Hidden quasi one-dimensional superconductivity in Sr$_2$RuO$_4$

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Using an asymptotically exact weak coupling analysis of a multi-orbital Hubbard model of the electronic structure of Sr$_2$RuO$_4$, we show that the interplay between spin and charge fluctuations leads unequivocally to triplet pairing which originates in the quasi-one dimensional bands. The resulting superconducting state spontaneously breaks time-reversal symmetry and is of the form $\Delta \sim (p_x + ip_y) \hat{z}$ with sharp gap minima and a d-vector that is only weakly pinned. The superconductor is topologically trivial and hence lacks robust chiral Majorana fermion modes along the boundary. The absence of topologically protected edge modes could explain the surprising absence of experimentally detectable edge currents in this system.

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Introduction - Sr$_2$RuO$_4$ is a layered perovskite material, isostructural to the hole-doped 214 family of cuprate superconductors. Below $T \sim 50K$, it exhibits Fermi liquid behavior and undergoes a superconducting transition at $T_c = 1.5K$. There is compelling experimental evidence which suggests that this superconducting state has odd parity and spontaneously breaks time-reversal symmetry. One of the simplest superconducting gap functions which meets both of these requirements is the chiral $p$-wave state, $\Delta(p) \propto (p_x + ip_y) \hat{z}$, a quasi-two-dimensional version of superfluid $^3$He-A.

In its simplest form, this chiral pairing gives rise to a topological superconductor: all Bogoliubov quasiparticle excitations are gapped in the bulk whereas topologically protected chiral Majorana fermion modes exist at the edge of the system and in vortex cores. These modes are robust against all perturbations, including disorder, so long as the BCS pairing gap in the bulk remains finite. In addition, spontaneous supercurrents are expected at sample edges and domain walls.

However, scanning squid and Hall bar imaging studies have revealed that edge currents of the expected magnitude are not found in Sr$_2$RuO$_4$. Moreover, low temperature power laws in the electronic specific heat and the nuclear spin relaxation $1/T_1$ suggest that this material is not a simple chiral superconductor, which would exhibit exponentially activated behavior in both of these quantities. The form of the superconducting order parameter which accounts for all of the observed phenomena remains unknown. Resolution of this puzzle could come from a careful consideration of the normal state properties, which are known with unprecedented detail.

The Fermi surface of Sr$_2$RuO$_4$ consists of 3 sheets, denoted $\alpha, \beta, \gamma$. The $\alpha$ and $\beta$ sheets are hole and electron pockets respectively; they are comprised primarily of the Ru $d_{xz}, d_{yz}$ orbitals which form quasi one dimensional bands. The $\gamma$ sheet is composed mainly of the Ru $d_{xy}$ orbital, which forms a quasi two dimensional band. A variety of experiments have shown that the system behaves as a quasi two dimensional Fermi liquid with considerable effective mass enhancements. Therefore, it is likely that electron correlations play a significant role in influencing the pairing mechanism of this system.

In this paper, we present a microscopic theory of superconductivity in Sr$_2$RuO$_4$. Using a simple extension of a recently developed asymptotically exact weak-coupling analysis of the Hubbard model, we show that the dominant superconducting instability is in the triplet channel and occurs on the quasi-1D Fermi surfaces of Sr$_2$RuO$_4$. The resulting superconducting state spontaneously breaks time-reversal symmetry. It exhibits node-like behavior since it possesses points on the Fermi surface where the gap is parametrically small. It supports Andreev bound states at domain walls and at the edges of the system. However, it is a topologically trivial superconductor without chiral Majorana fermion modes, or detectable spontaneous supercurrents at the edges.

Microscopic model - We consider a simple Hamiltonian with three bands derived from the Ru $t_{2g}$ orbitals

$$H = H_0 + U \sum_{i\alpha} n_{i\alpha \uparrow} n_{i\alpha \downarrow} + \frac{V}{2} \sum_{i,\alpha \neq \beta} n_{i\alpha} n_{i\beta} + \delta H$$ (1)
Here, we introduce vector indices such that $\alpha = x, y, \text{ and } z$, refer, respectively, to the Ru $d_{\alpha z}$, $d_{\alpha y}$, and $d_{\alpha x}$ orbitals, $n_{i\alpha\sigma}$ is the density of electrons having spin $\sigma$ at position $i$ in orbital $\alpha$ and $n_{i\alpha} = \sum_\sigma n_{i\alpha\sigma}$. The strength of the repulsive interaction between two electrons on like (distinct) orbitals at the same lattice site is given by $U(V)$. 

$$H_0 = \sum_\alpha \sum_\sigma (\epsilon_{\alpha\hat{k}} - \mu) c^\dagger_{\alpha\hat{k}\sigma} c_{\alpha\hat{k}\sigma}$$

is the dominant intra-orbital kinetic energy and gives rise to three decoupled energy bands at the Fermi level as shown in Fig. 1. Here, we make use of the following tight-binding parametrization of these energies:

$$\epsilon^0_{x(y)}(\hat{k}) = -2t \cos k_x(y) - 2t^\perp \cos k_x(x)$$

$$\epsilon^0_\alpha(\hat{k}) = -2t' (\cos k_x + \cos k_y) - 4t'' \cos k_x \cos k_y$$

where we take $(t, t^\perp, t'', \mu) = (1.0, 0.1, 0.8, 0.3, 1.0)$ [14] [15]. The quantity $\delta H$ represents smaller terms such as longer range hopping and spin orbit coupling (SOC) which mix the distinct orbitals. It plays a relatively minor role in determining the superconducting transition temperature. However, $\delta H$ plays a crucial role in selecting a superconducting state which breaks time-reversal symmetry, as will be discussed below. When $\delta H = 0$, the non-interacting susceptibilities of the normal state are separate functions for each orbital:

$$\chi_\alpha(\vec{q}) = \int \frac{d^2 k}{(2\pi)^2} \frac{f(\epsilon_{\alpha\hat{k}+\vec{q}}) - f(\epsilon_{\alpha\hat{k}})}{\epsilon_{\alpha\hat{k}+\vec{q}} - \epsilon_{\alpha\hat{k}}}$$

(3)

where $f(\epsilon)$ is the Fermi function. Since the quasi-two dimensional band is almost circular with a radius $k_f^{2d}$, its susceptibility is nearly constant: $\chi_\alpha \approx 1/4\pi t'$ for $\vec{q} < 2k_f^{2d}$. In contrast, the quasi-1D bands have susceptibilities that are peaked at $\vec{q}_\alpha = (2k_f^{2d}, \pi)$ and $\vec{q}_\alpha = (\pi, 2k_f^{2d})$ for the x and y orbitals, respectively. It is the structure of $\chi_x$ and $\chi_y$ which gives rise to the incommensurate spin fluctuations in the material [17].

Since the superconductivity in Sr$_2$RuO$_4$ evolves out of a Fermi liquid and $T_c \ll E_f$, it is reasonable to carry out a weak coupling analysis which treats the limit $U, V \ll W$ where $W$ is the bandwidth. In this limit, superconductivity is the only instability of the Fermi liquid, and it can be treated in an asymptotically exact manner via a two-stage renormalization group analysis [13]. In the first stage, high energy modes are perturbatively integrated out above an unphysical cutoff, and an effective particle-particle interaction in the Cooper channel is derived:

$$\Gamma_s(\hat{k}, \hat{q}, \alpha) = U + U^2 \chi_\alpha(\hat{k} + \hat{q}) - 2V^2 \sum_{\beta \neq \alpha} \chi_\beta(\hat{k} - \hat{q})$$

$$\Gamma_I(\hat{k}, \hat{q}, \alpha) = -U^2 \chi_\alpha(\hat{k} - \hat{q}) - 2V^2 \sum_{\beta \neq \alpha} \chi_\beta(\hat{k} - \hat{q})$$

(4)

where $\Gamma_\alpha(\hat{k}, \hat{q}, \alpha)$ ($a = s \text{ or } t$) is the effective interaction in the singlet(triplet) channel. In the second stage, the renormalization group flows of these effective interactions are computed and the superconducting transition temperature is related to the energy scale at which an effective interaction grows to be of order 1. Following this prescription, one obtains

$$T_c \sim W e^{-1/|\lambda_0^{(a,\alpha)}|}$$

(5)

where $\lambda_0^{(a,\alpha)}$ is the most negative eigenvalue of the matrix

$$\delta \Gamma_{k,\hat{q}}^{(a,\alpha)} = \sqrt{\frac{v_f}{v_f(k)}} \Gamma_s(\hat{k}, \hat{q}, \alpha) \sqrt{\frac{v_f}{v_f(q)}}$$

(6)

with $\hat{k}$ and $\hat{q}$ constrained to lie on the Fermi surface of band $\alpha$. The pair wavefunction in the superconducting state is proportional to the associated eigenfunction [13].

The values of $\lambda^{(a,\alpha)}$, obtained by numerical diagonalization, are presented in Fig. 2. When $V = 0$, the two dimensional z band has its dominant pairing instability in the singlet $d_{x^2-y^2}$ channel and a substantially lower pairing strength in the triplet p-wave channel. By contrast, the pairing tendencies of the x and y bands are stronger, and exhibit a close competition between singlet and triplet pairing [22]. When $V > 0$, only triplet pairing in the quasi-one dimensional bands is enhanced. Since the solutions with weaker pairing strengths have exponentially smaller transition temperatures in the weak-coupling limit, the effect of subdominant orders is negligible. Thus, in the asymptotically weak coupling limit, the dominant superconducting instability occurs in the quasi-one dimensional bands in the spin-triplet channel. For
\[ \delta H = \sum_{k,\sigma} \left[ g(\vec{k}) c_{\alpha, k, x, \sigma}^\dagger c_{\alpha, k, y, \sigma} + \text{H.C.} \right] + \eta \sum_{\alpha, \beta} \sum_{\sigma, \sigma'} \sum_{\vec{k}} c_{\alpha, k, x, \sigma}^\dagger c_{\beta, k, y, \sigma'} \ell_{\alpha, \beta} \cdot \vec{\sigma} \sigma' \]

where \( g(\vec{k}) = -2t'' \sin k_x \sin k_y \), the second quantity above is the SOC, and the angular momentum operators are expressed in terms of the totally anti-symmetric tensor as \( \ell_{\alpha, \beta} = \imath \epsilon_{\alpha \beta} \). Recent electronic structure calculations have produced the estimates \( t'' \approx 0.1t \) and \( \eta \approx 0.1t \) \[16, 20\].

There are several important qualitative effects of including these additional terms in the Hamiltonian: 1) Non-zero \( t'' \) or \( \eta \) pins the relative phase, \( \theta_x - \theta_y \), and relative orientation, \( \Omega_x, \Omega_y \), of the \( d \) vectors. 2) Non-zero \( \eta \) defines a preferred ordering direction for \( \Omega_a \). 3) The nodes on the \( xz \) and \( yz \) Fermi surfaces are gapped, although the gap is parametrically small for small \( \delta H \). To understand the role of \( \delta H \) in selecting among the large number of possible ordered phases, it is simplest to consider the Landau free energy \( F \) to low order in powers of the order parameter which is a valid approximation near \( T_c \). Since any order induced on the \( x \) band is slaved to the primary order on the \( x \) and \( y \) bands, we keep explicitly only \( \alpha = x, y \), in which case

\[ F = \sum_{\alpha} \left[ r |\tilde{d}_\alpha(\vec{k})|^2 + u |\tilde{d}_\alpha(\vec{k})|^4 + \gamma |\tilde{d}_\alpha(\vec{k}) \times \tilde{d}_\alpha(\vec{k})|^2 \right] \]

where the terms in the first line survive the \( \delta H \rightarrow 0 \) limit, \( a_1 \sim \mathcal{O}(\eta^2/t^2) \), and \( v_1 \) and \( J \) have contributions of order \( (\eta/t)^2 \) and \( (t''/t)^2 \). To quadratic order in the order parameters and to order \( (\eta/t)^2 \), \( (t''/t)^2 \), this expression is the most general one consistent with symmetry, but for the quartic terms, in the interest of simplicity, we have assumed that the SOC is weaker than the band-mixing, and so have enforced spin rotational symmetry. Since \( |v_1| \ll u \), the terms on the third line are not qualitatively important. When the action is derived from any form of BCS theory, it is possible to show that \( \gamma \) and \( J_1 > 0 \).

Thus, there are two possible phases depending on the sign and magnitude of \( a_3 \): (a) For \( a_3 > \text{Min}[0, a_2] \), there are time-reversal symmetry preserving “B” phase states (analogous to the B-phase in \( ^3\text{He} \)) in which \( \Omega_x \cdot \hat{z} = \Omega_y \cdot \hat{z} = 0 \) and \( \theta_x = \theta_y \). Depending on the sign of \( a_2 \), either \( \Omega_x = \hat{x} \) or \( \Omega_x = \hat{y} \). (b) For \( a_3 > \text{Min}[0, a_2] \), there is a “chiral p+ip” state (analogous to the A phase in \( ^3\text{He} \)) with \( \Omega_x = \Omega_y = \hat{z} \) and \( \theta_x - \theta_y \pm \pi/2 \). All other configurations have a higher Free energy and can be neglected.

The parameters \( a_j \) can be related to differences of susceptibilities of the non-interacting system, and so can be computed directly from the assumed band-structure. For the stated parameters, we find that \( a_1 < \text{Min}[0, a_2] \), so the chiral state is preferred. However, the balance is delicate, and this conclusion is not robust against small changes to the model.

Next, we address the fate of the gap nodes when \( \delta H \neq 0 \). We have studied the BdG Hamiltonian for the chiral state using the gap functions derived in the

FIG. 3: (Color online) (a) In the absence of any band mixing, the triplet state within the \( xz \) orbital (red) has \( k_x \)-wave symmetry and has line nodes near \( k_y = \pi/2 \) (dashed line). The condensate on the \( yz \) orbital (grey) is related to the one shown here by a 90-degree rotation. (b) The chiral state which results when small band mixing perturbations are taken into account. The relative phase factors on different portions of the Fermi surface are shown.
previous section. Generically, the resulting state is nodeless. However, although the nodes are not topologically stable, they are parametrically small: where a gap node occurs for \( \delta H = 0 \), the induced gap is \( \sim \Delta_0 \left[ O(t^2/|t|^2) + O(\eta^2/|t|^2) \right] \). The energy scale of these gap minima is therefore two orders of magnitude smaller than the transition temperature.

**Topological properties and edge currents -** Next, we consider the topological properties of the system assuming that \( a_1 < \min\{0, a_2\} \), so the chiral state is preferred. The BdG Hamiltonian for the quasiparticle excitations in the superconducting state can then be expressed in terms of Anderson pseudo-spins as

\[
H_{\text{BdG}} = \sum_{\nu, \vec{k}} \Psi_{\nu \vec{k}}^\dagger \left[ \hat{\delta}_\nu(\vec{k}) \cdot \vec{\tau} \right] \Psi_{\nu \vec{k}}. \tag{11}
\]

where \( \Psi_{\nu \vec{k}} \) are Nambu spinors, \( \nu = \alpha, \beta \) runs over the two quasi-1D bands, \( \vec{\tau} \) are the Pauli matrices, and the pseudo-Zeeman field is

\[
\hat{\delta}_\nu(\vec{k}) = \left( \text{Re}[\Delta_\nu(\vec{k})], \text{Im}[\Delta_\nu(\vec{k})], \epsilon_\nu(\vec{k}) - \mu \right) . \tag{12}
\]

For the chiral p-wave state, the pseudospin has the form of a skyrmion in momentum space: it points along the \(-\hat{z} (+\hat{z})\)-direction inside(outside) the Fermi surface, and on the Fermi surface, it lies in plane, winding by \( 2\pi \) around the Fermi surface. The topological properties of the chiral state come from the integer skyrmion number

\[
N_\nu = \frac{1}{4\pi|\tilde{\delta}_\nu(\vec{k})|^3} \int d^2\vec{k} \tilde{\delta}_\nu \cdot \left( \partial_\alpha \tilde{\delta}_\nu \times \partial_\beta \tilde{\delta}_\nu \right) \tag{13}
\]

where \( |\tilde{\delta}_\nu(\vec{k})| = \sqrt{\epsilon_\nu(\vec{k}) - \mu)^2 + |\Delta_\nu(\vec{k})|^2} \). The net number of chiral quasiparticle modes at the edge of the superconductor is given by the skyrmion number, and so long as \( N_\nu \neq 0 \), these modes are topologically protected, and cannot be localized by backscattering.

As \( N_\nu \) is an integer, small changes in the spectrum do not affect it. However, it is odd under \( \Delta_\nu \rightarrow \Delta_\nu^* \) (i.e. upon transforming \( p_x + ip_y \rightarrow p_x - ip_y \)) or under a particle-hole transformation, \( \epsilon_\nu - \mu \rightarrow \mu - \epsilon_\nu \). As can be seen in Fig. 1, hybridization between the two quasi-1D bands results in the closed \( \alpha \) and \( \beta \) Fermi surfaces, the former electron-like and the latter hole-like. Consequently, in a chiral \( p_x + ip_y \) state, \( N_\alpha = -N_\beta \), or in other words the net skyrmion number is zero so it is not a topological superconductor! The chiral edge modes along the boundary of the superconductor and along domain walls are not protected: in the presence of disorder or interactions that scatter a pair from one Fermi surface to the other, the counter-propagating edge modes from the two bands are localized [19].

The existence of edge currents in a chiral p-wave superconductor follows from symmetry, but whether or not it is large enough to detect is still an issue. There is a bulk contribution to the edge current which originates from the multi-component nature of the order parameter, and one from the chiral quasiparticle modes near the edge of the system. We will address the question of how the highly non-circular band structure of the quasi 1D bands affects the bulk contribution in a future publication [19]. Since the chiral quasiparticle modes travel with velocity \( v = v_f(\Delta/E_f) \), they would, by themselves, make a readily detectable contribution \( O(\Delta/E_f) \) to the edge current, were they not localized.

**Discussion -** It follows from general arguments [21] that near \( T_c \), superconductivity can arise either in the \( \{\alpha, \beta\} \) pockets or in the \( \gamma \) pocket; below \( T_c \), superconductivity is induced in the subdominant Fermi surfaces via a proximity effect

\[
\delta H_{\text{prox}} = J' \sum_{\nu, \nu'} c_{\nu \downarrow}^\dagger c_{\nu' \uparrow} c_{\nu' \downarrow} c_{\nu \uparrow}, \tag{14}
\]

with \( J' \ll U \). Due to the weakness of this proximity effect, it can be expected that for a range of temperatures \( J'(\Delta/E_f) \ll T < T_c \), superconductivity is present essentially only on the dominant portions of the Fermi surfaces. Nonetheless, in the present case, this coupling produces a small gap on the \( xy \) Fermi surface, which then adds to the skyrmion number; while the energy scales involved are likely too small to affect the results of any practical experiment, ultimately the proximity effect restores the topological character of the chiral superconducting state.

As we have shown, it is unavoidable, given the bandstructure of \( \text{Sr}_2\text{RuO}_4 \), and assuming the interactions are weak, that the superconductivity arises primarily on the quasi-1D bands. Within this framework, there is a natural explanation for the surprising absence of superconductivity in the closely related bilayer compound \( \text{Sr}_3\text{Ru}_2\text{O}_7 \); the bilayer splitting in \( \text{Sr}_3\text{Ru}_2\text{O}_7 \) primarily affects the quasi-1D bands, leaving the 2D \( d_{xy} \) band essentially unchanged. If pairing occurred primarily on the quasi-2d band, both compounds ought to be similarly superconducting. (An analysis of superconductivity in the bilayer system will be presented in a separate publication [19]).

Admittedly, we cannot rule out the possibility that strong coupling effects will change this conclusion. However, the absence of experimentally detectable edge currents is difficult to reconcile with a state which primarily involves the 2D bands. Further analysis of the experimental evidence concerning this issue will be postponed to a future paper [19]. We will also discuss the nature of the collective modes which reflect the near independence of the superconducting state on each of the quasi-1d bands, especially near the transition temperature.

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