Physica C 469 (2009) 640–650

Contents lists available at ScienceDirect

Physica C

journal homepage: www.elsevier.com/locate/physc

Renormalization group analysis of competing orders and the pairing symmetry in Fe-based superconductors

A.V. Chubukov

Department of Physics, University of Wisconsin-Madison, Madison, WI 53706, USA

ARTICLE INFO

Article history:
Available online 19 March 2009

PACS:
74.20.Mn
74.20.Rp
74.25.Jb
74.25.Ha

Keywords:
Superconductivity
Magnetism
Pairing symmetry

ABSTRACT

We analyze antiferromagnetism and superconductivity in novel Fe-based superconductors within the weak-coupling, itinerant model of electron and hole pockets near $(0,0)$ and (π,π) in the folded Brillouin zone. We discuss the interaction Hamiltonian, the nesting, the RG flow of the couplings at energies above and below the Fermi energy, and the interplay between SDW magnetism, superconductivity and charge orbital order. We argue that SDW antiferromagnetism wins at zero doping but looses to superconductivity upon doping. We show that the most likely symmetry of the superconducting gap is A_{1g} in the folded zone. This gap has no nodes on the Fermi surface but changes sign between hole and electron pockets. We also argue that at weak coupling, this pairing predominantly comes not from spin fluctuation exchange but from a direct pair hopping between hole and electron pockets.

1. Introduction

Recent discovery of superconductivity (SC) in the iron-based layered pnictides with T_c ranging between 26 and 52 K generated enormous interest in the physics of these materials, which also hold strong potential for applications [1]. SC has been observed in oxygen containing 1111 systems RFeAsO, where R = La, Nd, Sm, Pr, Gd, in oxygen-free 122 systems AFe_2As_2, where A = Ba, Sr, Ca, and in several other classes of materials like LiFeAs with 111 structure and α-FeSe with 11 structure [2–8].

In several respects, the pnictides are similar to the cuprates. Like the cuprates, the pnictides are highly two-dimensional, their parent materials show antiferromagnetic long-range order below 150 K [2,9–12], and superconductivity occurs upon doping of either electrons [2–5] or holes [6] into FeAs layers. This lead to early conjectures that the physics of the pnictides is similar to that of the cuprates and involves insulating Mott behavior [13–16]. Resistivity measurements, however, showed that iron pnictides remain itinerant down to zero doping, although the jury is still deliberating whether some signatures of Mott physics have been observed at higher energies (see e.g., [16,17]). Other evidences for itinerant behavior include

- a relatively small value of the observed magnetic moment per Fe atom in the magnetically ordered phase – 12–16% of $2\mu_B$ in 1111 materials [12,10],
- a good agreement between electronic band structure calculations [18–23] and ARPES and magneto-oscillation measurements of the Fermi surface (FS) and electronic states [24–29],
- drude-like behavior of the optical conductivity at small frequencies [30].

Although there are certain variations in the crystal structure between different classes of pnictides, the low-energy electronic structure is likely the same for all systems and consists of two small hole pockets at the center of the Brillouin zone (BZ) and two small electron pockets centered around M points (Fig. 1). The M points are located $q_1 = (0,\pi/a)$ and $q_2 = (\pi/a,0)$ in the unfolded BZ (one Fe atom in the unit cell) and at identical points $k_1 = (\pi/\bar{a},\pi/\bar{a})$ and $k_2 = (\pi/\bar{a},-\pi/\bar{a})$ in the folded BZ (two Fe atoms in the unit cell, $\bar{a} = a\sqrt{2}$) (see Fig. 2). The relations between the momenta in the folded and unfolded zones are $k_x = (q_x + q_y)/\sqrt{2}, k_y = (q_x - q_y)/\sqrt{2}$. The unfolded BZ includes only Fe states, the folded BZ (the correct zone) takes into account the fact that only a half of Fe states are actually identical in pnictides because of *As* which resides either above or below Fe plane (Fig. 2). Below we will use the folded BZ. Throughout the paper we define M point as $\mathbf{Q} = (\pi/\bar{a},\pi/\bar{a})$ and set $\bar{a} = 1$.

The goal of this paper is to summarize recent work done in collaboration with Efremov and Eremin [31] and by myself on the weak-coupling, Fermi-liquid analysis of magnetic and superconducting instabilities in the pnictides. I will address several issues:

- What interactions cause magnetism and SC?
- Are SC and magnetism competing orders?

E-mail address: chubukov@physics.wisc.edu

0921-4534/$ - see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.physc.2009.03.023

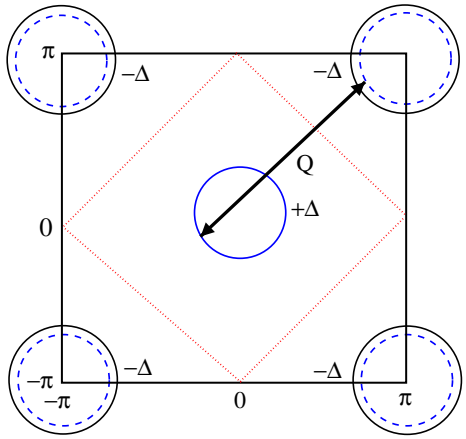

Fig. 1. A simplified geometry of Fe-based superconductors used in the present work. The Fermi surface consists of an electron pocket around (π,π) (black solid circle), and a hole pocket of roughly equal size around (0,0) (blue solid circle). A near-perfect nesting between hole and electron pockets means that, by moving a hole FS by (π,π), one obtains a near-perfect match with an electron FS. Upon electron doping, the size of the electron pocket increases (dashed blue → black), what breaks the nesting. Upon hole doping, the size of a hole FS increases, what again breaks the nesting. $+\Delta$ and $-\Delta$ are the values of the superconducting gaps on the two FS for an s^+ superconducting state. (From Ref. [31]). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

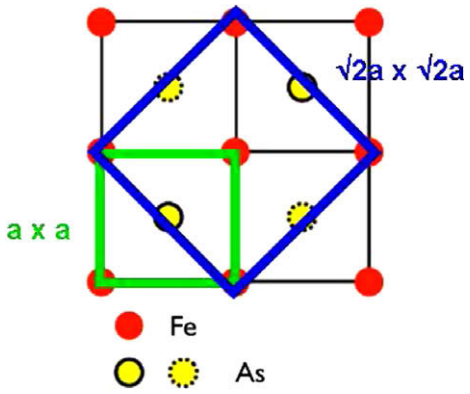

Fig. 2. Elementary unit cells for unfolded and folded BZ. The unit cell for the unfolded BZ is $a \times a$ square (one Fe atom per unit cell). The elementary cell for the folded zone (the correct one) is constructed to take into account the fact that only a half of Fe states are actually identical because *As*, whose projection onto an *Fe* plane is at a center of a square, is located either above or below an *Fe* plane. The elementary cell for the folded zone contains two Fe atoms and is a square with dimensions $\sqrt{2}a \times \sqrt{2}a$, rotated by 45^0 compared to the unit cell for the unfolded zone.

- Is charge order possible?
- What is the symmetry of the SC gap and how to overcome intra-pocket repulsion.
- Is the pairing magnetically mediated?

Central to weak coupling analysis is the idea of a near-nesting between electron and hole pockets at zero doping. The nesting does not mean that any of the FS has parallel pieces but rather implies that, by moving a hole FS by **Q**, one obtains a near-perfect match with an electron FS. This FS geometry is in a reasonable agreement with ARPES and magneto-oscillation measurements [24–29]. It has been known from the studies of chromium and its alloys in the 70th [32,33] and from generic theoretical studies of "excitonic insulators" [34] that such nesting leads to a spin-density-wave (SDW) order with momentum **Q** already at weak coupling in the same way as SC order appears at weak coupling in a BCS superconductivity. For pnictides, the role of nesting for SDW order was emphasized by Cvetkovic and Tesanovic [35] and Barzykin and Gorkov [36]. Upon doping, either by holes or by electrons, one of the two pockets gets relatively larger and the nesting breaks down. In this situation, SDW order gets weaker [35,37–39], and at some doping superconductivity emerges. How pnictides evolve from a magnet to a superconductor is not clear at the moment, and there are experimental evidences for both first order and continuous transitions. Theoretically, both situations are possible [40].

What interaction causes superconductivity and what is the symmetry of the superconducting gap are the two most intriguing issues for the pnictides. A conventional phonon-mediated *s*-wave superconductivity is an unlikely possibility because electron–phonon coupling calculated from first principles is quite small [41]. An electronic mechanism is therefore more likely. Mazin et al. [21] conjectured, by analogy with the cuprates, that SC in pnictides is mediated by antiferromagnetic spin fluctuations. This pairing mechanism is most effective if the superconducting gap changes the sign under the momentum shift by **Q**. For the cuprate FS, this unambiguously leads to $d_{x^2-y^2}$ superconductivity. For pnictides, the requirement is that the gap must change sign between hole and electron FS. This does not unambiguously determines the gap structure, but most natural would be the gap which is a constant Δ along a hole FS and a constant $-\Delta$ along an electron FS. In the classification of the eigenfunctions of the tetragonal D_{4h} group, this gap belongs to A_{1g} representation and is roughly $\Delta(\mathbf{k}) = \Delta(\cos k_x + \cos k_y)/2$ [36]. We will refer to this gap symmetry as s^+. The s^+ gap has been found as the most likely candidate in some of the RPA studies based on a 5-orbital Hubbard model [42], a 2-band spin-fluctuation model [43], and in the renormalization group (RG) analysis [44,31] (see below). The s^+ gap structure also emerges in the analysis based on localized spin models [45].

There are, however, two potential problems with the spin-fluctuation mechanism. First, the close proximity to a magnetic phase does not a'priori guarantee that the pairing is magnetically mediated. This is particularly true for pnictides because of two separate FS in which case there are multiple interactions between hole and electron states, and the interaction which gives rise to magnetism is not necessary the same interaction that gives rise to SC. This has to be verified in the calculations. We will argue below that the full pairing interaction does have a component which represents the exchange by soft dynamic magnetic fluctuations peaked at **Q**. However, we will argue that this component is subleading at weak coupling, and the dominant pairing component is a direct pair-hopping term. This does not change the outcome, though, that the pairing is in the s^+ channel.

Second, intra-pocket repulsion does not cancel out from the s^+ pairing problem because average gap along either hole or electron FS is non-zero. The intra-pocket interaction term in the Hamiltonian is quite likely stronger than the pair-hopping term [44,31] such that at this level s^+ channel is repulsive. One has to see to where the interactions flow at small energies and whether the renormalized pair-hopping term eventually becomes larger than intra-pocket repulsion.

This flow of couplings is outside RPA in which the interactions have the same values as in the Hamiltonian [46]. Whether or not s^+ superconductivity is favored in RPA then likely depends on the values of the bare interactions in the underlying 5-orbital model (intra-and inter-orbital Hubbard interactions, intra-orbital exchange and pair-hopping terms). While some researchers found the s^+ state [42], others [37] found that more likely candidates are two nearly degenerate states in which the gap has nodes on one of the FS sheets and no nodes on the other. One such state is another extended *s*-wave state with $\Delta(\mathbf{k}) \approx \Delta \cos\frac{k_x}{2} \cos\frac{k_y}{2}$, the sec-