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Magnetic interactions in iron superconductors: A review

Revue des interactions magnétiques dans les supraconducteurs à base de fer

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ABSTRACT

High-temperature superconductivity in iron pnictides and chalcogenides emerges when a magnetic phase is suppressed. The multi-orbital character and the strength of correlations underlie this complex phenomenology, involving magnetic softness and anisotropies, with Hund's coupling playing an important role. We review here the different theoretical approaches used to describe the magnetic interactions in these systems. We show that taking into account the orbital degree of freedom allows us to unify in a single phase diagram the main mechanisms proposed to explain the $(\pi, 0)$ order in iron pnictides: nesting-driven superconductivity, exchange between localised spins, and Hund-induced magnetic state with orbital differentiation. Comparison of theoretical estimates and experimental results helps locate the Fe superconductors in the phase diagram. In addition, orbital physics is crucial to address the magnetic softness, the doping-dependent properties, and the anisotropies.

RÉSUMÉ

La supraconductivité à haute température dans les pnictures et les chalcogénures de fer émerge quand une phase magnétique est supprimée. Le caractère multi-orbital et la force des corrélations sont sous-jacents à cette phénoménologie complexe, faisant appel à la douceur magnétique et aux anisotropies, dans lesquelles le couplage de Hund joue un rôle important. Nous passons ici en revue les différentes approches théoriques utilisées pour décrire les interactions magnétiques dans ces systèmes. Nous montrons que la prise en compte du degré de liberté orbital nous permet d'unifier dans un seul diagramme de phases les principaux mécanismes proposés pour expliquer l'ordre $(\pi; 0)$ dans les pnictures de fer : supraconductivité *nesting-driven*, échange entre spins localisés et état magnétique induit par couplage de Hund avec différenciation orbitale. La comparaison des estimations théoriques et des résultats expérimentaux nous permet de localiser les supraconducteurs à base de fer dans le diagramme de phases. De plus, la physique orbitale est cruciale pour approcher la douceur magnétique, les propriétés dépendant du dopage ainsi que les anisotropies.

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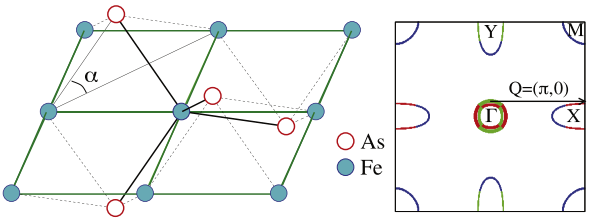

Fig. 1. (Left) The crystal structure of all the families of Fe superconductors share planes with Fe in a square lattice with a pnictogen or a chalcogen (here As) located out of plane in a tetrahedral coordination. The relative position of the out-of-plane anions with respect to the plane can be described by the angle α. Reproduced from [31]. (Right) Typical Fermi surface defined in the unfolded Brillouin zone (which corresponds to a single Fe unit cell with the x and y directions defined along the Fe nearest neighbours). This Fermi surface has been calculated with the tight-binding proposed in [31] with the α corresponding to a regular tetrahedron. The arrow indicates the wave-vector of the columnar ordering $(\pi, 0)$. The pockets at Γ and M are hole pockets and the ones at X and Y are electron pockets. The colour code refers to the orbital with the highest weight on a particular part of the Fermi surface: blue for xy, red for zx and green for yz. The e_g orbitals $3z^2 - r^2$ and $x^2 - y^2$ are also present at the Fermi surface though with a smaller weight [31]. For interpretation of the references to colour in this figure caption, please see the online version of this article.

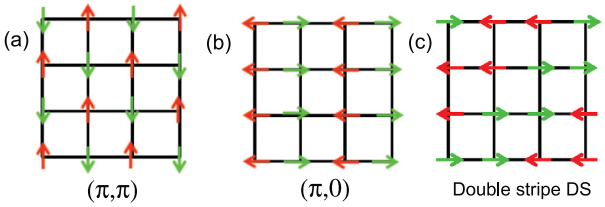

Fig. 2. (Colour online.) Some of the different antiferromagnetic orders within the Fe plane that appear in Fe-based superconductors. Each arrow represents the magnetic moment on an Fe ion. (a) The $\mathbf{Q} = (\pi, \pi)$ order, (b) the columnar order $\mathbf{Q} = (\pi, 0)$, the most common order in the Fe-pnictides, and (c) the double stripe order as in FeTe.

1. Introduction

The discovery of iron superconductors [1,2] challenged the uniqueness of cuprates as high T_c superconductors, triggering the search for new materials in previously unexplored directions. Most iron superconductors are magnetic when undoped, and the suppression of the magnetism via doping, pressure or isoelectronic substitution is accompanied by the appearance of a superconducting phase [3–5]. There is also a structural phase transition that may coincide with the magnetic transition or occur at a higher temperature. Details may depend on the particular structure or chemical composition but the general trends are robust. All the families of iron superconductors have atomic layers with Fe in a square lattice and a pnictogen (P, As) or a chalcogen (Se, Te) out of plane in tetrahedral coordination [6], see Fig. 1. Understanding the magnetism and electronic correlations in these systems may be the clue for elucidating the yet unknown pairing mechanism for high T_c superconductivity [5,7].

Superficially, the iron superconductors phase diagram resembles very much that of the cuprates in the sense that a magnetic phase is replaced by a superconducting one with doping [8]. However, there are some deep differences whose relevance for superconductivity is still to be determined. Undoped cuprates are well known for being Mott insulators and (π, π) order antiferromagnets. On the other hand, undoped Fe superconductors are generally metallic and show different types of magnetic arrangements [3,7]. The one that dominates is the columnar $(\pi, 0)$ one (with axis defined in the Fe–Fe first neighbours direction): antiferromagnetic in the x-direction and ferromagnetic in the y-direction, see Fig. 2. This order (or related magnetic fluctuations) is usually accompanied by a tetragonal to orthorhombic structural transition and in-plane (x/y) anisotropies.

The $(\pi, 0)$ order is found in the undoped iron arsenides, a denomination that includes different chemical compositions and structures – all with FeAs planes. The arsenides mainly comprise the 1111 family, like LaOFeAs, the 122, like $BaFe_2As_2$, and the 111, like LiFeAs and NaFeAs. The related phosphides (with FeP planes) are non-magnetic and their superconducting T_cs are low [1]. Most of the arsenides show the columnar order with a small magnetic moment, with typical values under $1\,\mu_B$ per Fe, and are metals [9]. LiFeAs is an exception to the rule as it does not order magnetically, it does not go through a structural transition and it is superconductor [10]. The iron chalcogenide FeTe has a different magnetic order, the double stripe, namely a double FM column along the diagonals (the Fe–Fe second-neighbour direction) and a larger magnetic moment $\sim 2\,\mu_B$ per Fe [11]. On the other hand, bulk FeSe suffers a structural transition at a much higher temperature than the superconducting one but bulk static magnetism only arises under pressure [12,13]. Related systems arise when some spacer is introduced between the FeSe layers [14–19]. The parent compounds of the alkaline Fe selenides $A_yFe_{2-x}Se_2$ (A = K, Rb, Cs, Tl), with Fe vacancies arranged in a particular pattern, have a block antiferromagnetic order with a large magnetic moment of $\sim 3\,\mu_B$ per Fe, and are insulators [20,21]. Transitions between different magnetic orders have been observed as a function of doping [22] and pressure [23,24].

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