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Vortex core excitations in superconductors with frustrated antiferromagnetism

Jian-Xin Zhu *, A.V. Balatsky

Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

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Abstract

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 $Na_{0.35}CoO_2 \cdot 1.3H_2O$ below ~5 K was discovered by Takada et al. [1] and confirmed immediately by several groups [2–5]. 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 κ-(BEDT-TTF)$_2$X 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 [9–12] 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 [14–16] 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. Note that both $d + id'$ and $p_x + ip_y$ support a full gap in the quasiparticle spectrum. So far, the nature of pairing symmetry in cobalt oxide superconductors and the issue of whether such kind of time-reversal-symmetry-broken pairing state exists are still hotly debated. For example, the data from both muon spin rotation/relaxation [17] and nuclear quadrupole resonance [18] measurements in the superconducting state are most consistent with a gapless pairing symmetry.

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 $Na_xCoO_2 \cdot 1.3H_2O$ similar to that of the cuprate superconductors [5], we consider in this paper 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. [19] can be explained successfully in

* Corresponding author.
E-mail address: jxzhu@lanl.gov (J.-X. Zhu).

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terms of the low-lying quasiparticle bound states as shown by Caroli et al. [20]. In copper-oxide cuprates, the condensate has a d-wave pairing symmetry [21]. Theoretical study based on d-wave BCS model suggested [22] 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 [23,24] or even no clear peak structure within the superconducting gap [25]. The discrepancy between the earlier theoretical prediction and the experimental observation stimulated various explanations. Recent intensive experimental [26–30] and theoretical [31–36] studies seem to converge on an explanation in terms of the field-induced AF around the vortex core. When the AF is frustrated on a triangular lattice [37,38], 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 superconductors. This model generates such rich physics as the commensurate AF spin density wave ordering at undoped systems, stripes at low doping, as well as the superconducting states at optimal and overdoped regimes [39]. Especially, within this model, it was found [32] that the AF ordering is induced around the vortex core, which explains several experimental observations on cuprates. Here, we extend this effective model to a lattice as shown in Fig. 1, which interpolates between the square and triangular lattices. 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

$$H = -\sum_{ij,\sigma} t_{ij} e^{i\varphi_{ij}} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i,\sigma} (U n_{i,\bar{\sigma}} + \epsilon_{\rm i} - \mu) c^{\dagger}_{i\sigma} c_{i\sigma} + \sum_{ij} (\Delta_{ij} c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow} + \Delta^{*}_{ij} c_{j\downarrow} c_{i\uparrow}). \quad (1)$$

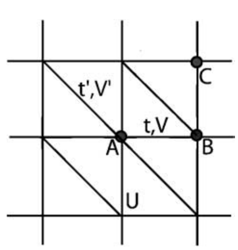

Fig. 1. Lattice structure of a superconductor with frustrated antiferromagnetism. It has a nearest-neighbor hopping t and pairing interaction V on the bonds forming the two-dimensional lattice, a next-nearest-neighbor hopping integral t' and V' along *one* diagonal of each plaquette, and an on-site Hubbard interaction U on each site. The sites A, B, and C labelled by filled circles are the vortex core center and its neighbors when the superconductor is in the mixed state.

Here $c_{i\sigma}$ annihilates an electron of spin σ at the ith 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 $n_{i\sigma} = \langle c^{\dagger}_{i\sigma} c_{i\sigma} \rangle$, $\epsilon_{\rm i}$, and μ, are the electron density with spin σ, the single site potential describing the scattering from impurities, and the chemical potential. The spin-singlet order parameter $\Delta_{ij} = \frac{V_{ij}}{2} \langle c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow} \rangle$ 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 $\varphi_{ij} = \frac{\pi}{\Phi_0} \int_{\mathbf{r}_j}^{\mathbf{r}_i} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r}$, where the superconducting flux quantum $\Phi_0 = hc/2e$ and the vector potential $\mathbf{A} = \frac{1}{2} \mathbf{H} \times \mathbf{r}$ in the symmetric gauge. The Hamiltonian (1) can also be derived from the t–U–J model [13,40]. We diagonalize Eq. (1) by solving self-consistently the Bogoliubov–de Gennes equation [41]:

$$\sum_j \begin{pmatrix} \mathscr{H}_{ij,\sigma} & \Delta_{ij} \\ \Delta^{*}_{ij} & -\mathscr{H}^{*}_{ij,\bar{\sigma}} \end{pmatrix} \begin{pmatrix} u^n_{j\sigma} \\ v^n_{j\bar{\sigma}} \end{pmatrix} = E_n \begin{pmatrix} u^n_{i\sigma} \\ v^n_{i\bar{\sigma}} \end{pmatrix}, \quad (2)$$

subject to the self-consistency conditions for the electron density and the superconducting order parameter: $n_{i\uparrow} = \sum_n |u^n_{i\uparrow}|^2 f(E_n)$ and $n_{i\downarrow} = \sum_n |v^n_{i\downarrow}|^2 [1 - f(E_n)]$, and $\Delta_{ij} = \frac{V_{ij}}{4} \sum_n (u^n_{i\uparrow} v^{n*}_{j\downarrow} + v^{n*}_{i\downarrow} u^n_{j\uparrow}) \tanh(\frac{E_n}{2k_{\rm B}T})$. Here the quasiparticle wavefunction, corresponding to the eigenvalue E_n, consists of the component $u^n_{i\sigma}$ for an electron of spin σ and the component $v^n_{i\bar{\sigma}}$ for a hole of opposite spin $\bar{\sigma}$. The single particle Hamiltonian reads $\mathscr{H}_{ij,\sigma} = -t_{ij} e^{i\varphi_{ij}} + (U n_{i\bar{\sigma}} + \epsilon_{\rm i} - \mu) \delta_{ij}$. The Fermi distribution function is $f(E) = 1/[e^{E/k_{\rm B}T} + 1]$. 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. The clean limit, i.e., $\epsilon_{\rm i} = 0$, is considered throughout the work. 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 [1,5], we choose the filling factor $n_f = \sum_{i,\sigma} n_{i\sigma} / N_x N_y = 0.65$, 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 $x = 0.35$ [13]. We use an exact diagonalization method to solve the BdG Eq. (2) self-consistently. In zero field, the solution is found to be uniform: there exits no AF spin density wave (SDW) and the superconducting bond order parameters exhibit the relation that $\Delta_x = |\Delta_0| e^{-i\theta}$, $\Delta_y = |\Delta_0| e^{i\theta}$, $\Delta_{xy} = |\Delta_0|$ with $\theta = 2\pi/3$, consistent with the results based on the t–J model (see, e.g., [12]). We find typically $|\Delta_0| = 0.07$ and 0.15 for $V = 2.5$ and 3.0, respectively. This complex order parameter forms a broken-time-reversal-symmetry chiral pairing state. We then use this zero-field solution as the initial condition for iteration for the vortex problem.