SO(5) theory of insulating vortex cores in high-$T_c$ materials

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We study the fermionic states of the antiferromagnetically ordered vortex cores predicted to exist in the superconducting phase of the proposed SO(5) model of strongly correlated electrons. Our model calculation gives a natural explanation of the recent STM measurements on BSCCO, which in surprising contrast to YBCO revealed completely insulating vortex cores.

During the past decade the vastly improved STM technique has led to detailed measurements of the electronic excitation spectrum of superconductors, in particular the local electronic density of states in Abrikosov vortices. The metal cores predicted by Caroli et al. were observed in both standard $s$-wave superconductors (sSC) and in the high-$T_c$ $d$-wave superconductors (dSC) YBCO. The experimental advances naturally led to intensified theoretical studies of SC vortices. Following initial calculations on sSC vortex cores, the focus soon turned to dSC cores, and it was observed that the vortex cores of the high-$T_c$ superconductor BSCCO were completely devoid of low-lying electronic excitations. In this paper we offer an explanation of the 41 meV magnetic resonance in the superconducting state of YBCO observed by Zhang

\[ \Psi_\uparrow(\mathbf{r}) = \{ c^\dagger_1(\mathbf{r}), c^\dagger_d(\mathbf{r}), d_1(\mathbf{r}), d_d(\mathbf{r}) \}. \]

The $d_\sigma(\mathbf{r})$ operators are associated with the sites on the opposite sublattice of the one to which $\mathbf{r}$ belongs:

\[ d_\sigma(\mathbf{r}) = e^{-i\mathbf{Q} \cdot \mathbf{R}} \sum_\mathbf{R} \varphi(\mathbf{R}) c_{\sigma}(\mathbf{r} + \mathbf{R}), \]

where $\varphi(\mathbf{R})$ is given by

\[ \varphi(\mathbf{R}) = \sum_\mathbf{k} e^{i\mathbf{k} \cdot \mathbf{R}} \text{sgn}(\cos k_x - \cos k_y) = \frac{2}{\pi^2} \frac{1 - e^{i\mathbf{Q} \cdot \mathbf{R}}}{R_x^2 - R_y^2}, \]

which is only nonzero on the sublattice not including the origin. The long range nature of $\varphi(\mathbf{R})$ is crucial for the existence of strict SO(5) symmetry. $\Psi(\mathbf{r})$ transforms like a spinor under SO(5) transformations, i.e., under rotations in the $ab$ plane generated by the operators $L_{ab} = \frac{1}{2} \sum_\mathbf{R} \Psi^*(\mathbf{r}) \Gamma^{ab} \Psi(\mathbf{r})$, where $\Gamma^{ab}$ is a 4x4 matrix given in terms of tensor products of the standard 2x2 Pauli matrices: $\Gamma^1 = \sigma_x \otimes \sigma_y$, $\Gamma^2 = \sigma_y \otimes \sigma_x$, $\Gamma^3 = \sigma_z \otimes \sigma_z$, $\Gamma^4 = I \otimes \sigma_x$, $\Gamma^5 = \sigma_x \otimes \sigma_y$. The indices 2, 3, and 4 are written as $x$, $y$, and $z$ referring to the real space directions of the AF order parameter. It can be shown that $L_{15}$ corresponds to the charge counting operator $Q$, that $L_{yz} = L_{zy}$, and $L_{xz}$ correspond to the spin operators $S_x$, $S_y$, and $S_z$, and that $L_{1(x,y,z)}$ are related to the $\pi(x,y,z)$ operators rotating between the dSC and
AF sectors. As in Ref. 15 we now focus on the vector interaction, which in the real space representation takes the form

$$H_{\text{int}} = \sum_{\mathbf{r}, \mathbf{s}} V(\mathbf{r} - \mathbf{s}) \left\{ |\Psi(\mathbf{r})|^2 \Gamma^a \Psi(\mathbf{r})^\dagger \right\} |\Psi(\mathbf{s})|^2 \Gamma^a \Psi(\mathbf{s}). \quad (5)$$

In reality the SO(5) symmetry is broken. However, both the interpretation of the 41 meV excitation as a pseudo Goldstone mode relating to a rotation of the dSC phase into the AF phase, as well as the fact that the coupling strengths in the dSC and AF sectors are almost identical, make it plausible that the SO(5) breaking is weak. The long-range correlations of the $d$-operators apparent in Eqs. (3) and (4) lead to rather unphysical infinite-range hopping. A natural way to break the SO(5) symmetry is thus to truncate the sum, and we choose to maintain only nearest neighbor correlations,

$$d_{\sigma}(\mathbf{r}) - \overline{d}_{\sigma}(\mathbf{r}) = \frac{1}{2} e^{-iQ\cdot \mathbf{r}} \sum_{j=1}^{4} \varphi_{j} c_{\sigma}(\mathbf{r} + \delta_{j}), \quad (6)$$

where $\varphi_{j} = (-1)^{\delta_{j}}$. Not only does this truncation constitute a simple form relating both to SO(5) symmetry and to Hubbard-like models for dSC, but, as we shall see below, it also leads, in the homogeneous phases, to the expected (and observed) quasiparticle excitation spectra of the gapless antiferromagnet and the $d$-wave superconductor, respectively. We emphasize that our approximation is designed for this reason and not for our present purpose of explaining the vortex core excitations. Rather, the latter is a consequence of the former. Now follow two approximations. First, we make the usual assumption of a point interaction, $V(\mathbf{r} - \mathbf{s}) = -\frac{1}{2} V \delta(\mathbf{r} - \mathbf{s})$. And second, we utilize the standard mean-field approximation. These approximations result in the following SO(5) symmetry broken mean-field interaction Hamiltonian:

$$H_{\text{int}}^{\text{mf}} = -\sum_{\mathbf{r}} V[\mathbf{m}(\mathbf{r}) \cdot (\mathbf{m}(\mathbf{r})) + 2\{\Delta(\mathbf{r})(\Delta^\dagger(\mathbf{r})) + \text{H.c.}\}], \quad (7)$$

with the dSC and AF order parameters given by

$$\Delta(\mathbf{r}) = c_{\uparrow}(\mathbf{r}) \overline{d}_{\uparrow}(\mathbf{r}) + \overline{d}_{\uparrow}(\mathbf{r}) c_{\uparrow}(\mathbf{r}), \quad (8)$$

where

$$\mathbf{m}(\mathbf{r}) = \frac{1}{2} e^{iQ \cdot \mathbf{r}} \left[ (c_{\uparrow}(\mathbf{r}), c_{\uparrow}(\mathbf{r})) \right] \mathbf{a} \left[ (\overline{d}_{\uparrow}(\mathbf{r}), \overline{d}_{\uparrow}(\mathbf{r})) \right]. \quad (9)$$

We find that in $H_{\text{int}}^{\text{mf}}$ of Eq. (7) the SO(5) symmetry is broken in such a way that a $d$-wave gap function results in the pure SC phase, $E_k^2 = \epsilon_k^2 + [2V\Delta(\cos k_x - \cos k_y)]^2$, while a full ($d$-wave modulated) gap develops in the pure AF phase, $E_k^2 = \epsilon_k^2 + [\frac{1}{2} Vm[1 + (\cos k_x - \cos k_y)]^2]$. We elude the role of the gap in the AF sector we first study the continuum limit of our model. The important low-lying excitations in the fermionic sector are concentrated in the regions near the four $d$-wave gap nodes $Q_{\lambda} = (\pi/2)(\cos[\pi(\lambda/2 - 1/4)], \sin[\pi(\lambda/2 - 1/4)])$, where $\lambda = 1, 2, 3, 4$. We get rid of the rapid variations by local gauge transformations in each of the four quadrants $\lambda$ in $\mathbf{k}$ space: $c_{\sigma}(\mathbf{r}) = \sum_{\lambda} e^{iQ_{\lambda} \cdot \mathbf{r}} \psi_{\lambda, \sigma}(\mathbf{r})$. The gauge transformation is then used on $H_0$ (with $\mathbf{A} = 0$) and $H_{\text{int}}^{\text{mf}}$. Upon summing over $\mathbf{r}$ we keep only slowly varying terms, i.e., terms where $\exp[i(Q_{\lambda} \cdot \mathbf{r})] \mathbf{r}$ vanish. Not surprisingly, the only surviving terms are either diagonal in $\lambda$ or have $Q_{\lambda} = Q_{\lambda} + \mathbf{Q}$. This means that $\psi_{1, \sigma}(\mathbf{r})$ and $\psi_{3, \sigma}(\mathbf{r}) = \psi_{1, \sigma}(\mathbf{r})$ form one subspace, and $\psi_{2, \sigma}(\mathbf{r})$ and $\psi_{4, \sigma}(\mathbf{r}) = \psi_{2, \sigma}(\mathbf{r})$ form the other. It thus becomes natural to consider the spinors

$$\Psi_{\lambda}^{\dagger}(\mathbf{r}) = \{ \psi_{\lambda, \uparrow}^{\dagger}(\mathbf{r}), \psi_{\lambda, \downarrow}^{\dagger}(\mathbf{r}), \psi_{\lambda, \uparrow}^{\dagger}(\mathbf{r}), \psi_{\lambda, \downarrow}^{\dagger}(\mathbf{r}) \}. \quad \text{The gauge factor} \quad e^{iQ_{\lambda} \cdot \mathbf{r}} \text{leads to a sign change between the terms} \quad \psi_{\lambda, \sigma}(\mathbf{r} + \delta_{j}) \text{and} \quad \psi_{\lambda, \sigma}(\mathbf{r} - \delta_{j}) \text{in} \ H_0 \text{and} \ \Delta. \text{The difference terms arising from this become derivatives in the continuum limit. Further care is necessary regarding extra} \ Q_{\lambda} \text{-dependent signs. For simplicity we assume} \ \mathbf{m}(\mathbf{r}) = m(\mathbf{r}) \mathbf{e}_z \text{and obtain a final Hamiltonian for the} \ \Psi^{\dagger}_{\lambda}(\mathbf{r}):}$$

$$H = \int d\mathbf{r} \Psi^{\dagger}_{\lambda}(\mathbf{r}) \left( \begin{array}{cccc} -t(i\partial_z + i\partial_y) & -2V(i\partial_z - i\partial_y)\Delta(\mathbf{r}) & -\frac{1}{2} Vm(\mathbf{r}) & 0 \\
\frac{1}{2} Vm(\mathbf{r}) & t(i\partial_z + i\partial_y) & 0 & \frac{1}{2} Vm(\mathbf{r}) \\
0 & -t(i\partial_z + i\partial_y) & 2V(i\partial_z - i\partial_y)\Delta(\mathbf{r}) & 2V \Delta(\mathbf{r})(i\partial_z - i\partial_y) \\
0 & \frac{1}{2} Vm(\mathbf{r}) & 2V \Delta(\mathbf{r})(i\partial_z - i\partial_y) & -t(i\partial_z + i\partial_y) \end{array} \right) \Psi_{\lambda}(\mathbf{r}). \quad (10)$$

With the ansatz $\Psi^{\dagger}_{\lambda}(\mathbf{r}) = (a_1, a_2, a_3, a_4)e^{-i\mathbf{k} \cdot \mathbf{r}}$, and $k_z = k_x \pm k_y$ for $\mathbf{k} = (k_x, k_y)$ the eigenvalue problem becomes...
A pure SC phase has a constant $\Delta$, while $m=0$, and the spectrum becomes $E = \pm (r^2 k_+^2 + |2V| J^2 k_+^2)^{1/2}$. The corresponding eigenstates are easily found. For a pure AF phase $m$ is a constant and $\Delta=0$, and the spectrum now becomes $E = \pm (r^2 k_+^2 + (\frac{1}{2}Vm)^2)^{1/2}$, with associated eigenstates.

We now imagine the plane to be divided into two parts. For $x<0$ the system is in the SC phase while for $x>0$ it is in the AF phase. It is now simple to study the scattering problem where a particle with energy $|E| < Vm$ in the SC sector is moving towards the barrier formed by the AF sector. The result is not surprising: if the particle starts out with a momentum near, say, $Q_0$, it is completely reflected by the AF sector (where it only acquires an exponentially damped probability), and it ends up with a momentum near either $Q_0$ or $Q_0^\perp$. The process resembles Andreev reflection in the quantum number $\lambda$. The conclusion of this exactly solvable model is clear: low energy particles in the SC sector can be confined by a surrounding AF sector, or conversely, the AF sector expels low energy particles.

We now proceed to discuss dSC vortices, first briefly mentioning the case of normal cores followed by our SO(5) model calculation of vortices with AF cores. In his semiclassical analysis of the electronic density of states produced by $d$-wave vortices, Volovik showed that only a small part of the density of states results from quasiparticles localized at the vortex cores, and that that part is a function of the vortex density. Hence, in any realistic calculation of quasiparticle results, the density of states comes from quasiparticles localized at magnetic unit cell. Our unit cell contains two ordinary vortices on one diagonal and two vortices penetrated by Dirac antivortices on the other. Periodic forms of strings will have no physical consequences at all when placed between lattice sites. However, they allow for the construction of a vector potential periodic in the magnetic unit cell, through which the magnetic flux is zero.

We now construct a square Abrikosov lattice with a Dirac antivortex added to the center of every second vortex. Since each vortex carry half a flux quantum, the smallest magnetic unit cell possible consists of two vortices. However, due to better convergence properties in obtaining the periodic vector potential and a periodic representation of the SC order parameter [especially its phase $\theta(r)$], we choose to double the magnetic unit cell. Our unit cell contains two ordinary vortices on one diagonal and two vortices penetrated by Dirac antivortices on the other. Periodic forms of $\Delta(r)$, $\theta(r)$, and $m(r)$ are then easily found by adding up contributions from a large number of unit cells (typically 64) surrounding the one we are studying. From this we obtain a mean field lattice Hamiltonian $H = H_0 + H_{\text{int}}$ given by Eqs. (1) and (7), which is periodic in our unit cell. Based on the Bogoliubov transformation for the operators within our unit cell

$$A' = \sum_j A_0 (r - R_j),$$

$$\Delta (r) = f(r) e^{i\theta (r)} = \prod_j f_0 (r - R_j) e^{i \sum_j \arg (r - R_j)},$$

$$m (r) = \sum_j m_0 (r - R_j),$$

where $\arg (r - R_j)$ is the polar angle between $r$ and $R_j$. In a lattice model a particularly simple way to construct the magnetic unit cell is the following. For each area penetrated by one flux quantum $\hbar/e$ a Dirac antivortex string carrying a flux $-\hbar/e$ is added. The strings will have no physical consequences at all when placed between lattice sites. However, they allow for the construction of a vector potential periodic in the magnetic unit cell, through which the magnetic flux is zero.

where $\alpha = \pm 1$ is the spin index and $\tilde{\sigma} = -\sigma$, the equation of motion for the $\gamma^\alpha$ operators using the periodic Hamiltonian $H$ leads to the Bogoliubov–de Gennes equation for the eigenenergies and eigenstates of the fermionic quasiparticles:

$$\begin{pmatrix} T + \sigma M & D \\ D^* & -T^* + \sigma M \end{pmatrix} \begin{pmatrix} u^\alpha \\ \chi^\alpha \end{pmatrix} = E^\alpha \begin{pmatrix} u^\alpha \\ \chi^\alpha \end{pmatrix},$$
FIG. 1. LDOS in the vortex core (solid line) and in the bulk SC (dashed line) for (a) BCS s-wave SC, (b) BCS d-wave SC, and (c) SO(5) SC with an AF vortex core.

Here $E^a$ is the quasiparticle energy, $u^a$ and $v^a$ are vectors containing the values of $u^a(\mathbf{r})$ and $v^a(\mathbf{r})$ on each lattice site in our unit cell, while the block matrices $T$, $D$, and $M$ are given by

$$
(T)_{rr'} = -i e^{-i(e/\hbar)} \sum_{j=1}^{4} \delta_{r', r} \delta - \mu \delta_{r', r},
$$

$$
(D)_{rr'} = \sum_{j=1}^{4} \varphi_j [D(r') + D(r)] \delta_{r', r} + \delta_j,
$$

$$
(M)_{rr'} = \sum_{j,j'} \varphi_j \varphi_{j'} M(r') \delta_{r', r} + \delta_j - M(r) \delta_{r', r},
$$

with $D(r) = \frac{1}{2} V(\Delta(r))$ and $M(r) = \frac{1}{2} e^{\mathbf{Q} \cdot \mathbf{r}} V(\mathbf{m}(r))$.

In the numerical calculation we use a $N \times N$ lattice with $N=44$. The origin is put in the center and the four vortices in the center of each of the quadrants. The periodicity is ensured by having $H(\mathbf{r} + \mathbf{N} \delta_r) = H(\mathbf{r} + \mathbf{N} \delta_r) = H(\mathbf{r})$. The Bogoliubov–de Gennes equation, Eq. (16), becomes a $2N^2 \times 2N^2$ eigenvalue problem yielding for a given value of the spin variable $\sigma$ the spectrum $E^a$ and the Bogoliubov coefficients $u^a$ and $v^a$. To compare our calculations with the experimental STM measurements on vortices and with the existing calculations on ordinary sSC and dSC vortices we compute the temperature dependent local density of states (LDOS) according to the standard minimal model:

$$
N(\mathbf{r}, E) = \sum_a \left[ |u^a(\mathbf{r})|^2 \{ -f'(E^a - E) \} + |v^a(\mathbf{r})|^2 \{ -f'(E^a + E) \} \right],
$$

where $f(e) = [\exp(e/k_B T) + 1]^{-1}$, and where we have neglected the dispersion in the magnetic Brillouin zone. The calculation yields the LDOS shown in Fig. 1. In all cases $V=0.8t$, $k_B T=0.1r$, and $\mu = -0.6r$, which due to the band structure leads to an asymmetric LDOS.

First, to check our calculations, we change the model from SO(5) to ordinary sSC and dSC. The latter is produced by setting $M_{\mathbf{r}, \mathbf{r}'} = 0$ in Eq. (19), and the former by furthermore setting $(D)_{\mathbf{r}, \mathbf{r}'} = \frac{1}{2} V(\Delta(\mathbf{r})) \delta_{\mathbf{r}, \mathbf{r}'}$ in Eq. (18). As shown in Figs. 1(a) and 1(b) we confirm qualitatively the main conclusions of Refs. 7–9. In the bulk of the sSC phase a full gap is observed, while a midgap peak (which splits at $T=0$) develops in the center of a sSC vortex. In the bulk of the dSC phase a steady rise of the LDOS is seen around the midgap position, while a midgap peak develops in the center of a dSC vortex. Our model calculation captures mainly generic features and can therefore not be used in the ongoing debate of the detailed form of the LDOS in the dSC vortex core. However, this issue is not important for our main observation in the SO(5) case: instead of a midgap peak the LDOS is dramatically suppressed in the AF vortex core resembling bulk behavior as shown in Fig. 1(c). This confirms the conclusion of the dSC/AF interface in the SO(5) model studied in the first part of this paper. The AF phase effectively suppresses any fermionic low energy states.

We thus reach our main conclusion. The experimentally observed lack of electronic quasiparticle states in the center of Abrikosov vortices in BSCCO (Ref. 10) as opposed to the measurements of a normal metallic core of vortices in YBCO (Ref. 3) finds a natural explanation in the framework of the SO(5) model. As already pointed out by Arovas et al., the nature of the SO(5) vortex cores are governed by the parameters (e.g., doping level and coupling strengths) of the given high-$T_c$ material. The cores can either become metallic, i.e., a pure dSC behavior, or insulating, i.e., a mixed dSC/AF behavior. At the present stage of the SO(5) theory it is difficult to predict which materials will in fact develop AF vortex cores. For example, as is studied in the striped phase, the insulating vortex cores are negatively charged, since they must be at half filling, in contrast to the hole doped bulk material maintained at lower filling. Such a charging energy must be taken into account in a detailed calculation of the energy gained by forming an AF vortex core. Our calculation of the generic features in the fermionic sector of the SO(5) model shows that the measured LDOS can be explained if one simply assumes that YBCO with its metallic vortex cores is a pure dSC SO(5) superconductor, while BSCCO is a dSC/AF SO(5) superconductor. We obtained our results by studying both the analytically solvable model of a perfect SC/AF interface and by exact numerical diagonalization of an Abrikosov lattice model. Clearly, further theoretical insight in the dual dSC/AF nature of the high-$T_c$ compounds can be obtained from studies of the striped phases, where alternating stripes of SC phases and AF phases occur.

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12 S.-C. Zhang, Science 275, 1089 (1997).
19 For experimental observation of this modulation see F. Ronning et al., Science 282, 2067 (1998).
20 Mathematically, the Dirac string is added to a point $r_0$ by the gauge transformation $\chi(r) = -(\hbar/e) \arg(r-r_0)$.