Theory of Magnetic excitations in High-T_c Cuprates: Two Component Spin-Fermion Model

Yunkyu Bang

Department of Physics, Chonnam National University, Kwangju 500-757, and Asia Pacific Center for Theoretical Physics, Pohang 790-784, Korea
E-mail: ykbang@jnu.ac.kr

Abstract. Recent neutron scattering experiments have revealed that the generic form of the magnetic excitations in the high-T_c cuprates has the so-called "hourglass" shape; it features both upward and downward excitations at the incommensurate (IC) momenta merging to the resonance peak at the commensurate momentum (π, π). We propose the two-component spin-fermion model as a minimal phenomenological model which has both local spins and itinerant fermions as independent degrees of freedom. Our calculations of the dynamic spin correlation function provide good agreement with experiments and show: (1) the upward dispersion branch of magnetic excitations is mostly due to the local spin excitations; (2) the downward dispersion branch is from collective spin excitations of fermions; (3) the resonance mode is a mixture of both degrees of freedom.

1. Introduction
Since the discovery of the high-T_c superconductors (HTSC), the understanding of spin dynamics has been a key issue because it is expected that the spin correlation holds crucial information for the mechanism of the high-T_c superconductivity. For long the two main observations in the neutron scattering experiments of high-T_c cuprates are (1) the incommensurate (IC) peaks at low energy or at quasielastic excitations [1, 2] and (2) the so-called resonance peak at commensurate wave vector at relatively high energy (30 ∼ 50 meV) [3]. With more recent experiments[4, 5, 6, 7, 8, 9], an unifying picture of the magnetic excitations in the cuprate superconductors has emerged as "hourglass" shape of excitations around the wave vector (1/2,1/2) (hereafter in units of 2π/a), in which the low energy IC excitations form the downward dispersion branch and the high energy IC excitations form the upward dispersion branch, and the two branches of excitations merge at the commensurate momentum and at the resonance frequency.

In this paper, we propose a two component spin-fermion model [10] as a minimal phenomenological model to provide a natural and unifying explanation for the above mentioned neutron experiments of high-T_c cuprates. In this phenomenological model, the minimal set of low energy degrees of freedom are the spin wave excitations of local spins and the continuum particle-hole excitations of fermions. Despite a gross similarity to the one component model [11], we argue that the necessity of the presence of local spins in the minimal model of HTSC is impelling from the neutron experiments.
2. Model

In a mixed momentum and real-space representation the corresponding Hamiltonian is written as

\[ H = \sum_{\mathbf{k}, \alpha} c_{\alpha}^\dagger(\mathbf{k}) \varepsilon(\mathbf{k}) c_{\alpha}(\mathbf{k}) + \sum_{\mathbf{r}, \alpha, \beta} g \mathbf{S}(\mathbf{r}) \cdot c_{\alpha}^\dagger(\mathbf{r}) \mathbf{\sigma}_{\alpha\beta}(\mathbf{r}) + H_S, \]  

(1)

where the first term is the fermionic kinetic energy and the second term describes the coupling between local spins \( \mathbf{S}(\mathbf{r}) \) and the spin density of the conduction electrons. The last term represents the phenomenology of the effective low-energy Hamiltonian for the local spins. When the local spins have a short range AFM correlation, the bare (before coupling to the fermions) spin correlation function has the general form as follows[12].

\[ \chi_{0,S}^{-1}(\mathbf{q}, \Omega) = \chi_{0,S}^{-1}(\mathbf{q}, 0) \cdot [1 + \xi^2q^2 - \Omega^2/\Delta_{SG}^2], \]  

(2)

where \( \mathbf{Q} \) the 2D AFM ordering vector, and the spin gap energy \( \Delta_{SG} \) and the magnetic correlation length \( \xi \) combine to give the spin wave velocity \( v_s = \Delta_{SG} \cdot \xi \). Counting the coupling term to one loop order, the dressed spin correlation functions of the model are written as follows.

\[ \chi_S^{-1}(\mathbf{q}, \Omega) = \chi_{0,S}^{-1}(\mathbf{q}, \Omega) - g^2 \cdot \chi_{0,f}(\mathbf{q}, \Omega) \]  

(3)

\[ \chi_f^{-1}(\mathbf{q}, \Omega) = \chi_{0,f}^{-1}(\mathbf{q}, \Omega) - g^2 \cdot \chi_{0,S}(\mathbf{q}, \Omega) \]  

(4)

where \( \chi_{0,f} \) is the noninteracting spin susceptibility of the conduction band of the fermions and \( \chi_{0,S} \) is introduced in Eq.(2). Having two degrees of freedom in the model, it is very important to treat the two spin susceptibilities \( \chi_S \) and \( \chi_f \) on equal footing.

To make a contact with experiments, we use a tight binding model for the fermion dispersion

\[ \varepsilon(\mathbf{k}) = -2t(\cos(k_x) + \cos(k_y)) - 2t' \cos(k_x) \cdot \cos(k_y) - \mu. \]  

(5)

For calculations in this paper, we chose \( t' = -0.4t \), and \( \mu = -0.81t \). The fermion susceptibility \( \chi_{0,f} \) is calculated both in normal state (NS) and in superconducting state (SS) assuming a canonical d-wave pairing \( \Delta(\mathbf{k}) = \Delta_0[\cos(k_x) - \cos(k_y)] \).

3. Results and Discussions

Fig.1(a) shows \( \text{Im} \chi_f(q, \Omega) \) scanned along \( q = (h, 1/2) \) in the superconducting state. The superconducting gap \( \Delta_0 = 0.2t \) and the bare spin gap \( \Delta_{SG} = 1.1t \) is chosen; the physical spin gap is strongly renormalized by coupling with fermions. The dimensionless coupling constant is defined as \( \lambda \equiv g^2 \cdot \chi_{0,f}(Q, 0) \cdot \chi_{0,S}(Q, 0) \), and we choose \( \lambda = 0.80 \) for calculations in this paper. The main effect of the coupling is to pull down the bare spin gap \( \Delta_{SG} \) below the particle-hole excitation gap of \( \chi_{0,f}(q, \Omega) \sim 2\Delta_0 \), which then forms a sharp resonance peak at \( Q = (1/2, 1/2) \). Centering from this resonance mode, both the downward dispersion branch and the upward dispersion branch span out. The origin of the upward dispersion is apparently from the local spin wave mode and the origin of the downward dispersion is the itinerant spin excitations of \( \chi_{0,f} \). This fact is identified in Fig.1(b) which shows \( \text{Im} \chi_{0,f}(q, \Omega) \) scanned along \( q = (h, 1/2) \) in the superconducting state. The shape and strength of the downward whisher like excitations in \( \text{Im} \chi_{0,f} \) is quite sensitive to the band structure (controlled by \( t, t' \), etc), Fermi surface curvature (controlled by \( \mu, t' \)), and the size of the d-wave gap \( \Delta(\mathbf{k}) \).

With the coupling strength \( \lambda = 0.8 \), the dressed susceptibility \( \chi_f(q, \Omega) \) obtains features of both the local spin susceptibility \( \chi_{0,S} \) and the itinerant spin susceptibility \( \chi_{0,f} \), and the behavior of the dressed susceptibility \( \chi_S(q, \Omega) \) is qualitatively similar to the one of \( \chi_f(q, \Omega) \) in this
Figure 1. (a) The dressed spin susceptibility $\text{Im}\chi_f(q, \Omega)$ in superconducting state. Parameters are $\Delta_{SC} = 1.1t$, $\Delta_0 = 0.2t$, and $\lambda = 0.8$ (b) The bare spin susceptibility $\text{Im}\chi_{0,f}(q, \Omega)$ in superconducting state. (c) $\text{Im}\chi_f(q, \Omega)$ in normal state ($\Delta_0 = 0$). (d) $\text{Im}\chi_{0,f}(q, \Omega)$ in normal state.

coupling strength. Therefore we show only the results of $\chi_f(q, \Omega)$ in Fig.1.; the experimental data of neutron scattering should be the sum of the contributions from both susceptibilities. With a smaller coupling strength ($\lambda < 0.5$) the two spin susceptibilities retain more of their original characteristics of the spin wave and the itinerant fermion susceptibility, respectively.

Fig.1(c,d) are the same plots as in Fig.1(a,b) but in normal state. First, the resonance peak becomes a completely overdamped mode having only a hump like structure in $\text{Im}\chi_f(q, \Omega)$. Second, the downward whisker like dispersion disappears because the free fermion susceptibility $\chi_{0,f}(q, \Omega)$ in normal state has no such structure as seen in Fig.1(d). Lastly, the upward dispersion remains almost similar to the case of the superconducting state. In experiments the upward dispersion in normal state appears more smeared [9]. This could be due to the effect of enhanced damping process at higher temperatures which is not included in our calculations. The results of Fig.1(a,c) successfully reproduce the main features of recent neutron scattering experiments in high-$T_c$ cuprates [4, 5, 6, 7, 8, 9], i.e., the resonance mode in superconducting state, the hourglass shape of the upward and downward dispersions, and their drastic change in normal and superconducting states. In particular, these results are in excellent agreement with the data of YBCO$_{6.6}$ [9]. However, we need reservation for applying our result to L$_{1.875}$B$_{x=0.125}$CO$_4$ [6]. L$_{1.875}$B$_{0.125}$CO$_4$ has a static stripe order and extremely low $T_c = 2.5$ K [14]. In particular, the presence of the stripe ordering will change the spin dynamics significantly and therefore our model should not be directly applied to this compound.

3.1. Conclusion
In conclusion, we proposed a two-component spin fermion model to explain the neutron scattering experiments in high-$T_c$ cuprates. With the two spin degrees of freedom of the local spins and the itinerant spins, our calculations of the spin correlations reproduced the essential features of the experiments: the hourglass dispersions, resonance mode, their changes in normal and superconducting states. With the success of the two-component spin fermion model to
describe the neutron scattering experiments, the pressing question is now what microscopic theory is behind the phenomenological two-component spin fermion model; specifically how the local spin degree of freedom survives after doping from the parent insulating cuprate compounds. Another issue is how these two component spin excitations (in particular, the high energy spin wave type excitation) would affect other physical properties. Recent ARPES experiment by T. Valla et al. [14], indicates the presence of high energy spin excitations (∼340 meV), which is consistent with our model. The consequences of this high energy spin wave type excitations to the superconducting pairing and other normal state properties are also very important and will be studied in future works.

Acknowledgments
We thank A. Chubukov, I. Eremin, and B. Keimer for discussions. This work is supported by the KOSEF through the Grant No. KRF-2007-070-C00044, KRF-2007-521-C00081.

References
[1] S-W. Cheong et al., Phys. Rev. Lett. 67, 1791 (1991).
[2] P. Dai, H. A. Mook, and F. Dogan, Phys. Rev. Lett. 80, 1738 (1998).
[3] H. A. Mook et al., Phys. Rev. Lett. 70, 3490 (1993); H. Fong et al., Phys. Rev. Lett. 75, 316 (1995); P. Dai, H. A. Mook, G. Aeppli, S. M. Hayden, and F. Dogan et al., Nature 406, 965 (2000).
[4] M. Arai et al., Phys. Rev. Lett. 83, 608 (1999)
[5] S. M. Hayden et al., Nature 429, 531 (2004).
[6] J.M. Tranquada et al., Nature 429, 534 (2004).
[7] S. Pailhes, Y. Sidis, P. Bourges, V. Hinkov, A. Ivanov, C. Ulrich, L. P. Regnault, and B. Keimer, Phys. Rev. Lett. 93, 167001 (2004)
[8] V. Hinkov et al., Nature 430, 650 (2004).
[9] V. Hinkov et al., cond-mat/0601048.
[10] Y. Bang, I. Martin, and A. V. Balatsky Phys. Rev. B 66, 224501 (2002); Y. Bang, M. J. Graf, N. J. Curro, and A. V. Balatsky, Phys. Rev. B 74, 054514 (2006); M.V. Eremin et al., JETP Lett. 84, 167 (2006).
[11] A.V. Chubukov, D.Pines, J. Schmalian, in The Physics of Superconductors , ed. K.H. Benneman and J. B. Ketterson, Berlin, Springer, 2003, and references therein.
[12] S. Sachdev, A. V. Chubukov, and A. Sokol, Phys. Rev. B 51, 14874 (1995).
[13] T. Valla et al, Science 314, 1914 (2006).
[14] T. Valla et al., 2007 Phys. Rev. Lett. 98, 167003