Physica E 41 (2009) 1281–1284

Contents lists available at ScienceDirect

Physica E

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

Hidden SDW order and effective low-energy theory for FeAs superconductors

Zheng-Yu Weng

Center for Advanced Study, Tsinghua University, Beijing 100084, China

ARTICLE INFO

Article history:
Received 17 February 2009
Received in revised form
18 February 2009
Accepted 19 February 2009
Available online 28 February 2009

Keywords:
Low-dimensional
Multibands
Magnetism
Superconductivity

PACS:
71.10.Hf
74.20.Mn
71.27+a
75.20.Hr

ABSTRACT

We propose a simple effective model to describe FeAs superconductors. This model is based on the assumption of a *local* spin-density-wave (SDW) order, with its magnetization direction allowed to fluctuate. It is shown that the long-range order with momentum $\mathbf{Q}=(\pi,\pi)$ is generally unstable in competing with the kinetic energy of the charge carriers. A true weak SDW order is formed in the undoped case with an additional momentum shift $\mathbf{Q}_s=(\pi,0)$ due to the peculiar Fermi surface nesting. In the doped case, the fluctuating long-range order driven by kinetic energy can naturally result in a d-wave superconducting condensation. Such low-energy physics is protected by the presence of the local SDW which sustains some kind of "Mott gaps" for the multiband d-electrons near the Fermi energy.

1. Introduction

The recent discovery of the iron-based superconductors [1–5] has stimulated a lot of interest concerning underlying mechanism for superconductivity in this new superconductor family. It has been established by various measurements [6–8] that there exists an spin-density-wave (SDW) order in the undoped LaOFeAs compound below $T\sim150$ K, which quickly disappears with the electrons doped into the system, where the superconducting phase starts to set in with transition temperatures being raised beyond 50 K [5,9]. While the general phase diagram [1–4,9] reminds us some interesting similarities with the cuprate superconductors, the d-electrons on Fe seem much more itinerant with multi-orbitals crossing the Fermi level as indicated by the band structure calculations [10–16], compared to the isolated $Cu_{3d_{x^2-y^2}}$–$O_{2p_{x,y}}$ antibonding orbitals in the cuprates. Many theoretical proposals are based on itinerant approaches [17–20] with the emphasis on the important role played by various magnetic fluctuations, while some conjectures are also made from the side of large-spin Mott insulators [21].

The LDA calculations [14,15] have found an energetically *robust* SDW state at the antiferromagnetic (AF) momentum $\mathbf{Q}=(\pi,\pi)$ with a large Fe moment $\sim2.3\mu_B$ per site, but experimentally only a *weak* SDW ordering with a different magnetic momentum $\mathbf{Q}_s=(\pi,0)$, which further doubles the unit cell of the former SDW state composed of two Fe per cell, has been identified [7,8] in the undoped case. The latter SDW (called stripe type below) was predicted by the first principle band structure calculation [6] due to the nesting Fermi surfaces of the hole and electron pockets, which is much more "fragile" and easily destroyed as the doped electrons fill up the small hole pockets at small doping.

In this paper, we will make a very simple proposal by assuming that the SDW state with an AF momentum $\mathbf{Q}$ remains strong *locally* in both the undoped and small doped regime. The corresponding profile of the electron density of states is schematically illustrated in Fig. 1. Based on this minimal model, we can show that the long-range part of this SDW is actually generically unstable, by coupling to the charge carriers near the Fermi level. Such instability can result in a weak stripe-type SDW order in the undoped case where the nesting Fermi surfaces are present, and naturally a superconducting condensation when the former is destroyed at small doping. In this whole regime, however, the local order of such an SDW remains robust to "protect" the low-energy physics, which resembles the role of the "Mott gap" in the cuprate superconductors [22].

2. Minimal model

In our model Hamiltonian $H_{\rm eff}=H_{\rm band}+H_{\rm I}$, the first term is a tight-binding model

$$H_{\rm band}=-\sum_{ij,a,b,\sigma}t_{ij}^{a,b}c_{ia\sigma}^{\dagger}c_{jb\sigma} \quad (1)$$

E-mail address: weng@tsinghua.edu.cn

1386-9477/$ - see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.physe.2009.02.015

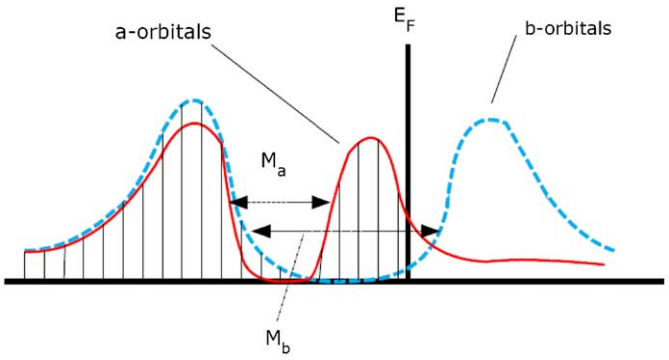

Fig. 1. (color online) Schematic profile of the density of states near the Fermi energy in the presence of the local SDW mean-fields M_a and M_b, which decide the "charge gaps" for the a-orbital and b-orbital bands according to H_0 (9). The lower half of each band (the so-called α-band, see text) is assumed below the Fermi energy E_F and is filled, while the upper half (the β-band) is only partially filled. Here a-bands refer to the bands passing the Fermi level, which are more d_{xy}, d_{xz}, d_{yz} like, and b-bands are more of $d_{x^2-y^2}$ character according to the LDA result [14,15].

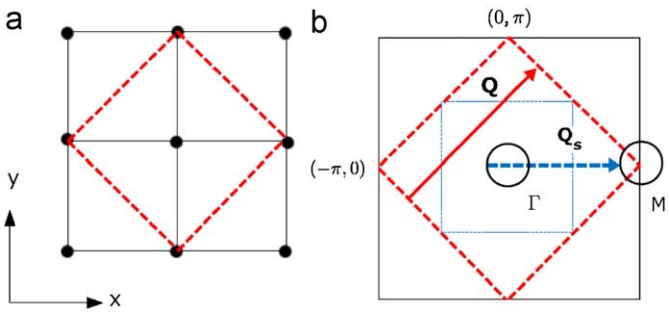

Fig. 2. (color online) (a) The iron atoms form a square lattice with the dashed diamond denoting the unit cell of the SDW order state with magnetic momentum **Q**. (b) The magnetic Brillouin zone (BZ) is illustrated by the dashed diamond shape. Two circles at the Γ and M points are hole and electron pockets connected by a momentum $\mathbf{Q}_s$. The smaller square is a reduced BZ corresponding to an enlarged unit cell indicated by the largest square in (a).

which describes the electron effective hoppings between the d-orbitals of the Fe ions on square lattice (Fig. 2(a)) at the nearest neighboring (NN) and next nearest neighboring (NNN) sites, including intra- and inter-orbital hoppings with the superscripts a, b specifying the orbitals. There have been several proposals [14,16,19,20] for $H_{\rm band}$ based on the LDA calculations in order to capture the relevant bands near the Fermi energy.

The second term $H_{\rm I}$ reflects the effective influence of the Coulomb interaction on the d-electrons, which includes the on-site and NN repulsions as well as the Hund's rule ferromagnetic coupling, and has the following "mean-field" look:

$$H_{\rm I} = -\sum_{i,a} \mathbf{M}_{ia} \cdot \mathbf{S}_{ia} \tag{2}$$

where $\mathbf{M}_{ia}$ denotes an effective SDW mean-field felt by the electron spin $\mathbf{S}_{ia}$ of the orbital a at site i. In an SDW ordered state, one would have $\mathbf{M}_{ia} \propto \sum_{b(\neq a)} J_H^{a,b} \langle \mathbf{S}_{ib} \rangle + U_a \langle \mathbf{S}_{ia} \rangle$, where $J_H^{a,b}$ is the Hund's rule coupling constant and U_a is the on-site repulsion. We shall make the following ansatz:

$$\mathbf{M}_{ia} = M_a (-1)^i \mathbf{n}_i \tag{3}$$

where a *single* unit vector $(-1)^i \mathbf{n}_i$ will describe the true polarization direction of $\mathbf{M}_{ia}$. Here the staggered factor $(-1)^i$ is introduced such that $\mathbf{n}_i = \hat{\mathbf{n}}$ will correspond to a true AF order, but in a general case $\mathbf{n}_i$ will not be fixed around a particular direction as only the relative change $\Delta_\alpha \mathbf{n}_i \equiv \mathbf{n}_{i+\hat{\alpha}} - \mathbf{n}_i$ ($\hat{\alpha} = \hat{x}, \hat{y}$) will enter the Hamiltonian as shown below.

The local SDW field M_a will be assumed large according to the LDA calculation [14,15] with the magnetization at different orbitals tightly aligned together by the Hund's coupling. Under this assumption, the long-wavelength, low-energy fluctuations of $\mathbf{n}_i$ may be treated as an independent degree of freedom. $\mathbf{n}_i$ will be self-consistently determined by coupling to the electrons near the Fermi level in $H_{\rm eff}$.

3. Effective theory

One may redefine $\mathbf{n}_i$ as the new $\hat{\mathbf{z}}$-axis for the spin index of the electron spinor operator:

$$\hat{c}_{ia} = U_i \hat{a}_{ia} \tag{4}$$

with $\hat{a}_{ia}^\dagger = (\hat{a}_{ia,\uparrow}^\dagger, \hat{a}_{ia,\downarrow}^\dagger)$ by an SU(2) rotation

$$U_i^\dagger \mathbf{n}_i \cdot \hat{\boldsymbol{\sigma}} U_i = \hat{\sigma}_z \tag{5}$$

Then $H_{\rm I}$ simply reduces to

$$H_{\rm I} = -\sum_{i,a} M_a (-1)^i S_{ia}^z \tag{6}$$

while $H_{\rm band}$ becomes

$$H_{\rm band} = -\sum_{ij,a,b} t_{ij}^{a,b} \hat{a}_{ia}^\dagger (U_i^\dagger U_j) \hat{a}_{jb} \tag{7}$$

We may further rewrite

$$H_{\rm eff} = H_0 + H_1 \tag{8}$$

where $H_0 \equiv H_{\rm I} + H_{\rm band}[U_i^\dagger U_j = 1]$ is simply an SDW mean-field Hamiltonian for the multibands, which can be diagonalized as

$$H_0 = \sum_{\mathbf{k},a} \xi_{\mathbf{k}}^{a+} (\hat{\alpha}_{\mathbf{k}a}^\dagger \hat{\alpha}_{\mathbf{k}a} + \hat{\beta}_{\mathbf{k}a}^\dagger \hat{\beta}_{\mathbf{k}a}) - \sum_{\mathbf{k},a} E_{\mathbf{k}}^a (\hat{\alpha}_{\mathbf{k}a}^\dagger \hat{\alpha}_{\mathbf{k}a} - \hat{\beta}_{\mathbf{k}a}^\dagger \hat{\beta}_{\mathbf{k}a}) + \text{const.} \tag{9}$$

by a canonical transformation $\hat{a}_{\mathbf{k}a} = u_{\mathbf{k}}^a \hat{\alpha}_{\mathbf{k}a} - v_{\mathbf{k}}^a \hat{\sigma}_z \hat{\beta}_{\mathbf{k}a}$, $\hat{a}_{\mathbf{k}+\mathbf{Q}a} = v_{\mathbf{k}}^a \hat{\sigma}_z \hat{\alpha}_{\mathbf{k}a} + u_{\mathbf{k}}^a \hat{\beta}_{\mathbf{k}a}$ with $u_{\mathbf{k}}^a = [(1 - \xi_{\mathbf{k}}^{a-}/E_{\mathbf{k}}^a)/2]^{1/2}$, $v_{\mathbf{k}}^a = [(1 + \xi_{\mathbf{k}}^{a-}/E_{\mathbf{k}}^a)/2]^{1/2}$. Here $\xi_{\mathbf{k}}^{a\pm} \equiv (\varepsilon_{\mathbf{k}}^a \pm \varepsilon_{\mathbf{k}+\mathbf{Q}}^a)/2$ and

$$E_{\mathbf{k}}^a = \sqrt{(\xi_{\mathbf{k}}^{a-})^2 + (M_a/2)^2} \tag{10}$$

where $\varepsilon_{\mathbf{k}}^a$ denotes the bare spectrum determined by (1) (setting the chemical potential $\mu = 0$). Note that the band label a here can be different from the original orbital label in (1) because of the mixture of orbitals, and in obtaining (10), the same M_a is assumed for the mixed orbitals. Here $\mathbf{k}$ is defined in the magnetic Brillouin zone (BZ) with the magnetic momentum $\mathbf{Q} = (\pi, \pi)$, which coincides with the BZ of two irons per unit cell (Fig. 2(b)).

Now let us consider the term with $U_i^\dagger U_j \neq 1$:

$$H_1 = -\sum_{ij,a,b} t_{ij}^{a,b} \hat{a}_{ia}^\dagger (U_i^\dagger U_j - 1) \hat{a}_{jb} \tag{11}$$

We shall focus on the case in which the α-bands are all filled up by the electrons, and the Fermi energy is located in some of β-bands, which corresponds to both the undoped and electron-doped (or slightly hole-doped) situations as illustrated in Fig. 1. After integrating out the α-bands and by assuming $\Delta_\alpha \mathbf{n}_i$ is small, H_1 may be simplified [23] (at large M_a) to

$$H_1 \simeq \frac{1}{2} \sum_{\mathbf{k},\mathbf{q},\sigma} \nabla \varepsilon_{\mathbf{k}} \cdot (\mathbf{D}_{\mathbf{q}})_{\sigma,-\sigma} (-\theta_{\mathbf{k}+\mathbf{q}} + \sigma \bar{\theta}_{\mathbf{k}+\mathbf{q}}) \beta_{\mathbf{k}+\mathbf{q},\sigma}^\dagger \beta_{\mathbf{k},-\sigma} + \text{H.c.} + \frac{J_{\rm eff}}{8} \sum_i (\Delta \mathbf{n}_i)^2 \tag{12}$$