Spin-roton excitations in the cuprate superconductors

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We identify a 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, $k_B T_c \simeq E_g/6$, 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 resonancelike mode and the Raman A_{1g} mode observed in the high-T_c cuprates.

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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 ρ_s by[1,2]

$$\rho_s(T) = \rho_s(0) - aT, \tag{1}$$

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.[3]

On the other hand, in view of the small superfluid density in the cuprates, which are widely considered to be a doped Mott insulator,[4] the phase fluctuation of the superconducting order parameter has been suggested[5] to play an important role in the transition regime, which can be characterized by the following London action:

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

where ϕ specifies the $U(1)$ phase of the order parameter of condensate carrying charge q, and $\mathbf{A}^e$ is the external electromagnetic field. In this point of view, the superconducting transition is of a Kosterlitz-Thouless (KT) type[6] with the proliferation of topological vortices

$$\oint d\mathbf{r}\cdot\nabla\phi = \pm 2\pi, \tag{3}$$

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,[7–11] which is simply given by

$$k_B T_c = \frac{E_g}{\kappa}, \tag{4}$$

where $\kappa \sim 6$ and E_g denotes the characteristic energy scales observed in inelastic neutron scattering (INS)[7–9,12–17] and electronic Raman scattering (ERS)[10,18–28] measurements, as illustrated in Fig. 1. Here, E_g in INS corresponds to the well-known *resonance* energy[12] in the literature, which is a *spin-triplet* excitation at momentum centered on the antiferromagnetic (AF) wave vector $\mathbf{Q}_{\mathrm{AF}}=(\pi,\pi)$. By contrast, E_g in ERS corresponds to a *singlet* mode in the A_{1g} channel near momentum $\mathbf{Q}_0=(0,0)$. The ERS data in B_{1g} and B_{2g} channels have provided the compelling evidence for the d-wave pairing symmetry in the cuprate superconductors, however, the A_{1g} peak at E_g remains an unresolved mystery.[18] As shown in Fig. 1, more materials can be accessible by ERS than INS, including the $La_{2-x}Sr_xCuO_4$ 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 Eq. (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 probed 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.[1] 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 quasidegenerate 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 toward 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 $\mathbf{Q}_{\mathrm{AF}}$ should have some kind of profound effect on the

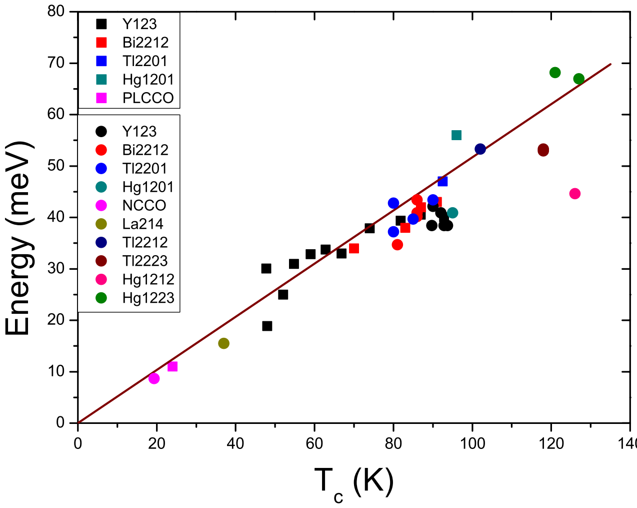

FIG. 1. (Color online) The characteristic energies observed by inelastic neutron scattering (INS) and electron Raman scattering (ERS) experiments versus the superconducting transition temperature T_c for the high-T_c cuprates. The straight line shows the empirical formula (4), which will be derived in the present work. Here, the solid squares represent the INS resonance mode, with different colors indicating different families including hole-doped Y123 (Ref. 13), Bi2212 (Ref. 14), Tl2201 (Ref. 15), and Hg1201 (Ref. 16), and electron doped $Pr_{0.88}LaCe_{0.12}CuO_{4-\delta}$ (Ref. 17); the solid circles represent the ERS A_{1g} mode, including the hole doped Y123 (Refs. 19 and 20), Bi2212 (Ref. 21), Tl2201 (Refs. 22 and 23), Hg1201 (Ref. 20), La214 (Ref. 24), Tl2212 (Ref. 23), Tl2223 (Ref. 25), Hg1212 (Ref. 26), Hg1223 (Ref. 27), and the electron doped NCCO compound (Ref. 28).

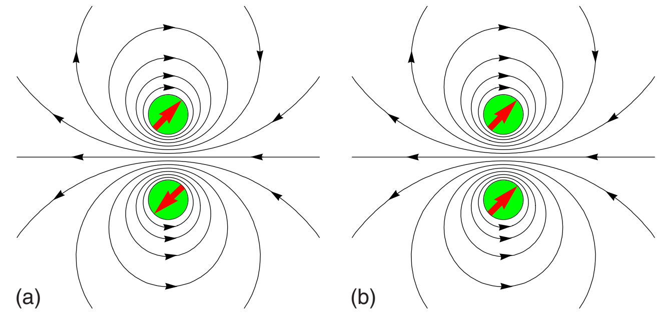

FIG. 2. (Color online) Schematic illustration of an $S=0$ (singlet) and an $S=1$ (triplet) spin rotons. Each of them is composed of a supercurrent vortex-antivortex bound pair, with a pair of neutral free spins sitting at the two poles of the two-dimensional roton. Such a spin-roton composite is an elementary excitation in the superconducting state of a doped Mott insulator described by the phase string theory (Refs. 32 and 33).

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.[2] 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 $\mathbf{Q}_0$, to play an equally important role. Lastly, the simple scaling relation [Eq. (4)] with a universal κ 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 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 supercurrents.[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 Eq. (4). We will show that the singlet and triplet spin rotons can be indeed directly probed by ERS in A_{1g} channel at $\mathbf{Q}_0$ and INS near $\mathbf{Q}_{\mathrm{AF}}$. 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 δ 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 (TR) and spin rotational symmetry breakings, one is naturally led to a modified action for superconductivity. In Sec. II B, 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. II C, the T_c formula (4) determined by the spin-roton excitations is obtained. Finally, in Sec. III, 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,[4] 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 [Eq. (2)] should be modified in order to properly reflect the Mott physics.

For example, in the U(1) slave-boson gauge theory description,[34] the charge carriers are described by spinless bosons known as holons. The superconducting state corresponds to the Bose condensation of the holons, with Eq. (2) replaced by

$$L_h = \frac{\rho_s}{2}\int d^2\mathbf{r}(\nabla\phi + \mathbf{A}^s + e\mathbf{A}^e)^2, \tag{5}$$

where ρ_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 $\mathbf{A}^s$. In the U(1) slave-boson gauge theory,[34] $\mathbf{A}^s$ 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 $\mathbf{A}^s$ 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 $\mathbf{A}^s$ gains a mass and cannot play a role as a new source to effectively reduce T_c.[34]

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 mathematical structure,[32,33] 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 $\mathbf{A}^s$ will only minimally couple to the holon matter field as given in Eq. (5), not to spinon currents. Instead its strength will be generated from the spinon matter field according to the following gauge-invariant relation

$$\oint_c d\mathbf{r}\cdot\mathbf{A}^s(\mathbf{r}) = \phi_0\int_{\Sigma_c} d^2\mathbf{r}[n^b_\uparrow(\mathbf{r}) - n^b_\downarrow(\mathbf{r})]. \tag{6}$$

Here the flux of $\mathbf{A}^s$ 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 $n^b_{\uparrow\downarrow}(\mathbf{r})$ denoting the local density of spinons where the integration runs over the area Σ_c enclosed by c.

Due to the sign change between the ↑ and ↓ spins on the r.h.s. of Eq. (6), $\mathbf{A}^s(\mathbf{r})$ will explicitly preserve the TR symmetry, as $\uparrow\leftrightarrow\downarrow$ under the TR transformation. This is in contrast to a conventional electromagnetic vector potential $\mathbf{A}^e$,

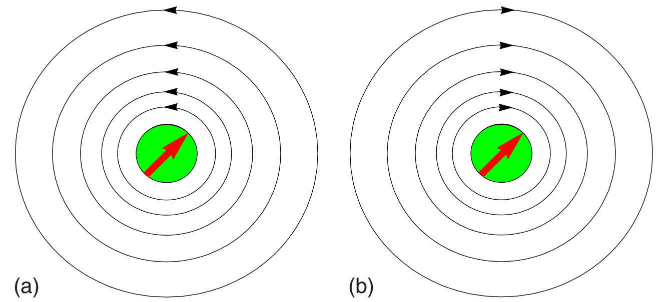

FIG. 3. (Color online) Schematic illustration of single spinon vortices. An isolated neutral spin (spinon) in the superconducting state will always induce a vortexlike supercurrent response from the charge condensate according to the generalized London action [Eq. (5)]. Notice that the vorticity sign of the vortex is actually independent of the spin orientation as long as $\phi_0=\pi$ in Eq. (6), which preserves the spin rotational symmetry.

which breaks the TR symmetry. However, since the path c is oriented, the spin rotational symmetry may be broken for a general ϕ_0. But under a specific choice

$$\phi_0 = \pi, \tag{7}$$

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 $\oint_c d\mathbf{r}\cdot\mathbf{A}^s = \pm\phi_0 = \pm\pi$, which is still spin dependent. However, such a spin-dependence sign change can be effectively compensated in Eq. (5) by combining with a proper topological vortex of the holon condensate given in Eq. (3). Such a "large" gauge transformation will not cost any energy in Eq. (5) when $\mathbf{A}^e=0$. It is also "legal" to precisely bind such a holon vortex core of Eq. (3) with the spinon because the no double occupancy constraint in the doped Mott insulator dictates that a site without a holon must be always occupied by a neutral spin. Hence, based on some general physical considerations, the London action for a superconducting state can be modified in a fundamental way in a doped Mott insulator, with an internal vector potential $\mathbf{A}^s$ emerging as a topological gauge field without breaking the time-reversal and spin rotational symmetries.

According to Eq. (5), the charge current will be determined by the London equation

$$\mathbf{J}_h = \rho_s(\nabla\phi + \mathbf{A}^s + e\mathbf{A}^e). \tag{8}$$

For an isolated neutral spin, in terms of Eq. (6), there will be vortexlike charge currents induced from the charge condensate with $\oint d\mathbf{r}\cdot\mathbf{J}_h = \pm\rho_s\pi$ in the absence of $\mathbf{A}^e$, where $\pm$ will be independent of the spin index based on the above discussion. Namely each neutral spin can induce a current vortex with two opposite vorticities as illustrated in Fig. 3, which is known as a spinon vortex.[32,33]

According to a general argument given by Haldane and Wu,[35] 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 Σ_c enclosed by c, as if it sees an effective "magnetic field" described by a vector potential $\mathbf{A}^h$,

$$\Delta\Phi_{\text{Berry}}(c) = \phi_0 \int_{\Sigma_c} d^2\mathbf{r}\rho_h(\mathbf{r}) \equiv \oint_c d\mathbf{r}\cdot\mathbf{A}^h(\mathbf{r}). \tag{9}$$

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

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

$$H_s = -J_s \sum_{\langle ij\rangle\sigma} b^\dagger_{i\sigma} b^\dagger_{j-\sigma} e^{i\sigma A^h_{ij}} + \text{H.c.}, \tag{10}$$

where $b^\dagger_{i\sigma}$ defines the bosonic creation operator for a spinon at site i with a spin index σ. Here, A^h_{ij} is the lattice version of the gauge potential $\mathbf{A}^h(\mathbf{r})$ introduced in Eq. (9) and the sign σ in front of the gauge phase in Eq. (10) will ensure the TR invariance.

Although one can alternatively write down an effective model with the hopping term $b^\dagger_{i\sigma} b_{j\sigma} e^{i\sigma A^h_{ij}}$ replacing the RVB pairing term $b^\dagger_{i\sigma} b^\dagger_{j-\sigma} e^{i\sigma A^h_{ij}}$ in Eq. (10), without breaking the gauge and TR symmetries, Eq. (10) is physically more meaningful because in the ground-state spinons will be all paired up with $\langle b^\dagger_{i\sigma} b^\dagger_{j-\sigma} e^{i\sigma A^h_{ij}}\rangle \equiv \Delta^s/2 \neq 0$, which automatically satisfies the spinon-confinement requirement to ensure superconducting phase coherence as to be discussed below. Furthermore, $\oint_c d\mathbf{r}\cdot\mathbf{A}^h=0$ at half filling, where H_s [Eq. (10)] reduces to the Schwinger-boson mean-field Hamiltonian, which well captures the AF correlations including the long-range AF order at $T=0$.[36]

Therefore, the London action [Eq. (2)] for superconductivity has been phenomenologically modified for the doped Mott insulator in Eq. (5). Here, the charge condensate will be generally coupled to neutral spin excitations, ubiquitously presented in a doped Mott insulator governed by Eq. (10), via an emergent topological gauge field [Eq. (6)]. Such a self-consistent description based on Eqs. (5), (6), (9), and (10) can be justified[32,33] in the phase string theory of the *t-J* model, with the superfluid stiffness $\rho_s \equiv \rho_h/m_h$ (m_h is the effective mass for holons) and effective coupling constant J_s in Eq. (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,[34] 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.

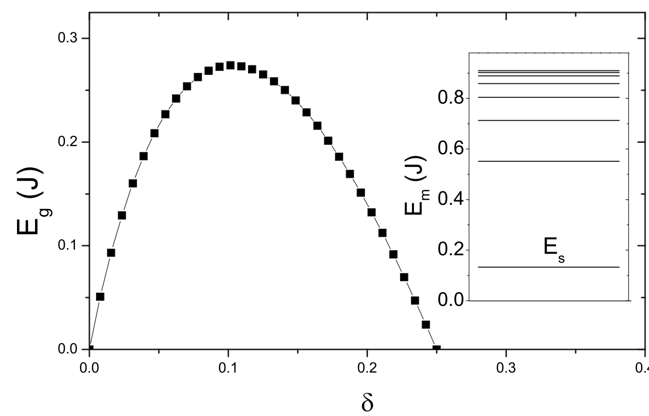

FIG. 4. The doping dependence of the characteristic energy scale E_g of the spin rotons is shown. Here, $E_g=2E_s$ with E_s as the lowest excited energy of the spinon spectrum shown in the inset, obtained based on Eq. (10) at a specific doping concentration $\delta=0.125$.

1. Resonancelike characteristic energy E_g

The spinon Hamiltonian [Eq. (10)] can be easily diagonalized[37] under the condition that the holons are uniformly condensed with $\rho_h=\delta a^{-2}$ (a is the lattice constant) as outlined in Appendix A. The solution of Eq. (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 $E_s \equiv E_g/2$ for simplicity. In the main panel of Fig. 4, $E_g=2E_s$ is shown as a function of doping. Note that in the calculation, the magnitude of J_s in Eq. (10) has to be determined self consistently as $J_s \propto J\Delta^s$ based on the microscopic theory as mentioned above, and here we have directly used its doping dependence previously obtained in Ref. 38. The corresponding spinon wave packet looks like

$$|w_{m\sigma}(\mathbf{r}_i)|^2 \simeq \frac{a^2}{2\pi a_c^2}\exp\left\{-\frac{|\mathbf{r}_i-\mathbf{R}_m|^2}{2a_c^2}\right\}, \tag{11}$$

with a "cyclotron length" $a_c \equiv a/\sqrt{\pi\delta}$. Namely, the lowest spinon excitations governed by Eq. (10) are nonpropagating modes of an intrinsic size in order of a_c. Here the degenerate levels are labeled by the coordinates $\mathbf{R}_m$,[39] the centers of the spinon wave packet Eq. (11), 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 $\mathbf{r}_i$ in the modified London action [Eq. (5)] at $\mathbf{A}^e=0$, one can obtain (see Appendix B) an effective interaction term for spinon vortices on the von Neumann lattice

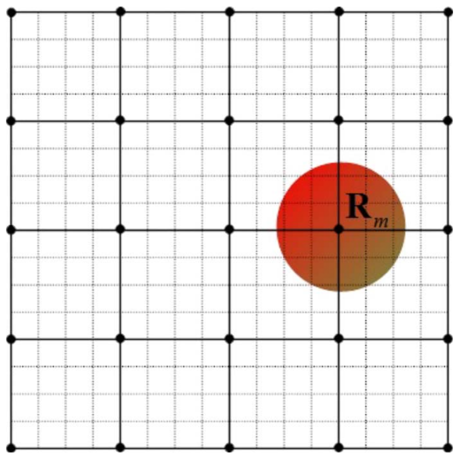

FIG. 5. (Color online) The degenerate spinon modes in the lowest-energy level, shown in the inset of Fig. 4, are labeled by $\mathbf{R}_m$, which form the von Neumann lattice with a lattice constant $\xi_0 = \sqrt{2\pi} a_c$ with the cyclotron length $a_c = a/\sqrt{\pi\delta}$ as the size of each spinon wave packet. Here, the case $\delta = 1/8$ and $\xi_0 = 4a$ is shown. For each $\mathbf{R}_m$, there is an additional degeneracy $g=4$, corresponding to orthogonal wave functions: $w_{m\uparrow}(\mathbf{r}_i)$, $w_{m\downarrow}(\mathbf{r}_i)$, $(-1)^{\mathbf{r}_i} w_{m\uparrow}(\mathbf{r}_i)$ and $(-1)^{\mathbf{r}_i} w_{m\downarrow}(\mathbf{r}_i)$ (Ref. 37).

$$U_{\mathrm{int}} = -\frac{\pi}{4}\rho_s \sum_{\mathbf{R}_m \mathbf{R}_{m'}} \ln \frac{|\mathbf{R}_m - \mathbf{R}_{m'}|}{\xi_0} q_m q_{m'}, \qquad (12)$$

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

$$H_v = \frac{E_g}{2} \sum_m |q_m| + U_{\mathrm{int}}. \qquad (13)$$

It is noted that there is a fourfold 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 Eq. (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 Eq. (5) will be decoupled from the neutral RVB spin background as $A^s \approx 0$ and the excited spinon vortices are effectively described by Eq. (13).

Hence, the spin-roton structure shown in Fig. 2 will emerge as the bound pair of the excited spinons, which are of spin triplet ($S=1$) and singlet ($S=0$), respectively, and *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 $U_{\mathrm{int}}=0$.

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 *magnetically*. However, we have also seen that these spinons must be confined *spatially* in pairs, appearing at the poles of roton supercurrent structure and subjected to logarithmic attraction U_{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_{int} becomes negligible and the spinons are still "asymptotically free."

2. INS and ERS probes

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

$$\chi_{zz}(\tau, \mathbf{r}_i - \mathbf{r}_j) = -\langle T_\tau S_i^z(\tau) S_j^z(0)\rangle, \qquad (14)$$

where τ denotes the imaginary time, $S_i^z = \frac{1}{2}\Sigma_\sigma \sigma b_{i\sigma}^\dagger b_{i\sigma}$. Similarly a density-density correlation function, which can be detected by the electron Raman scattering[40] is defined as follows

$$\chi_{\mathrm{ERS}} = -\langle T_\tau \tau_{A_{1g}}(\tau) \tau_{A_{1g}}(0)\rangle, \qquad (15)$$

where the A_{1g} density operator[40] $\tau_{A_{1g}} \equiv -\frac{1}{2}\Sigma_{\langle ij\rangle\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \mathrm{H.c.}$ Here, $c_{i\sigma}^\dagger$ is the electron operator whose relation with the holon and spinon operators is given in Appendix A.

Based on the Bogolivbov transformation [Eq. (A1)] and the phase string representation for the electron operator $c_{i\sigma}$, one can express S_i^z and $c_{i\sigma}$ in terms of $\gamma_{m\sigma}^\dagger$ 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_v Eq. (13), in which the interaction term U_{int} can be also neglected because S_i^z and $\tau_{A_{1g}}$ only create a pair of spinons locally within a von Neumann lattice site (Fig. 5),

$$S_i^z \sim -\frac{1}{2}\sum_{mn\sigma} u_m v_n w_{m\sigma}^*(\mathbf{r}_i) w_{n\sigma}(\mathbf{r}_i) \sigma \gamma_{m\sigma}^\dagger \gamma_{n-\sigma}^\dagger + \mathrm{H.c.} \qquad (16)$$

and

$$\tau_{A_{1g}} \sim -\delta \sum_{m\sigma} u_m |v_m| \gamma_{m\sigma}^\dagger \gamma_{m-\sigma}^\dagger + \mathrm{H.c.}, \qquad (17)$$

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

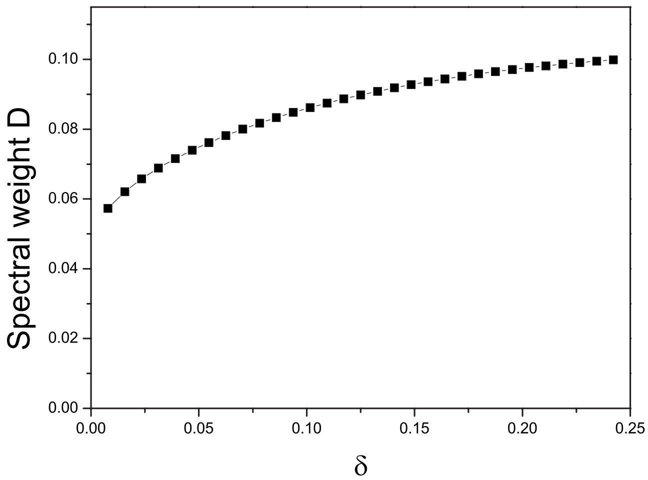

FIG. 6. The doping dependence of the spectral weight D for the spin rotons appearing in Eqs. (20) and (21).

It is straightforward to obtain

$$\chi_{zz}(\tau,\mathbf{r}) = -D(-1)^{\mathbf{r}}e^{-\mathbf{r}^2/2a_c^2}e^{-E_g\tau} \tag{18}$$

and

$$\chi_{\mathrm{ERS}}(\tau) \simeq -\delta D e^{-E_g\tau}, \tag{19}$$

with $D=\frac{\delta^2}{2u_m^2v_n^2}$ is the spectral weight whose doping dependence is shown in Fig. 6. In χ_{zz} we have used the relation[39] $|\Sigma_m w^*_{m\sigma}(\mathbf{r})w_{m\sigma}(\mathbf{r}')|=\frac{1}{2\pi a_c^2}e^{-(\mathbf{r}-\mathbf{r}')^2/4a_c^2}$.

Correspondingly the dynamic spin susceptibility is obtained by

$$\chi''_{zz}(\mathbf{q},\omega) = \frac{2a_c^2}{\pi}De^{-2a_c^2(\mathbf{q}-\mathbf{Q}_{\mathrm{AF}})^2}\delta(\omega-E_g) \tag{20}$$

and the A_{1g} Raman scattering cross section

$$I_{\mathrm{ERS}}(\omega) \propto \chi''_{\mathrm{ERS}}(\omega) \simeq \delta D\,\delta(\omega-E_g). \tag{21}$$

So the triplet spin-roton will appear as a resonancelike mode in $\chi''_{zz}(\mathbf{q},\omega)$ at $\omega=E_g$, with momentum $\mathbf{q}$ peaked at the AF wave vector $\mathbf{Q}_{\mathrm{AF}}$ and a width inversely proportional to the RVB pairing size a_c which thus determines the spin-spin correlation length $\propto a/\sqrt{\delta}$. Similarly, in $I_{\mathrm{ERS}}(\omega)$ 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_{int} in Eq. (13) 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. 4, whose effect[37] 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 Eq. (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, $I_{\mathrm{ERS}}(\omega)=0$ 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[37] at $\delta\to 0$ with the spinon spectrum shown in the inset of Fig. 4 becomes a continuous energy spectrum described by the Schwinger boson mean-field theory.[36]

C. T_c 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 ρ_s will be renormalized by spin-roton excitations via the internal gauge field $\mathbf{A}^s$ in the London action Eq. (5). Such spin-rotons shown in Fig. 2 resemble the conventional vortex-antivortex pairs in the XY model,[6] except that the unit vorticity of each spinon-vortex is π instead of 2π 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. 5, 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_v in Eq. (13), is expected to be similar to a conventional KT transition, but the T_c formula should be quantitatively different due to the peculiar internal structure of a spin-roton excitation outlined above.

In the following, we shall follow a standard textbook mathematical procedure[41] in dealing with a conventional KT transition. Define the reduced stiffness $K\equiv\frac{\rho_s}{k_BT}$. and then the renormalized reduced stiffness K_R, obtained by averaging over the spin-roton excitations governed by Eq. (13), is found by

$$K_R = K + \frac{\pi^2K^2}{4Na^2}g^2\sum_{\mathbf{R}_m\mathbf{R}_{m'}}(\mathbf{R}_m-\mathbf{R}_{m'})^2\langle q_mq_{m'}\rangle, \tag{22}$$

where N is the original total lattice number. The correlation $\langle q_mq_{m'}\rangle$ can be easily evaluated in terms of Eq. (13) to lowest order in fugacity y (Ref. 41),

$$\langle q_mq_{m'}\rangle = -2y^2[|\mathbf{R}_m-\mathbf{R}_{m'}|/\xi_0]^{-(\pi/2)K}. \tag{23}$$

such that

$$K_R = K - g^2\pi^3y^2K^2\int_{\xi_0}^{\infty}\frac{dR}{\xi_0}\left(\frac{R}{\xi_0}\right)^{3-(\pi/2)K}, \tag{24}$$

where the lattice constant ξ_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

$$\frac{dK^{-1}}{dl} = g^2\pi^3y^2 + O(y^4), \tag{25}$$

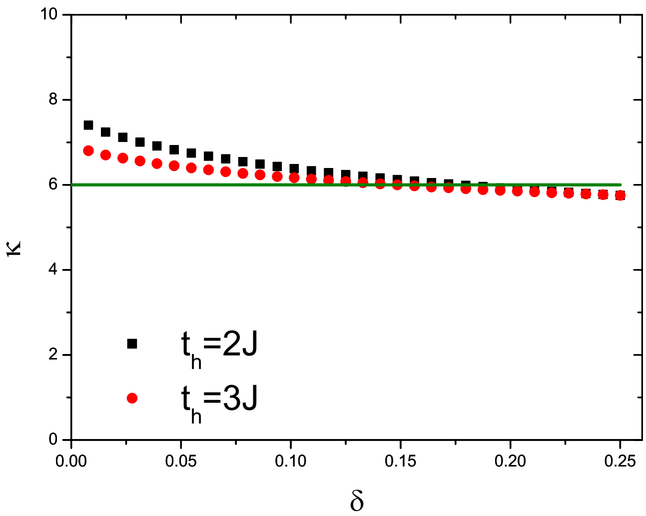

FIG. 7. (Color online) The coefficient κ defined in Eq. (29) is calculated at some typical values of the parameter: $t_h/J=2$ and 3, and is weakly doping dependent around $\kappa=6$.

$$\frac{dy}{dl} = \left(2 - \frac{\pi}{4}K\right) y + O(y^3), \tag{26}$$

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

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

$$\frac{8}{\pi} = \frac{\rho_s}{k_B T_c} + g^2 \pi^3 y_c^2 \frac{\left(\frac{\rho_s}{k_B T_c}\right)^2}{4 - \frac{\pi}{2}\frac{\rho_s}{k_B T_c}} \tag{27}$$

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

$$y_c^2 = \frac{1}{2\pi^2}\frac{n^2}{g^2}\left(1-\frac{8}{n^2\pi}\frac{k_BT_c}{\rho_s}\right)^2, \tag{28}$$

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

$$\frac{E_g}{k_BT_c} = 2\ln\frac{4\sqrt{2}\pi}{1-\frac{8k_BT_c}{\pi\rho_s}} \equiv \kappa, \tag{29}$$

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

$$\kappa \simeq 2\ln 4\sqrt{2}\pi = 5.76. \tag{30}$$

Generally, κ can be determined self-consistently according to Eq. (29) with using $m_h=1/(2t_ha^2)$ and $E_g(\delta)$ presented in Fig. 4. The result is shown in Fig. 7 as a function of doping concentration δ at $t_h=2J$ and $t_h=3J$, respectively. Figure 7 indicates that the value of κ 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 straighten in Fig. 1. It is noted that $y_c^2=e^{-\kappa}\ll 1$ 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,[42] T_c was calculated without properly considering both the singlet and triplet spin-roton excitations, which resulted in somewhat higher and nonuniversal 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 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 wave vector 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 Eq. (4), 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.[43] Similarly, the resonant inelastic x-ray scattering (RIDS)[44] should be also able to detect such a singlet spin-roton excitation if a higher resolution (≤ 40 em V) 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 overtopping because the underlying RVB pairing $\Delta^s \equiv \sum_\sigma \langle b_{i\sigma}^\dagger b_{j-\sigma}^\dagger e^{i\sigma A_{ij}^h}\rangle=0$,[38] while E_g vanishes at $\delta=0$ where the spin-rotons 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 or the lower pseudogap phase,[32,33] which may explain the Nernst regime discovered[45] in the cuprates.

However, if E_g vanishes at a finite but small doping concentration, then the AF order may persist over in a finite regime where $T_c=0$. As a matter of fact, if the non-uniform charge distribution is allowed, E_g as the solution of Eq. (10) can indeed be softened to zero at some small finite doping. A case considering some Z_2 topological excitation at low doping does lead to the result that E_g vanishes as $\sqrt{\delta - x_c}$ at a critical doping $x_c \simeq 0.043$.[46] Below x_c, either an AF spin glass state or charge stripe phases has been shown[46,47] 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 $E_g \to 0$. 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.

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APPENDIX A: DIAGONALIZATIONS OF H_s (10)

The spinon Hamiltonian H_s Eq. (10) can be easily diagonalized[37] 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

$$b_\sigma(\mathbf{r}) = \sum_m (u_m \gamma_{m\sigma} - v_m \gamma^\dagger_{m-\sigma}) w_{m\sigma}(\mathbf{r}) \tag{A1}$$

we obtain the spinon Hamiltonian H_s as follows:

$$H_s = \sum_{m\sigma} E_m \gamma^\dagger_{m\sigma}\gamma_{m\sigma} + \text{const.}, \tag{A2}$$

where

$$u_m = \frac{1}{\sqrt{2}}\sqrt{\frac{\lambda}{E_m}+1}, \quad v_m = \text{sgn}(\xi_m)\frac{1}{\sqrt{2}}\sqrt{\frac{\lambda}{E_m}-1} \tag{A3}$$

and

$$E_m = \sqrt{\lambda^2 - \epsilon_m^2}. \tag{A4}$$

Here, the quantum number m denotes an eigenstate $w_{m\sigma}(\mathbf{r}_i)$ with the eigenvalue ξ_m

$$\epsilon_m w_{m\sigma}(\mathbf{r}_i) = -J_s \sum_{j=\text{NN}(i)} e^{i\sigma A^h_{ij}} w_{m\sigma}(\mathbf{r}_j). \tag{A5}$$

The spinon excitation spectrum Eq. (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 $J_s = J(1-4\delta)\Delta^s/2$ (Ref. 38) and the chemical potential λ in E_m by enforcing $\sum_{i\sigma} b^\dagger_{i\sigma} b_{i\sigma} = (1-\delta)N$.

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

$$O_m(\mathbf{r}_i) = |w_{m\sigma}(\mathbf{r}_i)|^2 \simeq \frac{a^2}{2\pi a_c^2}\exp\left\{-\frac{1}{2a_c^2}|\mathbf{r}_i - \mathbf{R}_m|^2\right\}, \tag{A6}$$

with the degenerate states labeled[39] by the site $\mathbf{R}_m$ in a von Neumann lattice shown in Fig. 5. Note that for each $\mathbf{R}_m$, there are four degenerate states $(g=4)$ corresponding $w_{m\uparrow}(\mathbf{r}_i)$, $w_{m\downarrow}(\mathbf{r}_i)$, $(-1)^{\mathbf{r}_i} w_{m\uparrow}(\mathbf{r}_i)$, and $(-1)^{\mathbf{r}_i} w_{m\downarrow}(\mathbf{r}_i)$ due to the time reversal and bipartite lattice symmetry.[37]

Finally one can express the spin operator $S_i^z = \frac{1}{2}\sum_\sigma \sigma b^\dagger_{i\sigma} b_{i\sigma}$ in terms of $\gamma^\dagger_{m\sigma}$ and $\gamma_{m\sigma}$

$$S_i^z = \frac{1}{2}\sum_{mn\sigma} \sigma(u_m \gamma^\dagger_{m\sigma} - v_m \gamma_{m-\sigma})(u_n \gamma_{n\sigma} - v_n \gamma^\dagger_{n-\sigma}),$$

$$w^*_{m\sigma}(\mathbf{r}_i) w_{n\sigma}(\mathbf{r}_i) \simeq -\frac{1}{2}\sum_{mn\sigma} \sigma u_m v_n w^*_{m\sigma}(\mathbf{r}_i) w_{n\sigma}(\mathbf{r}_i)\gamma^\dagger_{m\sigma}\gamma^\dagger_{n-\sigma} + \text{H.c.} \tag{A7}$$

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,[40] $\tau_{A_{1g}} \equiv -\frac{1}{2}\sum_{\langle ij\rangle\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}$, one can use the phase string representation[30,31] for the electron operator in the t-J model and the holon condensation condition to obtain

$$\begin{aligned}\tau_{A_{1g}} &= -\frac{1}{2}\sum_{\langle ij\rangle\sigma} h_i h_j^\dagger e^{-i(\phi^0_{ij}+A^s_{ij})} b^\dagger_{i\sigma} b_{j\sigma} e^{i\sigma A^h_{ij}} + \text{H.c.} \\ &\simeq -\frac{1}{2}\delta\sum_{\langle ij\rangle\sigma} b^\dagger_{i\sigma} b_{j\sigma} e^{i\sigma A^h_{ij}} + \text{H.c.} \\ &\propto -\delta\sum_{m\sigma} u_m |v_m| \gamma^\dagger_{m\sigma}\gamma^\dagger_{m-\sigma} + \text{H.c.}\end{aligned} \tag{A8}$$

APPENDIX B: DERIVATION OF U_{int} IN EQ. (12)

According to the discussion in Sec. II A, an excited spinon will always induce a π vortex as shown in Fig. 3. The vortex core will be determined by the spinon wave packet $O_m(\mathbf{r}_i)$ in Eq. (A6) with a core energy $E_s = E_g/2$. Introduce $\mathbf{m} = \nabla \times \tilde{\mathbf{A}}$ with $\tilde{\mathbf{A}} \equiv \nabla\phi + \mathbf{A}^s$ to describe the winding number for the spinon vortices:

$$\mathbf{m}(\mathbf{r}) = \hat{z}\pi\sum_m \sum_{\mathbf{r}_i} O_m(\mathbf{r}_i)\delta(\mathbf{r}-\mathbf{r}_i) q_m, \tag{B1}$$

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 $\mathbf{r}$ in Eq. (5) in the absence of the external electromagnetic field, one can determine an effective interaction between the spinon-vortices,

$$\begin{aligned}U_{\text{int}} &= \frac{1}{2}\rho_s \int \frac{d^2\mathbf{q}}{(2\pi)^2}\tilde{\mathbf{A}}(\mathbf{q})\cdot\tilde{\mathbf{A}}(-\mathbf{q}) \\ &= \frac{1}{2}\rho_s \int \frac{d^2\mathbf{q}}{(2\pi)^2}\frac{\mathbf{m}(\mathbf{q})\cdot\mathbf{m}(-\mathbf{q})}{q^2} \\ &= Q^2\frac{\pi}{4}\rho_s \ln L - \frac{\pi}{4}\rho_s \sum_{\mathbf{R}_m\mathbf{R}_{m'}} q_m q_{m'} I_{mm'}.\end{aligned} \tag{B2}$$

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

$$I_{mm'} = \sum_{i,j} O_m(\mathbf{r}_i) O_{m'}(\mathbf{r}_j) \ln|\mathbf{r}_i - \mathbf{r}_j|$$
$$= \sum_{\mathbf{r}_i', \mathbf{r}_j'} \left(\frac{a^2}{2\pi a_c^2}\right) \exp\left\{-\frac{a^2}{2a_c^2}(\mathbf{r}_i'^2 + \mathbf{r}_j'^2)\right\} \times \ln|(\mathbf{r}_i' - \mathbf{r}_j') + (\mathbf{R}_m - \mathbf{R}_{m'})| \simeq \ln|(\mathbf{R}_m - \mathbf{R}_{m'})|, \tag{B3}$$

which leads to Eq. (12).

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