Theory of chiral $p$-wave superconductivity with near-nodes for Sr$_2$RuO$_4$

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We use functional renormalization group method to study a three-orbital model for superconducting Sr$_2$RuO$_4$. Although the pairing symmetry is found to be chiral $p$-wave, the atomic spin-orbit coupling induces near-nodes for quasiparticle excitations. Our theory explains a major experimental puzzle between $d$-wave-like feature observed in thermal experiments and the chiral $p$-wave triplet pairing revealed in nuclear-magnetic-resonance and Kerr effect.

PACS numbers: 74.20.-z, 71.27.+a, 74.20.Rp

Introduction: The layered perovskite ruthenate Sr$_2$RuO$_4$ is one of the rare candidate materials that is expected to carry chiral $p$-wave pairing in the superconducting (SC) state. Nuclear magnetic resonance (NMR) [1–4] and spin polarized neutron scattering [5] measurements show absence of drop in the spin susceptibility below the SC transition temperature $T_c$, providing identification of spin-triplet pairing in Sr$_2$RuO$_4$. Muon spin relaxation [6] and polar Kerr effect [7] experiments reveal that time reversal symmetry in Sr$_2$RuO$_4$ is spontaneously broken below $T_c$, suggesting chiral $p$-wave triplet pairing. The $d$-vector of the triplet is proposed as $\hat{z}(k_x \pm ik_y)$, [8, 9] which is analogous to that in the superfluid $^3$He-A phase. [10] In this case, the SC state is likely fully gapped, since no symmetry forces the chiral $p$-wave gap function to vanish on the quasi two-dimensional Fermi surface (FS) of the layered Sr$_2$RuO$_4$.

In experiments, however, low-energy quasi-particle excitations deep in the SC state, characteristic of gap nodes on the FS (forming nodal lines along the direction perpendicular to the RuO$_2$ plane), are observed in specific heat, [11–13] superfluid density, [14] spin-lattice relaxation rate, [15] thermal conductivity [16–18] and ultrasound attenuation [19] at low temperatures. To explain the nodal-like behavior, a simple scenario is to assume $d$-wave pairing symmetry, so that the gap nodes are symmetry protected. This scenario is, however, inconsistent with the compelling signatures of chiral $p$-wave triplet mentioned above. An alternative scenario is the chiral $p$-wave gap function may have deep minima or accidental nodes.[20–24] The linear specific heat and thermal conductivity below $T_c/2$ suggest that the gap minimum $\Delta_{\text{min}}$ should be much smaller than the gap maximum $\Delta_{\text{max}}$.[21, 22] The recent thermal conductivity measurement [18] sets an upper bound $\Delta_{\text{min}}/\Delta_{\text{max}} \leq 1/100$, and the field dependence suggests $d$-wave pairing, or $d$-wave-like $f$-wave pairing in the form of $(k_x + ik_y)g(k)$, where $g(k) \sim k_xk_y$ or $k_x^2 - k_y^2$.[25–27]

Sr$_2$RuO$_4$ has three energy bands ($\alpha$, $\beta$ and $\gamma$, derived from the $d_{x^2,y^2,z^2,yz}$ orbitals) crossed by the Fermi level, with the $\gamma$ Fermi pocket closer to the van Hove singularity (vHS) on the zone boundary. The singular-mode functional renormalization group (SMFRG) study of the three-orbital model without spin-orbit coupling (SOC) [24] showed that the gap function on the $\gamma$ pocket is largest and strongly anisotropic, with $\Delta_{\text{min}}/\Delta_{\text{max}} \sim 1/10$. However, such a gap structure is not yet enough to explain the linear specific heat and thermal conductivity at the measured low temperatures. Models with SOC were previously studied by using weak coupling RG and random phase approximation.[28, 29] But to our knowledge, close and systematic comparisons to experiments have not been reported.

The outstanding puzzle of the chiral $p$-wave pairing revealed in NMR and Kerr effect and the $d$-wave-like behavior indicated in thermal experiments motivates us to perform more careful microscopic investigations. We consider a comprehensive model including all of the three orbitals and the atomic SOC. We adopt the band structure (with the effect of SOC) that best fits the angular-resolved photo-emission spectroscopy measurement.[30] We apply the spin-resolved version of SMFRG [31–34] and treat all possible ordering tendencies on equal footing.

Our main results are summarized in Figs.4 and 5. We find that chiral $p$-wave pairing is dominant and can be related to the small-momentum spin fluctuations derived from the $d_{xy}$ orbital, similarly to the case in Ref.[24]. However, SOC induces near-nodes on the $\gamma$ pocket, with $\Delta_{\text{min}}/\Delta_{\text{max}} < 1/100$. SOC also induces sizable and anisotropic gaps on the $\alpha$ and $\beta$ pockets. The calculated specific heat, superfluid density, Knight shift, spin-lattice relaxation rate and thermal conductivity are in excellent agreement with experimental data, superior to the $d$-wave fits. Our theory reconciles the $d$-wave-like feature in thermal measurement and chiral $p$-wave spin triplet pairing in NMR and Kerr effect in Sr$_2$RuO$_4$. 
Here $\psi$ can be written as $H$ Hamiltonian dispersion in the complete energy window.

Also indicated roughly by the colored linewidth. Inset: The $d$ derived from the black lines) along high-symmetry cuts. The spectral weight (color scale) dominates,

FIG. 1: Main panel: Low energy band dispersion (thin black lines) along high symmetry.

Model and method: We now specify the model Hamiltonian $H = H_0 + H_1$ for Sr$_2$RuO$_4$. The free part can be written as

$$H_0 = \sum_k \psi_k^\dagger h_k \psi_k, \quad h_k = \epsilon_k \sigma_0 - \lambda \mathbf{L} \cdot \mathbf{\sigma}/2. \quad (1)$$

Here $\psi_k = (c_{k1}, c_{k2}, c_{k31}, c_{k31}, c_{k21}, c_{k34})^T$ is the fermion spinor, with $c_{s\alpha}$ annihilating an electron of momentum $k$ and spin $s \in \{\uparrow, \downarrow\}$ on orbital $\alpha \in (1, 2, 3) \leftrightarrow (d_{xz}, d_{yz}, d_{xy})$. In the single-particle Hamiltonian $h_k$, $\epsilon_k$ is a matrix in the orbital basis, $\mathbf{L}$ is the orbital angular momentum, and $\mathbf{\sigma}/2$ is the spin angular momentum. The SOC parameter is $\lambda = 0.032 eV.$ [30] and the other details can be found in Ref. [30] and also in the Supplemental Material (SM). [35]

FIG. 1 shows the band dispersion (thin black lines) along high symmetry

cuts. Each band is degenerate in pseudo-spin, forming a Kramers doublet at each momentum. Notice that near the Fermi level the $d_{xy}$-weight (color scale) dominates, implying its importance in driving instabilities in the presence of interactions, but it is missing along G-M on the $\gamma$-pocket. We will come back to these features below.

The interacting part of the Hamiltonian $H$ is given by, in real space,

$$H_I = U \sum a \ n_{ia\uparrow} n_{ia\downarrow} + J \sum_{i,a>b} \mathbf{c}_{ia}^\dagger \mathbf{c}_{ib} \mathbf{c}_{ib}^\dagger \mathbf{c}_{ia},$$

where $i$ denotes the lattice site, $n_{ia} = \sum \mathbf{c}_{ia}^\dagger \mathbf{c}_{ia}$, $U$ is the intra-orbital repulsion, $U'$ is the inter-orbital repulsion, $J$ is Hund’s rule coupling, and $J'$ is the pair hopping term. The interactions can lead to competing collective fluctuations in particle-hole (PH) and particle-particle (PP) channels, which we handle by SMFRG. The idea of FRG [36] is to obtain the one-particle-irreducible 4-point interaction vertices $\Gamma_{1234}$ (where numerical index labels single-particle state) for quasi-particles above a running infrared energy cut off $\Lambda$ (which we take as the lower limit of the continuous Matsubara frequency). Starting from $\Lambda = \infty$ where $\Gamma$ is specified by the bare parameters in $H_I$, the contribution to the flow (toward decreasing $\Lambda$) of the vertex, $\partial \Gamma_{1234}/\partial \Lambda$, is illustrated in Fig. 2. At each stage of the flow, we decompose $\Gamma$ in terms of eigen scattering modes (separately) in the PP and PH channels to find the negative leading eigenvalue (NLE), the divergence of which signals an emerging order at the associated collective momentum, with the internal microscopic structure described by the eigenfunction. The technical details can be found elsewhere.[24, 31–34, 37–41] and also in the self-contained SM.[35]

Discussions: We consider the bare interaction parameters $(U, U', J, J') = (0.4, 0.16, 0.04, 0.04) eV$. The results are qualitatively robust against fine tuning around this setting, see SM.[35] Fig. 3 shows the flow of NLE $S_{PP}$ in the PH channel (a), and $S_{PP}$ in the PP channel (b). At high energy scales, $S_{PP}$ dominates over $S_{PP}$. The corresponding collective momentum in the PH channel changes from $Q_1 \sim (0.719, 0.719) \pi$ at high energy scale to $Q_2 \sim (0.219, 0.219) \pi$ in the intermediate stage. The eigenfunction shows the scattering mode describes site-local spin. The $d_{xz,yz} (d_{xy})$ orbitals dominate before (after) the level crossing. The inset shows the NLE $S_{PH}(q)$ as a function of momentum $q$ at the final stage of the FRG flow. We see a strong peak at $Q_2$ and also a secondary peak at $Q_1$. These peaks are consistent with that observed in neutron scattering experiments.[42] Our results provide clear origins of such peaks: spin fluctuations at $Q_1 (Q_2)$ arise mainly from the $d_{xz,yz} (d_{xy})$ orbital, similarly to the case without SOC.[24]

Here the dominant $d_{xy}$ component is made possible by the prevalence of the $d_{xy}$ spectral weight near the
reduces the amplitude (at zone boundary known previously,[24] but the SOC can be ascribed to the proximity to the vHS on the d-wave amplitude), but that on the \( \beta \) and \( \alpha \) pockets follows the usual \( k_x + i k_y \) pattern (with modulated amplitude), but that on the \( \gamma \) pocket is more complicated. The phase changes very fast across G-X, but converges along G-M slowly. This follows from anti-phase pairing between \( d_{xy} \)-electrons on first- and second-neighbor bonds, see SM.[35] (ii) Fig.4(b) shows a gap minimum at \( \theta = 0 \) on the \( \gamma \) pocket, the gap also vanishes at \( \theta = 45^\circ \) (or along G-M), which would have been the maximum without SOC. This feature is related to the fact that the \( d_{xy} \)-weight is missing on the Fermi pocket along G-M (see Fig.1), whereas the dominant pairing component involves \( d_{xy}-orbital.[35] \) (iv) SOC also induces sizable gaps on the \( \alpha \) and \( \beta \) pockets, but with large anisotropy. The relative gap size (to that on the \( \gamma \) pocket) is significantly larger than that without SOC.[24]

We calculate various properties of the SC state using the FRG-derived mean field theory,[35] and compare to the experimental data. No other tuning parameters are invoked regarding the gap structure.[43] The results are presented in Fig.5. In the experimental regime, our gap structure behaves effectively nodal, and could in fact fit the data better than that in the \( d \)-wave case, e.g., for the thermal conductivity. The details are as follows.

The numerical result for the specific heat (solid line) is presented in Fig.5(a), along with the experimental data (symbols) extracted from Ref.[11], where a high-quality sample with \( T_c = 1.48 \)K was investigated. We find excellent agreement both in the linear behavior below \( T_c/2 \) and the jump at \( T_c \).

The calculated superfluid density \( \rho \) (solid lines) is shown in Fig.5(b), along with experimental data (symbols) with \( T_c = 1.39 \)K.[14] for scattering rate \( \zeta/T_c = 0.1 \) and 0.5, respectively. We estimate the elastic scattering rate \( \zeta \) from nonmagnetic impurities in the experimental situation as,[44, 45]

\[
\ln(T_{c0}/T_c) = \Psi(1/2 + \zeta/2\pi T_c) - \Psi(1/2), \tag{3}
\]

where \( \Psi(x) \) is the digamma function, \( T_{c0} = 1.5K \).
is assumed to be the transition temperature in the disorder-free material. We get \( \zeta / T_c \sim 0.1 \) for \( T_c = 1.39 \) K according to Eq.3. Using this value of \( \zeta \), the result (green line) deviates from the data (symbols) in view of the curvature in the intermediate temperature window. (The same curvature problem occurs in the d-wave case not shown here.) However, if we assume \( \zeta / T_c = 0.5 \), the result (blue line) is in much better agreement with the data, suggesting that either the sample in the experiment is dirtier than the estimate according to Eq.3, or the clean limit \( T_0 \) might be even higher than 1.5K.

The calculated spin-lattice relaxation rate \( 1 / T_1 \) (solid lines) is shown in Fig.5(c), along with the experimental data (symbols) from Ref.15, where \( T_c = 1.48K \) corresponds to \( \zeta / T_c = 0.26 \) via Eq.3. We find good agreement: both experimental and theoretical results show \( 1 / T_1 \propto T^3 \) at low temperatures. The Knight shift \( K_{\mu \nu} \) depends on the probed spin direction \( \mu \), see Fig.5(d). \( K_{xx,yy} \) barely changes, while \( K_{zz} \) is suppressed below \( T_c \). This is the anticipated behavior of triplet Cooper pairing with its d-vector along z, which is indeed dominant in our pairing function.[35] In experiment, \( K_{zz} \) is also unchanged below \( T_c \), and this might be understood if the z-direction field could align the spin of the Cooper pair (or rotate the d-vector toward the plane), given the small energy gap. [2, 46]

Finally, we address the thermal conductivity \( \kappa \). Fig.5(e) shows the calculated \( \kappa / T \) versus \( \zeta \) (solid line) at the fixed low temperature \( T = T_0 = T_c / 30 \), compared to the experimental data (symbols) from Refs.[16–18]. We see our chiral p-wave case (solid line) fits the data very well, including the universal behavior \( \kappa / T \propto 1 / \zeta \) at \( \zeta / T_0 = 30 \), \( \zeta / T_c \gg 1 \), and the mild decrease near and below \( \zeta / T_c = 0.4 \). In contrast, in the d-wave case (dashed line) \( \kappa / T \) increases monotonically with decreasing \( \zeta \), although it also shows universal behavior on the large-\( \zeta \) side. (Note the eventual rise as \( \zeta / T_0 \to 0 \) is beyond the realm of the theory of universal conductance even for the d-wave case,[35, 47] but in both cases can be explained by Boltzman equation for well-defined quasiparticles, which predicts \( \kappa / T \propto 1 / \zeta \). On the other hand, we have normalized the numerical \( \kappa / T \) by \( \gamma_n \), the value of \( \kappa / T \) with \( T = T_0 \), \( \zeta = 0.6T_c \), and zero gap. This leaves the relative size of \( \kappa / T \) in the p- and \( d \)-wave cases unambiguous.) Therefore, the experimental data, rather than implying \( d \)-wave pairing, actually supports a gap structure with various gap minima on the three Fermi pockets, as in our chiral p-wave case. This is supported by further discussions in SM.[35] Of course, if the probing temperature \( T_0 \) is reduced further, so that \( T_0 \ll \Delta_{\min} \), \( \kappa / T \) is eventually suppressed.[35] At this stage the \( d \)-wave and chiral p-wave behave most differently. Measurement at such low temperatures is important to close the issue, but might be a challenge in experiment.

**Summary and remarks:** We studied the superconductivity of Sr₂RuO₄ by the state-of-art SMFRG. We find that chiral p-wave pairing is dominant, but SOC induces deep near-nodes on the \( \gamma \) pocket and also sizable and anisotropic gaps on the \( \alpha \) and \( \beta \) pockets. The microscopic theory is in excellent agreement with

![Figure 5](image-url)
experiments, resolving the outstanding puzzle between the d-wave-like feature in thermal measurements and the chiral p-wave superconductivity revealed in NMR and Kerr effect experiments.

Remarkably, the simultaneous presence of deepest near-nodes along G-X and less deep ones along G-M (both on the γ pocket in our case) is exactly the gap structure speculated to explain the systematic angle-dependent specific heat under in-plane as well as conical magnetic fields in Ref.[48], where the near-nodes along G-M were assumed (but do not have) to be on the α and β pockets. The near-nodes may also be an important factor to reduce the spontaneous edge current (not detected so far[49]) at finite temperatures and under impurity scatterings,[50] We leave these as future topics.

The project was supported by the National Key Research and Development Program of China (under Grant No. 2016YFA0300401), the National Basic Research Program of China by MOST (under Grant No. 2014CB9221203), and the National Natural Science Foundation of China (under Grant Nos.11604168, 11574134, 11674278, and 11404383). FCZ also acknowledges the support by K. C. Wong Magna Fundation of Ningbo University.

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