Spin-roton excitations in the cuprate superconductors

J. W. Mei and Z. Y. Weng
Institute for Advanced Study, Tsinghua University, Beijing, 100084, China

(Dated: September 30, 2009)

We identify a new kind of elementary excitations, spin-rotons, in the doped Mott insulator. They play a central role in deciding the superconducting transition temperature $T_c$, resulting in a simple $T_c$ formula, $k_B T_c \simeq E_g/\kappa$, with $E_g$ as the characteristic energy scale of the spin rotons. We show that the degenerate $S = 1$ and $S = 0$ rotons can be probed by neutron scattering and Raman scattering measurements, respectively, in good agreement with the magnetic Raman mode and the Raman $A_{1g}$ mode observed in the high-$T_c$ cuprates.

PACS numbers: 74.20.Mn, 71.10.Hf, 71.10.Li

I. INTRODUCTION

To fully understand the nature of high-$T_c$ superconductivity in the cuprates, one essential task is to identify the most important elementary excitation which controls the superconducting transition. In a conventional BCS superconductor, the Bogoliubov quasiparticle constitutes the most crucial low-lying excitation. In a d-wave state, nodal quasiparticle excitations generally lead to a linear-temperature reduction of the superfluid stiffness $\rho_s$ by

$$\rho_s(T) = \rho_s(0) - aT$$

which, however, would be normally extrapolated to a transition temperature ($\rho_s(T_c) = 0$) much higher than the factual $T_c$ in the cuprates, based on the microwave measurements of the penetration depth which determines the superfluid density.

On the other hand, in view of the small superfluid density in the cuprates, which are widely considered to be a doped Mott insulator, the phase fluctuation of the superconducting order parameter has been suggested to play an important role in the transition regime, which can be characterized by the following London action

$$L = \frac{\rho_s}{2} \int d^2 r (\nabla \phi + q A^e)^2$$

where $\phi$ specifies the $U(1)$ phase of the order parameter of condensate carrying charge $q$, and $A^e$ is the external electromagnetic field. In this point of view, the superconducting transition is of a Kosterlitz-Thouless (KT) type with the proliferation of topological vortices

$$\int d^2 r \cdot \nabla \phi = \pm 2\pi$$

which destroy the phase coherence of superconductivity resulting in $k_B T_c \simeq \rho_s(T_c)$.

However, a striking and puzzling empirical $T_c$ formula for the cuprate superconductors has been known experimentally, which is simply given by

$$k_B T_c = \frac{E_g}{\kappa}$$

where $\kappa \sim 6$ and $E_g$ denotes the characteristic energy scales observed in inelastic neutron scattering (INS) and electronic Raman scattering (ERS) experiments versus the superconducting transition temperature $T_c$ for the high-$T_c$ cuprates. The straight line shows the empirical formula, which will be derived in the present work. Here the solid squares represent the INS resonance mode, with different colors indicating different families including hole-doped Y123, Bi2212, Tl2201 and Hg1201, and electron doped Fr0.88LaCe0.12CuO4, the solid circles represent the ERS $A_{1g}$ mode, including the hole-doped Y123, Bi2212, Tl2201, Hg1201, La214, and the electron doped NCCO compound.

FIG. 1: [Color online] The characteristic energies observed by inelastic neutron scattering (INS) and electron Raman scattering (ERS) experiments versus the superconducting transition temperature $T_c$ for the high-$T_c$ cuprates. The straight line shows the empirical formula, which will be derived in the present work. Here the solid squares represent the INS resonance mode, with different colors indicating different families including hole-doped Y123, Bi2212, Tl2201 and Hg1201, and electron doped Fr0.88LaCe0.12CuO4, the solid circles represent the ERS $A_{1g}$ mode, including the hole-doped Y123, Bi2212, Tl2201, Hg1201, La214, and the electron doped NCCO compound.
cessible by ERS than INS, including the La$_{2-x}$Sr$_x$CuO$_4$ compound in which there is no direct INS evidence for a sharp resonancelike mode but a singlet mode in ERS$^{24}$, has been still found with $E_g$ well fit by (4). The above empirical scaling law of $T_c$ vs. $E_g$ implies that the elementary excitations controlling the superconducting transition in the cuprates should be composed of two degenerate modes, with quantum number $S = 0$ and 1, respectively, as proved in ERS and INS. Note that in the literature the magnetic resonancelike mode observed in INS has been sometimes interpreted as the bound state of a Bogoliubov quasiparticle pair near the antinodal regime due to the residual superexchange interaction$^{11}$. In this picture it would be hard to understand the necessity for the existence of a singlet bound state with the roughly degenerate energy. The further challenging and fundamental question is, given the presence of two degenerate modes observed in ERS and INS, how can they directly influence the superconducting coherence?

A proposal made by Uemura$^{11}$ recently is that the two quasi-degenerate modes observed in INS and ERS may originate from soft modes in spin and charge channels in an incommensurate stripe state, which are called$^{11}$ twin spin/charge roton mode, in analogy with the soft phonon-roton mode towards solidification in superfluid $^4$He. Hence the mechanism for superconducting transition is due to the substantial reduction of the superfluid density by thermal excitations of such twin spin-charge soft mode at $T_c/2 < T < T_c$, whereas the quasiparticle excitations mainly dominate at lower temperature $< T_c/2$.

Nevertheless, according to the experimental results shown in Fig. 1, it seems that the $T_c$ formula (4) holds more generally than simply in a neighborhood of stripe states$^{29}$. It calls for an intrinsic “spin-charge entanglement” in the superconducting phase of the cuprates. Namely, magnetic excitations at $Q_{AF}$ should have some kind of profound effect on the superconducting condensation such that thermal excitations of the former can be destructive to the latter, much more effective than the usual nodal quasiparticles in the BCS theory. Furthermore, the mechanism should allow for a degenerate singlet mode, which may be not associated with a soft mode of any charge order as its characteristic momentum is around $Q_0$, to play an equally important role. Lastly, the simple scaling relation (4) with a universal $\kappa$ should be independent of the details of materials including the charge inhomogeneity. Or more precisely, all the detailed properties of the system should influence $T_c$ mainly through the characteristic energy scale $E_g$.

In this paper, we will demonstrate that a self-consistent mathematical description of superconductivity in doped Mott insulators can give rise to a systematic account for the above-mentioned novel properties including the $T_c$ formula (4). In the superconducting state, besides the emergent quasiparticles as the recombination of charge and spin, the most nontrivial elementary excitations are the vortex-antivortex bound pairs locking with free spins at the poles, with total spin $S = 0$ or 1, as illustrated in Fig. 2. We shall call these excitations spin-rotons in the following, which are distinguished from those proposed by Uemura$^{11}$ as they are not slaved with any charge and spin orders, but a direct consequence of the phase string effect$^{30,31}$ in the $t$-$J$ model with a peculiar nonlocal spin-charge entanglement: neutral spins locking with charge supercurrent$^{32,33}$.

These spin-rotons will naturally include two degenerate excitations. The degeneracy of these modes with spin quantum number $S = 0$ and 1 is due to the fact that the pair of neutral spins are excited “spinons” from an underlying resonating-valence-bond (RVB) spin background. The degenerate spin-roton modes thus indicate spin-charge separation, but with a twist. That is, a stable spin-roton object in the superconducting phase also implies a spinon-confinement as two spinons cannot be separated freely in space due to the logarithmic potential between the vortex and antivortex. Such rotonlike supercurrents will play a central role in deciding the superconducting phase coherence transition as in (4). We shall show that the singlet and triplet spin-rotons can be indeed directly probed by ERS in A$_{1g}$ channel at $Q_0$ and INS near $Q_{AF}$. They have the minimal characteristic energy $E_g \sim \delta J$ in the low-doping regime with the magnitude in good agreement with the experimental data where $\delta$ denotes the doping concentration and $J$ is the superexchange coupling constant determined in the undoped case.

The remainder of the paper is arranged as follows. In Sec. II A, we introduce the description of a doped-Mott-insulator superconductor, obtained previously$^{32,33}$ based on the phase string theory$^{30,31}$ of the $t$-$J$ model, by using a phenomenological construction. We argue that in order to incorporate the influence of spin degrees of freedom (which is important in a lightly doped Mott insulator where spins constitute the majority of low-lying degrees of freedom) under the requirement of no time-reversal and spin rotational symmetry breakings, one is naturally
led to a modified action for superconductivity. In Sec. 11B, the spin-roton excitations as a direct consequence of this formulation are discussed. Then, how the spin-roton excitations as the resonancelike modes can be probed by INS and ERS are discussed. In Sec. 11C, the $T_c$ formula determined by the spin-roton excitations is obtained. Finally, in Sec. 11D, a general discussion will be given.

II. SPIN-ROTON EXCITATIONS

A. Phenomenological description of a doped-Mott-insulator superconductor

From a doped Mott insulator point of view, the superconductivity in the cuprates occurs in a small doping regime where the charge carrier number is greatly reduced as compared to the total electron number. Namely, the strong on-site Coulomb interaction will make the charge degrees of freedom partially frozen, while the full spin degrees of freedom of the electrons remain at low energy. Thus the London action in order to properly reflect the Mott physics.

For example, in the U(1) slave-boson gauge theory description, the charge carriers are described by spinless bosons known as holons. The superconducting state corresponds to the Bose condensation of the holons, with replaced by

$$ L_h = \frac{\rho_s}{2} \int d^2 r (\nabla \phi + A^s + eA^c)^2 $$

where $\rho_s$ is proportional to the density of condensed holons and $q = +e$, in contrast to the conventional London action where the condensate of Cooper pairs of the electrons is involved with $q = -2e$. As a component of the electron fractionalization, holons are no longer gauge neutral and are generally coupled to an internal emergent gauge field $A^s$. In the U(1) slave-boson gauge theory, $A^s$ will be also minimally coupled to the other component of the electron fractionalization, i.e., neutral spins called spinons. However, since the latter are in RVB pairing, the internal gauge field $A^s$ is expected to be suppressed due to the “Meissner effect” of the RVB state, whose mean-field transition temperature is presumably much higher at low doping. Consequently in such a mean-field “pseudogap” regime $A^s$ gains a mass and cannot play a role as a new source to effectively reduce $T_c$.

However, the U(1) slave-boson gauge theory is not the only possible theoretical description for the doped Mott insulator. In the following, we shall elucidate in a phenomenological way an alternative self-consistent construction. It will reveal the existence of a new mathematical structure, in which the charge condensate can become strongly correlated with spin excitations.

The key distinction will be that, instead of minimally coupling to both the holon and spinon currents in the U(1) slave-boson gauge theory, here $A^s$ will only minimally couple to the holon matter field as given in [3], not to spinon currents. Instead its strength will be generated from the spinon matter field according to the following gauge-invariant relation

$$ \oint_c d r \cdot A^s(r) = \phi_0 \int_{S_c} d^2 r \left[ n^1_s(r) - n^{\uparrow}_s(r) \right] $$

Here the flux of $A^s$ within an arbitrary loop $c$ on the left-hand-side (l.h.s.) is contributed by $\pm \phi_0$ flux-tubes bound to individual spinons on the right-hand-side (r.h.s.), with $n^1_s(r)$ denoting the local density of spinons where the integration runs over the area $S_c$ enclosed by $c$.

Due to the sign change between the $\uparrow$ and $\downarrow$ spins on the r.h.s. of (6), $A^s(r)$ will explicitly preserve the time-reversal (TR) symmetry, as $\uparrow \leftrightarrow \downarrow$ under the TR transformation. This is in contrast to a conventional electromagnetic vector potential $A^e$, which breaks the TR symmetry. However, since the path $c$ is oriented, the spin rotational symmetry may be broken for a general flux $\phi_0$. But under a specific choice

$$ \phi_0 = \pi $$

one finds that the spin rotational symmetry can be still maintained: without loss of generality, one can consider a loop $c$ which encloses a single spin such that $\oint_c d r \cdot A^s = \pm \phi_0 = \pm \pi$ which is still spin-dependent.

According to a general argument given by Haldane and Wu, since a spinon behaves like a supercurrent vortex, its motion through a closed path $c$ must then pick up a Berry’s phase which is determined by the number of superfluid particles of the condensate in the area $S_c$.
enclosed by $c$, as if it sees an effective “magnetic-field” described by a vector potential $A^h$:  

$$
\Delta \Phi_{\text{Berry}}(c) = \phi_0 \int_{\Sigma_c} d^2 \mathbf{r} \ \rho_h(\mathbf{r}) 
= \int_c d\mathbf{r} \cdot \mathbf{A}^h(\mathbf{r})
$$

where $\rho_h(\mathbf{r})$ denotes the local superfluid density of condensed holons, with $\phi_0 = \pi$ instead of $2\pi$.

Thus, one may write down a minimal gauge-invariant Hamiltonian for spinons simply as

$$
H_s = -J_s \sum_{\langle ij \rangle > \sigma} b_{i\sigma}^\dagger b_{j\sigma} e^{i \sigma A^h_{ij}} + \text{h.c.} 
$$

where $b_{i\sigma}^\dagger$ defines the bosonic creation operator for a spinon at site $i$ with a spin index $\sigma$. Here $A^h_{ij}$ is the lattice version of the gauge potential $A^h(\mathbf{r})$ introduced in [3] and the sign $\sigma$ in front of the gauge phase in (10) will ensure the TR invariance.

Although one can alternatively write down an effective model with the hopping term $b_{i\sigma}^\dagger b_{j\sigma} e^{i \sigma A^h_{ij}}$ replacing the RVB pairing term $b_{i\sigma}^\dagger b_{j\neg\sigma} e^{i \sigma A^h_{ij}}$ in (10), without breaking the gauge and TR symmetries, (10) is physically more meaningful because in the ground state spinons will be all paired up with $b_{i\sigma}^\dagger b_{j\neg\sigma} e^{i \sigma A^h_{ij}} \equiv \Delta^s/2 \neq 0$ which automatically satisfies the spinon-confinement requirement to ensure superconducting phase coherence as to be discussed below. Furthermore, $\frac{1}{\hbar} \int d\mathbf{r} \cdot \mathbf{A}^h = 0$ at half-filling, where $H_s$ (10) reduces to the Schwinger-boson mean-field Hamiltonian which well captures the antiferromagnetic (AF) correlations including the long-range AF order at $T = 0$.

Therefore, the London action [2] for superconductivity has been phenomenologically modified for the doped Mott insulator in [3]. Here the charge condensate will be generally coupled to neutral spin excitations, ubiquitously presented in a doped Mott insulator governed by (10), via an emergent topological gauge field [3]. Such a self-consistent description based on [3], [3], [3] and (10) can be justified in the phase string theory of the $t$-$J$ model, with the superfluid stiffness $\rho_s \equiv \rho_n/m_h$ ($m_h$ is the effective mass for holons) and effective coupling constant $J_s$ in (10) determined microscopically. One is referred to Ref. [33] and the references therein for details. Although it is not a unique construction for a doped Mott insulator (one can alternatively have other possible mathematical constructions like the $U(1)$ slave-boson gauge theory description for example, as mentioned before), some very unique consequences will follow from such a self-consistent approach, which can be directly compared with experiments.

### B. Spin-roton excitations

A direct physical consequence is that a single spinon excitation in the superconducting state will not be permitted because the self energy of a vortex shown in Fig. 3 is logarithmically divergent. Then all the spinons in the superconducting state must appear in pairs, with the associated supercurrent vortices forming vortex-antivortex bound pairs, as illustrated in Fig. 2. These bound objects are referred to as spin-rotons, which carry total spin 0 (singlet) and 1 (triplet), charge 0, together with a supercurrent structure analogous to a two-dimensional roton excitation in a Bose condensate. In this sense, the spinons must be “confined” and only integer spin excitations are allowed in the superconducting state.

#### 1. Resonance-like characteristic energy $E_g$

The spinon Hamiltonian (10) can be easily diagonalized under the condition that the holons are uniformly condensed with $\rho_n = \delta a^{-2}$ (a is the lattice constant) as outlined in Appendix A. The solution of (10) has an uneven Landau-level-like spectrum for spinon excitations as shown in the inset of Fig. 4, which are excited by breaking up RVB pairs in the ground state.

At low temperature, we shall focus on the lowest excited level at $E_g = E_g/2$ for simplicity. In the main panel of Fig. 4, $E_g = 2E_s$ is shown as a function of doping under a proper consideration of the doping dependence of $J_s^{38}$. The corresponding spinon wavepacket looks like

$$
|w_{ns}(\mathbf{r}_1)|^2 \simeq \frac{a^2}{2\pi \alpha_c^2} \exp \left\{ - \frac{|\mathbf{r}_1 - \mathbf{R}_m|^2}{2\alpha_c^2} \right\}
$$

with a “cyclotron length” $\alpha_c \equiv a/\sqrt{\pi \delta}$. Namely, the lowest spinon excitations governed by (10) are non-propagating modes of an intrinsic size in order of $\alpha_c$. 

**FIG. 3:** [Color online] Schematic illustration of single spinon-vortices. An isolated neutral spin (spinon) in the superconducting state will always induce a vortexlike supercurrent response from the charge condensate according to the generalized London action [5]. Notice that the vorticity sign of the vortex is actually independent of the spin orientation as long as $\phi_0 = \pi$ in [4], which preserves the spin rotational symmetry.
Here the degenerate levels are labeled by the coordinates \( \mathbf{R}_m \), the centers of the spinon wavepacket, which form a von Neumann lattice with a lattice constant \( \xi_0 = \sqrt{2\pi a_c} \), as shown in Fig. 5.

After integration over the original lattice index \( r_i \) in the modified London action \( (5) \) at \( A^e = 0 \), one can obtain (see Appendix [13]) an effective interaction term for spinon-vortices on the von Neumann lattice

\[
U_{\text{int}} = -\frac{\pi}{4} \rho_s \sum_{\mathbf{R}_m, \mathbf{R}_m'} \ln \frac{|\mathbf{R}_m - \mathbf{R}_m'|}{\xi_0} q_m q_{m'} \tag{12}
\]

where \( q_m \) (\( = \pm 1 \) or 0) denotes the vorticity for each spinon-vortex on the site \( \mathbf{R}_m \), and to avoid the logarithmic divergence, the neutral constraint \( \sum_m q_m = 0 \) will be imposed. So the total energy of the spinon-vortices is given by

\[
H_v = \frac{E_g}{2} \sum_m |q_m| + U_{\text{int}}. \tag{13}
\]

It is noted that there is a four-fold degeneracy, \( g = 4 \), at each site \( \mathbf{R}_m \) as mentioned in the caption of Fig. 5.

Note that a conventional vortex-antivortex pair in a KT system will normally shrink at low temperature and be annihilated in the ground state. But a spin-roton in the present case cannot literally disappear in the ground state because the two spins sitting at the poles of a roton in Fig. 2 cannot annihilate each other. Nevertheless, the roton supercurrents surrounding the neutral spins will have minimal effect on the ground state. In fact, as the solution of (10), spins will form short-range RVB pairs in the ground state, of a characteristic length scale \( \sim a_c \), which is comparable to the finite core size of each pole of a spin-roton in Fig. 2 (the spin trapped at the core cannot sit still due to the uncertainty principle and the intrinsic core size is set by the cyclotron length \( a_c \)). Thus, the surrounding rotonlike supercurrents around an RVB pair will be effectively canceled out in the ground state. In other words, the London action \( (5) \) will be decoupled from the neutral RVB spin background as \( A^e \approx 0 \) and the excited spinon-vortices are effectively described by (13).

Hence the spin-roton structure shown in Fig. 2 will emerge as the bound pair of the excited spinons, which of are of spin triplet \( (S = 1) \) and singlet \( (S = 0) \), respectively, and \emph{degenerate} in energy. The spin-rotons here will have a minimal energy scale \( E_g \) when two excited spinons are located at the same von Neumann lattice site such that the vortex-antivortex supercurrent structure is effectively annihilated with \( U_{\text{int}} = 0 \).

The degenerate singlet and triplet spin-rotons imply the spin-charge separation: i.e., the existence of single spinons carrying \( S = 1/2 \) and zero charge as individual excitations, which do not interact with each other \emph{magnetically}. However, we have also seen that these spinons must be confined \emph{spatially} in pairs, appearing at the poles of roton supercurrent structure and subjected to logarithmic attraction \( U_{\text{int}} \). Therefore, in such a non-BCS superconducting state the spin-charge separation has a twist, which is characterized by new elementary excitations of degenerate spin-rotons instead of individual spinons. In other words, the spinon confinement does not mean a spin-charge tight recombination like in a conventional Fermi liquid or BCS superconductor of the electrons. Rather, at a short distance scale \( \sim \xi_0 \), the confining force \( U_{\text{int}} \) becomes negligible and the spinons are still “asymptotically free”.

2. \textit{INS and ERS probes}

Experimentally, the neutron and Raman scattering measurements can provide direct means to probe such
novel excitations, in spin triplet and singlet channels, respectively.

Define the spin-spin correlation function

\[ \chi_{zz}(\tau, r_i - r_j) = -\langle T_\tau S^z_i(\tau) S^z_j(0) \rangle \]  

(14)

where \( \tau \) denotes the imaginary time, \( S^z_i = \frac{1}{2} \sum_\sigma \sigma_i \) and \( h.c. \). Similarly a density-density correlation function which can be detected by the electron Raman scattering is defined as follows

\[ \chi_{\text{ERS}} = -\langle T_\tau \tau_{A_{1g}}(\tau) \tau_{A_{1g}}(0) \rangle \]  

(15)

where the \( A_{1g} \) density operator \( \tau_{A_{1g}} = -\frac{1}{2} \sum_{\langle i,j \rangle, \sigma} c_i^{\dagger} c_j + h.c. \). Here \( c_i^{\dagger} \) is the electron operator whose relation with the holon and spinon operators is given in Appendix A.

Based on the Bogolimbobb transformation and the phase string representation for the electron operators, one can express \( S^z_i \) and \( \tau_{A_{1g}} \) in terms of \( \gamma^{m}_{\sigma} \) and \( \gamma^{m}_{\sigma} \) as shown in Appendix A. We shall mainly concentrate on energies near the minimal \( E_g \), where the total Hamiltonian reduces to \( H_\text{int} \) in which the interaction term \( H_\text{int} \) can be also neglected because \( S^z_i \) and \( \tau_{A_{1g}} \) only create a pair of spinons locally within a von Neumann lattice site (Fig. 5):

\[ S^z_i \sim -\frac{1}{2} \sum_{m,n,\sigma} u_m v_n w^*_m(a_i) w_n(a_i) \gamma^m_{\sigma} \gamma^{n}_{\sigma} + h.c. \]  

(16)

and

\[ \tau_{A_{1g}} \sim -\delta \sum_{m,n} u_m v_n \gamma^{m}_{\sigma} \gamma^{n}_{\sigma} + h.c. \]  

(17)

where \( u_m v_n \) is the coherent factor due to the R VB paring, with \( m \) and \( n \) denoting the degenerate lowest energy states shown in the inset of Fig. 4 with the degenerate \( E_m = E_s \).

It is straightforward to obtain

\[ \chi_{zz}(\tau) = -D(-1)^e \exp \left( -\frac{T}{T_c} e^{-E_g \tau} \right) \]  

(18)

and

\[ \chi_{\text{ERS}}(\tau) \simeq -\delta D e^{-E_g \tau} \]  

(19)

with \( D = \frac{\delta^2}{2a_c^2} \) is the spectral weight whose doping dependence is shown in Fig. 6. In \( \chi_{zz} \) we have used the relation

\[ \sum_m w^*_m(a_i) w_n(a_i) = \frac{1}{2a_c^2} \frac{e^{-r_i \sqrt{m-n \pi}}}{r_i} \]  

Correspondingly the dynamic spin susceptibility is obtained by

\[ \chi''_{zz}(q, \omega) = \frac{2a_c^2}{\pi} D e^{-2\delta^2 q^2 E_g^2} \delta(\omega - E_g) \]  

(20)

and the \( A_{1g} \) Raman scattering cross-section

\[ I_{\text{ERS}}(\omega) \propto \chi''_{\text{ERS}}(\omega) \simeq \delta D \delta(\omega - E_g) \]  

(21)

So the triplet spin-roton will appear as a resonancelike mode in \( \chi''_{zz}(q, \omega) \) at \( \omega = E_g \), with momentum \( q \) peaked at the AF wavevector \( q_{AF} \) and a width inversely proportional to the RVB pairing size \( a_c \), which thus determines the spin-spin correlation length \( \propto a_c/\sqrt{\delta} \). Similarly, in \( I_{\text{ERS}}(\omega) \) a "resonance mode" at \( E_g \) will also be exhibited, which corresponds to the singlet spin-roton excitation. It should be emphasized that in the neutron and Raman scattering measurements only local spinons at the same von Neumann lattice are involved and the correction from the logarithmic potential \( U_\text{int} \) is always negligible. Of course, high-energy spin-roton excitations can be also detected by these experiments at \( \omega > E_g \), which will involve spinons at higher energy levels shown in the inset of Fig. 6 whose effect will not be considered in the present work for simplicity.

At half-filling, the minimal roton energy will be softened to zero: i.e., \( E_g = 0 \) with \( a_c \to \infty \). As shown in Fig. 6 the spectral weight \( D \) in (20) remains finite at \( \delta \to 0 \) and characterizes the weight of the Néel order as the triplet rotons at \( E_g = 0 \) are condensed into the AF ordering. By contrast, \( I_{\text{ERS}}(\omega) = 0 \) in this limit as there is no more charge density fluctuation to couple with the incident light in the Raman scattering measurement. Furthermore, high-energy triplet spin-roton excitation is expected to be reduced to the gapless spin wave at \( \delta \to 0 \) with the spinon spectrum shown in the inset of Fig. 6 becomes a continuous energy spectrum described by the Schwinger boson mean-field theory.

\[ C. \quad T_c \text{ formula} \]

We now discuss how thermally excited spin-rotons can effectively destroy the phase coherence of the superconducting condensation and determine the transition temperature \( T_c \).

The long-wavelength superfluid stiffness \( \rho_s \) will be
renormalized by spin-roton excitations via the internal gauge field $A^z$ in the London action (5). Such spin-rotons shown in Fig. 2 resemble the conventional vortex-antivortex pairs in the $XY$ model, except that the unit vorticity of each spinon-vortex is $\pi$ instead of $2\pi$ of a conventional vortex. A further difference is that the low-energy spinon-vortices will distribute on a von Neumann lattice with the degeneracy $g = 4$ as illustrated in Fig. 3 instead of $g = 1$ on the original lattice in the $XY$ model. Corresponding to the minimal energy $E_g$ of a spin-roton, the fugacity is $y = e^{-E_g/2k_BT}$ as each spinon effectively contributes to a core energy $E_g/2$. Compared to the $XY$ model, such a vortex core energy is much cheaper as $E_g \sim \delta J$ at low doping. Thus, the superconducting phase transition controlled by spin-rotons, which are governed by $H_s$ in (13), is found by averaging over the spin-roton excitations governed by (14), is expected to be similar to a conventional vortex in the $XY$ model. A further difference is that the low-$K$ $K_{0v}$, is obtained by averaging over the spin-roton excitations governed by (14), is found by

$$K_R = K + \frac{\pi^2 K^2}{4N a^2 g^2} \sum_{R_m R_m'} (R_m - R_m')^2 \langle q_{m q_{m'}} \rangle $$

(22)

where $N$ is the original total lattice number. The correlation $\langle q_{m q_{m'}} \rangle$ can be easily evaluated in terms of (13) to lowest order in fugacity $y^{(1)}$:

$$\langle q_{m q_{m'}} \rangle = -2y^2 |R_m - R_m'|/\xi_0 \sim 8K$$

(23)

such that

$$K_R = K - g^2 \pi^3 y^2 K^2 \int_0^\infty \frac{dR}{\xi_0} \left( \frac{R}{\xi_0} \right)^3 \sim 8K$$

(24)

where the lattice constant $\xi_0$ of the von Neumann lattice provides the short distance cutoff. Again following the steps in Ref. 41, one arrives at differential renormalization group (RG) equations

$$\frac{dK^{-1}}{dt} = g^2 \pi^3 y^2 + O(y^4)$$

(25)

$$\frac{dy}{dt} = \left( 2 - \frac{\pi}{4} K \right) y + O(y^3)$$

(26)

with $K_R = K_{R}^{(1)}[l, y(l)]$ remaining as a constant, which results in the fixed point at $K^* = 8/\pi$ and $y^* = 0$.

Thus, by substituting $K_R = \lim_{l \rightarrow \infty} K(l) = K^*$ into (24), one gets

$$\frac{8}{\pi} = \frac{\rho_{s}}{k_BT_c} + g^2 \pi^3 y^2 \left( 4 - \frac{\pi}{4} \frac{\rho_{s}}{k_BT_c} \right)$$

(27)

\[\text{FIG. 7: [Color online] The coefficient $\kappa$ defined in (28) is calculated at some typical values of the parameter: $t_h/J = 2$ and 3, and is weakly doping dependent around $\kappa = 6$.} \]

with $y^2 = e^{-E_g/k_BT_c}$, which can be further rewritten as

$$y^2 = \frac{1}{2\pi^2 g^2} \left( 1 - \frac{8}{n^2 \pi} \frac{k_BT_c}{\rho_s} \right)^2$$

(28)

in which $n\pi$ with $n = 1$ denotes the unit vorticity of the vortex. (For the sake of comparison, we have introduced $n$ in (28) such that the case of $n = 2$ is also allowed which corresponds to the conventional $2\pi$ vortex in the $XY$ model.) Equation (28) indicates that the rigidity of the superconducting state can only sustain the amount of vortex-antivortex pairs with $y^2 \leq \frac{1}{2\pi^2 g^2}$. Using $n = 1$ and $g = 4$, one finally finds

$$\frac{E_g}{k_BT_c} = 2 \ln \frac{4\sqrt{2}\pi}{1 - \frac{8n^2 k_BT_c}{\pi \rho_s}} \approx \kappa$$

(29)

which at $k_BT_c \ll \pi \rho_s/8$ results in

$$\kappa \approx 2 \ln 4\sqrt{7}\pi = 5.76$$

(30)

Generally, $\kappa$ can be determined self-consistently according to (29) with using $m_h = 1/(2t_h a^2)$ and $E_g(\delta)$ presented in Fig. 4. The result is shown in Fig. 7 as a function of doping concentration $\delta$ at $t_h = 2J$ and $t_h = 3J$, respectively. Fig. 7 indicates that the value of $\kappa$ is roughly a universal value at 6 which is weakly dependent on the choice of $t_h$ as well as the doping concentration. So we obtain the $T_c$ formula (4), which is in excellent agreement with the high-$T_c$ cuprates as shown by the straightline in Fig. 1. It is noted that $y^2 = e^{-\kappa} < 1$ is consistent with the small fugacity condition used in the above derivation of the RG equations. Finally, we comment that in a previous more complicated approach, $T_c$ was calculated without properly considering both the singlet and triplet spin-roton excitations, which resulted in somewhat higher and non-universal value of $T_c$. 

III. DISCUSSION

In this work, we have proposed a consistent understanding of some intriguing experimental facts concerning high-$T_c$ superconductivity in the cuprates. The key concept is the presence of a new type of elementary excitations in the superconducting state, i.e., spin-rotons, in addition to conventional nodal quasiparticle excitations. Such novel modes are composed of supercurrent vortex-antivortex pairs (rotons) locking with free spins at the two poles, which form degenerate spin singlet and triplet spin states. We have found that they are indeed measurable by ERS in the $A_{1g}$ channel and INS at the AF wavevector as resonancelike modes, which are consistent with the experimental observations. In particular, we have shown that it is this new kind of excitation that determines superconducting phase coherence transition with $T_c \propto E_g$ in $\Omega$, in excellent agreement with the cuprate superconductors. It should be noted that the $A_{1g}$ peak has also been probed in the resonant electronic Raman scattering experiment. Similarly, the resonant inelastic X-ray scattering (RIXS) should be also able to detect such a singlet spin-roton excitation if a higher resolution ($\leq 40\text{meV}$) can be achieved.

So the “resonance energy” $E_g$ as the characteristic energy scale of these spin-roton excitations will play an important role in the superconducting phase, in contrast to the BCS theory in which quasiparticle excitations dominate. To leading order approximation, $E_g$ vs. doping in Fig. 4 will decide the phase diagram of superconductivity. Here $E_g$ (thus $T_c$) vanishes at overdoping because the underlying RVB pairing $\Delta^s \equiv \sum_{\sigma} \langle b^\dagger_{i\sigma} b^\dagger_{j\bar{\sigma}} e^{i\sigma A_{ij}} \rangle = \Omega^\dagger$, while $E_g$ vanishes at $\delta = 0$ where the spin-rovers experience Bose condensation to form an AF Néel order at $T = 0$. The phase above $T_c$ will be full of free spinon-vortices known as the spontaneous vortex phase, which may explain the Nernst regime discovered.

Below $x_c$, either an AF spin glass state or charge stripe phases has been shown to be competitive before the system becomes a commensurate AF ordered state near the half-filling.

Furthermore, there is no physical reason to protect the degeneracy of singlet and triplet spin-roton excitations as $E_g \rightarrow 0$. In other words, the residual interaction may decide which mode will be softened more quickly to result in a competing charge or spin order at low doping, as conjectured in Refs. 11 and 48. The bottomline here is that the spin-roton excitations are expected to be essential in describing the quantum phase transition of superconductivity to other low-doping phases at $T = 0$. Detail investigation along this line is beyond our current scope and will be discussed elsewhere.

Acknowledgments

We acknowledge helpful discussions with P. W. Anderson, D. H. Lee, P. A. Lee, T. Li, N. P. Ong, T. Senthil, and X. G. Wen. This work is supported by the NSFC grant nos. 10688401, 10834003 and the National Program for Basic Research of MOST grant no. 2009CB929402.

APPENDIX A: DIAGNOLIZATIONS OF $H_s$ (10)

The spinon Hamiltonian $H_s$ (10) can be easily diagonalized under a uniform distribution of the holon condensate $\rho_h = \delta a^{-2}$. To be self-contained, in the following we briefly outline the main results.

By using the Bogoliubov transformation

$$b_\sigma (r) = \sum_m (u_m \gamma_{m\sigma} - v_m \gamma_{m\bar{\sigma}}) w_{m\sigma} (r)$$

we obtain the spinon Hamiltonian $H_s$ as follows

$$H_s = \sum_{m\sigma} E_m \gamma_{m\sigma} \gamma_{m\bar{\sigma}} + \text{const.}$$

where

$$u_m = \frac{1}{\sqrt{2}} \sqrt{\frac{\lambda}{E_m}} + 1, \quad v_m = \text{sgn}(\xi_m) \frac{1}{\sqrt{2}} \sqrt{\frac{\lambda}{E_m}} - 1$$

and

$$E_m = \sqrt{\lambda^2 - c_m^2}$$

Here the quantum number $m$ denotes an eigen-state $w_{m\sigma} (r_1)$ with the eigen-value $\xi_m$.

The spinon excitation spectrum (A4) exhibits an uneven Landau-level-like form as shown in the inset of Fig. 4. To obtain this spectrum, we have used a self-consistent condition for $J_s = J(1 - 4\delta)/(2\sqrt{A})$ and the chemical potential $\Lambda$ in $E_m$ by enforcing $\sum_{\sigma} b^\dagger_{i\sigma} b_{i\bar{\sigma}} = (1 - \delta)N$.

Focusing on the lowest energy level $E_s = E_g/2$, the corresponding wave package as the solution of (A5) can be express as

$$O_m (r_i) = |w_{m\sigma} (r_i)|^2 \simeq \frac{a^2}{2\pi a_c^2} \exp \left\{ -\frac{1}{2a_c^2} |r_i - R_m|^2 \right\}$$

with the degenerate states labeled by the site $R_m$ in a von Neumann lattice shown in Fig. 4. Note that for each
Finally one can express the spin operator $S^z_i = \frac{1}{2} \sum^{m}_{\sigma} \gamma^{\dagger}_{m \sigma} \gamma_{m \sigma}$ in terms of $\gamma^{\dagger}_{m \sigma}$ and $\gamma_{m \sigma}$

\[ S^z_i = \frac{1}{2} \sum^{m}_{m \sigma} \sigma(u_m \gamma^{\dagger}_{m \sigma} - v_m \gamma_{m - \sigma})(u_m \gamma_{m \sigma} - v_m \gamma^{\dagger}_{m - \sigma}) \]

\[ w^*_m(r_i) w_m(r_i) \]

\[ \simeq - \frac{1}{2} \sum^{m}_{m \sigma} \sigma u_m v_m w^*_m(r_i) w_m(r_i) \gamma^{\dagger}_{m \sigma} \gamma_{m - \sigma} + \text{h.c.} \]

(A7)

Here we discard the $\gamma \gamma$ terms because they have vanishing contribution at the low temperature. And for the Raman tensor in the $A_{1g}$ channel \cite{21}, $\tau_{A_{1g}} \equiv \frac{1}{b} \sum_{i<j>\sigma} \epsilon_{i\sigma} c_{i\sigma}^\dagger + \text{h.c.}$, one can use the phase string representation \cite{22} for the electron operator in the $t$-$J$ model and the holon condensation condition to obtain

\[ \tau_{A_{1g}} = - \frac{1}{2} \sum_{i<j>\sigma} h_i h_j e^{-i\phi_{ij} + A_{ij}'} b_{i\sigma}^\dagger b_{j\sigma} e^{i\sigma A_{ij}'} + \text{h.c.} \]

\[ \approx - \frac{1}{2} \sum_{i<j>\sigma} b_{i\sigma}^\dagger b_{j\sigma} e^{i\sigma A_{ij}'} + \text{h.c.} \]

\[ \cong - \delta \sum_{m \sigma} v_m |\gamma_{m \sigma}^{\dagger} \gamma^{\dagger}_{m - \sigma} + \text{h.c.} \]

(A8)

APPENDIX B: DERIVATION OF $U_{\text{int}}$ IN (12)

According to the discussion in Sec. II A an excited spinon will always induce a $\pi$-vortex as shown in Fig.

\[ \Phi \]

The vortex core will be determined by the spinon wavepacket $O_m(r_i)$ in (A0) with a core energy $E_\gamma = E_g/2$. Introduce $m = \nabla \times \vec{A}$ with $\vec{A} \equiv \nabla \phi + A'$ to describe the winding number for the spinon vortices:

\[ \mathbf{m}(r) = \frac{\varepsilon}{\pi} \sum_i \sum_{m} O_m(r_i) \delta(r - r_i) q_m \]

(B1)

where $q_m(= 0, \pm 1)$ denotes the vorticity of a spinon-vortex ($q_m = 0$ means no spinon excitation at state $m$). Then by integrating over $r$ in (B1) in the absence of the external electromagnetic field, one can determine an effective interaction between the spinon-vortices

\[ U_{\text{int}} = \frac{1}{2} \rho_s \int \frac{d^2 q}{(2\pi)^2} \vec{A}(q) \cdot \vec{A}(-q) \]

\[ = \frac{1}{2} \rho_s \int \frac{d^2 q}{(2\pi)^2} m(q) \cdot m(-q) \]

\[ = Q^2 \frac{\pi}{4} \rho_s \ln L - \frac{\pi}{4} \rho_s \sum_{m} q_m q_{m'} I_{mm'} \]

(B2)

The first term in $U_{\text{int}}$ leads to vortex neutrality $Q = \sum m q_m = 0$, and in the second term

\[ I_{mm'} = \sum_{i,j} O_m(r_i) O_{m'}(r_j) \ln |r_i - r_j| \]

\[ = \sum_{r_i,r_j} \left( \frac{a^2}{2\pi a^2} \right)^{1/2} \exp \left\{ - \frac{a^2}{2\pi a^2} r^2 \right\} \]

\[ \times \ln |r'_i - r'_j| + (R_m - R_{m'}| \right| \]

\[ \simeq \ln |R_m - R_{m'}| \]

(B3)

which leads to (12).

\[ \Phi \]

---

1. P.A. Lee, N. Nagaosa and X.G. Wen, Rev. Mod. Phys. 78, 17 (2006).
2. P.A. Lee, X.G. Wen, Phys. Rev. Lett. 78, 4111 (1997).
3. B.R. Boyce, J. Skinta, and T. Lemberger, Physica C 314-348, 561 (2000).
4. P.W. Anderson, Science 235, 1196 (1987).
5. V.J. Emery and S.A. Kivelson, nature 374, 434 (1995).
6. J.M. Kosterlitz and D.J. Thouless, J. Phys. C 6, 1181 (1973); J.M. Kosterlitz, ibid. 7, 1046 (1974).
7. P. Bourges et al, Physica B 215, 30 (1995); P. Bourges, in The Gap Symmetry and Fluctuations in High Temperature superconductors, edited by J.Bok et al, (Plenum Press, New York, 1998).
8. P.C. Dai et al, Phys. Rev. Lett. 77, 5425 (1996).
9. H.F. Fong et al., Phys. Rev. Lett. 83, 713 (1999).
10. Y. Gallais et al, Phys. Rev. Lett. 88, 177401 (2002).
11. Y.J. Uemura, J. Phys. Condens. Matter 16, S4515 (2004); Y.J Uemura, Physica B 374-375, 1 (2006).
12. H.F. Fong et al, Phys. Rev. Lett. 75, 316 (1995).
13. S.L. Li et al, Phys. Rev. B 77, 014523 (2008) and references therein.
14. H.F. Fong et al, Nature 398, 588 (1999); H. He et al. Phys. Rev. Lett. 86, 1610 (2001); B. Fuque et al, Phys. Rev. B 76, 214512 (2007); L. Capogna et al, Phys. Rev. B 75, R060502 (2007).
15. H. He et al, Science 295, 1045(2002).
16. G. Yu et al, cond-matt/0801.5719.
17. S.D. Wilson et al, Nature 442, 141523 (2008).
18. T.P. Devereaux and R. Hack, Phys. Mod. Rev. 79, 175 (2007) and references therein.
19. X.K. Chen, Phys. Rev. B 48, 10530 (1993); S.L. Cooper et al, Phys. Rev. B 37, 5920 (1988); S.L. Cooper et al, Phys. Rev. B 38, 11934 (1989).
20. M.L. Tacon et al, Phys. Rev. B 71, R100504 (2005).
21. A. Hoffmann et al, J. Low Temp. Phys. 99, 231 (1995); T.P. Devereaux et al, Phys. Rev. Lett. 72, 396 (1994); T. Stauffer et al, Phys. Rev. Lett. 68, 1069 (1992).
22. L.V. Gasparov et al, Phys. Rev. B 55, 1223 (1997).
23. M. Kang et al, Phys. Rev. B 56, R11427 (1997).
24. X.K. Chen et al, Phys. Rev. Lett. 73, 3290 (1994).
25. A. Hoffmann et al, Physica C 235-240, 1897 (1994); L.V. Gasparov et al, Physica B 223-244, 481 (1996).
A. Sacuto et al, Europhys. lett. 39, 207 (1997).
A. Sacuto et al, Phys. Rev. B 58, 11721 (1998); A. Sacuto et al, Phys. Rev. B 61, 7122 (2000).
B. Stadlober et al, Phys. Rev. Lett. 74, 4911 (1995).
S.A. Kivelson et al, Rev. Mod. Phys. 75, 1201 (2003) and references therein.
K. Wu, Z.Y. Weng and J. Zaanen, Phys. Rev. B 77, 155102 (2008); Z.Y. Weng, et al, Phys. Rev. B 55, 3894 (1997); D.N. Sheng, Y.C. Chen and Z.Y. Weng, Phys. Rev. Lett. 77, 5102 (1996).
For a review, Z.Y. Weng, Int. J. Mod. Phys. B 21, 773 (2007), cond-matt/0704.2875.
V.N. Muthukumar and Z.Y. Weng, Phys. Rev. B 65, 174511 (2002).
Z.Y. Weng and X.L. Qi, Phys. Rev. B 74, 144518 (2006).
N. Nagaosa and P.A. Lee, Phys. Rev. Lett. 64, 2450 (1990); P.A. Lee and N. Naogaosa, Phys. Rev. B 46, 5621 (1992).
F.D.M. Haldane and Y.S. Wu, Phys. Rev. Lett. 55, 2887 (1985).
D.P. Arovas and A. Auerbach, Phys. Rev. B 38, 316 (1988).
W.Q. Chen and Z.Y. Weng, Phys. Rev. B 71, 134516 (2006).
Z.C. Gu and Z.Y. Weng, Phys. Rev. B 72, 104520 (2005).
E.I. Rashba, L.E. Zhukov and A.L. Efros, Phys. Rev. B 55, 5306 (1997).
B.S. Shastry and B.I. Shraiman, Phys. Rev. Lett. 65 1068 (1990).
P.M. Chaikin and T.C. Lubensky in Principles of condensed matter physics, Cambridge, 1995.
M. Shaw, Z.Y. Weng and C.S. Ting, Phys. Rev. B 68, 014511 (2003).
O.V. Mischenko and E.Y. Sherman, J. Phys.: Condens. Matter 12 (2000), 9905; M. Limonov et al, Phys. Rev. B 66, 054509 (2002).
L. Braicovich et al, Phys. Rev. Lett. 102, 167401 (2009); C. Ulrich et al, Phys. Rev. Lett. 103, 107205 (2009); L.J.P. Ament et al, Phys. Rev. Lett. 103, 117003 (2009).
Z.A. Xu et al, Nature (London) 406, 486 (2000); Y. Wang et al, Phys. Rev. B 64, 224519 (2001).
S.P. Kou and Z.Y. Weng, Phys. Rev. Lett. 90, 157003 (2003).
S.P. Kou and Z.Y. Weng, Phys. Rev. B 67, 115103 (2003).
C.F. Henry, J.C. Davis and D.H. Lee, cond-matt/0403001.