Vortex Core Excitations in Superconductors with Frustrated Antiferromagnetism

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Motivated by recent discovery of cobalt oxide and organic superconductors, we apply an effective model with strong antiferromagnetic and superconducting pairing interaction to a related lattice structure. It is found that the antiferromagnetism is highly frustrated and a broken-time-reversal-symmetry chiral $d+id'$-wave pairing state prevails. In the mixed state, we have solved the local electronic structure near the vortex core and found no local induction of antiferromagnetism. This result is in striking contrast to the case of copper oxide superconductors. The calculated local density of states indicates the existence of low-lying quasiparticle bound states inside the vortex core, due to a fully gapped chiral pairing state. The prediction can be directly tested by scanning tunneling microscopy.

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Recently, superconductivity in the oxyhydrate Na$_{0.35}$CoO$_2$·1.3H$_2$O below $\sim 5K$ was discovered by Takata et al. [1] and confirmed immediately by several groups [2, 3, 4, 5]. Interesting features of this material include: (i) It is believed that the superconductivity comes from CoO$_2$ layers, similar to that in copper-oxide cuprates. (ii) Co$^{4+}$ atoms have spin $\frac{1}{2}$ but form a triangular lattice, which frustrates the antiferromagnetism (AF) and thus is a promising candidate for the occurrence of spin-liquid phases [6]. There are also organic superconductors like the $\kappa$-(BEDT-TTF)$_2X$ materials which have a lattice structure very similar to the triangular lattice [7, 8]. (iii) Theoretically, the analysis based on the resonant valence bond theory in the framework of the $t$-$J$ model [9, 10, 11, 12] or on the renormalization group theory within the framework of $t$-$U$-$J$ model [13] indicates a wide window of broken-time-reversal-symmetry (BTRS) $d+id'$-wave pairing state in the phase diagram. Other theoretical groups [14, 15, 16] proposed a $p_x+ip_y$-wave pairing state mediated by ferromagnetic fluctuations. Since the ferromagnetism is insensitive to the detailed lattice structure, no frustration effect is expected on a triangular lattice. At this stage, we are not at a position to resolve the pairing state issue. Motivated by recent observation of a superconducting phase diagram of Na$_x$CoO$_2$·1.3H$_2$O similar to that of the cuprate superconductors [2], we consider in this Letter a spin-singlet pairing and study the nature of low-lying excitations around a vortex in these new superconductors with frustrated antiferromagnetism. The results can be directly tested by further experiments such as scanning tunneling microscopy (STM), which likely will be carried out soon.

In conventional $s$-wave superconductors such as NbSe$_2$, the observed quasiparticle tunneling spectrum at the vortex core by Hess et al. [15] can be explained successfully in terms of the low-lying quasiparticle bound states as shown by Caroli, de Gennes, and Matricon [16]. In copper-oxide cuprates, the condensate has a $d$-wave pairing symmetry. Theoretical study based on $d$-wave BCS model suggested [17] that, due to the existence of nodal quasiparticles, the local density of states (LDOS) at the $d$-wave vortex core exhibits a single broad peak at zero energy. However, the STM-measured local differential tunneling conductance at the vortex core center only exhibits a subgap double-peak structure [20, 21] or even no clear peak structure within the superconducting gap [22]. The discrepancy between the earlier theoretical prediction and the experimental observation stimulated various explanations. Recent intensive experimental [22, 24, 25, 26, 27, 28] and theoretical [24, 26, 30, 31, 32, 33] studies seem to converge on an explanation in terms of the field-induced AF around the vortex core. When the AF is frustrated in a triangular lattice [34, 35], one would expect a different nature of electronic excitations near the vortex. Previously, we have applied an effective microscopic mean-field model with competing AF and superconducting interactions to a square lattice, as relevant to the copper-oxide supercon-
bonds forming the two-dimensional (2D) lattice and formation is along \( t \) and \( U \). 

Analysis of this paper is also directly applicable to organic conductors that have such a lattice structure.

The model consists of an on-site repulsion and off-site attraction. The former is solely responsible for the antiferromagnetism while the latter causes the superconductivity. The mean-field Hamiltonian is written as:

\[
H = - \sum_{ij,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i (Un_{i\sigma} + \epsilon_i - \mu)c_{i\sigma}^\dagger c_{i\sigma} + \sum_{ij} (\Delta_{ij} c_{i\sigma}^\dagger c_{j\uparrow} + \Delta_{ij}^* c_{j\sigma} c_{i\uparrow}).
\] (1)

Here \( c_{i\sigma} \) annihilates an electron of spin \( \sigma \) at the \( i \)th site. The hopping integrals are respectively \( t_{ij} = t \) on the bonds forming the two-dimensional (2D) lattice and \( t' \) along one diagonal of each plaquette. The on-site repulsion is \( U \) on each site. The quantities \( n_{i\sigma} = \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle \), \( \epsilon_i \), and \( \mu \) are the electron density with spin \( \sigma \), the single site potential describing the scattering from impurities, and the chemical potential. The spin-singlet order parameter \( \Delta_{ij} = \frac{\Delta}{\sqrt{2}} (c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow}) \) comes from the pairing interactions on the bond \( (V_{ij} = V) \) and along one diagonal of each plaquette \( (V_{ij} = V') \). The case of \( t' = 0 \) and \( V' = 0 \) correspond to the model on a square lattice. With the application of an external magnetic field \( \mathbf{H} \), the Peierls phase factor is given by the integral \( e^{i\mathbf{r} \cdot \mathbf{F}_0} \), where the superconducting flux quantum \( \Phi_0 = hc/2e \) and the vector potential \( \mathbf{A} = \frac{i}{2} \mathbf{H} \times \mathbf{r} \) in the symmetric gauge. The Hamiltonian \( H \) can also be derived from the \( t-U-J \) model \[13, 37\]. We diagonalize Eq. (1) by solving self-consistently the Bogoliubov-de Gennes equation:

\[
\sum_{j} \left( \begin{array}{cc}
H_{ij,\sigma} & \Delta_{ij} \\
\Delta_{ij}^* & -H_{ij,\sigma}
\end{array} \right) \left( \begin{array}{c}
u_{j\sigma}^n \\
\nu_{j\sigma}^{\dagger n}
\end{array} \right) = E_n \left( \begin{array}{c}
u_{j\sigma}^n \\
\nu_{j\sigma}^{\dagger n}
\end{array} \right),
\] (2)

subject to the self-consistency conditions for the electron density and the superconducting order parameter: \( n_{i\uparrow} = \sum_n |\nu_{i\uparrow}^n|^2/2f(E_n) \) and \( n_{i\downarrow} = \sum_n |\nu_{i\downarrow}^n|^2|1 - f(E_n)| \), and \( \Delta_{ij} = \frac{\nu_{ij}^e}{\nu_{ij}^c} \sum_k (u_{ik}^e v_{kj}^c + v_{ik}^e u_{kj}^c) \tanh \left( E_n / 2k_B T \right) \). Here the quasiparticle wavefunction, corresponding to the eigenvalue \( E_n \), consists of the component \( u_{ik}^e \) for an electron of spin \( \sigma \) and the component \( v_{ik}^c \) for a hole of opposite spin \( \bar{\sigma} \). The single particle Hamiltonian reads \( H_{ij,\sigma} = -t_{ij} e^{i\phi_{ij}} + (Un_{i\bar{\sigma}} + \epsilon_i - \mu)\delta_{ij} \). The Fermi distribution function is \( f(E) = 1/[e^{E/k_B T} + 1] \). Hereafter we measure the length in units of the lattice constant \( a_0 \) and the energy in units of \( t(>0) \). As relevant to the superconductivity in the cobalt oxides, we report results below for the case with \( t' = t \) and \( V' = V \). As a model calculation, we choose \( U = 4 \) and various values of \( V \). We find that the antiferromagnetism is highly frustrated even when \( V = 0 \) and the filling factor is one electron per site. Since the experiments on cobalt oxides were performed in the optimal or slightly overdoped regime \[11, 12\], we choose the filling factor \( n_f = \sum_i n_{i\sigma}/N_x N_y = 0.65 \), where \( N_x, N_y \) are the linear dimensions of the unit cell under consideration. The chosen band filling factor corresponds to an electron doping \( x = 0.35 \). We use an exact diagonalization method to solve the BdG equation \( H \) self-consistently. In zero field, the solution is found to be uniform: There exists no AF spin density wave (SDW) and the superconducting bond order parameters exhibit the commensurate AF spin density wave ordering at un-
FIG. 2: The three-dimensional display of the amplitude distribution of (a-c) the three superconducting bond order parameters, (d) the staggered magnetization $M_i$, and (e) the electron density $n_i = \sum_\sigma n_{i\sigma}$ in a magnetic unit cell containing two vortices. The size of the unit cell is $32 \times 32$. Parameter values: $U = 4$, $V = 3$, $n_f = 0.65$, and $T = 0$.

FIG. 3: The local density of states as a function of energy at three selected sites A (red line), B (green line), and C (blue line) for (a) $V = 3$ and (b) $V = 2.5$. The relative positions of the selected sites are indicated on Fig. 1. Also shown is the density of states for the zero-field uniform case. The energy is scaled to the maximum superconducting gap $\Delta_{\text{max}}$. The other parameter values are the same as in Fig. 2 except for $T = 0.02$.

The LDOS is defined by

$$\rho_i(E) = -\frac{1}{M_x M_y} \sum_{k,n,\sigma} |u_{i\uparrow}^n,k|^2 f'(E^n_{\sigma,k} - E) + |u_{i\downarrow}^n,k|^2 f'(E^n_{\sigma,k} + E),$$

where $f'(E)$ is the derivative of the Fermi distribution function. The $\rho_i(E)$ is proportional to the local differential tunneling conductance which could be measured by STM experiments. In Fig. 3 we plot the LDOS as a function of energy at the three selected sites around the vortex core center, which are labelled in Fig. 1 for various values of $V$. For comparison, we have also displayed the density of states for the zero-field uniform case, which is peaked at the maximum superconducting energy gap $\Delta_{\text{max}}$. The coherent peaks at the gap edge are smeared out in the LDOS at the vortex core. Instead there are
sharp subgap resonance peaks in the LDOS. Due to the energy level quantization of the bound states, the small gap around the Fermi energy follows approximately the relation, $\Delta_1 \sim \Delta_{\text{max}}^2/E_F$, similar to the s-wave case. For a strong pairing interaction, which leads to a large magnitude of the superconducting order parameter, the energy level spacing is wide (Fig. 4). For a weak pairing interaction, the level spacing is so small that only a thermally broadened peak is observed. This result is dramatically different from that in a BCS d-wave superconductor. In the latter, due to the existence of nodal quasiparticles, there always appears a broadened single peak around the Fermi energy regardless of how short the superconducting coherence length is. We propose to use the STM to investigate the core structure in these materials. For cobalt oxides, the superconducting energy would be very small, since $T_c \sim 5K$ at slightly overdoped regime. It is expected that a broadened single peak should be observed. It is a possibility that cobalt oxide superconductors have a spin-triplet pairing symmetry mediated by ferromagnetic fluctuations. One would expect therefore a competition between ferromagnetism and superconductivity in this case and vortex core excitations analogous to the ones in copper oxide cuprates may occur. This question is reserved for an interesting future study.

We now look into the nature of the vortex states. In Fig. 4, we display the spatial distribution of the local density of states at a resonant energy level. It shows no long-range tails, in striking contrast to the case of d-wave superconductors, where tails runs along the gap nodal directions. Instead, the LDOS at the core level is trapped in an area characterized by the superconducting coherence length, indicating that the core states are completely localized.

In conclusion, we have studied the vortex core excitations in superconductors with frustrated antiferromagnetism. This investigation is relevant to recently discovered cobalt oxide and organic superconductors. We find no local induction of antiferromagnetism around the vortex core. Low-lying quasiparticle bound states are found inside the vortex core due to a fully gapped chiral pairing state. These core states can be directly measured by STM experiments regardless of the magnitude of the level spacing between them. To our knowledge, this is the first theoretical investigation of the nature of vortex core states in superconductors with frustrated antiferromagnetism.

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