Competitions in layered ruthenates: ferro- vs. antiferromagnetism and triplet vs. singlet pairing

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Ru based perovskites demonstrate an amazing richness in their magnetic properties, including 3D and quasi-2D ferromagnetism, antiferromagnetism, and unconventional superconductivity. Tendency to ferromagnetism, stemming from the unusually large involvement of O in magnetism in ruthenates, leads to ferromagnetic spin fluctuations in Sr$_2$RuO$_4$ and eventually to $p$-wave superconductivity. A related compound Ca$_2$RuO$_4$ was measured to be antiferromagnetic, suggesting a possibility of antiferromagnetic fluctuations in Sr$_2$RuO$_4$ as well. Here we report first principles calculations that demonstrate that in both compounds the ferro- and antiferromagnetic fluctuations coexist, leading to an actual instability in Ca$_2$RuO$_4$ and to a close competition between $p$-wave and $d$-wave superconducting symmetries in Sr$_2$RuO$_4$. The antiferromagnetism in this system appears to be mostly related with the nesting, which is the strongest at $Q \approx (2\pi/3a, 2\pi/3a, 0)$. Surprisingly, for the Fermiology of Sr$_2$RuO$_4$ the $p$-wave state wins over the $d$-wave one everywhere except in close vicinity of the antiferromagnetic instability. The most stable state within the $d$-wave channel has vanishing order parameter at one out of three Fermi surfaces in Sr$_2$RuO$_4$, while in the $p$ channel its amplitude is comparable at all three of them.

In the last few years an understanding emerged, thanks to the progress in the high-$T_c$ problem, that $s$-wave and $d$-wave pairing are not entirely antagonistic. It is possible to obtain either symmetry in the framework of one and the same model, depending on the actual values of parameters. It is, however, commonly believed that the triplet ($p$) and singlet ($s, d$) pairings are so different in their nature that more than just changing numerical parameters of a model is needed to switch between these symmetries. Here we show that a realistic model of the superconducting layered ruthenate Sr$_2$RuO$_4$ is in fact unstable with respect to both $p$- and $d$-wave pairing and it is a close competition between the two that determines the actual ground state.

It was suggested a few years ago that Sr$_2$RuO$_4$ may be a $p$-wave superconductor. The main consideration was that the sister 3D compound, SrRuO$_3$, is a strong ferromagnet, so one could expect substantial ferromagnetic spin fluctuations in Sr$_2$RuO$_4$. It was also known that superconductivity in the canonical triplet superconductor, $^3$He, is due to ferromagnetic spin fluctuations, so it was natural to conjecture that the pairing in Sr$_2$RuO$_4$ was also triplet. At that time there was hardly any experimental evidence and no microscopic calculations to support this idea. Since then convincing experimental evidence has been collected (for review, see Ref. [3]) that the superconductivity in Sr$_2$RuO$_4$ is indeed unconventional (not $s$-wave) and most likely triplet. Microscopic calculations revealed the mechanism for ferromagnetism in SrRuO$_3$ and demonstrated that a tendency to ferromagnetism is still present in Sr$_2$RuO$_4$, although it is weaker and does not result in an actual magnetic instability.

The recent discovery of antiferromagnetism in Ca$_2$RuO$_4$ forces us to reconsider this simple picture. This compound differs from Sr$_2$RuO$_4$ only in that the RuO$_6$ octahedra are tilted and rotated $\pi/3$, as it is common in perovskites (cf. La$_2$CuO$_4$). This causes some modification of the hopping amplitudes compared to Sr$_2$RuO$_4$, but this modification has a tremendous effect on magnetic properties: the material becomes antiferromagnetic with a substantial ($> 1 \mu_B$/ Ru) magnetic moment. This suggests that there should be some latent tendency to antiferromagnetism in Sr$_2$RuO$_4$ itself, and casts doubt on the basic assumptions of Refs. [1,2] and others that the spin fluctuations in this material are predominantly of the ferromagnetic type. To answer this question one cannot rely upon analogies with other materials, but needs quantitative (at least semiquantitative) calculations.

Fortunately, and unlike cuprates and most 3$d$-oxides, the conventional local density approximation (LDA) provides a very good description of magnetic properties of the ruthenate-based perovskites. Previously we have performed calculations for various ruthenates for which crystal structure and magnetic properties are known experimentally, and we found excellent agreement with the experiment: SrRuO$_4$ comes out ferromagnetic with the total magnetization $1.59 \mu_B$/f.u. (experiment: 1.6), CaRuO$_3$ is a paramagnet on a verge of ferromagnetism, and the double perovskite Sr$_2$RuYO$_6$ is antiferromagnetic with $3 \mu_B$/f.u., again in accord with the experiment. Finally, in Sr$_2$RuO$_4$ the paramagnetic state comes out more stable in the LDA calculations than either ferro- or antiferromagnetic one.

The reason for ferromagnetism in SrRuO$_3$ (and antiferromagnetism in CaRuO$_3$) is now well understood: There is substantial oxygen density of states at the Fermi level in these ruthenates (due to strong $p-d$ hybridization), and the difference between the FM and the AFM state is that in the latter case the oxygen
is not spin-polarized. The oxygen ion has considerable Stoner energy, which is lost in the AFM case. Furthermore, this additional energy is entirely lost for the $q = \{\pi, \pi, \pi\}$ AFM ordering, two thirds of that is lost for $q = \{\pi, \pi, 0\}$, and one third for $q = \{\pi, 0, 0\}$, compared with the FM ordering ($q = (0, 0, 0)$). This allows one to construct a $q$-dependent Stoner interaction, $I(q) \approx 0.46 \text{eV}/(1 + 0.08q^2)$, where $q$ is measured in units of $\pi/a$. This interaction strongly favors a FM instability, and whether or not the actual instability occurs depends on the density of states at the Fermi level, according to the Stoner criterion, $I(0)N(0) \approx 1$. It appears that in SrRuO$_3$ this condition is satisfied, $IN = 1.23$, and the material is a FM. In CaRuO$_3$ the smaller ionic radius of Ca leads to a smaller Ru-Ru distance and thus to larger distortion. A peak in the density of states that exists in SrRuO$_3$ is washed out and the material is on the border line, $IN \approx 1$.

The same mechanism is operative in Sr$_2$RuO$_4$ : for an individual RuO$_2$ plane we obtain a (2D) Stoner factor $I(q) \approx 0.43 \text{eV}/(1 + 0.08q^2)$, favoring ferromagnetic spin fluctuations in the plane. However, the 2D character of the band structure of Sr$_2$RuO$_4$ introduces additional complications. As discussed in Refs. 5, 6, of the three Fermi surface sheets one ($\gamma$) is quasi-isotropic 2D, and two ($\alpha$ and $\beta$) are quasi-1D. The latter can be visualized (cf. Fig.1 in Ref. 5) as a system of parallel planes separated by $Q = 2\pi/3a$, running both in the $x$ and $y$ directions. This is true in the nearest neighbor $dd\pi$ tight-binding model, while in reality due to the next hoppings the planes are warped and reconnected at the crossing lines, to form two pseudo-square prisms, obtained in LDA calculations and observed experimentally. Naturally, such a Fermi surface should give rise to sizable nesting effects at the wave vectors $k = (Q, k_y)$, $k = (k_x, Q)$, and especially at $k = Q = (Q, Q)$. This would lead to AFM spin fluctuations at these vectors, in addition to the FM fluctuations discussed above. To check, we have integrated the LDA band structure of Sr$_2$RuO$_4$ to get the bare RPA susceptibility,

$$\chi_0(q) = \sum_{k_{ij}} \frac{M_{k_{ij}, k_{ij}q}f(\varepsilon_{k_{ij}}) - f(\varepsilon_{k_{ij}q})}{\varepsilon_{k_{ij}q} - \varepsilon_{k_{ij}}}.$$  

where $f$ is the Fermi distribution function, $i$ and $j$ label the three bands. All $|k_i >$ states were classified according to the maximal $t_{2g}$ character, $xy$, $yz$, and $zx$, and the matrix element $M$ is taken to be 1 between two states which have the same maximal character and 0 otherwise. This is, of course, a rather crude approximation, but it should reveal the qualitative behavior of $\chi_0$. The results are shown in Fig.1. Roughly speaking,

$$\chi_0(q) = N(0) + \chi_n(q),$$  

where $\chi_n$ is the nesting-dependent contribution. The total susceptibility can then be expressed as

$$\chi(q) = \frac{\chi_0(q)}{1 - I(q)\chi_0(q)} = \frac{\chi_0(q)}{1 - I(q)N(0) - I(q)\chi_n(q)}.$$  

This form implies two different kinds of spin fluctuations: FM ones, $q = 0$, and AFM ones, at $q = Q$. If $I(Q)N(0) + I(Q)\chi_n(Q) > I(0)N(0)$, the AFM fluctuations are stronger. This seems to be the case in Sr$_2$RuO$_4$ : our calculations yield $I(0)N(0) = 0.82$, in good agreement with the experimentally observed susceptibility enhancement, and $I(Q)N(0) + I(Q)\chi_n(Q) = 1.02$ (which actually corresponds to an instability with respect to tripling of the unit cell both in $x$ and in $y$). Since no instability is observed in the experiment, nor in the direct calculations, we conclude that the approximate treatment of the matrix elements in Eq.4 leads to an overestimation of $\chi_n$ by at the very least 2%, but the conclusion that AFM fluctuations are stronger or at least comparable with the FM ones likely holds.

![FIG. 1. Calculated bare susceptibility for Sr$_2$RuO$_4$](Image)

The direct way to test this experimentally is via neutron scattering. There is, however, an indirect argument in favor of strong AFM spin fluctuations. Increasing the effective dimensionality by adding additional RuO$_2$ layers, one can increase $N(0)$ and eventually get a FM instability. Experimentally this happens when the number of layers is 3 or maybe even 2. Another possible (but not guaranteed) effect of adding layers is increased $z$-dispersion and thus deteriorated nesting. On the other hand, reducing the next-nearest-neighbor hopping should improve nesting and make an AFM transition more likely. One expects such a reduction from rotating the RuO$_6$ octahedra, as for instance in Ca$_2$RuO$_4$. Indeed, experimentally Ca$_2$RuO$_4$ is an AFM with a magnetization of 1.2–1.3 $\mu_B$/Ru and $T_N \approx 150$ K. Moreover,
this AFM state is remarkably different from typical Mott-Hubbard insulators, driven by strong Coulomb correlations. First, although the conductivity grows with temperature, the functional dependence is consistent with a variable-range hopping and not with activation. Second, there is substantial density of states at the Fermi level, as evidenced by specific heat measurements. These two facts indicate that Ca$_2$RuO$_4$ is not a simple insulator, but a metal with disorder localized carriers (which might explain why it has been discussed above, and they are the Stoner ferromagnetism. The calculated density of states is sizable, although the conductivity grows with temperature, the functional dependence is consistent with variable-range hopping and not with activation.

We performed LDA calculations for Ca$_2$RuO$_4$ similar to those reported in Refs. [3,4] and found a magnetic moment of $\approx 1.5 \mu_B$ (of which $\approx 1 \mu_B$ is inside the the Ru MT sphere and the rest mostly residing on the apical oxygens) for Ca$_2$RuO$_4$ (in agreement with the experimental $M = 1.3 \mu_B$). In fact, we also find a FM instability, and that the FM and the AFM states Ca$_2$RuO$_4$ degenerate within the LDA to within a few meV/atom, indicating a close competition between these two magnetic states [11]. For genuine Mott insulators the LDA either fails to reproduce the magnetic instability, or underestimates the magnetization. The calculated density of states is sizable, $N(E_F) = 1.6$ st./eV spin f.u., but the corresponding effective mass is large (the in-plane average $n/m = 7.5 \times 10^{20}$ cm$^{-3}$/m$_0$), because Ru is strongly spin polarized and thus Ru-Ru nearest neighbor hopping is suppressed with AFM order. This also facilitates localization.

We now enumerate the relevant magnetic interactions in the (Sr,Ca)$_2$RuO$_4$ system. The first two have been discussed above, and they are the Stoner ferromagnetism ($Q = 0$), nesting-derived antiferromagnetism ($Q \approx \{2\pi/3, 2\pi/3\}$). As usually, there is also superexchange ($Q = \{\pi, \pi\}$). One should be reminded at this point, that superexchange per se is not a strong correlation phenomenon. In a quasi-one-electron approach like LDA, for sufficiently large exchange splittings, an AFM state is lower in energy than the FM one by roughly $Zt^2/\Delta$, where $Z$ is coordination, $t$ is the hopping, and $\Delta$ is the exchange splitting. Since $t$ is usually overestimated in LDA, and $\Delta$ is usually smaller than Hubbard $U$, the effect of superexchange is usually overestimated, not underestimated in LDA (see Ref. [8] for more).

While superexchange is a universal mechanism and should also be operative in Ca$_2$RuO$_4$, it hardly plays a leading role. Otherwise, the LDA calculations that gave the right Ru moment would have overstabilized the AFM state, while in reality the opposite is true (they come out degenerate instead of the AFM being the ground state). The most likely cause for the instability is nesting. Furthermore, superexchange is of less relevance for Sr$_2$RuO$_4$ because it manifests itself for finite amplitude spin fluctuations, and not in the low-energy spectrum.

Assuming that the LDA gives a reasonable description of the spectrum of spin fluctuations in Sr$_2$RuO$_4$, we can discuss the consequences that the AFM spin fluctuations may have on superconductivity. Recall that in $p$-wave superconductivity only the small $q$ spin fluctuations are pairing, while in the $d$-wave case they are mostly pair-breaking. For a spectrum with a complicated $q$ dependence, as the one described by Eq.3, the most favorable state is defined by an interplay of the Fermi surface geometry and the structure of the effective interaction. In the weak coupling near $T_c$ the gap equation looks like

$$\Delta_{ki} = \sum_{k'j} V_{ki,k'j} \Delta_{k'j},$$

where for the singlet ($d$) pairing $\Delta$ is the order parameter, and $V_{ki,k'j}$ is (negative) pairing interaction, which in the same approximation as the one used in Ref. [9] is given by

$$V(q = k - k') = -\frac{I^2(q)\chi_0(q)}{1 - I^2(q)\chi_0^2(q)}.$$  

For the triplet ($p$) pairing $\Delta$ is the amplitude of the order parameter, usually denoted as $d$, and $V_{ki,k'j}$ now includes the sign-changing angular factor:

$$V(q = k - k') = \frac{\nu_k \cdot \nu_{k'}}{\nu_k \cdot \nu_{k'}} \frac{I^2(q)\chi_0(q)}{1 - I^2(q)\chi_0^2(q)}.$$  

The largest eigenvalue of the matrix $V$ in Eq.4 defines the critical temperature, and the corresponding eigenvector defines the anisotropy of the gap near $T_c$. Correspondingly, the instability in the singlet channel is defined by the same matrix, but with the opposite sign (the interaction is repulsive in singlet channel), and without the angular factor $\frac{\nu_k \cdot \nu_{k'}}{\nu_k \cdot \nu_{k'}}$. We have solved these eigenvalue problems numerically using a discrete mesh of $k$ points at the Fermi line. We used model susceptibility [8], adding an adjustable reduction $\alpha$ for the nesting.
part, \( \chi_0(\mathbf{q}) = N(0) + \alpha \chi_\alpha(\mathbf{q}) \), and look for the solutions at different \( \alpha < 0.98 \) (i.e., below actual AFM instability). Furthermore, to simplify the calculations, we used an analytical form for \( \chi_\alpha(\mathbf{q}) \) that recovers the main qualitative characteristics of the numerical result of Fig.1, namely \( \chi_\alpha(\mathbf{q}) = A(\cos(aq_x) + \cos(aq_y)) + B(\cos(2aq_x) + \cos(2aq_y)) + C(\cos(aq_x) + \cos(aq_y)) \).

The results are shown in Fig. 2. Amazingly, only in close vicinity to the actual AFM instability (0.85 < \( \alpha < 0.98 \)) the superconducting transition happens in the \( d \)-wave channel. For smaller \( \alpha \) the \( p \)-wave state is favored. An interesting question is, what is the angular and/or interband anisotropy of the gap. We illustrate this anisotropy for the critical value of \( \alpha \) (Fig. 3). The \( p \)-wave state is relatively isotropic, indicating that at least in the Fermiology there is no reason for substantial interband anisotropy (“orbital-dependent superconductivity”), suggested in Ref. \([4]\). The \( d \)-wave, to the contrary, is substantially anisotropic beyond the standard anisotropy associated with the nodes along the \( \{\pi, \pi\} \) direction, namely the so-called \( \alpha \) pocket of the Fermi surface has nearly vanishing order parameter.

Our conclusions are as follows: (1) LDA calculations yield a self-consistent solution with the AFM ordering for \( \text{Cs}_2\text{RuO}_4 \), degenerate with a FM solution. The non-magnetic state is considerably higher in energy, in agreement with the experiment. The calculated magnetization value of \( \approx 1 \mu_B \) is in agreement with the experiment as well. (2) This fact suggests that besides the known tendency to ferromagnetism, there is an intrinsic tendency to antiferromagnetism in \( \text{Ru} \) based layered perovskites. (3) Analysis of the Fermi surface geometry of \( \text{Sr}_2\text{RuO}_4 \), as well as direct calculations, indicate a strong nesting at \( \mathbf{Q} = \{\pm 2\pi/3, \pm 2\pi/3\} \), as well as a weaker nesting for the wave vectors connecting these four points (Fig. 1). This result also suggests that the AFM ordering in \( \text{Ca}_2\text{RuO}_4 \) is mostly due to nesting, although superexchange may play some role as well. It is, however, unlikely that this compound is a Mott-Hubbard insulator. (4) The spin fluctuations in \( \text{Sr}_2\text{RuO}_4 \) have both a FM and an AFM component, of comparable magnitude, thus making \( d \)-wave superconductivity a strong competitor with the \( p \)-wave state. It is possible that the system may be driven to the \( d \)-wave superconductivity by an external force, for instance by pressure. (5) Spin fluctuation spectrum combined with the actual fermiology of \( \text{Sr}_2\text{RuO}_4 \) produced a \( p \)-wave state with little angular or interband anisotropy. (6) The sister compound \( \text{Cs}_2\text{RuO}_4 \) is a low carrier density metal, where carrier are localized due to disorder and electron-magnon scattering, and where antiferromagnetism is primarily due to the nesting effects.

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\[ \text{FIG. 3. Relative magnitude of the order parameter in} \]

\[ \text{the singlet (left) and the triplet (right) states. Parameter} \]

\[ \alpha \]

\[ \text{is the same for both panels (0.83), corresponding to the} \]

\[ \text{coupling constant in both channels} \lambda \approx 0.5. \]

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\[ \text{the Office of the Naval Research.} \]

\[ [1] \text{T.M. Rice and M. Sigrist, J. Phys. Condens. Matter 7, L643 (1995).} \]
\[ [2] \text{M. Sigrist et al, Proc. of the conference “Anomalous Complex Superconductors”,} \]
\[ \text{Crete, 1998, to be published.} \]
\[ [3] \text{D. J. Singh, J. Appl. Phys. 78, 4819 (1996).} \]
\[ [4] \text{I. I. Mazin and D. J. Singh, Phys. Rev. B 56, 2556 (1997).} \]
\[ [5] \text{I. I. Mazin and D. J. Singh, Phys. Rev. Lett. 79, 733 (1997).} \]
\[ [6] \text{M. Braden, G. Andre, S. Nakatsuji, and Y. Maeno, Phys. Rev. B 58, 847 (1998).} \]
\[ [7] \text{D.J. Singh, Planewaves Pseudopotentials and the LAPW} \]
\[ \text{method (Kluwer, Boston, 1994) and references therein.} \]
\[ [8] \text{Imai et al (preprint submitted to PRL) recently reported} \]
\[ \text{NMR relaxation rate measurements which they interpreted as indication of the absence of} \]
\[ \text{AFM spin fluctuations. However, their data only relate with the spin} \]
\[ \text{susceptibility at} \] \[ \mathbf{q} = \{\pi, \pi\} \text{, while our calculations predict spin fluctuations at} \]
\[ \mathbf{q} = \mathbf{Q} = \frac{2}{5}(\pi, \pi). \]
\[ [9] \text{In the calculation (to be published elsewhere) the} \]
\[ \text{n = 2} \]
\[ \text{compound} \] \[ \text{Sr}_3\text{Ru}_2\text{O}_7 \text{is not yet ferromagnetic; experimental reports are contradictory, but the} \]
\[ \text{n = 3} \]
\[ \text{material,} \] \[ \text{Sr}_4\text{Ru}_3\text{O}_10 \text{is positively FM.} \]
\[ [10] \text{We do not discuss here the smearing of the density of} \]
\[ \text{states due to additional Bragg reflections in a distorted} \]
\[ \text{structure, an effect that controls the loss of magnetic} \]
\[ \text{ordering from} \] \[ \text{SrRuO}_3 \text{to} \] \[ \text{Ca}_2\text{RuO}_4. \]
\[ [11] \text{We used crystal and magnetic structure of} \] \[ \text{Ca}_2\text{RuO}_4 \text{as recently measured by means of neutron scattering} \]
\[ \text{[3]. The full-potential linear augmented plane wave method, as described in} \]
\[ \text{[4]} \text{was utilized. The ferromagnetic structure appeared lower than the AFM one by} \]
\[ \approx 0.5 \text{mRy/Ru. While the technical accuracy of the computations is better than that, the} \]
\[ \text{LDA itself is not as accurate in magnetic energy differences; LDA and GGA} \]
\[ \text{results, for instance, usually differ by a larger margin. It is not excluded that on top of the} \]
\[ \{\pi, \pi\} \text{AFM structure reported in Ref. [4] there is an incommensurate super-} \]
structure with $\mathbf{Q} \simeq 0.6(\pi/a, \pi/b)$. This would lower the energy slightly and probably render this AFM state more stable than the FM one. A more detail account of these calculations will be published elsewhere.

[12] The effective mass has substantial (factor of 3) in-plane anisotropy.