A Consistent Picture for Resonance Neutron Peak and ARPES Spectra in High-\textit{T}_c Superconductors

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The spectra observed in ARPES measurements are examined together with the resonance peak observed in neutron scatterings, based on the slave-boson approach to \textit{t} - \textit{t}‘ - \textit{J} model. We show that the peak/dip/hump features arise from the scattering of electrons by collective spin excitations which, at the same time, give rise to the neutron resonance mode. The doping dependences and the dispersions of the peak/dip/hump positions are shown to be consistent with experiments. Our results indicate that recently observed \cos(6\theta) deviation from the pure \textit{d}-wave also result from the renormalization by spin fluctuations.

PACS number: 71.10.-w, 74.25.Jb, 74.25.Ha, 79.60.Fy

Both angle resolved photoemission spectroscopy (ARPES) and neutron scattering experiments have played important roles in the studies of high-\textit{T}_c superconductors. It has been shown by ARPES that the spectral lineshape possesses a peak/dip/hump structure in the superconducting (SC) state. The anomalous momentum, temperature and doping dependences of the spectral lineshape suggest that electrons are strongly coupled to collective excitations centered at (π, π) and these collective excitations are related to the pairing interaction. On the other hand, the most prominent feature of the spin susceptibility observed in neutron scattering studies is the sharp resonance peak at (π, π) in the superconducting or pseudogap states. It has been speculated, from a comparison of these two kinds of experimental data, that the collective excitations are the resonance modes in the neutron scattering experiments. This idea has been further explored qualitatively in a phenomenological spin-fermion model, in which the resonance mode is identified as the propagating collective spin excitations and the scattering of electrons by these spin modes gives rise to the anomalous spectral lineshape. Using the slave-boson theory for the \textit{t} - \textit{t}‘ - \textit{J} model, Brinckmann and Lee have investigated the spin resonance and its evolution with doping.

Recent ARPES study reveals the specular dependences of the peak, dip and hump energies with doping. Furthermore, a small \cos(6\theta) (θ is the Fermi surface angle) deviation from the pure \textit{d}-wave structure is observed. These results and their correlation with the mode energy inferred from neutron data are the essential ingredient for a consistent picture of the ARPES lineshape and the neutron data. In this paper, we examine these issues and show that they can be quantitatively reproduced based on the slave-boson approach to the 2D \textit{t} - \textit{t}‘ - \textit{J} model. The model reads,

\[ H = - \sum_{<ij>,\sigma} t_{i\alpha} c_{i\sigma}^+ c_{j\sigma} - \sum_{<ij>',\sigma} t'_{i\alpha} c_{i\sigma}^+ c_{j\sigma} + \frac{J}{2} \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j, \]

where \( <ij> \) denotes the nearest-neighbor (n.n.) bond and \( <ij>' \) the next n.n. bond. In the slave-boson method, the physical electron operators \( c_{i\sigma} \) are expressed by slave bosons \( b_{i\sigma} \) carrying the charge and fermions \( f_{i\sigma} \) representing the spin: \( c_{i\sigma} = b_{i\uparrow}^\dagger f_{i\sigma} \). We consider the \textit{d}-wave SC state with the order parameters \( \Delta_{ij} = -f_{i\uparrow} f_{j\downarrow}^+ > 0 > f_{i\downarrow} f_{j\uparrow}^+ > 0 > f_{i\uparrow} f_{j\downarrow}^+ > 0 > f_{i\downarrow} f_{j\uparrow}^+ > 0 \), and \( \chi_{ij} = \sum_\alpha < f_{i\alpha}^+ f_{j\alpha} > \), in which bosons condense \( b_i \rightarrow <b_i> = 1/(\delta) \) (δ is the hole concentration). Then, the mean-field Hamiltonian of Eq.(1) is,

\[ H_m = \sum_{k\sigma} \epsilon_k f_{k\sigma}^+ f_{k\sigma} - \sum_k \Delta(k) (f_{k\uparrow}^+ f_{-k\downarrow} + c.c.) + 2 NJ' (\chi_0^2 + \Delta_0^2), \]

where the dispersion for fermions \( \epsilon_k = -2(\delta t + J'\chi_0)[\cos(k_x) + \cos(k_y)] - 4\delta t' \cos(k_x) \cos(k_y) - \mu \), and the gap \( \Delta(k) = 2J'\Delta_0[\cos(k_x) - \cos(k_y)] \), with \( J' = 3J/8 \).

The mean-field parameters \( \chi_0, \Delta_0 \) and the chemical potential \( \mu \) for different doping \( \delta \) are obtained from a self-consistent calculation.

In the above mean-field calculation, we have set \( <S_i> = 0 \). In order to consider the response to external magnetic and electric fields, we include the antiferromagnetic (AF) fluctuation by writing \( H = H_m + H' \), where \( H' \equiv H - H_m \), and treating \( H' \) as a perturbation to \( H_m \). In the Hartree-Fock approximation, this reproduces the mean-field results. To investigate the AF fluctuations, we consider the scattering of electrons off spin fluctuations in \( H' \). As a first step, we calculate the spin susceptibility in the random-phase approximation (RPA) as shown in Fig.1(a),

\[ \chi(q, \omega) = \chi_0(q, \omega)/[1 + \alpha J(q)\chi_0(q, \omega)]. \]
Here $J(q) = J(\cos q_x + \cos q_y)$ and $\chi_0(q, \omega)$ is the unperturbed spin susceptibility which is calculated from the fermionic bubbles representing particle-hole excitations. Following Ref. [3], we choose $\alpha = 0.34$ in order to set the AF instability at $\delta = 0.02$, which is the experimental observed value. This is the only adjusted parameter throughout the paper. The fermionic self-energy is obtained from the lowest-order contribution of the scatterings of fermions off spin fluctuations. In the SC state, there are two different self-energies $\Sigma_s$ and $\Sigma_w$, as shown in Fig.1(b) and (c), which renormalize the fermionic dispersion and the SC gap, respectively. In the previous study [5], only $\Sigma_s$ is included in their calculations. We will show that the inclusion of $\Sigma_w$ lead the otherwise flat doping dependence of the ARPES peak to be consistent with experiments. The fermionic Green’s function is calculated by

$$G_f(k, \omega) = \left[ G_{f0}^\omega(k, \omega) + (\Delta_s + \Sigma_w) G_{f0}^\omega(−k, −\omega)\right]^{-1}$$

with $G_{f0}(k, \omega) = [\omega − ε_k − \Sigma_w(k, ω)]^{-1}$. In the SC state, bosons condense and the electronic Green’s function can be approximated by $G(k, \omega) ≈ \delta G_f(q, \omega)$. Then, the spectral function of electrons is calculated from $A(k, \omega) = -(1/π)\text{Im}G(k, \omega)$. Numerical calculations are performed at low temperature $T = 0.005J$, with $t = 2J, t' = −0.45t$, and $J = 0.13eV$.

We first analyze the imaginary part of the spin susceptibilities at $Q = (π, π)$. It develops sharp resonance peaks for various doping densities. This result has been reported in Ref. [4]. In the framework of the d-wave BCS theory, the origin of these peaks has been discussed [6,7,9]. Essentially the peak arises from a collective spin excitation mode corresponding to $1 + αJ(Q)\text{Re}\chi_0(Q, ω) = 0$ and negligibly small $\text{Im}\chi_0(Q, ω)$. It is due to a step-like rise of $\text{Im}\chi_0$ at its gap edge and then a logarithmic singularity in $\text{Re}\chi_0$ via the Kramers-Kroening relation. This singularity shifts downward the collective mode energy and leads it to situate in the spin gap, so no damping is expected for the mode. The step-like rise in $\text{Im}\chi_0$ arises from the flat band(extended van Hove singularity) which is observed near $(π, 0)$ and the property that $Δ_k + Σ_s = −Δ_k$ for transition momentum $Q$ due to the d-wave gap symmetry [1].

The lineshape $A(q, ω)f(ω)$ ($f(ω)$ is the Fermi distribution function) of electrons coming from the scatterings by spin fluctuations for doping $δ = 0.12$ are shown in Fig.2. The results are plotted for several wavevectors $k = (π, 0), (π, 0.15π), ...$, down to $(π, 0.5π)$. Clear peak/dip/hump structures are present at and near $(π, 0)$. In order to understand the origin of the peak/dip/hump structure, we plot the self-energy $\Sigma_s[\Sigma_s]$ is qualitatively similar to $\Sigma_s$ at the Fermi wavevector $k_F$ for doping $δ = 0.12$ in the inset of Fig.2. The solid line denotes its real part $\Sigma'_s$, while the dashed line its imaginary part $\Sigma''_s$. The corresponding lineshape at $k_F$ is expressed by the line with open squares in the main panel. Due to the coupling to the spin resonance mode, the whole structure of the self-energy $\Sigma_s$ is very similar to that of the unperturbed spin susceptibility $\chi_0$ (for a comparison, see Fig.2 in Ref. [5]). When frequency $|ω|$ is below about $0.5J$, $\Sigma''_s$ is equal to zero. Above $0.5J$, a step-like rise can be seen and is followed by a decrease. Consequently, $\Sigma'_s$ has a peak at about the center of the step-like rise of $\Sigma'_s$. The quasiparticle energy is given by the pole of the Green’s function, which is the solution $ω$ of the equation $P(k_F, ω) = ω − Σ_s(k, ω))^{2} (Δ_s + Σ_w(k, ω)) = 0$. We also show $P(k_F, ω)$ (dotted line) in the inset of Fig.2. The lowest binding-energy solution of the pole equation $P(k_F, ω) = 0$ is $ω = −0.42J$. Meanwhile, the damping of this mode which is proportional to $Σ''_s$ and $Σ''_w$ approaches to zero. Therefore, it gives rise to a quasiparticle mode which is denoted by the sharp low binding-energy peak in the lineshape shown in Fig.2. As $|ω|$ increases further, the pole equation does not satisfy anymore. Near the end of the step-like rise in $\Sigma'_s$, $P(k_F, ω)$ reaches its local maximum, meanwhile the imaginary part of the self-energy is also near its maximum, therefore a dip appears. It indicates that the dip is caused by the step-like rise in the imaginary part of the self-energy. After the dip, $P(k_F, ω)$ decreases with $|ω|$ and near $ω = −1.0J$, it reaches a local minimum. This leads to the broad higher binding-energy hump.

We now discuss the dispersion of the hump/dip/peak structure. At the momentum range below and slightly above the Fermi wavevector $(π, 0.15π)$, the low binding-energy peak nearly does not disperse with $k$. Above $(π, 0.3π)$, the peak starts to move to higher binding-energy but cannot move further than that dip seen around $k_F$. Then, it disappears gradually with the further increasing of $k$, due to the unavailable quasiparticle states above the Fermi surface at low temperatures. As a result, the dip also disappears gradually. These behaviors were observed in experiments [1]. The position of the peak determines the normalized gap size due to spin fluctuations. In Fig.3, we show a typical dependence of the renormalized gap magnitude on the Fermi surface angle $θ$, which is the angle between $k_F$ and $k_z$. In general, the next order deviation from the d-wave starts from $\cos(6θ)$ and can be described by the form $Δ(θ) = Δ_1 \cos(2θ) + Δ_2 \cos(6θ)$. However, our results indicate that the best fit is $Δ(θ) = Δ_{max}[B \cos(2θ) + (1 − B) \cos(6θ)]$ with $B$ being around 0.88-0.94. This particular form was also used in Ref. [1] to fit their ARPES data with roughly the same range of $B$.

In Fig.4(a), we show the doping dependence of the positions of the hump and the peak, and compare our results with the experiment [1]. One can see that our result for the peak is in reasonably good agreement with the experiment. We note that, if we just include the self-energy $Σ_s$ in our calculation as was done in Ref. [8], a doping independence for the peak positions is obtained. Hence the renormalization of the gap by including $Σ_w$ is
important. The magnitude of the position of the hump and its trend with the doping variation are also consistent with the experiment. However, the slope of the curve of hump versus hole density is flatter than the experimental result. Considering that all parameters in our calculations are chosen according to the well-known values and the only adjusted parameter $\alpha$ is fixed by the experimental observation on AF instability, these results are quite satisfactory. The dependence of the ratio between the hump and peak energy at $(\pi, 0)$ on doping concentrations is shown in Fig.4(b). A flat variation for a wide doping level is seen. This result again agrees with the experiment [10].

An important quantity addressed in the ARPES experiments is the peak-dip separation, which is shown to be close to the mode energy of the neutron peak [10]. From a comparison of Fig.2 in Ref. [1] and Fig.3, one can see that the peak-dip separation in our calculations is lower than the neutron peak. However, we would like to point out that this separation is sensitive to the experimental energy resolution simulated to be $\Gamma = 0.02J$ here. When $\Gamma$ increases, the self-energy $\Sigma''$ decreases and the quasiparticle peak broadens, consequently the peak-dip separation increases. However the position of the neutron scattering peak does not change for different $\Gamma$, it just becomes broad. So, this comparison is also sensitive to $\Gamma$. But, as noted above, the dip stems from the step-like edge in $\Sigma''$, which is in turn caused by the coupling to the collective spin mode. On the other hand, this spin resonance mode also arises from the step-like edge in $\text{Im} \chi_0$ which is due to the extended van Hove singularity near $(\pi, 0)$ and the $d$-wave symmetry. Therefore, an intimate relation between them is suggested. Thus, our result seems to provide a consistent picture for the spin resonance peak and the hump/dip/peak structure based on the spin excitations in a $d$-wave superconductor.

Recently, P.J. White et al. [17] have investigated the effect of nonmagnetic Zn impurities on the lineshape of $Bi_2Sr_2Ca(Cu_{1-x}Zn_x)O_{8+\delta}$ by ARPES experiment. They found that the dip is diminished with Zn doping. According to the previous studies by one of the authors (Li) [15], Zn doping will wash out the van Hove singularity and cause the decays of quasiparticle states. So, the enhancement in $\text{Re} \chi_0$ and the step-like rise in $\text{Im} \chi_0$ will be suppressed. As a result, no clear resonance neutron peak appears at certain Zn doping concentration [15]. Because the dip is suggested to come from the coupling to the spin resonance mode here, the disappearance of the dip upon Zn doping may be naturally explained in the present framework.

It is quite encouraging that our results fit various kinds of ARPES and neutron scattering data with correct trend and reasonable magnitude. There is only one adjustable parameter which is fixed by the experimentally observed AF instability. Therefore, our investigation represents a natural extension to the work of Brinckmann and Lee [9], which addressed the doping dependence of the resonance peak in neutron scatterings. In addition, in comparison to the qualitative study by Abanov and Chubukov [8], our study further furnishes a quantitative basis.

In summary, based on the slave-boson approach to the $\hat{t} - \hat{t}' - J$ model, we show that the anomalous peak/dip/hump structure observed in the ARPES experiments arises from the coupling of quasiparticle to the collective spin excitations which gives rise to the resonance peak in the neutron scattering experiments. Our investigation seems to give a consistent explanation for the resonance neutron peak and the ARPES spectra based on the spin excitations in a $d$-wave superconductor.

We acknowledge the support from NSC of Taiwan under Grant Nos.88-2112-M-001-004 and 89-2112-M-007-024. J.X.Li was support in part by the National Science Foundation of China. He would also like to thank Laboratory of Physics, Academia Sinica (Taiwan) for support during the initial stages of this work and C.D.Gong for helpful discussion.

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is independent of the photon energy [H.M.Fretwell et al., cond-mat/9910221 (unpublished)]
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FIGURE CAPTIONS

Fig.1 Feynman diagrams for: (a) the RPA approximation to the spin susceptibility coming from particle-hole excitations. (b) and (c) the lowest-order contribution to the self-energy from fermion-spin excitation scatterings.

Fig.2 Photoemission spectra $A(k,\omega)f(\omega)$ at $k = (\pi,0), (\pi,0.15\pi), (\pi,0.225\pi), (\pi,0.3\pi), (\pi,0.4\pi), (\pi,0.5\pi)$ (from the up to down lines). Inset shows the frequency dependence of the fermion’s self-energy $\Sigma_s$ at $k_F = (\pi,0.15\pi)$ (Fermi wavevector). The solid line corresponds to its real part and the dashed line to its imaginary part. Also shown in the inset is $P(k_F,\omega)$ (see text) which is denoted by the dotted line.

Fig.3 The renormalized gap size versus the Fermi surface angle $\theta$ for $\delta = 0.08$. The open circles are our results, while the solid line is the fit using the gap function $\Delta(\theta) = \Delta_{\text{max}}[B\cos(2\theta) + (1-B)\cos(6\theta)]$ with $B = 0.94$.

Fig.4 Doping dependences of the energy scales for the hump and the peak at $(\pi,0)$. (a) Doping dependences of the hump and peak positions. The open squares and the solid triangles are experimental data for the hump and peak positions from Ref. [10], respectively. (b) Doping dependence of the ratio of the hump position to the peak position.
$$\chi = \bigcirc + \bigcirc + \cdots \quad (a)$$

$$\Sigma_s(q,\omega) =$$

$$\Sigma_w(q,\omega) =$$

Fig.1, Li, Mou and Lee
Fig. 2, Li, Mou and Lee
Fig. 3, Li, Mou and Lee

\[ \frac{\Delta(\theta)}{J} \]
Fig. 4 Li, Mou, and Lee

Hump/Peak vs. Hole Density

Peak Position ($x \times 10^{-3} K$)

Hump Position ($x \times 10^{-3} K$)