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The role of spin-orbit coupling for the superconducting state in Sr_2RuO_4

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Abstract. – The odd-parity spin-triplet Cooper pairing states show a six-fold degeneracy for a quasi–two-dimensional electron system. In this article we show how spin-orbit coupling can lift this degeneracy for Sr_2RuO_4 taking the band structure based on the three relevant t_{2g}-orbitals of the Ru-ions into account. The stabilized state depends on the relative strength of the pairing interaction. We show that under reasonable assumptions the chiral pairing state $\boldsymbol{d}(\boldsymbol{k}) = \hat{\boldsymbol{z}}(k_x \pm ik_y)$ is favored against the others.

The search for new superconducting transition metal oxide systems has lead a few years ago to the discovery of Sr_2RuO_4 [1]. Despite the low transition temperature ($T_{\mathrm{cmax}} \approx 1.5\,\mathrm{K}$) which is, in addition, very sensitive to disorder [2], the unusual properties of the superconductor have attracted much interest. During the last year it has been experimentally established that this compound is a spin-triplet superconductor as initially suggested on theoretical basis [3,4]. The superconducting state is characterized by the violation of time-reversal symmetry [5] and equal spin pairing within the basal plane of the tetragonal crystal lattice [6]. The single candidate consistent with all presently known experimental data is described by the gap function of the symmetry $\boldsymbol{d}(\boldsymbol{k}) = \hat{\boldsymbol{z}}(k_x \pm ik_y)$ in the standard vector notation [7]. This state is two-fold degenerate and has chiral symmetry, *i.e.* the Cooper pairs possess an orbital angular momentum. There are various possible other candidates for spin-triplet pairing which might be rather close in energy as we will show below. The question arises what is the microscopic reason to favor the chiral phase compared to the others. It is the aim of this paper to show that the chiral state is a natural consequence of the electronic structure of Sr_2RuO_4 and the presence of spin-orbit coupling.

Sr_2RuO_4 is, like several of the high-temperature superconductors, a layered perovskite system of stacking RuO_2-planes with a single layer per unit cell [1]. Like Cu in the high-temperature superconductors, Ru forms a square lattice. While a single-band description seems to be adequate for the CuO_2-system, the case of RuO_2 requires at least three bands originating from the three 4d-t_{2g}-orbitals of Ru occupied by four electrons on the average. All bands cross the Fermi energy and give rise to three Fermi surfaces, two electron-like and one hole-like, all of nearly cylindrical shape owing to the weak dispersion along the c-axis [8–10].

The low-temperature normal state of Sr_2RuO_4 is that of a strongly correlated, nearly two-dimensional Fermi liquid. In this sense this system resembles to some extent the nature of the Fermi liquid ^{3}He [3].

Starting from this assumption we show that the ordinary weak-coupling theory for spin-triplet pairing yields a six-fold degenerate superconducting state if the spin space is completely rotation symmetric. This degeneracy is lifted through spin-orbit coupling as suggested in ref. [3,7]. In this letter we describe the effect of spin-orbit coupling based on the orbital origin of the three electron bands. For this purpose we introduce a simple model taking the basic structure of the three orbitals into account and leading to spin-triplet superconductivity. The three t_{2g}-orbitals, d_{yz}, d_{zx}, d_{xy}, will be labeled as $1, 2, 3$, respectively. The kinetic energy is then given by

$$\mathcal{H}_{\rm kin} = \frac{1}{N}\sum_{\boldsymbol{k},s} C^\dagger_{\boldsymbol{k}s} \begin{pmatrix} \varepsilon_{\boldsymbol{k}1} & g_{\boldsymbol{k}} & 0 \\ g_{\boldsymbol{k}} & \varepsilon_{\boldsymbol{k}2} & 0 \\ 0 & 0 & \varepsilon_{\boldsymbol{k}3} \end{pmatrix} C_{\boldsymbol{k}s}\,, \tag{1}$$

with $C^\dagger_{\boldsymbol{k}s} = (c^\dagger_{\boldsymbol{k}1s} c^\dagger_{\boldsymbol{k}2s} c^\dagger_{\boldsymbol{k}3s})$, $(\varepsilon_{\boldsymbol{k}1}, \varepsilon_{\boldsymbol{k}2}) = -2t_1(\cos k_y, \cos k_x) - \mu$, $\varepsilon_{\boldsymbol{k}3} = -2t_2(\cos k_x + \cos k_y) - 4t_3 \cos k_x \cos k_y - \mu'$ and $g_{\boldsymbol{k}} = -4t_4 \sin k_x \sin k_y$ (N: number of lattices sites). The parameters will be later chosen to fit the band structure as close as possible [9, 11]. Through the hybridization of the orbitals 1 and 2 the Hamiltonian leads to the bands α and β corresponding to the hole-like and electron-like Fermi surface, respectively. The band belonging to orbital 3 is called γ in accordance with the band structure literature [8,9,11].

We now turn to the discussion of the pairing interaction yielding spin-triplet pairing. The on-site interaction is definitely repulsive suppressing pairing in the standard s-wave channel. Therefore we focus on nearest-neighbor-site interactions. Furthermore, the zero-momentum pairing requires that two paired electrons are on the same Fermi surface. Interband pairs have, in general, a finite net momentum. As a possible candidate for pairing ferromagnetic spin fluctuations were discussed [7,12]. Experimental studies show, however, that the ferromagnetic components of the spin fluctuations are rather weak [13] and, in additions, if they are enhanced, *e.g.* by pressure, superconductivity is actually suppressed [14]. Alternatively, Hund's rule coupling was mentioned as another cause for parallel spin pairing [3,4]. Standard Hund's rule coupling on the Ru-ion, however, yields an on-site interaction and would not be available for spin-triplet pairing. There is, however, a spin-dependent interaction mediated via orthogonal oxygen orbitals between different nearest-neighbor orbitals. For example, on a bond between site 1 and 2 along the x-axis spins on the Ru-d_{xy}- and d_{xz}-orbitals on different sites interact ferromagnetically as they hybridize with orthogonal p-orbitals on the intermediate oxygens. This is a variant of the Goodenough-Kanamori mechanism for ferromagnetic exchange based on Hund's rule effect on oxygen in transition metal oxides. It is easy to see that the d_{xy}-orbital couples in this way to the d_{zx}- and d_{yz}-orbitals of the Ru-ions on neighboring sites along the x- and y-direction,

$$H_{\rm int} = J' \sum_i [\boldsymbol{S}_{i3} \cdot \boldsymbol{S}_{i+\hat{\boldsymbol{x}},2} + \boldsymbol{S}_{i+\hat{\boldsymbol{x}},3} \cdot \boldsymbol{S}_{i2} + \boldsymbol{S}_{i3} \cdot \boldsymbol{S}_{i+\hat{\boldsymbol{y}},1} + \boldsymbol{S}_{i+\hat{\boldsymbol{y}},3} \cdot \boldsymbol{S}_{i1}]\,. \tag{2}$$

This is an interorbital interaction and by itself for pairing not so effective. However, the local spin polarization generated by this interaction can be transferred via on-site Hund's rule coupling to the other orbitals and lead to an effective spin-dependent nearest-neighbor

intraorbital pairing interaction which has the form

$$H_{\rm p} = \sum_i [J_1\{\boldsymbol{S}_{i1}\cdot\boldsymbol{S}_{i+\hat{\boldsymbol{x}}1}+\boldsymbol{S}_{i2}\cdot\boldsymbol{S}_{i+\hat{\boldsymbol{y}}2}\}+J_2\{\boldsymbol{S}_{i1}\cdot\boldsymbol{S}_{i+\hat{\boldsymbol{y}}1}+\boldsymbol{S}_{i2}\cdot\boldsymbol{S}_{i+\hat{\boldsymbol{x}}2}\}+ +J_3\{\boldsymbol{S}_{i3}\cdot\boldsymbol{S}_{i+\hat{\boldsymbol{x}}3}+\boldsymbol{S}_{i3}\cdot\boldsymbol{S}_{i+\hat{\boldsymbol{y}}3}\}], \tag{3}$$

where J_1 is ignored as it has no contribution in our model. The effective coupling strengths depend on the on-site polarizability of the spins in the different orbitals:

$$J_2 = -\frac{J'J_H}{N}\sum_{\boldsymbol{q}}\chi_{33}(\boldsymbol{q}) \qquad \text{and} \qquad J_3 = -\frac{J'J_H}{N}\sum_{\boldsymbol{q}}[\chi_{11}(\boldsymbol{q})+\chi_{12}(\boldsymbol{q})], \tag{4}$$

where $\chi_{\mu\nu}(\boldsymbol{q}) = -\frac{i}{N}\int_0^\infty {\rm d}t\langle[\boldsymbol{S}_{\mu\boldsymbol{q}}(t),\boldsymbol{S}_{\nu-\boldsymbol{q}}(0)]\rangle$ is the static spin susceptibility (ignoring retardation effects) of the orbital μ with the field acting on the orbital ν.

Besides this spin-dependent contribution we introduce also a spin-independent part of the attractive intraorbital interaction of unknown origin. This can be done by replacing $\boldsymbol{S}_{i\mu}\cdot\boldsymbol{S}_{j\mu}$ by $\boldsymbol{S}_{i\mu}\cdot\boldsymbol{S}_{j\mu}+v_\mu n_{i\mu}n_{j\mu}/4$. Decomposed into spin-singlet and spin-triplet channels, this does not change the structure of the interaction. For simplicity, we will take $v_1 = v_2 = v_3$ for our calculation. To lift the degeneracy completely we have also to include the pair scattering between different Fermi surfaces. This interaction is mediated by Coulomb interaction [15]. For unconventional Cooper pairs the on-site scattering is ineffective. Thus we include the scattering via nearest-neighbor interaction also here,

$$H_{ib} = \sum_{i,\mu,\mu'}\sum_{s,s',\hat{\boldsymbol{r}}} g c^\dagger_{i\mu s}c^\dagger_{i+\hat{\boldsymbol{r}},\mu s'}c_{i+\hat{\boldsymbol{r}},\mu' s'}c_{i\mu' s}\,, \tag{5}$$

for $\mu \neq \mu'$. Including all terms and changing to momentum space we obtain in a pairing interaction of the form

$$H_{\rm pair} = \frac{1}{N}{\sum}' V^r_{\mu\mu',s_1,\ldots s_4}\cos(k_r-k'_r)c^\dagger_{\boldsymbol{k}\mu s_1}c^\dagger_{-\boldsymbol{k}\mu s_2}c_{-\boldsymbol{k}'\mu' s_3}c_{\boldsymbol{k}'\mu' s_4}\,, \tag{6}$$

where $\sum'$ indicates that we sum over all repeated indices ($r = x, y$) and the coefficients $V^r_{\mu\mu',s_1,\ldots s_4}$ are easily obtained from the above interactions. The decomposition of $\cos(k-k')$ into $\cos k\cos k' + \sin k\sin k'$ yields the wave functions of the possible states: "extended s-wave" ($\cos k_x + \cos k_y$), "$d_{x^2-y^2}$-wave" ($\cos k_x - \cos k_y$) for the spin-singlet channel and the p-wave" spin-triplet states ($\sin k_x, \sin k_y$) which are degenerate by symmetry [16]. While both spin-singlet states have, in general, zero-nodes in the gap, it is possible to combine the two degenerate p-wave components to form a nodeless gap. In this sense the p-wave channel is expected to be favored, if the spin-dependent part of the interaction does not suppress the triplet spin configuration.

The degeneracy of the two Cooper pair channels with the orbital wave functions $\sin k_x$ and $\sin k_y$ is independent of the spin wave function. Thus, we may choose the spin configuration to optimize the condensation energy. The gap function is given by

$$\hat{\Delta}_\mu(\boldsymbol{k}) = i\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{d}_\mu(\boldsymbol{k})\hat{\sigma}^y = i\sum_{\nu=x,y,z}\hat{\sigma}^\nu\hat{\sigma}^y\hat{\boldsymbol{\nu}}(a_{\nu\mu}\sin k_x + b_{\nu\mu}\sin k_y)\,, \tag{7}$$

where $\hat{\boldsymbol{\nu}}$ is the unit vector in ν-direction. The quasiparticle energy gap in each band is given by $\sqrt{|\boldsymbol{d}_\mu(\boldsymbol{k})|^2}$. States with the same gap have within the weak-coupling theory the same

TABLE I – *Degenerate stable spin-triplet pairing states listed according to the irreducible representations of the tetragonal point group D_{4h} assuming simultaneous rotations of spin and orbital part.*

Γ	$\boldsymbol{d}_\mu(\boldsymbol{k})$	P	Q
A_{1u}	$\hat{\boldsymbol{x}}\sin k_x + \hat{\boldsymbol{y}}\sin k_y$	$+1$	$+1$
A_{2u}	$\hat{\boldsymbol{x}}\sin k_y - \hat{\boldsymbol{y}}\sin k_x$	$+1$	-1
B_{1u}	$\hat{\boldsymbol{x}}\sin k_x - \hat{\boldsymbol{y}}\sin k_y$	-1	$+1$
B_{2u}	$\hat{\boldsymbol{x}}\sin k_y + \hat{\boldsymbol{y}}\sin k_x$	-1	-1
E_u	$\hat{\boldsymbol{z}}(\sin k_x \pm i\sin k_y)$	± 1	-

condensation energy and are consequently degenerate. The combinations given in table I have all the same gap $\sqrt{\sin^2 k_x + \sin^2 k_y}$ so that we find six degenerate pairing states [3, 7, 16]. This is a special feature of a two-dimensional Fermi liquid. In three dimensions one finds only one stable state, the Balian-Werthamer state, $\boldsymbol{d}(\boldsymbol{k}) = \hat{\boldsymbol{x}}\sin k_x + \hat{\boldsymbol{y}}\sin k_y + \hat{\boldsymbol{z}}\sin k_z$. Note that this result is general and does not depend on the details of the Hamiltonian as long as it favors p-wave pairing. It was shown that going beyond weak coupling by including the renormalization of the spin fluctuation spectrum the state $\boldsymbol{d}(\boldsymbol{k}) = \hat{\boldsymbol{z}}(\sin k_x \pm i\sin k_y)$ would be favored analogously to the spin fluctuation feedback mechanism stabilizing the A-phase of superfluid ^{3}He [7]. This is a secondary effect and does not affect the degeneracy of T_c, but is connected with the condensation energy at low temperature.

The degeneracy of T_c can be lifted by removal of spin rotation symmetry, *i.e.* by taking spin-orbit coupling into account. The spin-orbit coupling is connected with the heaviest ion —Ru in our case— where it acts as an on-site term in the Hamiltonian, $\mathcal{H}_{\rm so} = \lambda\sum_i \boldsymbol{L}_i\cdot\boldsymbol{S}_i$. The angular momentum $\boldsymbol{L}_i$ operates on the three t_{2g}-orbitals on the site i. If we restrict ourselves to these three orbitals, ignoring the e_g-orbitals, we can write the spin-orbit Hamiltonian as

$$\mathcal{H}_{\rm so} = i\frac{\lambda}{2}\sum_{l,m,n}\epsilon_{lmn}\sum_{\boldsymbol{k},s,s'} c^\dagger_{\boldsymbol{k}l,s}c_{\boldsymbol{k}ms'}\sigma^n_{ss'}\,, \tag{8}$$

where ϵ_{lmn} is the completely antisymmetric tensor and λ is a coupling constant such that the t_{2g}-states behave like an $\ell = 1$ angular-momentum representation (we use for l, m, n either $\{x, y, z\}$ or equivalently $\{1, 2, 3\}$). Together with eq. (1) the spin-orbit coupling leads to new quasiparticles which are now labeled by pseudo-orbital and pseudo-spin indices connected with the original ones by the unitary transformation defined for each wave vector $\boldsymbol{k}$,

$$(a_{\boldsymbol{k}1s}, a_{\boldsymbol{k}2s}, a_{\boldsymbol{k}3s})^\dagger = (c_{\boldsymbol{k}1s}, c_{\boldsymbol{k}2s}, c_{\boldsymbol{k}3-s})^\dagger\hat{U}_{\boldsymbol{k}s}\,, \tag{9}$$

where the spin-orbit coupling mixes the up-spins of the orbital 1 and 2 with down-spin of orbital 3 and vice versa. We find that the matrix elements of $\hat{U}_{\boldsymbol{k}s}$ of opposite spin are related as $u_{\boldsymbol{k}\mu\nu s} = u^*_{\boldsymbol{k}\mu\nu,-s}$ for $\mu = 1, 2$ and $u_{\boldsymbol{k}3\nu s} = -u^*_{\boldsymbol{k}3\nu,-s}$ for $\mu = 3$. Note that the inclusion of spin-orbit coupling affects the band structure so that the chemical potential of the orbitals has to be adjusted for different values of λ to produce the proper Fermi surface shape.

Cooper pairing has now to be defined and analyzed concerning the symmetry based on these new quasiparticles. We proceed, therefore, by rewriting the original pairing interaction $H_{\rm pair}$ in terms of these quasiparticles,

$$H_{\rm pair} = \frac{1}{2N}{\sum}' \mathcal{V}^{\nu\nu'}_{s_1s_2s_3s_4}(\boldsymbol{k},\boldsymbol{k}')a^\dagger_{\boldsymbol{k}\nu s_1}a^\dagger_{-\boldsymbol{k}\nu s_2}a_{-\boldsymbol{k}'\nu' s_3}a_{\boldsymbol{k}'\nu' s_4}\,, \tag{10}$$

where

$$\begin{aligned}
\mathcal{V}^{\nu\nu'}_{s_1s_2s_3s_4}(\boldsymbol{k},\boldsymbol{k}') &= \left(K^{mm'}_{s_1s_2s_3s_4}\mathcal{U}^{P*}_{\boldsymbol{k}m\nu s_1s_2}\mathcal{U}^{P}_{\boldsymbol{k}'m'\nu' s_3s_4} + \tilde{K}^{mm'}_{s_1s_2s_3s_4}\mathcal{U}^{P*}_{\boldsymbol{k}m\nu s_1s_2}\mathcal{U}^{-P}_{\boldsymbol{k}'m'\nu' s_3s_4}\right),\\
K^{mm'}_{s_1s_2s_3s_4} &= \tilde{J}_m\delta_{mm'}\boldsymbol{\sigma}_{s_1s_4}\boldsymbol{\sigma}_{s_2s_3} + \tilde{g}_{mm'}\delta_{s_1s_4}\delta_{s_2s_3} + \tilde{g}'_{mm'}\delta_{s_1,-s_4}\delta_{s_1,-s_2}\delta_{s_3,-s_4},\\
\tilde{K}^{mm'}_{s_1s_2s_3s_4} &= \tilde{g}'_{mm'}\delta_{s_1,-s_4}\delta_{s_1,s_2}\delta_{s_3,s_4}. \qquad (11)
\end{aligned}$$

Here we introduced the abbreviation $\tilde{J}_m = (J_m/4)(1+v)$. $\tilde{g}$ and $\tilde{g}'$ are symmetric with non-vanishing elements $\tilde{g}_{12} = \tilde{g}'_{13} = \tilde{g}'_{23} = g$. The functions $\mathcal{U}^P$, $P = \pm 1$, are used to express the pairing states and shall be constructed according to the symmetries listed in table I where P for each state is given,

$$\begin{aligned}
\mathcal{U}^{P}_{\boldsymbol{k}1\nu s_1s_2} &= u_{\boldsymbol{k}1\nu s_1}u_{\boldsymbol{k}1\nu s_2}\sin k_x + iPu_{\boldsymbol{k}2\nu s_1}u_{\boldsymbol{k}2\nu s_2}\sin k_y,\\
\mathcal{U}^{P}_{\boldsymbol{k}2\nu s_1s_2} &= u_{\boldsymbol{k}2\nu s_1}u_{\boldsymbol{k}2\nu s_2}\sin k_x + iPu_{\boldsymbol{k}1\nu s_1}u_{\boldsymbol{k}1\nu s_2}\sin k_y,\\
\mathcal{U}^{P}_{\boldsymbol{k}3\nu s_1s_2} &= u_{\boldsymbol{k}3\nu s_1}u_{\boldsymbol{k}3\nu s_2}(\sin k_x - is_1s_2P\sin k_y). \qquad (12)
\end{aligned}$$

A 90° rotation acting on the orbital part only (*i.e.*, $\boldsymbol{k}$) leads to $\mathcal{U}^{P}_{\boldsymbol{k}m\nu s_1s_2} \to -iP\mathcal{U}^{P}_{\boldsymbol{k}m\nu s_1s_2}$ following table I. Note that in $H_{\rm pair}$ different signs of P are coupled through the pair scattering between orbital 3 and orbital 1 or 2 only. These interband pair scatterings are responsible for the lifting of degeneracy of the $A_{1,2u}$ and $B_{1,2u}$ pairing states.

The standard BCS-type mean-field approach leads to the definition of the quasiparticle gap,

$$\Delta_{\nu s_2s_1}(\boldsymbol{k}) = \frac{1}{4N}{\sum}' \mathcal{V}^{\nu\nu'}_{s_1,s_2,s_3,s_4}(\boldsymbol{k},\boldsymbol{k}')f_{\nu' s_3s_4}(\boldsymbol{k}') \qquad (13)$$

with $f_{\nu' s_3s_4}(\boldsymbol{k}') = \langle a_{-\boldsymbol{k}'\nu' s_3}a_{\boldsymbol{k}'\nu' s_4}\rangle$ which is readily calculated after diagonalizing the mean-field Hamiltonian. After some algebra, we formulate the self-consistent gap equation for pairing in the odd-parity (pseudo spin-triplet) channel for the $\boldsymbol{d}$-vector,

$$\begin{aligned}
d^x_\nu(\boldsymbol{k}) &= \frac{1}{2N}{\sum}' \left(\tilde{J}_m\delta_{mm'} + \tilde{g}_{mm'} - Q\tilde{g}'_{mm'})\right)\left(Q\mathcal{U}^{-P*}_{\boldsymbol{k}m\nu\downarrow\downarrow} + \mathcal{U}^{P*}_{\boldsymbol{k}m\nu\uparrow\uparrow}\right)D^{PQ}_{m'},\\
d^y_\nu(\boldsymbol{k}) &= \frac{i}{2N}{\sum}' \left(\tilde{J}_m\delta_{mm'} + \tilde{g}_{mm'} - Q\tilde{g}'_{mm'}\right)\left(-Q\mathcal{U}^{-P*}_{\boldsymbol{k}m\nu\downarrow\downarrow} + \mathcal{U}^{P*}_{\boldsymbol{k}m\nu\uparrow\uparrow}\right)D^{PQ}_{m'},\\
d^z_\nu(\boldsymbol{k}) &= -\frac{1}{N}{\sum}' \left(\tilde{J}_m\delta_{mm'} + \tilde{g}_{mm'} + \tilde{g}'_{mm'}\right)\mathcal{U}^{P*}_{\boldsymbol{k}m\nu\uparrow\downarrow}D^{P}_{m'}, \qquad (14)
\end{aligned}$$

with $D^{PQ}_{m'}$ and $D^{P}_{m'}$ are, respectively, the eigenvectors of

$$\begin{aligned}
D^{PQ}_{m'} &= -\frac{1}{N}{\sum}' \left(\tilde{J}_m\delta_{mm''} + \tilde{g}_{mm''} - Q\tilde{g}'_{mm'}\right)\mathcal{U}^{P}_{\boldsymbol{k}m'\nu'\uparrow\uparrow}\mathcal{U}^{P*}_{\boldsymbol{k}m\nu'\uparrow\uparrow}F_{\nu'\boldsymbol{k}}D^{PQ}_{m''},\\
D^{P}_{m'} &= -\frac{1}{N}{\sum}' \left(\tilde{J}_m\delta_{mm''} + \tilde{g}_{mm''} + \tilde{g}'_{mm'}\right)\mathcal{U}^{P}_{\boldsymbol{k}m'\nu'\uparrow\downarrow}\mathcal{U}^{P*}_{\boldsymbol{k}m\nu'\uparrow\downarrow}F_{\nu'\boldsymbol{k}}D^{P}_{m''}, \qquad (15)
\end{aligned}$$

where $F_{\nu,\boldsymbol{k}} = \tanh(\beta E_{\nu'\boldsymbol{k}}/2)/2E_{\nu'\boldsymbol{k}}$ and $P, Q = \pm 1$ corresponding to table I. These six eigenequations (4 for $D^{PQ}_{m'}$ and 2 for $D^{P}_{m'}$) have solutions with the symmetries corresponding to the pairing states as in table I. Note that $D^{P}_{m'}$ is independent of Q and is the same for both $P = \pm 1$ (because $\mathcal{U}^{-P}_{\boldsymbol{k}m\nu\uparrow\downarrow} = \mathcal{U}^{P*}_{\boldsymbol{k}m\nu\uparrow\downarrow}$), which is, therefore, always doubly degenerate. If $D^{P}_{m'}$

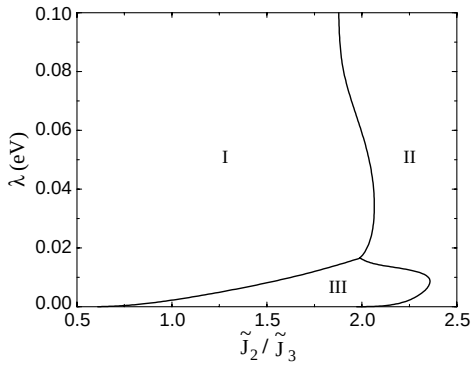

Fig. 1 – Phase diagram of stable states, with phase I representing $\hat{\boldsymbol{z}}(k_x \pm ik_y)$, phase II $\hat{\boldsymbol{x}}k_y - \hat{\boldsymbol{y}}k_x$ and phase III $\hat{\boldsymbol{x}}k_x + \hat{\boldsymbol{y}}k_y$. The parameters used are $t_1 = 0.18\,\mathrm{eV}$, $t_2 = 0.17\,\mathrm{eV}$, $t_3 = 0.08\,\mathrm{eV}$, $t_4 = 0.02\,\mathrm{eV}$, $\mu' - \mu = 0.1\,\mathrm{eV}$, $\tilde{J}_3 = -0.1\,\mathrm{eV}$ and $g = 0.02\,\mathrm{eV}$.

gives the highest transition temperature T_c after solving the eigen-equations self-consistently, then all $D^{PQ}_{m'}$ have only trivial solutions at T_c. Hence the pairing state has only a d^z component and is doubly degenerate, which is consistent with the chiral state. On the other hand, there will be no d^z component in the pairing state when one of the $D^{PQ}_{m'}$ gives the highest T_c.

Our calculation shows that the spin-orbit coupling lifts the degeneracy in favor of different pairing states depending on the relative strength of the pairing interactions, $\tilde{J}_2$ and $\tilde{J}_3$. In fig. 1 we present the phase diagram of spin-orbit coupling λ *vs.* the ratio $\tilde{J}_2/\tilde{J}_3$. Among the three states occurring in the phase diagram we find also the time reversal symmetry breaking state $\hat{\boldsymbol{z}}(k_x \pm ik_y)$ which is most stable, if the pairing interaction is dominant in the d_{xy}-orbital. The other two phases corresponding to the irreducible representations A_{1u} (phase II) and A_{2u} (phase I) in table I, require either substantially stronger pairing interaction in the bands of the orbitals d_{yz} and d_{zx} or rather weak spin-orbit coupling. The values of λ of the Ru^{4+}-ion in the literature are of the order of 0.07 eV. In view of the effect the spin-orbit coupling has on the quasiparticle spectrum we may argue that its strength is moderate, since the band structure calculations ignoring spin-orbit coupling are in reasonable agreement with the de Haas-van Alphen data [8–10]. There are also experimental indications which suggest that superconductivity in Sr_2RuO_4 is carried mainly by the d_{xy}-band [17]. Clearly also the electronic density of states of this band makes up 43% of the whole system. (In the choice of parameters used in this calculation we have taken the ratios of density of states into account.) The role of the interband pair scattering in eq. (5) is to distinguish between the A_{1u}- and A_{2u}-state which would be degenerate for $g = 0$.

Our approach is based on the assumption that spin-orbit coupling is not too strong so that we can deal with it essentially by changing only the character of the quasiparticles. This procedure is complicated due to the itinerant character of the electrons. In our discussion we have not taken into account the modification of the spin-dependent matrix elements of the interaction. For this purpose we would need more detailed knowledge about the pairing mechanism. Nevertheless, for the mechanism based on the extended Hund's rule coupling we can test the effect of spin-orbit coupling. Calculating the free-quasiparticle spin susceptibilities including spin-orbit coupling shows that the anisotropy in the spin interaction in eq. (3) is only of the order of 1% in the range of λ important for, considerably smaller than the above effect.

Calculating the static spin susceptibility for all bands we obtain within our model a very similar form as calculated from LDA [12] and measured recently by neutron scattering [13]. Both theory and experiment agree well in the aspect that the strongest spin correlation is not ferromagnetic, $q = 0$, but has a finite wave vector associated with the rather strong nesting feature of the nearly one-dimensional bands of the d_{yz}- and d_{zx}-orbitals which in this way dominate the q-dependence of the susceptibility. The large density of states, however, leads to the strongest contribution to the overall susceptibility by the d_{xy}-band. In calculating the coupling strengths J_2 and J_3 we find that their ratio is of the order 1.7 in favor of J_2 which still would lead to the chiral superconducting state in the phase diagram. However, also the spin-independent interactions have to be taken into account, which we cannot estimate at present. The main conclusion of our study is that spin-orbit coupling plays an important role in stabilizing the time-reversal symmetry-breaking p-wave pairing state in Sr_2RuO_4 and is strongly connected with the orbital structure of the electron bands.

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