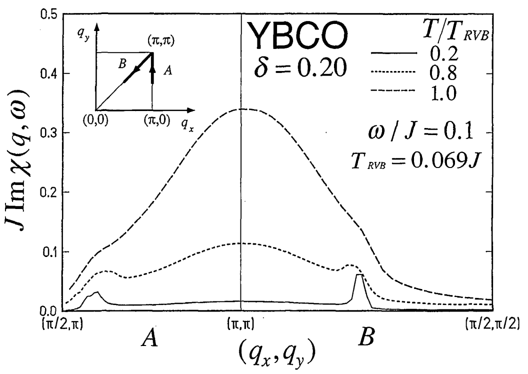


Fig. 5. The $\boldsymbol{q}$-dependences near $\boldsymbol{q}=\boldsymbol{Q}$ for $\omega=0.1J$ both in the uniform ($T=T_{\mathrm{RVB}}=0.069J$) and the singlet RVB states ($T/T_{\mathrm{RVB}}=0.8$, 0.2) for YBCO, $\delta=0.20$.

have appreciable dependences on ω and T, but they are not strongly modified through the onset of the singlet RVB state, which corresponds to the onset of the superconducting state if the doping rate is near optimal but in the high-doping region. The latter feature is in qualitative agreement with experiments.[22,23] However, the present ω- and T-dependences appear to be stronger than the experimental findings.[23] In particular, $\mathrm{Im}\,\chi(\boldsymbol{q}, \omega)$ at the incommensurate peaks of ref. 23 (Fig. 4) is not proportional to ω for small ω (1.5 meV $<\omega<$ 6 meV), as opposed to the linear dependence on ω in the present results. Such a weak dependence on ω of $\mathrm{Im}\,\chi(\boldsymbol{q}, \omega)$ has actually been observed in $YBa_2Cu_{2.9}Zn_{0.1}O_{6.6}$,[24] and also in spin-glass systems.[25] These facts lead us to the conclusion that neutron scattering in LSCO may have been affected by some kind of randomness whose microscopic origin, however, is not clear at present.

II. YBCO

The ω-dependence at $\boldsymbol{q}=\boldsymbol{Q}$ in the uniform RVB state is linear for small ω with an extended tail at high energies more or less in accordance with experiments on YBCO for $T\gtrsim 100$ K.[26] In the singlet RVB state, however, there is a gap-like behaviour at low energies, whose spectral weight is pushed up to the apparent cutoff energy $\omega\sim 0.5$–$0.6\,J$, together with structures in the intermediate energies. These share common features with experiments on $YBa_2Cu_3O_{6.92}$.[26] The relative intensities of the two broad peaks in the intermediate-energy region are, however, opposite between the present theoretical results and experiments. Although we can think of several possible causes of this discrepancy, such as more details of the energy bands or lifetime broadening, we cannot decide which at present.

As regards the $\boldsymbol{q}$-dependence, it is interesting to note that the peak at $\boldsymbol{q}=\boldsymbol{Q}$ seen in the uniform RVB state is easily suppressed by the onset of the singlet RVB state as seen in Fig. 5. This may explain the apparent contradiction between two experimental findings;[26,27] the sample ($YBa_2Cu_3O_{6.92}$ at $T=150$ K) of ref. 26 is located in the uniform RVB state while that ($YBa_2Cu_3O_{6.9}$ at $T=150$ K) of ref. 27 is in the singlet RVB state. This kind of difference is possible because of the subtlety of the phase diagram, Fig. 1, near the optimal T_c, as has been seen in the experiment of nuclear magnetic relaxation rate on $YBa_2Cu_3O_{6+x}$ with $x=0.92$ and $x=1$.[28]

Irrespective of the overall agreement between experiments and the present theoretical results for YBCO, we note that the theoretical prediction of the doping dependence of the "spin gap," ω_g, defined as the threshold energy for the finite intensity at $\boldsymbol{q}=\boldsymbol{Q}$, is weaker than experimental findings. It is possible that the present mean-field theory does not correctly describe the region near its magnetic instability point. This is the reason why we focus on samples near optimal doping. This problem will be further explored elsewhere in the context of nuclear magnetic relaxation.

In summary, we have explored the implications of the slave-boson mean-field theory of the *t-J* model by examining the dynamical properties of the spin excitations. It is found that various unusual features seen in experiments are understood by the present theory, at least qualitatively and in some cases even semi-quantitatively.

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