Spin Dynamics of t-J Model on Triangular Lattice

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Abstract

We study the spin dynamics of t-J model on triangular lattice in the Slave-Boson-RPA scheme in light of the newly discovered superconductor Na$_x$CoO$_2$. We find resonant peak in the dynamic spin susceptibility in the $d+id'$-wave superconducting state for both hole and electron doping in large doping range. We find the geometrical frustration inherent of the triangular lattice provide us a unique opportunity to discriminate the SO(5) and RPA-like interpretation of the origin of the resonant peak.
The newly discovered superconductor Na$_x$CoO$_2$ has aroused many interests$^{[1, 2, 3, 4, 5]}$. It is believed that its low energy physics is analogous to high temperature superconductor and is another example of doped 2D Mott insulator. Another interesting aspect of this material is that it has a triangular lattice and is geometrically frustrated and non-bipartite. An effective model for this material is the t-J model on a triangular lattice. Historically, triangular lattice was used by Anderson to introduce the concept of resonant valence bond (RVB) state which is now widely used in the study of high temperature superconductivity, with the hope that the geometrical frustration can help to stabilize the RVB state over the ordered state. Hence it is believed that the study of Na$_x$CoO$_2$ superconductivity may shed new light on the study of high temperature superconductivity.

The most prominent feature of a doped Mott insulator is its spin dynamics, since its charges are largely frozen by the strong correlation effect at low energy. In high temperature superconductor, the spin dynamics plays a very important role in our understanding of its physics. The most remarkable thing in the spin dynamics of a high temperature superconductor is the appearance of the so called resonant neutron peak in the superconducting state$^6$. The origin of this remarkable phenomena (the dramatic change of spin dynamics accompanying the appearance of coherence in charge motion) is still not well understood. Two frequently discussed scenarios are an anti-bonding collective mode in the particle-particle channel related to a SO(5) symmetry between antiferromagnetism and d-wave superconductivity$^{[7, 8]}$, and a particle-hole bonding collective mode that manifests the internal structure of the Cooper pair as in the RPA-like theory$^{[9, 10, 11]}$.

In this paper, we study the spin dynamics of t-J model on the triangular lattice. We work in the Slave-Boson-RPA scheme and find resonant neutron peak in the spin dynamics of the $d + i d'$-wave superconducting state. This is expected since the resonant neutron peak is a manifestation of the internal structure of the Cooper pairs$^{[11]}$ and it should be visible when the measuring wavelength is comparable to the size of the pair (for $d + i d'$-wave pairing this length scale is just the lattice size near half filling). Since Cooper pair on the triangular lattice differ in detail from that on the square lattice, we expect the resonant peak on the triangular lattice will be different from that of high temperature superconductors.

The geometric frustration of the triangular lattice also provide us the opportunity to discriminate the SO(5) and the RPA explanation of the origin of the resonant peak. For
the SO(5) explanation to apply, the two particle continuum must collapse at some point in
the Brillouin Zone in order to make room for antibonding collective mode in the particle-
particle channel to be well defined at low energy. For a non-frustrated bipartite lattice, this
requirement is automatically met at \((\pi, \pi)\) point in the Brillouin Zone (this property is used to
show the SO(4) symmetry of the negative-U Hubbard model, which is the origin of the SO(5)
idea\cite{12}). For the non-bipartite triangular lattice, the two particle continuum never collapse
and SO(5) explanation dose not apply (it is easy to prove that the physical requirement of
collapse of the two particle continuum is equivalent to bipartite of the lattice for a general
tight binding Hamiltonian\cite{13}). Hence if we do detect resonant peak on triangular lattice,
it must be caused by some mechanism other than SO(5). In other words, the SO(5) idea is
not appropriate for a non-bipartite system.

Our starting point is the t-J model on a triangular lattice

\[ H = -t \sum_{<i,j>,\sigma} (\hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.}) + J \sum_{<i,j>} S_i \cdot S_j \]

here \(\hat{c}_{i,\sigma}\) is the constrained Fermion operator \(\sum_{\sigma} \hat{c}^\dagger_{i,\sigma} \hat{c}_{i,\sigma} \leq 1\). To treat such constraint
we work in the Slave Boson scheme. This scheme is convenient for the discussion of singlet
superconductivity (for triplet pairing this scheme is not convenient since the exchange term
is repulsive in the triplet channel). According to this scheme, we write \(\hat{c}_{i,\sigma} = f_{i,\sigma} b^\dagger_i\), in
which \(f_{i,\sigma}\) is the chargeless Fermionic spinon operator and \(b^\dagger_i\) is the spinless bosonic holon
operator. Then, we make the usual RVB mean-field decoupling (assuming uniform solution)
and arrive at the mean field Hamiltonian in the spinon sector (for simplicity we only consider
zero temperature and the holon is condensed in this case),

\[ H_{MF} = -tx \sum_{<i,j>,\sigma} (f^\dagger_{i,\sigma} f_{j,\sigma} + \text{h.c.}) - \frac{3J}{8} \sum_{<i,j>} (\chi_{i,j} f^\dagger_{i,\sigma} f_{j,\sigma} + \Delta_{i,j} f^\dagger_{i,\uparrow} f^\dagger_{j,\downarrow} + \text{h.c.}) - \mu \sum_{i,\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} \]

here \(x\) is the holon concentration, \(\chi_{i,j} = \langle f^\dagger_{j,\uparrow} f_{i,\uparrow} + f^\dagger_{j,\downarrow} f_{i,\downarrow} \rangle\) and \(\Delta_{i,j} = \langle f_{i,\downarrow} f_{j,\uparrow} + f_{j,\downarrow} f_{i,\uparrow} \rangle\)
are RVB order parameter, \(\mu\) is the chemical potential constraining the total Fermion number.
Symmetry consideration (rotational symmetry and the even parity of the singlet pairing)
shows that the pairing order parameter \(\Delta_{i,j}\) has only two solution: a \(d+i\bar{d}\)-wave solution and
a extended s-wave solution (the same conclusion is also reached by unconstrained Hartree-
Fock search\cite{4}). Since the s-wave solution is always higher in free energy, we neglect it. The
$d + id'$-wave solution is an analog of the d-wave solution on square lattice. That is, the pairing extend over only nearest neighbors, and a $\frac{2\pi}{z}$ rotation give to a $\frac{4\pi}{z}$ (or $-\frac{4\pi}{z}$) phase change, where $z$ is the coordinate number of the corresponding lattice ($z = 4$ for square lattice and $z = 6$ for triangular lattice). In square lattice case, such a pairing pattern is responsible for the appearance of the resonant peak at $(\pi, \pi)$. Similarly, we expect the triangular lattice can also support resonant peak but at a somewhat different momentum region in the Brillouin Zone.

We first solve the self-consistent equation for the RVB order parameter. In the triangular lattice, the particle-hole symmetry is broken and we solve for both hole doping ($t > 0$) and electron doping ($t < 0$) case. The result is shown in Figure 1. Here we present the result only for $|t|/J = 3$ (which is the value for the high temperature superconductors) since the exact value of this parameter is still unknown [4, 5]. In general, the doping range in which the $d + id'$-wave pairing order exists enlarge with decreasing $|t|/J$ value, with the qualitative features unchanged.

The calculation of the spin dynamics is straightforward. We first calculate the mean field susceptibility according to the BCS formula:

$$\chi_0(q, \omega) = \frac{1}{4} \sum_k (1 - \xi_k \xi_{q-k} + \text{Re}(\Delta_k \Delta^*_{q-k}))(\frac{1}{\omega + E_k + E_{q-k} + i\delta} - \frac{1}{\omega - E_k - E_{q-k} + i\delta})$$

here $\xi_k = -2(tx + \frac{3J}{8}\chi)(\cos(k_x) + 2\cos(\frac{k_x}{2})\cos(\sqrt{3}k_y)) - \mu$ is dispersion of the nearest-neighbouring hopping Hamiltonian on the triangular lattice, $\Delta_k = \frac{3\Delta}{4}(\cos(k_x) - \cos(\frac{k_x}{2})\cos(\sqrt{3}k_y)) + i\sqrt{3}\sin(\frac{k_x}{2})\sin(\sqrt{3}k_y)$ is the $d + id'$-wave pairing order parameter which is complex (time reversal symmetry is broken and there is staggered current loop flowing in the superconducting state around every elementary triangular plaquette). $E_k = \sqrt{\xi_k^2 + |\Delta_k|^2}$ is the energy of the BCS quasiparticle. $\delta$ is its inverse life time. $1 - \frac{\xi_k \xi_{q-k} + \text{Re}(\Delta_k \Delta^*_{q-k})}{E_k E_{q-k}}$ is the BCS coherence factor. In the square lattice case, since $\Delta_k = -\Delta_{q-k}$ for $q = (\pi, \pi)$, the BCS coherence factor reach their maximum value at $(\pi, \pi)$. However, for the non-bipartite triangular lattice, there is no such special momentum.

The bare susceptibility should be renormalized by the RPA correction. The correction is given by
$$\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - J(q)\chi_0(q, \omega)}$$

Here $J(q) = J(\cos(q_x) + 2\cos(\frac{q_x}{2})\cos(\frac{\sqrt{3}q_y}{2}))$ is the Fourier transform of the exchange interaction on the triangular lattice. In general, the momentum dependence of the dynamic spin susceptibility in the RPA-like theory is determined by the Fermi surface, pairing gap (which together determine the BCS coherence factor that embody the internal structure of Cooper pair) and the RPA renormalization factor $J(q)$ (which determine the classical spin ordering tendency). For $d$-wave pairing on square lattice near half filling, both the BCS coherence factor and the RPA renormalization factor are largest at $(\pi, \pi)$. For triangular lattice, $J(q)$ reach its maximum at $(\frac{4\pi}{3}, 0)$ and symmetry related points $((\pm\frac{4\pi}{3}, 0), (\pm\frac{2\pi}{3}, \pm\frac{2\sqrt{3}}{3}))$. At the same time, although $\Delta_k = -\Delta_{q-k}$ dose not hold true generally for any given $q$, calculation shows on average this condition is least violated at the same set of momentum as $J(q)$ dose. Hence we expect to see resonant peak around these set of momentum.

For square lattice, the RVB state is unstable with respect to RPA correction in a large doping range. Two facts are responsible for this instability. First, the system is bipartite and the Fermi surface is nearly nested. Second, the exchange term is unfrustrated on square lattice. To cure this problem, some author introduced a artificial reduction factor for the RPA correction \[10\]. For the non-bipartite triangular lattice, the single particle dispersion is almost isotropic around the Fermi surface close to half filling. At the same time, the exchange interaction is also frustrated. Hence we expect RPA correction to give much weaker modification to the phase diagram. Calculation shows for $|t|/J = 3$ the ordering instability occurs at about 2% doping for hole doping and at about 2.5% for electron doping (the ordering instability is indicated by the divergence of the static spin susceptibility. For both hole and electron doping the ordering instability occur near $(\frac{4\pi}{3}, 0)$ and symmetry related momentum which correspond to the classical 3-sublattice $120^0$ spin order). Hence, the RVB state is much more stable on triangular lattice than on square lattice due to the geometrical frustration. For this reason we do not need to introduce the reduction factor for the RPA correction.

We now present the result for the dynamic spin susceptibility. For $|t|/J = 3$, we find resonant peak below about 12% doping for hole doping and below about 7.5% for electron doping. Hence there is a large doping range in which the resonant peak can be
detected, especially for hole doping. The doping range in which resonant peak exists increases(decreases) with decreasing (increasing) $|t|/J$. Figure.2 show the energy dependence of the spin susceptibility at 5% doping. The momentum is taken at $(\frac{4\pi}{3}, 0)$. The dispersion of the resonant peak is somewhat complicate. In Figure 3, we show momentum scans of the dynamic spin susceptibility at various energy for 7% hole doping. The result can be summarized as follow (1)there is an optimal energy at which the spin susceptibility reach its maximum. Above this energy, the resonant peak appears at symmetric position on the $k_x$ axis (and symmetry related momentum in the Brillouin Zone). Below the optimal energy, the resonant peak split into two and disperse away from the $k_x$ axis. (2)The range of energy below the optimal energy in which resonant peak exists shrinks with decreasing doping and vanishes when ordering instability occurs. Hence the ordering instability always occurs on the $k_x$ axis. (3)There is no qualitative difference between electron doping and hole doping.

In the study of high temperature superconductivity, the origin of the resonant peak and its role in the low energy physics are hotly debated. In the RPA-like perspective, the resonant peak is a collective mode in the particle-hole channel whose long life time is understood in kinematic manner. The existence of this peak is a consequence of the superconducting pairing and its property depends on the detailed form of the pairing. At the same time, this resonant peak can couple to many other degree of freedom and make it visible in many other experiments such as ARPES, STM, and optical conductivity\[14, 15, 16\]. Another interesting perspective of the resonant peak is the SO(5) theory of high temperature superconductivity. In this perspective, the resonant peak is a Goldstone mode relating the d-wave superconducting order and the antiferromagnetic order. The stability of the mode is guaranteed by the SO(5) symmetry. In fact, the existence of this particle-particle-channel anti-bonding(since it is a spin triplet) collective mode is totally independent of superconductivity in the SO(5) theory. Superconductivity only make it visible in the spin channel and in this way providing a driving force for superconductivity itself. Since it is a Goldstone mode related with a symmetry, it is not expected that the mode to couple strongly with other degree of freedom. However, even with these big differences, it is still hard to decide which perspective is more appropriate for the high-Tc physics. Here we argue that the study on the non-bipartite triangular lattice may provide the opportunity to discriminate the two perspectives. This is because a bipartite lattice is a prerequisite for the existence of SO(5) symmetry and of well defined anti-bonding particle-particle collective
mode at low energy. Historically, the SO(5) symmetry and the particle-particle collective mode are extensions of the SO(4) symmetry and the corresponding η pair mode relating CDW order and s-wave superconducting order in the negative U Hubbard model. In that case, the existence of SO(4) symmetry and the η pair rely on the bipartite property of the lattice ($\xi_k + \xi_{(\pi,\pi,...)k} = const$). That is, the two particle continuum must collapse at $(\pi,\pi,...)$. More directly, it is this collapse of the two particle continuum that makes a well defined antibonding particle-particle collective mode possible at low energy (as we have mentioned, bipartite of the lattice is equivalent to collapse of the two particle continuum at some momentum in the Brillouin Zone). For the geometrically frustrated triangular lattice, the collapse of two particle continuum never occur and there is no room for antibonding particle-particle collective mode to be well defined at low energy. To see this, we plot the momentum dependence of the band width of the two particle continuum for both the square and the triangular lattice in Figure. 4. From this plot, we find that the bandwidth of the two particle continuum only vary mildly in the Brillouin Zone and never collapse to a point for the triangular lattice. According to our discussion, this means the SO(5) idea does not apply for such a geometrically frustrated system. Hence if we do detect resonant peak on a triangular lattice system, its origin must not be SO(5). Put it in another way, the SO(5) theory can only be defined on a bipartite lattice.

The authors would like to thank members of the HTS group at CASTU for discussion.

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FIGURES

FIG. 1. Doping dependence of the $d + id'$-wave pairing order parameter for both electron and hole doping.

FIG. 2. Imaginary part of the dynamic spin susceptibility at $(\frac{4\pi}{a}, 0)$ for 5 lines are the bare and the RPA-corrected results.

FIG. 3. Momentum scans of the dynamic spin susceptibility at various energy for 7% hole doping. (a) $\omega = 0.39J$, (b) $\omega = 0.40J$, (c) $\omega = 0.405J$, (d) $\omega = 0.41J$, (e) $\omega = 0.415J$, (f) $\omega = 0.42J$, (g) $\omega = 0.425J$, (h) $\omega = 0.43J$. The maximum of the dynamic spin susceptibility occurs at $\omega = 0.415J$ at this doping rate.

FIG. 4. Momentum dependence of reduced band width of the two particle continuum for (a) the bipartite square lattice, (b) the non-bipartite triangular lattice.
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