Mixed-Parity Superconductivity in Sr$_2$RuO$_4$

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We show that in Sr$_2$RuO$_4$ the Fermi surface geometry as inferred from angle resolved photoemission experiments has important implications for a pairing interaction dominated by incommensurate, strongly anisotropic, spin fluctuations. For a spin fluctuation spectrum consistent with inelastic neutron scattering experiments the system is close to an accidental degeneracy between even parity spin singlet and odd parity spin triplet channels. This opens the possibility of a mixed parity order parameter state in Sr$_2$RuO$_4$. We determine the stable and metastable order parameter phases at low temperatures and discuss especially phases with order parameter nodes.

The study of the superconducting material Sr$_2$RuO$_4$ has attracted considerable experimental and theoretical attention because of its peculiar low energy electronic properties. It is a rare example of a multiband superconductor with possibly spin triplet pairing symmetry. Based on muon spin relaxation measurements an early suggestion for the order parameter symmetry was the time reversal symmetry breaking '$p_z \pm ip_y$'-state. Recent experiments on the contrary favor order parameter changes from $s^\pm$ to $d^\pm$.

As experimental results become more reliable, it becomes possible to test if a pairing mechanism via incommensurate, strongly anisotropic, spin fluctuations the order parameter state in Sr$_2$RuO$_4$ is close to two accidental degeneracies between ferromagnetic and anti-ferromagnetic fluctuations. The dominant contributions to the spin susceptibility, \( \chi (q) \), are located around \( Q = (1/4, 1/4, 0) \) with an incommensurability \( \delta \approx 0.4 \). Similar results have been also suggested theoretically finding \( \delta \approx 1/3 \). It was suggested that in the cross-over regime between ferromagnetic and anti-ferromagnetic spin fluctuations the order parameter changes from $p$-wave to $d$-wave.

As experimental results become more reliable, it becomes possible to test if a pairing mechanism via incommensurate spin fluctuations is consistent with a) the spin fluctuation spectrum measured in INS, b) the electronic structure as tested by angle resolved photoemission and de Haas-van Alphen spectroscopy, and c) the experimental implications for the order parameter symmetry.

In this Letter we study the possible pairing symmetries for the order parameter in Sr$_2$RuO$_4$ resulting from a pairing interaction dominated by incommensurate, strongly anisotropic, spin fluctuations. Given the measured Fermi surface geometry in Sr$_2$RuO$_4$, we find that the system is close to two accidental degeneracies between the triplet $E_{2u}$ superconducting state and one of the single superconducting states either in the $B_{1g}$ (predominantly $d$-wave) channel or in the $A_{1g}$ (predominantly $g$-wave) channel. This opens the possibility of a superconducting state with mixed parity order parameter in Sr$_2$RuO$_4$. The possibility of such superconducting states was discussed some time ago in connection with UPt$_3$. We also study the different possible stable and metastable low-temperature phases in Sr$_2$RuO$_4$ for the three cases that either of the three relevant order parameter symmetries $E_{2u}$, $B_{1g}$, or $A_{1g}$ is dominant. We find both nodeless solutions and order parameters with nodes.

NMR experiments suggest a strong anisotropic spin susceptibility, with only the $\chi_{zz}$ peaked around the incommensurate wave vector $Q$. Thus, we consider an anisotropic model with $\chi \approx \chi_{zz}$ suggests a strong anisotropic susceptibility, with only the $\chi_{zz}$ peaked around the incommensurate wave vector $Q$.

This model susceptibility has three parameters. The overall magnitude, $\chi_Q$, determines the coupling strength in the dominant pairing channel, and thus the superconducting transition temperature $T_c$. The other two parameters, the spin-spin correlation length, $\xi_{\parallel}$, and the degree of incommensurability, $\delta$, determine the relative coupling strengths in the different symmetry channels, defining the symmetry of dominant and sub-dominant components. The specific form of the susceptibility allows a smooth cross-over from anti-ferromagnetic fluctuations, $Q_{AF} = (1, 1, 0) \pi/a$, to ferromagnetic, $Q_{FM} = (0, 0, 0)$, by tuning $\delta$ from 0 to 1. Extracting the values of $\xi_{\parallel}$ and $\delta$ from the INS data gives $\xi_{\parallel} \approx 4.0a$ and $\delta \approx 0.4$. The effective pairing interaction via spin fluctuation exchange is determined by the coupling function $g(p) \chi^{i} (p - p') g(p')$. The coupling between spin fluctuations and quasiparticles, $g(p)$, is approximated in what follows by a constant, $g$. To reproduce the structure of the experimentally probed three-sheet Fermi surface we use the tight-binding dispersions

\[ t'_i^x = 2t_1^x \cos p_x + 2t^y \cos p_y - 4t_1^x \cos p_x \cos p_y - \mu^i. \]

The band index $i$ labels the $xy$, $xz$, and $yz$ bands. The parameters of the dispersions \((t_1^x, t_1^y, t_1^z, \mu^i)\) are taken from
the weak coupling gap equation reads

$$\Delta_{\alpha\beta}(p_f) = - \sum_{i=x,y,z} \sum_{\gamma\delta} \chi^{\delta} \langle \sigma_{\alpha\gamma} \hat{\chi}^{\delta}(p_f - p_f') \sigma_{\beta\delta} n(p_f') f_{\gamma\delta}(p_f') \rangle p_f'$$

where $f_{\gamma\delta}(p_f) = T \sum_{\epsilon} d \xi E_{\gamma\delta}(p_f, \epsilon; \xi_0)$, $F$ is the anomalous propagator, $\epsilon_0$ fermionic Matsubara frequencies, and $\xi_0$ is the usual frequency cut-off. The isotropic interaction in Eq. (3) breaks spin rotational symmetry, but since each $p_f$-state is doubly Kramers-degenerate in zero-field, we can still decompose $\Delta_{\alpha\beta}$ and $F_{\gamma\delta}$ into (pseudo-)spin singlet ($s$) and (pseudo-)spin triplet ($t$) components [19] and arrive, for $x = s, t$, at

$$\Delta_x(p_f) = - \left( V_x(p_f - p_f') n(p_f') f_x(p_f') \right) p_f'$$

with $V_s = \hat{\chi}^2 + \hat{\chi}^2/2$, $V_t = -\hat{\chi}^2 + \hat{\chi}^2/2$, $V_s = -\hat{\chi}^2/2$. Isotropic spin fluctuations ($\chi^2 = \chi^2$) support triplet superconductivity only for nearly ferromagnetic enhancement. In the case of extreme anisotropy the coupling functions for singlet and triplet pairing with $d$-vector in $\hat{z}$-direction have equal sign and magnitude, $V_s = V_t = \hat{\chi}^2/2$. In addition, a second triplet-pairing state with $d \perp \hat{z}$ is possible. It couples via $V_t = -\hat{\chi}^2/2$. In order to study the symmetry of the superconducting state near $T_{c\alpha}$, we determine numerically the eigenvalue spectrum of the integral kernel in Eq. (3) following Ref. [23]. The resulting complete orthogonal set of basis functions $\chi^{\delta}_{\gamma\delta}(p_f)$ can be classified according to the irreducible representations ($\Gamma$) of the crystal group $D_{4h}$. The corresponding eigenvalues, $\lambda^\Gamma$, determine the coupling constants for the $\mu$th basis function in the symmetry channel ($\Gamma$) [21]. The most attractive (negative) eigenvalue in representation (\(\Gamma\)), $\lambda^\Gamma = \min_{\mu}(\lambda^\Gamma)$, is eliminated in favor of a transition temperature for order parameter symmetry ($\Gamma$) in the usual way, $T_{c\xi} = 1.13c_0 \exp(-1/|\lambda^\Gamma|)$.

The dominant coupling constant $\lambda^{\Gamma_0}$ determines the superconducting transition temperature $T_{c\alpha}$ and the symmetry ($\Gamma_0$) of the superconducting phase near $T_{c\alpha}$. Once an order parameter component in a certain representation ($\Gamma$) nucleates, the other components $\mu(\Gamma)$ in the same representation are usually induced by the presence of the first component. Thus, physical transitions between different superconducting phases only occur when additional symmetries are spontaneously broken. Such subdominant transitions are suppressed below the value $T_{c\Gamma}$ in the presence of a dominant order parameter. In the following we study which of the different possible phases nucleates first at given $\xi_0$ and $\delta$ and determine points of accidental degeneracy between two different order parameter phases as a function of these parameters. In Fig. 1 we show the dependence of the attractive eigenvalues on $\delta$ for $\chi^2 = 0$, fixing $\xi_0$ at 4.0a, a value which should closely correspond to the actual value in $Sr_2RuO_4$ [9]. The relevant phases near $T_{c\alpha}$ are the even-parity one-dimensional irreducible representations $A_{1g}$ and $B_{1g}$, which give spin-singlet superconductivity, and the odd-parity two-dimensional irreducible representation, $E_{2u}$, rendering a spin-triplet channel for superconductivity. At small values of incommensuration, up to $\delta \approx 0.35$, the system prefers the $B_{1g}$-pairing channel. Above this point there is a region, $0.35 < \delta \lesssim 0.42$, of spin-triplet pairing in the $E_{2u}$ channel with $d \parallel \hat{z}$. Beyond $\delta \approx 0.42$, the pairing state is spin-singlet with $A_{1g}$ symmetry, bounded by a narrow region of $B_{1g}$-pairing starting around $\delta \approx 0.61$. In the large-$\delta$ range there is again triplet pairing, but now with $d \perp \hat{z}$. The two accidental degeneracy points of interest for us are $B_{1g} + E_{2u}$ for an incommensuration $\delta \approx 0.35$ and $A_{1g} + E_{2u}$ for $\delta \approx 0.42$. Both points are remarkably close to the experimental value of $\delta \approx 0.4$ and the theoretically predicted value of $\delta \approx 0.33$. Calculations with an additional component $\chi^2$ resulted into accidental degeneracies even closer to each other.

We also performed calculations for $\delta \approx 0.4$ and varying $\xi_0$. Additionally, a hybridization of the $xz$ and $yz$ bands is given by $t_{12} = 0.1$ eV [17].
showing that the presence of the accidental degeneracies near $\delta = 0.4$ is a robust feature for $\xi_a > 2a$.

In the following we study the possible low temperature superconducting phases close to the accidental degeneracies. We concentrate on the three cases where either of the three symmetry channels is slightly dominant. We chose $\delta = 0.3$ for a dominant $B_{1g}$ channel, $\delta = 0.4$ for a dominant $E_{2u}$ channel, and $\delta = 0.45$ for a dominant $A_{1g}$ channel. To determine the superconducting state at low temperatures we solve the non-linear gap equation (4). Expanding the order parameter with respect to the set of basis functions $\gamma^{(e)}(p_f)\delta$ we obtain the order parameter components $\Delta^{\mu}_{\pm}$ for each representation. In the case of a mixed parity state a mixture of even parity, $\Delta^{(e)}(p_f)$, and odd-parity, $\Delta^{(o)}(p_f)$, basis functions occurs as

$$\Delta_{\pm}(p_f) = \sum_{\mu} \Delta^{(e)}_{\mu}(p_f) \pm \sum_{\mu} \Delta^{(o)}_{\mu}(p_f).$$

Once parity is broken, each of the doublets, $\psi_\uparrow \psi_\uparrow$ and $\psi_\uparrow \psi_\downarrow$, acquire separate order parameters, $\psi_{\uparrow, \downarrow}$ with $\Delta^{\uparrow}(p_f)$ and $\Delta^{\downarrow}(p_f)$, and $\Delta(p_f)$ has the required anti-symmetry since $\Delta_{\pm}(p_f) = -\Delta_{\mp}(p_f)$. As there may be several possible superconducting states, each state being a local minima in the free energy, we compute the free energy of each candidate state using the Serene-Rainer free energy functional [22], and select the state of lowest energy as the superconducting phase.

As the temperature evolution of the order parameter depends on $T_c, T_{\alpha}$, that minimizes the free energy at $\delta = 0.4$ and with $\xi_a = 4a$. We find three local minima: one ground state (G) and two metastable states (M1 and M2). The free energy difference at zero temperature between M1 and G corresponds to only 9% of the ground state condensation energy (it amounts to 22% for M2). G is of pure $E_{2u}$-symmetry. M1 is symmetric around the $p_x$ and $p_y$ axis and has points with small gap values on the $\alpha$-sheet. M2 is symmetric around the diagonals $p_x \pm ip_y$ and has nodes on the $\alpha$ sheet. Also shown in Fig. 2 is the total (angle-averaged) density of states (DOS) at the Fermi surface. The DOS is fully gapped for the ground state. The first metastable state shows a DOS with a much smaller excitation gap, and the DOS for the second metastable state shows low energy nodal excitations originating from the $\alpha$ sheet. The metastable states break spin-rotation symmetry and parity. The amplitudes $\Delta^{(e,o)}_{\mu}$ have a zero relative phase for basis functions within the same parity, and a relative phase difference of ±$\pi/2$ for basis functions with opposite parity; thus, $\Delta_{\pm}(p_f) = \Delta_{\pm}(p_f)^*$. In the ground state the odd-parity basis functions with same eigenvalue have a $\pi/2$ relative phase difference, giving a ‘$p_x \pm ip_y$’-state. We emphasize: all three solutions break time-reversal symmetry.

Going to a $\delta$ where superconductivity nucleates first in either the $B_{1g}$ or the $A_{1g}$ channel, we find that already the ground states are mixed parity states. The lowest energy state is a nodeless time reversal symmetry breaking state with relative phases similar to the M1 state discussed above. For both $\delta = 0.3$ and $\delta = 0.45$ we find metastable states, with nodes on all three Fermi surface sheets, that are of slightly higher free energies (9.0% and 15.6% respectively) than the nodeless ground states. In Fig. 3 we show $|\Delta_{+}(p_f)|$ and the DOS for both states at $\delta = 0.3$ and $\delta = 0.45$. For the metastable states the odd-parity components can develop higher order nodes, and remarkably, even whole arcs with vanishing or very small order parameter magnitude at the positions of the nodes in the even-parity components. At $\delta = 0.3$, for instance, the odd parity component has nodes along a diagonal in the Brillouin zone, coinciding with the $d$-wave nodes of the even parity component. In this case such arcs of almost zero $\Delta^{(o)}_{\mu}(p_f)$ occur on the $\gamma$-sheet, extending all over the two quadrants which contain the nodes of the total order parameter.

The two components of the odd-parity order parameter transform like a vector in momentum space. Its direction is determined by the anisotropy introduced by a) the normal state DOS and b) the presence of the even-parity
by experiment, for an incommensuration near relation length of several lattice constants, as suggested
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In conclusion, we have shown that in the parameter
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ate $B_{1g} \oplus E_{2u}$ state and near $\delta = 0.42$ the state is
$A_{1g} \oplus \bar{E}_{2u}$. Both states are of mixed parity and break
the $D_{4h}$ crystal symmetry and time reversal symmetry. Within our model we find as ground states time reversal
symmetry breaking nodeless states. However, close
in free energy there exist metastable states of the order
parameter with nodes, which may be stabilized by addi-
tional interactions.

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![Diagram](image)

**FIG. 3.** The same as in Fig. 2 for $\delta = 0.3$ (left) and
and for $\delta = 0.45$ (right). Top to bottom: gap magnitude of the
metastable state (M), gap magnitude of the ground state (G),
and the density of states for each corresponding state.

$B_{1g}$ or $A_{1g}$ components. The mixed parity solutions
for each incommensurability correspond to the align-
ment of this vector with high symmetry directions in the Bril-
lovin zone. Because the energy difference between the
ground state and the state with nodes is only a fraction
of the ground state condensation energy, fluctuations in
the direction of this vector can be responsible for the
presence of nodal excitations. Analyzing data of specific
heat measurements [3] and of thermal conductivity [3],
prompts that the $Sr_2RuO_4$ order parameter should have
nodes. This conclusion is further strengthened by recen-
test measurements of the penetration depth showing a
non-exponential low-temperature behavior [3]. Based on
the presented calculations, this implies that a mixed parity
superconducting state, breaking spin-rotation symme-
try, may be a candidate state for $Sr_2RuO_4$, and maybe
even stabilized by additional interactions in the Hamil-
tonian not considered here.

In conclusion, we have shown that in the parameter
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