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# Fermiology and interaction in unconventional superconductors—Triplet vs singlet pairs

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#### Abstract

We give an overview on how the superconductivity is in general affected by the underlying electronic structure (spatial dimensionality, shape of the Fermi surface, etc.) and the form of the electron–electron interaction. We discuss: (i) Two-dimensional systems are generally more favourable. Disconnected Fermi surfaces greatly help, since we can insert nodes, required for anisotropic pairs arising from electron–electron repulsions, in between the Fermi sheets or pockets. (ii) When spin-fluctuation mediated, the pairing interaction is much larger in the singlet channel than in the triplet channel, while this can be altered when charge fluctuations are significant for longer-ranged interactions. We propose that a combined effect of (i) (quasi-1D Fermi surface) and (ii) favours an f pairing in an organic superconductor (TMTSF)<sub>2</sub>PF<sub>6</sub>. For Sr<sub>2</sub>RuO<sub>4</sub>, we propose a time-reversal-broken triplet  $p_{x+y} + ip_{x-y}$  pairing, which is again stabilised by the charge-fluctuation mediated interaction. External magnetic field can also give rise to a non-unitary pairing. (iii) We also point out that multi-orbital systems has a possibility, e.g., a spin-triplet, of orbital-singlet pair. These should have relevance to vortex structures. © 2006 Elsevier B.V. All rights reserved.

Keywords: Electron correlation; Triplet pair; Singlet pair; Spin fluctuations; Charge fluctuations; Ruthenate; TMTSF

## 1. Introduction

There is a growing realisation that the unconventional superconductors, exemplified by the cuprates, have an electronic mechanism, where anisotropic pairs arise from the repulsive electron–electron interaction. While superconductivity from electron repulsion is conceptually interesting in its own right, one prominent feature in the strongly correlated electron systems is that the way in which the correlation effects such as magnetism and superconductivity appear is very sensitive to the underlying band structure. We can then extend the idea to fermiology in correlated electron systems to explore the possibility of manipulating superconductivity and magnetism by choosing the shape of the Fermi surface [1].

Here we discuss how pairs with various symmetries, including both spin singlet and triplet pairs, can be

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favoured from the viewpoints of (i) dimensionality and fermiology, (ii) spin-fluctuation mediated vs chargefluctuation mediated interactions, and (iii) multi-orbital systems.

### 2. Dimensionality and fermiology

## 2.1. Singlet vs triplet pairings in 2D vs 3D

Arita et al. have examined typical two-dimensional (2D) and 3D lattices with various band filling or t' [2] with the fluctuation exchange approximation (FLEX). The conclusion is

	2D	3D
Singlet	V	V
Triplet	Х	Х

The reason why 2D is more favourable than 3D may be traced back [2,3] to Eliashberg's equation, where the height

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and width of the region both in the frequency  $(\omega)$  and momentum (q) sectors over which the interaction is appreciable turn out to be similar between 2D and 3D. This means that their phase volume fraction is much greater in 2D. This agrees with the empirical fact that there are many layered superconductors (cuprates, Co compound, Hf compound, CeCoIn<sub>5</sub>, etc.).

Why triplet p is weak even when ferromagnetic fluctuations dominate may be traced back to the pairing interactions in the singlet channel and triplet channel (characterised by the *d*-vector  $|| z \text{ or } \perp z$ ),

$$\begin{split} V_{\text{singlet}}(\boldsymbol{q}) &= +(1/2)V_{\text{spin}}^{zz}(\boldsymbol{q}) + V_{\text{spin}}^{+-}(\boldsymbol{q}), \\ V_{\text{triplet}}^{d\parallel z}(\boldsymbol{q}) &= +(1/2)V_{\text{spin}}^{zz}(\boldsymbol{q}) - V_{\text{spin}}^{+-}(\boldsymbol{q}), \\ V_{\text{triplet}}^{d\perp z}(\boldsymbol{q}) &= -(1/2)V_{\text{spin}}^{zz}(\boldsymbol{q}), \end{split}$$

where  $V_{\text{spin}}^{zz}(V_{\text{spin}}^{+-})$  is the longitudinal (transversal) spin-fluctuation-mediated interaction, and q is the momentum transfer. When the spin is isotropic  $|V_{\text{triplet}}| = (1/3)V_{\text{singlet}}$ , i.e., the pairing interaction in the singlet channel, which can exploit all the three (two transverse [+-] as well as longitudinal) components, is three times as large as in the triplet channel. This is consistent with a salient fact that triplet superconductors are very rare, found only in some heavy fermion compounds, organic metals, and a ruthenate, Sr<sub>2</sub>RuO<sub>4</sub>.

## 2.2. Why is $T_C$ so low?

 $T_{\rm C}$  in the electron mechanism is very low, in that  $T_{\rm C}$ , as estimated with FLEX [4] and more recently with DCA [5], is  $T_{\rm C} < 0.03t$ , two orders of magnitude smaller than the starting electronic energy scale, t. This is also the case with Uemura's experimental plot for  $T_{\rm C}$  against  $T_{\rm F}$  for all the known superconductors. Theoretically, there are good reasons why  $T_{\rm C}$  is low: (a) The effective attraction mediated by the fluctuation is much smaller than the starting repulsive interaction. (b) Quasi-particles have finite lifetimes due to the self-energy correction arising from the electron correlation. (c) Pairing in repulsive systems has to be anisotropic with nodes in the gap function, and the nodes, which usually intersect the Fermi surface, act to greatly suppress  $T_{\rm C}$ .

Recently, Kuroki and Arita [6] have proposed that we can overcome the difficulty (c) by considering disconnected Fermi surfaces, on which we can insert the nodes in between the Fermi pockets. Each pocket is then fully gapped, with opposite signs across the pockets.  $T_C \sim 0.08t$ , almost an order of magnitude higher, is indeed estimated with FLEX in the disconnected cases. Other lattices (plaquette lattices [7], bond-alternating lattices in 3D [8]) have also been shown to have similar  $T_C$ . The mechanism works for triplet [9] as well. Examples for triplet are triangular and honeycomb lattices, and Kuroki et al. [10] have recently examined its relevance to the Co compound superconductor, although complications such as multi-bands may be relevant in the compound [11].



Fig. 1. Pairs, formed within each piece of the Fermi surface, can exploit interband pair scattering (arrows).

## 2.3. Structure of $\chi(\mathbf{q},\omega)$

In the above mechanism pairs are formed within each pocket, and they exploit the interband pair scattering processes (Fig. 1). A question then is: Better the nesting, the better? In the simply connected Fermi surfaces, the pairing arises from the intraband nesting, and we have previously suggested [12] that the better nesting does not necessarily imply the more enhanced pairing correlation. This applies to the interband nesting as well. A physical picture is that the Fermi surface, or the band dispersion to be more precise, must be such that the peak position, height and width in the spin susceptibility  $\gamma(q,\omega)$  in both wave number and frequency sectors have to be right for the superconductivity to be optimised. Specifically, the susceptibility peak has to be blurred with a width comparable to the size of the Fermi pocket. This should be related to the energy spread of the k-dependent part of the spin fluctuation discussed in Moriya's SCR theory.

#### 3. Spin- vs charge-fluctuation mediated pairing

Even when the shape of the Fermi surface is right, we still have to overcome the difficulty of  $|V_{\text{triplet}}| = (1/3)|V_{\text{singlet}}|$  for the triplet pairing to be stable. We can then note that the interaction contains not only  $V_{\text{spin}}$ , which is the main component for the Hubbard model with an on-site repulsion, but also the charge-fluctuation mediated pairing interaction,  $V_{\text{charge}}$ , which can become significant when the interaction extends beyond the on-site, so the full expression is

$$V_{\text{singlet}}(q) = +(3/2)V_{\text{spin}}(q) - (1/2)V_{\text{charge}}(q),$$
  
$$V_{\text{triplet}}(q) = -(1/2)V_{\text{spin}}(q) - (1/2)V_{\text{charge}}(q).$$

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