Superconductivity in iron-based compounds (Scientific session of the Physical Sciences Division of the Russian Academy of Sciences, 29 January 2014)

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A scientific session of the Physical Sciences Division of the Russian Academy of Sciences (RAS), entitled 'Superconductivity in iron-based compounds', was held on 29 January 2014 at the conference hall of the Lebedev Physical Institute, RAS.

The agenda of the session, announced on the website www.gpad.ac.ru of the RAS Physical Sciences Division listed the following reports:

(1) **Eremin I M** (Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Deutschland; Kazan (Volga region) Federal University, Kazan, Russian Federation) "Antiferromagnetism in iron-based superconductors: interaction of the magnetic, orbital, and lattice degrees of freedom";

(2) **Korshunov M M** (Kirenskii Institute of Physics, Siberian Branch of the Russian Academy of Sciences, Krasnoyarsk) "Superconducting state in iron-based materials and spin-fluctuation pairing theory";

(3) **Kuzmicheva T E** (Lebedev Physical Institute, Russian Academy of Sciences, Moscow; Lomonosov Moscow State University) "Andreev spectroscopy of iron-based superconductors: temperature dependence of the order parameters and scaling of Δ_{LS} with T_c ";

(4) Eltsev Yu F (Lebedev Physical Institute, Russian Academy of Sciences, Moscow) "Synthesis and study of the magnetic and transport properties of iron-based superconductors of the 122 family".

Papers written on the basis of oral presentations 1–4 are published below.

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Antiferromagnetism in iron-based superconductors: magnetic order in the model of delocalized electrons

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In 2008, a group of Japanese materials scientists led by Hideo Hosono of Tokyo Institute of Technology discovered superconductivity in iron-based layered materials [1]. Understanding the interplay between magnetism and superconductivity in these *ferropnictides or iron pnictides* (as they are commonly referred to) requires insight into the main body of magneti-

Uspekhi Fizicheskikh Nauk **184** (8) 875–902 (2014) DOI: 10.3367/UFNr.0184.201408f.0875 Translated by E G Strel'chenko, S N Gorin, T E Kuzmicheva; edited by A Radzig cally ordered states in nonsuperconducting parent compounds and how these states evolve with the number of charge carriers (i.e., the doping level). Notably, a hot current topic is the origin of magnetism in parent iron-containing superconducting compounds, because it is believed that the magnetic interactions responsible for magnetic ordering are also responsible for Cooper pairing [2].

The phase diagrams of ferropnictides (FPs) are similar to those of high-temperature superconducting cuprates in showing neighboring antiferromagnetic (AFM) and superconducting phases. At low carrier concentrations, most ferropnictides are antiferromagnetic, and the suppression of the AFM state with increasing doping level, pressure, or degree of disorder leads to emerging of superconductivity. This fact is reminiscent of the phase diagram of cuprates and is often used as evidence of the interrelation between magnetism and superconductivity in iron-based materials.

There are, however, two important differences between ferropnictides and cuprates. First, the starting FP compounds are AFM metals, and second, in most FPs the superconducting Cooper pairing most likely exhibits extended S-wave symmetry, with or without zeros on the Fermi surface [2]. The electronic structures of paramagnetic FPs have been studied experimentally with angle-resolved photoemission spectroscopy (ARPES) [3-9] and de Haas-van Alphen oscillation measurements [10-12] and found to be in overall agreement with band calculations [13, 14]. In particular, the Fermi surface of a ferropnictide is two-dimensional and consists, when viewed in a plane, of two nearly spherical hole pockets of different sizes centered at the Γ point (0,0) of the Brillouin zone, and of two elliptical electron pockets centered at the points $(0, \pi)$ and $(\pi, 0)$ of the Brillouin zone in the unit cell containing a single Fe atom. Because of the tetragonal symmetry, the two electron pockets are equivalent under rotation through 90°. The Brillouin zone that was utilized in the experiments contains two Fe atoms per unit cell due to the nonequivalent positions of the As atom, and, hence, both electron pockets are centered at (π, π) . The electron dispersions near the electron pockets show behavior that is very similar to the analogous behavior near the hole pockets, except for the global change in sign [the so-called

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Uspekhi Fizicheskikh Nauk **184** (8) 875–882 (2014) DOI: 10.3367/UFNr.0184.201408g.0875 Translated by E G Strel'chenko; edited by A Radzig nesting property which allows the electron and hole bands to be mutually nested into each other through a shift by a wave vector (π, π)]. This dispersion property is characteristic of most (but not all) ferropnictides, as will be discussed later on.

This article presents a theoretical analysis of the magnetic ordering mechanisms in parent FPs [15, 16]. Inelastic neutron scattering measurements in such compounds have shown that the ordering of interest most commonly reveals itself on the wave vectors $(0, \pi)$ and $(\pi, 0)$ —that is, ferromagnetic chains along one of the crystallographic axes and antiferromagnetic chains in the other direction. Such a magnetic order originates, in principle, in the $J_1 - J_2$ model of localized spins with exchange interactions J_1 and J_2 between, respectively, the nearest and next-to-nearest neighbors for $J_2 > 0.5J_1$ [17–21].

The current discussion, however, concerns a different scenario, one taking into account that a ferropnictide remains metallic when it resides a magnetic state, and relies on a model that describes AFM order in terms of the spin density wave (SDW) for itinerant electrons.

The reason is that optical conductivity measurements reveal a transfer of spectral weight from the Drude peak to the middle of the infrared peak, in accordance with the itinerant electron model that leads to AFM order [22]. As is known, the nesting mechanism produces an incommensurate AFM order in Cr [23, 24]. Given the ferropnictide electronic structure, a natural conjecture is that AFM order is established, at least in part, due to nesting between the electron and hole energy dispersions. That this is indeed so may be supported by band structure calculations and also by a total energy analysis of the AFM state: it is strictly found that the total energy gain with respect to the paramagnetic state is mainly due to those regions of the Brillouin zone that contain electron and hole pockets [25]. Furthermore, ARPES experiments have demonstrated a direct relationship between nesting and the origin of AFM ordering [26]. Moreover, an incommensurate ordering wave vector is observed in neutron diffraction experiments with a varying number of carriers, again in agreement with the itinerant electron model [27]. The application of this mechanism to ferropnictides has been a subject of study for some years and is outlined below [15, 28-33].

Magnetic ordering and magnetic frustration effects. As noted above, the first evidence for magnetic order in FPs came from neutron scattering [34] and muon spin relaxation (μ SR) [35]. The Néel temperature of magnetic transition is about $T_N = 150$ K. In real space, magnetic ordering manifests itself in appearing ferromagnetic chains along one of the crystallographic axes in the square lattice of antiferromagnetically bonded Fe atoms. In momentum space, this ordering is defined by the wave vector $\mathbf{Q}_1 = (\pi, 0)$ or, alternatively, $\mathbf{Q}_2 = (0, \pi)$. In the localized scenario, this ordering arises in the context of the $J_1 - J_2$ model of localized electrons [17] for $J_2 > 0.5J_1$, and with allowance for quantum fluctuations.

Now let us have a look at the band theory interpretation of this order. Figure 1 shows the Fermi surface of a normalstate ferropnictide. This Fermi surface topology exhibits two equivalent wave vectors of instability, $\mathbf{Q}_1 = (\pi, 0)$ and $\mathbf{Q}_2 = (0, \pi)$, with respect to spin density wave formation due to the nesting of electronic and hole Fermi surfaces. For the idealized case of zero-ellipticity electron pockets and equal electron and hole effective masses, the situation is similar to that in the single-band Hubbard model on the square lattice with a half-filled conduction band. In particular, the



Figure 1. Schematics of the Fermi surface of a ferropnictide. Its unit cell contains one Fe atom, hole fermion pockets situated near the Γ -point of the Brillouin zone, and two elliptical electron pockets near (π , 0) and (0, π) points. **Q**₁ and **Q**₂ are two possible ordering vectors for the spin density wave.

electron-hole susceptibility in this case shows a logarithmic divergence, similar to what occurs in the particle-particle channel of Cooper pairing. The renormalization group analysis shows that the fundamental instability in this case develops in the magnetic channel [28, 29]. However, given the presence of two wave vectors, \mathbf{Q}_1 and \mathbf{Q}_2 , the question remains as to how one of two experimentally observed ordering vectors should be selected.

To formulate the problem, we start by describing the general spin configuration as determined by two magnetic order parameters Δ_i in the mean field approximation for each of the wave vectors \mathbf{Q}_i :

$$\mathbf{S}(\mathbf{R}) = \Delta_1 \exp\left(i\mathbf{Q}_1\mathbf{R}\right) + \Delta_2 \exp\left(i\mathbf{Q}_2\mathbf{R}\right). \tag{1}$$

This configuration divides the iron lattice into two antiferromagnetically ordered, mutually penetrating sublattices with respective magnetizations $\Delta_1 + \Delta_2$ and $\Delta_1 - \Delta_2$. In this case, however, neither the angle between nor the relative magnitude of the two Néel vectors is fixed. Shown in Fig. 2 are four of the set of all possible magnetic configurations, those in panels c and d corresponding to the experimental situation in which one of the order parameters Δ_i vanishes.

Let us consider a model of interacting fermions with circular Fermi contours centered at the Γ -point of the Brillouin zone (α zone) and two elliptical pockets around the points ($\pm \pi$, 0) and (0, $\pm \pi$) (β zone) (see Fig. 1):

$$H_{2} = \sum_{\mathbf{p},\sigma} \left[\varepsilon_{\mathbf{p}}^{\alpha_{1}} \alpha_{1\mathbf{p}\sigma}^{+} \alpha_{1\mathbf{p}\sigma} + \varepsilon_{\mathbf{p}}^{\beta_{1}} \beta_{1\mathbf{p}\sigma}^{+} \beta_{1\mathbf{p}\sigma} + \varepsilon_{\mathbf{p}}^{\beta_{2}} \beta_{2\mathbf{p}\sigma}^{+} \beta_{2\mathbf{p}\sigma} \right].$$
(2)



Figure 2. Possible magnetic ordering configurations in ferropnictides [16].

Here $\varepsilon_{\mathbf{p}}^{\alpha_1}$, $\varepsilon_{\mathbf{p}}^{\beta_1}$, and $\varepsilon_{\mathbf{p}}^{\beta_2}$ are the quasiparticle energies in the hole and electron bands, respectively:

$$\begin{split} \varepsilon_{\mathbf{p}}^{\alpha_{1}} &= -\frac{\hbar^{2}\mathbf{p}^{2}}{2m_{1}} + \mu, \quad \varepsilon_{\mathbf{p}}^{\beta_{1}} = \frac{\hbar^{2}p_{x}^{2}}{2m_{x}} + \frac{\hbar^{2}p_{y}^{2}}{2m_{y}} - \mu, \\ \varepsilon_{\mathbf{p}}^{\beta_{2}} &= \frac{\hbar^{2}p_{x}^{2}}{2m_{y}} + \frac{\hbar^{2}p_{y}^{2}}{2m_{x}} - \mu, \end{split}$$

the quasimomenta of the α fermions are counted from the point (0, 0), those of the β_1 and β_2 fermions are measured from (0, π) and (π , 0), respectively, and μ is the chemical potential. In the general case, the interaction Hamiltonian includes density-density type interactions, scattering with wave vectors (0, π), (π , 0) and (π , π), and quasiparticle pair hopping.

Consider first the density–density type interaction between α and β fermions and the quasiparticle pair hopping processes:

$$H_{4} = U_{1} \sum \alpha_{1\mathbf{p}_{3}\sigma}^{+} \beta_{j\mathbf{p}_{4}\sigma'}^{+} \beta_{j\mathbf{p}_{2}\sigma'} \alpha_{1\mathbf{p}_{1}\sigma} + \frac{U_{3}}{2} \sum \left(\beta_{j\mathbf{p}_{3}\sigma'}^{+} \beta_{j\mathbf{p}_{4}\sigma'}^{+} \alpha_{1\mathbf{p}_{2}\sigma'} \alpha_{1\mathbf{p}_{1}\sigma} + \text{h.c.} \right).$$
(3)

Here, the interaction parameters are assumed to be wave vector-independent; α , (α^+) , β , (β^+) are the annihilation (creation) operators for the hole and electron Fermi surfaces; the summation is assumed to be taken over all momenta ($\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, \mathbf{p}_4$) and spins (σ, σ') , and h.c. stands for 'Hermitian conjugate'. Because two β bands are involved, it is natural to introduce two SDW order parameters: $\Delta_1 \propto \sum_{\mathbf{p}} \langle \alpha^+_{1\mathbf{p}\delta} \sigma_{\delta\gamma} \beta_{1\mathbf{p}\gamma} \rangle$ (where $\sigma_{\delta\gamma}$ are the Pauli matrix elements) with a wave vector $\mathbf{Q}_1 = (\pi, 0)$, and $\Delta_2 \propto \sum_{\mathbf{p}} \langle \alpha^+_{1\mathbf{p}\delta} \sigma_{\delta\gamma} \beta_{2\mathbf{p}\gamma} \rangle$ with a wave vector $\mathbf{Q}_2 = (0, \pi)$. Without loss of generality, we may assume that the vector Λ_1 is directed along the *z*-axis, and that Λ_2 lies in the *xz* plane. For the purposes of further discussion, it is convenient to redefine these parameters in the following way:

$$\begin{split} \Delta_{1}^{z} &= -U_{\rm SDW} \sum_{\mathbf{p}} \left\langle \alpha_{1\mathbf{p}\uparrow}^{+} \beta_{1\mathbf{p}\uparrow} \right\rangle, \\ \Delta_{1}^{z(x)} &= -U_{\rm SDW} \sum_{\mathbf{p}} \left\langle \alpha_{1\mathbf{p}\uparrow}^{+} \beta_{1\mathbf{p}\uparrow(\downarrow)} \right\rangle, \end{split}$$
(4)

where $U_{\text{SDW}} = U_1 + U_2$. Assuming first a circular shape of the electron pockets ($m_x = m_y = m$ and $\varepsilon_{\mathbf{p}}^{\beta_1} = \varepsilon_{\mathbf{p}}^{\beta_2} = \varepsilon_{\mathbf{p}}^{\beta}$), the Hamiltonian is diagonalized by three consecutive Bogoliubov transformations, reducing the self-consistent equation for the order parameter to

$$1 = \frac{U_{\text{SDW}}}{2N} \sum_{\mathbf{p}} \frac{1}{\sqrt{(\varepsilon_{\mathbf{p}})^2 + \Delta^2}} \,. \tag{5}$$

Two important conclusions follow from the above. First, the self-consistent equation defines the order parameters not separately but in combination, $\Delta_1^2 + \Delta_2^2$, i.e., at this level of calculation a pair of vector order parameters, Δ_1 and Δ_2 , can be considered as a generalized six-component vector. Here, a state of spin density waves is characterized by spontaneous breaking of the O(6) symmetry, and this ordered state has five Goldstone modes. The degenerate ground state corresponds to two-sublattice states antiferromagnetically ordered along the $(0, \pi)$ and $(\pi, 0)$ diagonals for which $\Delta_1 = 0$ or $\Delta_2 = 0$, and also corresponds to many other situations, some of which are demonstrated in Fig. 2.

It should also be noted that the revealed degeneracy turned out greater than in the J_1-J_2 model of localized spins. In our case, not only can the angle between the two sublattices be arbitrary, but also the sublattices can have different ordered moments.

We note, in conclusion, that integration over momenta in Eqn (5) *extends beyond* the Fermi surface. The SDW order parameter also becomes finite when the Fermi surface disappears. This results from the fact that an electron-hole loop formed by α and β fermions is similar to the particle-particle loop because the α - and β -band dispersions differ in sign. As a consequence, the small sizes of hole and electron pockets are of no relevance to the formation of an SDW or, in other words, an SDW arises in this case due to the nesting between the α and β bands, but not due to nesting in individual Fermi surfaces.

Now let us switch on the interaction between two electron pockets — which we should because it is not weak and should be taken into account in a theoretical analysis — and see whether this can lift the degeneracy. Four types of interaction may be distinguished:

$$H_{4}^{ex} = U_{6} \sum \beta_{1p_{3\sigma}}^{+} \beta_{2p_{4}\sigma'}^{+} \beta_{2p_{2}\sigma'} \beta_{1p_{1}\sigma} + U_{7} \sum \beta_{2p_{3\sigma}}^{+} \beta_{1p_{4}\sigma'}^{+} \beta_{2p_{2}\sigma'} \beta_{1p_{1}\sigma} + \frac{U_{8}}{2} \sum \left(\beta_{1p_{3\sigma}}^{+} \beta_{2p_{4}\sigma'}^{+} \beta_{2p_{2}\sigma'} \beta_{1p_{1}\sigma} + \text{h.c.} \right)$$
(6)
$$+ \frac{U_{4}}{2} \sum \left(\beta_{1p_{3\sigma}}^{+} \beta_{2p_{4}\sigma'}^{+} \beta_{2p_{2}\sigma'} \beta_{1p_{1}\sigma} + \beta_{2p_{3}\sigma}^{+} \beta_{1p_{4}\sigma'}^{+} \beta_{2p_{2}\sigma'} \beta_{1p_{1}\sigma} \right)$$

(we use the notation of Ref. [16]). All the U_i are considered to be positive. Carrying out consecutive Bogoliubov transformations and averaging yields the following corrections to the ground state energy:

$$E_{\rm gr}^{\rm ex} = 2A^2 (U_6 + U_8 - U_7 - U_4) \frac{|\Delta_1|^2 |\Delta_2|^2}{\Delta^4} + 4A^2 U_7 \frac{(\Delta_1 \Delta_2)^2}{\Delta^4}.$$
(7)

It is seen that E_{gr}^{ex} now depends on both the magnitude and the relative direction of vectors Δ_1 and Δ_2 . When all the interactions are equal in strength, the first term on the righthand side vanishes, and the second has a minimum at $\Delta_1 \perp \Delta_2$. The O(6) symmetry is reduced, but not to lower than $O(3) \times O(2)$, i.e., the order parameters each have the same value at all sites because $(\Delta_1 + \Delta_2)^2 = (\Delta_1 - \Delta_2)^2$, but the angle between $\Delta_1 + \Delta_2$ and $\Delta_1 - \Delta_2$ is still arbitrary. This is exactly the same situation as in the classical $J_1 - J_2$ model. However, if $(U_6 + U_8 - U_7 - U_4) \neq 0$, the symmetry drops to O(3) even in the mean-field approximation. Because U_4 is reduced and indeed changes sign [14] — whereas the other U remain unchanged—under renormalization group transformations, the most likely situation to occur is one in which $U_6 + U_8 - U_7 - U_4 > 0$ and, hence, the minimum energy cases are consistent with $\Delta_1 = 0$ and $\Delta_2 = 0$, which in turn correspond to SDW with the wave vector $(0, \pi)$ or $(\pi, 0)$. This is exactly what is observed experimentally. If $U_6 + U_8 U_7 - U_4 < 0$, the minimum of E_{gr}^{ex} occurs at $|\Delta_1| = |\Delta_2|$, and the sublattice order parameters are orthogonal to each other. Figure 2 depicts the spin ordering pattern for this case. This type of spin ordering was found earlier when analyzing the two-orbit model.

Now let us take into account the fact that the electron pockets are not circular but elliptical, i.e., the effective masses m_x and m_y are not equal between themselves and $\varepsilon_{\mathbf{k}}^{\beta_1} \neq \varepsilon_{\mathbf{k}}^{\beta_2}$. For the problem to remain tractable analytically, we assume

that the departure from a circular shape of the electron pockets is small and introduce $m_x = (1 + \delta) m$ and $m_y = (1 - \delta) m$, with $\delta \leq 1$. Consecutive Bogoliubov transformations give

$$E_{\rm gr}^{\rm ellipt} = C |\Delta_1|^2 |\Delta_2|^2, \quad C = \delta^2 \frac{m\mu^2}{4\pi\Delta^4}.$$
(8)

From formula (8) it is seen that the ellipticity of the electron pockets lifts the degeneracy in favor of a $(0, \pi)$ or a $(\pi, 0)$ SDW. As already noted, this is precisely the situation corresponding to the experimental data. Thus, ellipticity gives rise to the effective interaction between the SDW order parameters, which for $\Delta \ll \mu$ favors the same ground state arising from the inclusion of interaction between two electron pockets.

For comparison, let us consider the same itinerant electron model, but with the conduction electrons interacting as in the J_1-J_2 model. Then, the model Hamiltonian takes the form

$$H^{J_1-J_2} = \sum_{\mathbf{p}} \mathbf{S}(\mathbf{p}) \, \mathbf{S}(-\mathbf{p}) \\ \times \left[J_1(\cos p_x + \cos p_y) + J_2 \cos p_x \cos p_y \right], \qquad (9)$$

where $S(\mathbf{p}) = (1/2) \sum a_{\mathbf{p},\alpha}^+ \sigma_{\alpha\beta} a_{\mathbf{p}_1+\mathbf{p},\beta}$, a^+ and a are the fermion operators that describe holes or electrons if \mathbf{p} resides, respectively, near (0, 0) and near (0, π) or (π , 0). The kinetic energy term is the same as that in Eqn (2). To avoid confusion, note that the model we are considering differs from the localized spin model, even if the parameters J_1 and J_2 are much larger than the Fermi energy. In particular, in this model states on the same lattice site cannot be filled twice—unlike the t-J model for the cuprates, where they can. A version of the J_1-J_2 model as applied to localized moments will be considered below.

Energy operator (9) can be put into correspondence with the potential energy operator in Eqn (3) by considering the values of the operator **p** in the neighborhoods of (0, 0), (0, π), and (π , 0) points. Writing the spin operators in a secondquantized form, we find that $U_3 = 3J_2$ and $U_1 = J_2 - J_1$. Thus, $U_{\text{SDW}} = U_1 + U_3 = J_{\text{SDW}} = 4J_2 - J_1$ in this model. As was the case with Eqn (3), it is logical to introduce vector of parameters with the components $\Delta_1^z = -J_{\text{SDW}} \sum \langle \alpha_{1\mathbf{p}\uparrow}^+ \beta_{1\mathbf{p}\uparrow} \rangle$ and $\Delta_2^{z(x)} = -J_{\text{SDW}} \sum \langle \alpha_{1\mathbf{p}\uparrow}^+ \beta_{2\mathbf{p}\uparrow\downarrow} \rangle$. A mean-field approximation calculation similar to that described above gives the following equation for the order parameter $\Delta^2 = |\Delta_1|^2 + |\Delta_2|^2$:

$$1 = \frac{J_{\text{SDW}}}{2N} \sum_{\mathbf{p}} \frac{1}{\sqrt{(\varepsilon_{\mathbf{p}})^2 + \Delta^2}} \,. \tag{10}$$

A solution for $\Delta^2 = |\Delta_1|^2 + |\Delta_2|^2$ exists for $J_2 > J_1/4$. Large values of J_2 produce antiferromagnetic ordering along diagonals. It is instructive to look at the condition $J_2 > J_1/4$ in relation to its counterpart inequality for the $J_1 - J_2$ model of localized spins — and thereby to see that they indeed differ from each other. The degeneracy between different SDW states with the same value of $\Delta^2 = |\Delta_1|^2 + |\Delta_2|^2$ is lifted by including the interaction between the electron pockets, which is described by the Fourier transforms for J_1 and J_2 at the momenta $\mathbf{p} = (0, 0)$ and $\mathbf{p} = (\pi, \pi)$. It is easily verified that the term with $\mathbf{p} = (\pi, \pi)$ mixes electronic states and this is equivalent to including the interactions U_6 , U_7 , and U_8 , whereas the presence of the term with $\mathbf{p} = (0, 0)$ is equivalent to including U_6 and U_4 .

By second-quantizing S(p) S(-p), we obtain an operator quadratic in β_1 and β_2 fermions in the same form with the

coefficients

$$U_6^s = J_1 - 3J_2, \quad U_7^s = -J_1 - 3J_2,$$

$$U_8^s = 3(J_1 - J_2), \quad U_4^s = -3(J_1 + J_2),$$
(11)

which, when substituted into the total energy expression, gives

$$E_{\rm gr}^{J_1-J_2} = 2A^2 \left[4J_1 \frac{|\mathbf{\Delta}_1|^2 |\mathbf{\Delta}_2|^2}{\Delta^4} - (J_1 + 3J_2) \frac{(\mathbf{\Delta}_1 |\mathbf{\Delta}_2|^2)}{\Delta^4} \right], \quad (12)$$

where A > 0. It is seen that the coefficient of $(\Delta_1 \Delta_2)^2$ is negative, i.e., the energy decreases when the vectors Δ_1 and Δ_2 become parallel. In this case, $|\Delta_1|^2 |\Delta_2|^2 = (\Delta_1 \Delta_2)^2$, and from Eqn (12) we obtain

$$E_{\rm gr}^{J_1 - J_2} = -2A^2 (J_2 - J_1) \, \frac{|\mathbf{\Delta}_1|^2 |\mathbf{\Delta}_2|^2}{\Delta^4} \,. \tag{13}$$

It is seen that the states with $\Delta_1 = 0$ or $\Delta_2 = 0$, corresponding, respectively, to SDW vectors with $(0, \pi)$ or $(\pi, 0)$ are stabilized only for $J_1/4 < J_2 < J_1$. For larger J_2 's, the energy has a minimum at $\Delta_1 = \pm \Delta_2$. In the corresponding SDW state, one sublattice is antiferromagnetically ordered, whereas the other is disordered (Fig. 2d), exemplifying that the Landau theory predicts magnetic ordering when extended to the case of a two-component order parameter. It is also interesting to note that, when J_2 stands for the dominant parameter, the spin– spin interaction between two electron bands stabilizes a different SDW from that due to the interaction in the charge channel.

We have established above that the magnetic stripe $(0, \pi)$ or $(\pi, 0)$ ordering is stabilized in a three-band (one hole and two electron) model by a usual charge interaction. In the discussion below, we will see how the introduction of the second hole pocket affects the stabilization of an SDW in a ferropnictide. The second hole Fermi contour is less strongly coupled to the electron contours than is the one already included in the three-band model, the reason being the differences in the strength of interaction and the degree of mixing with the electron Fermi contours. A discussion of these two factors follows.

Let us consider first a model constructed from two electronic and two hole Fermi surfaces, all circular. We assume that they are equal in size, but with two types of interaction existing between the electron and hole bands: $U_{\text{SDW}}^{(1)}$ for one hole band, and $U_{\text{SDW}}^{(2)}$ for the other. There are, in addition, four order parameters: Δ_{11} , Δ_{12} , Δ_{21} , and Δ_{22} , the first and the third corresponding to SDW with the wave vector \mathbf{Q}_1 , and two others with the vector \mathbf{Q}_2 . Without loss of generality, let Δ_{11} be directed along the z-axis, and Δ_{12} lie in the *xz* plane, but let Δ_{21} and Δ_{22} have arbitrary directions. To simplify matters, we assume the SDW configurations to be coplanar. Let Δ_{11} and Δ_{21} be directed along the z-axis, and Δ_{12} and Δ_{22} be along the x-axis. Under the above assumptions, we have, by analogy, the following relations:

$$\begin{aligned} \mathcal{A}_{11} &= \mathcal{A}_{1}^{z} = -U_{\text{SDW}}^{(1)} \sum \left\langle \alpha_{1\mathbf{p}\uparrow}^{+} \beta_{1\mathbf{p}\uparrow} \right\rangle, \\ \mathcal{A}_{12} &= \mathcal{A}_{1}^{x} = -U_{\text{SDW}}^{(1)} \sum \left\langle \alpha_{1\mathbf{p}\uparrow}^{+} \beta_{2\mathbf{p}\uparrow} \right\rangle, \\ \mathcal{A}_{21} &= \mathcal{A}_{2}^{z} = -U_{\text{SDW}}^{(2)} \sum \left\langle \alpha_{2\mathbf{p}\uparrow}^{+} \beta_{1\mathbf{p}\uparrow} \right\rangle, \\ \mathcal{A}_{22} &= \mathcal{A}_{2}^{x} = -U_{\text{SDW}}^{(2)} \sum \left\langle \alpha_{2\mathbf{p}\uparrow}^{+} \beta_{2\mathbf{p}\uparrow} \right\rangle. \end{aligned}$$
(14)

As before, we start by allowing one hole band to interact with electronic states (U_1 and U_3). Partially averaging in the four-fermion terms and separating the order parameters, we arrive at a Hamiltonian of the quadratic form: $H_{\text{eff}}^{(2)} = H^{\text{kin}} + H_{\alpha,\beta}^{(2)} + H_{\alpha_2\beta}^{(2)}$, where

$$H^{\rm kin} = \sum_{\mathbf{p},\sigma,i=1,2} \varepsilon_{\mathbf{p}} \left[\alpha_{i\mathbf{p}\sigma}^{+} \alpha_{i\mathbf{p}\sigma} - \beta_{i\mathbf{p}\sigma}^{+} \beta_{i\mathbf{p}\sigma} \right], \qquad (15)$$

$$H_{\alpha_{1}\beta}^{(2)} = -\sum_{p} \left[\alpha_{1\mathbf{p}\uparrow}^{+} (\varDelta_{1}^{z}\beta_{1\mathbf{p}\uparrow} + \varDelta_{1}^{x}\beta_{2\mathbf{p}\downarrow}) - \alpha_{1\mathbf{p}\downarrow}^{+} (\varDelta_{1}^{z}\beta_{1\mathbf{p}\downarrow} - \varDelta_{2}^{x}\beta_{2\mathbf{p}\uparrow}) \right] + \text{h.c.},$$

$$H_{\alpha_{2}\beta}^{(2)} = -\sum_{p} \left[\alpha_{2\mathbf{p}\uparrow}^{+} (\varDelta_{2}^{z}\beta_{1\mathbf{p}\uparrow} + \varDelta_{2}^{x}\beta_{2\mathbf{p}\downarrow}) - \alpha_{2\mathbf{p}\downarrow}^{+} (\varDelta_{2}^{z}\beta_{1\mathbf{p}\downarrow} - \varDelta_{2}^{x}\beta_{2\mathbf{p}\uparrow}) \right] + \text{h.c.}$$
(16)

That part involving α_1 holes and the parameters Δ_1^z and Δ_1^x can be diagonalized in the same manner as in the three-band model, i.e., by introducing new operators. The self-consistent equation for the gap Δ_1 ($\Delta_1 = [(\Delta_1^z)^2 + (\Delta_1^x)^2]^{1/2}$) has the form

$$1 = \frac{U_{\rm SDW}^{(1)}}{2N} \sum_{\mathbf{p}} \frac{1}{\sqrt{(\varepsilon_{\mathbf{p}})^2 + \Delta_1^2}},$$
 (17)

and the equation for the gap $\Delta_2 (\Delta_2 = [(\Delta_2^z)^2 + (\Delta_2^x)^2]^{1/2})$ is written down as

$$1 = \frac{U_{\rm SDW}^{(2)}}{2N} \sum_{\mathbf{p}} \frac{1}{\sqrt{(\varepsilon_{\mathbf{p}})^2 + \Delta_2^2}} \,. \tag{18}$$

Clearly, both equations (17) and (18) facilitate a reduction in the energy through their nonzero solutions for Δ_1 and Δ_2 —if, certainly, such exist. This means that the energy decreases still further if, in addition to states with $\Delta_1^z = \Delta_1 \cos \theta$ and $\Delta_1^x = \Delta_1 \sin \theta$, a state with $\Delta_{21}^z = -\Delta_2 \sin \theta$ and $\Delta_2^z = \Delta_2 \cos \theta$ forms. Furthermore, for equal circular Fermi contours, solutions for Δ_1 and Δ_2 exist at any $U_{\text{SDW}}^{(1)}$ and $U_{\text{SDW}}^{(2)}$. The resulting fermion excitations turn out to have energy gaps.

Thus, we come to the conclusion that an SDW state exhibits a dielectric nature in a four-band model with hole and electron pockets of equal size and a circular shape.

Let us see whether this conclusion is consistent with the observation of SDWs with wave vectors $(0, \pi)$ and $(\pi, 0)$. Because the angle θ does not enter explicitly into the quadratic forms, the ground state turns out to be degenerate again. A degenerate SDW multiplet can be described by the expression

$$S(\mathbf{R}) \propto n_z (\varDelta_1 \cos \theta - \varDelta_2 \sin \theta) \exp(i\mathbf{Q}_1 \mathbf{R}) + n_x (\varDelta_1 \sin \theta + \varDelta_2 \cos \theta) \exp(i\mathbf{Q}_2 \mathbf{R}).$$
(19)

This degenerate set contains no $(0, \pi)$ and $(\pi, 0)$ states with only a \mathbf{Q}_1 or only a \mathbf{Q}_2 SDW vector. These states are obtained by putting $\tan \theta = \Delta_1/\Delta_2$ or $\tan \theta = -\Delta_2/\Delta_1$. The question arises as to whether such states will be stabilized by other interactions, as was the case for the $(0, \pi)$ and $(\pi, 0)$ states in the three-band model. In our view, no, they won't. The reason is that the $(0, \pi)$ and $(\pi, 0)$ states in the four-band model occur for θ chosen such that Δ_1 and Δ_2 have components with both \mathbf{Q}_1 and \mathbf{Q}_2 wave vectors. The total spin component with either \mathbf{Q}_1 or \mathbf{Q}_2 vanishes as the components Δ_1 and Δ_2 cancel each other out. Indeed, for $U_{\text{SDW}}^{(2)} \ll U_{\text{SDW}}^{(1)}$, the angle θ is close to zero or $\pi/2$ but not equal to either of these values. Recall that the above discussion of a degeneracy lifting in the threeband model showed that the interaction between the β_1 and β_2 electrons leads, together with the ellipticity effect, to an energy of the form $E_{\rm gr}(\theta) = E_0 + E_1 \sin^2(2\theta)$, with a minimum at either $\theta = 0$ or $\theta = \pi/2$. To verify what the four-band model gives, we extended our analysis to finite $U_{\rm SDW}^{(2)}$ and analyzed the behavior of an $E_{\rm gr}(\theta)$ minimum perturbatively by adding the small parameter $U_{\rm SDW}^{(2)}/U_{\rm SDW}^{(1)}$. We omit here the details of the calculation, because they follow those for three bands, and only mention that the minimum of $E_{\rm gr}(\theta)$ does not shift from $\theta = 0$ and $\theta = \pi/2$.

Thus, we see that in the four-band model the interactions that lift the degeneracy of SDW states do not lead to the stabilization of $(0, \pi)$ or $(\pi, 0)$ states. For example, at $\theta = 0$ one obtains

$$S(\mathbf{R}) \propto n_z \varDelta_1 \exp(\mathrm{i}\mathbf{Q}_1\mathbf{R}) + n_x \varDelta_2 \exp(\mathrm{i}\mathbf{Q}_2\mathbf{R})$$

This SDW state corresponds to a two-sublattice structure with two equal order parameters but not with collinear spins.

To summarize the above analysis, the $(0, \pi)$ or $(\pi, 0)$ states occur only if Δ_2 is exactly zero and, hence, the second hole band has no relevance for the formation of an SDW. Only in this case do interactions and ellipticity lift the degeneracy in favor of $(0, \pi)$ or $(\pi, 0)$ states. Otherwise, the order parameter with necessity has both \mathbf{Q}_1 and \mathbf{Q}_2 components, and an SDW turns out to be modulated along both the *x*- and the *y*-axes. This conclusion is directly related to the electronic structure. At $\Delta_2 = 0$, one hole band and one electron band have no energy gaps, meaning that *the system remains metallic*.

As noted above, there is a perfect nesting for hole and electron pockets of a circular shape; therefore, $\Delta_2 \neq 0$ for any value of $U_{\text{SDW}}^{(2)}$. The situation changes when the hole Fermi contours differ in size and the electron pockets are elliptical. Then, repeating the calculation generally yields a state with four SDWs, which is described by the Hamiltonian

$$H_{\rm SDW} = \sum_{a,b} \sum_{\mathbf{p}} E_{1,2\mathbf{p}} (e^+_{a,b\mathbf{p}} e_{a,b\mathbf{p}} + p^+_{a,b\mathbf{p}} p_{a,b\mathbf{p}}) + \sum_{a,b} \sum_{\mathbf{p}} E_{3,4\mathbf{p}} (e^+_{a,b\mathbf{p}} e_{a,b\mathbf{p}} + p^+_{a,b\mathbf{p}} p_{a,b\mathbf{p}}).$$
(20)

Here, e^+ and e are the creation and annihilation operators for the new quasiparticles that are produced after the diagonalization of the Hamiltonian quadratic form with SDW order parameters:

$$E_{1,2\mathbf{p}} = \frac{1}{2} \left(\varepsilon_{\mathbf{p}}^{\alpha_1} + \overline{\varepsilon}_{\mathbf{p}} \right) \pm \frac{1}{2} \sqrt{\left(\varepsilon_{\mathbf{p}}^{\alpha_1} + \overline{\varepsilon}_{\mathbf{p}} \right)^2 + 4|\Delta_1|^2} ,$$

$$E_{3,4\mathbf{p}} = \frac{1}{2} \left(\varepsilon_{\mathbf{p}}^{\alpha_2} + \overline{\overline{\varepsilon}}_{\mathbf{p}} \right) \pm \frac{1}{2} \sqrt{\left(\varepsilon_{\mathbf{p}}^{\alpha_2} + \overline{\overline{\varepsilon}}_{\mathbf{p}} \right)^2 + 4|\Delta_2|^2} ,$$

where $\bar{\varepsilon}_{\mathbf{p}} = \varepsilon_{\mathbf{p}}^{\beta_1} \cos^2 \theta + \varepsilon_{\mathbf{p}}^{\beta_2} \sin^2 \theta$, and $\bar{\bar{\varepsilon}}_{\mathbf{p}} = \varepsilon_{\mathbf{p}}^{\beta_2} \cos^2 \theta + \varepsilon_{\mathbf{p}}^{\beta_1} \sin^2 \theta$. The self-consistent equations for the two gaps are as follows:

$$1 = U_{\rm SDW}^{(1)} \sum_{\mathbf{p}} \frac{n(E_{1\mathbf{p}}) - n(E_{2\mathbf{p}})}{\sqrt{(\varepsilon_k^{\alpha_1} - \bar{\varepsilon}_k)^2 + 4|\Delta_1|^2}},$$
 (21)

$$I = U_{\rm SDW}^{(2)} \sum_{\mathbf{p}} \frac{n(E_{3\mathbf{p}}) - n(E_{4\mathbf{p}})}{\sqrt{(\varepsilon_k^{\alpha_2} - \bar{\bar{\varepsilon}}_k)^2 + 4|\Delta_2|^2}} \,.$$
(22)

An analysis of this equation shows that, if the nesting is not perfect, the origination of magnetism with SDW shows itself as a threshold phenomenon in the sense that the interactions $U_{\rm SDW}$ should exceed a certain value for Δ_1 and Δ_1 to be nonzero. We found that the hole band with heavier carriers and, hence, with a larger Fermi contour, should be coupled more strongly to the electron bands. This band features as an α_1 band in our discussion. When $U_{\rm SDW}^{(1)}$ exceeds the threshold value $U_{\rm cr}^{(1)}$, an SDW with $\Delta_1 \neq 0$ arises in the system, which is a stripe ordering with a wave vector $(0, \pi)$ or $(\pi, 0)$. For the hole band — the α_2 band in our terminology — a $\Delta_2 \neq 0$ SDW arises when $U_{\rm SDW}^{(2)}$ exceeds the critical value of $U_{\rm cr}^{(2)} > U_{\rm cr}^{(1)}$. If this happens, an SDW with Q_1 and Q_2 components arises, as illustrated in Fig. 3a, b. The interaction regime characterized by inequalities $U_{\rm SDW}^{(1)} > U_{\rm cr}^{(1)}$, $U_{\rm SDW}^{(2)} > U_{\rm cr}^{(2)}$ and consistent with experimental data appears to be quite reasonable.

Our conclusion regarding the linkage of stripe ordering with $\Delta_1 \neq 0$ and $\Delta_2 = 0$ directly follows from the topology, and more specifically from the fact that both hole Fermi contours are situated around Γ point. To see this, assume that the hole and electron bands mix to form an SDW with the vector $\mathbf{Q}_1 = (0, \pi)$ (Fig. 3a). If the interaction is strong, an energy gap develops in the SDW excitation spectrum, thus blocking coupling with the other electron band. However, if the blocking is not strong enough, then another pair of bands coupled by the vector $\mathbf{Q}_1 = (0, \pi)$ will also undergo mixing, leading to the generation of an SDW and, hence, starting to destroy the stripe order $\mathbf{Q}_1 = (0, \pi)$. A different situation occurs if the second hole band is centered around (π, π) , not (0, 0) (Fig. 3c). In this case, the connecting wave vectors are about the same for both pairs; hence, the originally established stripe order remains intact. Figure 3c corresponds to the situation occurring in the t-t'-U model with a half-filled band. The Hamiltonian of the model has the form

$$H = t \sum_{i,\delta_{1},\sigma} c^{+}_{i\sigma} c_{i+\delta_{1}\sigma} + t' \sum_{i,\delta_{2},\sigma} c^{+}_{i\sigma} c_{i+\delta_{2}\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \quad (23)$$



Figure 3. Fermi contours and magnetic structure changes related to the appearance of a relatively small Δ_2 (a, b) for pnictides, and (c, d) for the t - t' model with $t \leq t'$.

where δ_1 and δ_2 are the distances to the nearest and next-tonearest neighbors, respectively, and $n_{i\sigma} = c^+_{i\sigma}c^-_{i_1\sigma}$. The quasiparticle energy $\varepsilon_p = 2t(\cos p_x + \cos p_y) + 4t' \cos p_x \cos p_y - \mu$ has maxima at (0, 0) and (π, π) points. For $t \neq 0$, the effective masses are different. The energy minima and, accordingly, the electron pockets are located near points $(0, \pi)$ and $(\pi, 0)$. The Fermi contour topology is illustrated in Fig. 3c. For large values of U, the model reduces to the Heisenberg $J_1 - J_2$ model. All quasiparticle excitations have gaps in this model. In the mean-field approximation, the order parameters of SDW states are degenerate.

It is instructive to consider in more detail the distinction between the four-band model and the t-t'-U model. Recall that in the four-band model the ellipticity of and interaction between electron pockets lift degeneracy already in the meanfield approximation. We will show below that in the meanfield approximation, the t-t'-U model does not allow the removal of degeneracy, even if $t \neq 0$ and the electron pockets are elliptical. In this case, the $(0, \pi)$ and $(\pi, 0)$ states remain degenerate with an unboundedly large number of sublattice states. Extending the J_1-J_2 model beyond the mean-field approximation, it is found that quantum fluctuations stabilize the $(0, \pi)$ or $(\pi, 0)$ states. To demonstrate that in the t-t'-U model the SDW order parameter is degenerate in the mean-field approximation, we consider the case of small t and introduce two order parameters:

$$\varDelta_{1} = -\frac{U}{2N} \sum_{\mathbf{k}} \left\langle c_{\mathbf{k},\alpha}^{+} \sigma_{\alpha\beta} c_{\mathbf{k}+\mathbf{Q}_{1},\beta} \right\rangle$$

with the wave vector \mathbf{Q}_1 , and

$$\varDelta_2 = -\frac{U}{2N} \sum_{\mathbf{k}} \left\langle c_{\mathbf{k},\alpha}^+ \sigma_{\alpha\beta} c_{\mathbf{k}+\mathbf{Q}_2,\beta} \right\rangle$$

with the wave vector \mathbf{Q}_2 . We further introduce four types of fermion operators with quasimomenta near (0, 0), $(0, \pi)$, $(\pi, 0)$, and (π, π) points and reformulate the t-t'-U model in correspondence with the concept of holes and electrons. Because the calculation is similar to that done above, we omit the details and only present the results. The additional term in the Hamiltonian quadratic form arises from the interaction between holes and electrons. For t = 0, all four dispersion relations turn out to be the same except for the sign, and the Hamiltonian is diagonalized as before. The ground state energy depends only on the sum $\Delta_1^2 + \Delta_2^2$, indicating degeneracy.

Let us now touch on the interaction effect between electron bands. There are four types of electron–electron interactions analogous to U_6 , U_7 , U_8 , and U_4 . They all originate from an initial U and have the same prefactor. The electron–electron interaction contributes the term of the type $E_{gr}^{ex} =$ $4A^2U(\Delta_1\Delta_2)^2/\Delta^4$ to the ground state energy, which 'brings into order' Δ_1 and Δ_2 and arranges them perpendicular to one another, with the result that the order parameters $\Delta_1 + \Delta_2$ and $\Delta_1 - \Delta_2$ have the same value in the two sublattices. In the absence of the term $|\Delta_1|^2 |\Delta_2|^2$, however, the angle between the two sublattices remains arbitrary.

Let us consider next the consequences of introducing electron pocket ellipticity. Recall that in our model the ellipticity effects were to introduce correction terms proportional to $|\Delta_1|^2 |\Delta_2|^2$. The t-t'-U model produces a very similar situation. The ground state energy $E_{\rm gr}$ again comprises two contributions, one of which is defined by the second-order perturbation theory allowing for off-diagonal Hamiltonian terms, and the other of which is due to the change in the dispersion relation. The contribution from the off-diagonal terms is given by the expression

$$E_{\rm gr}^{a, \rm ellipt} = 8t^2 \frac{|\Delta_1|^2 |\Delta_2|^2}{\Delta^4} \times \sum_{\bf p} \frac{(\cos^2 p_x + \cos^2 p_y) \Delta^2}{\left[\Delta^2 + 16(t')^2 \cos^2 p_x \cos^2 p_y\right]^{3/2}} + \dots, (24)$$

where, as before, the ellipsis refers to the terms that depend only on Δ . The contribution due to the change in the dispersion of the diagonal Hamiltonian terms is written out as follows:

$$E_{\rm gr}^{b, \, \rm ellipt} = -8t^2 \, \frac{|\mathbf{\Delta}_1|^2 \, |\mathbf{\Delta}_2|^2}{\Delta^4} \\ \times \sum_{\mathbf{p}} \frac{(\cos^2 p_x + \cos^2 p_y) \, \Delta^2}{\left[\Delta^2 + 16(t')^2 \cos^2 p_x \cos^2 p_y\right]^{3/2}} + \dots$$
(25)

Comparing Eqns (25) and (24), we see that the two contributions cancel out. Thus, including elliptical electron pockets into the t-t'-U model does not lift the degeneracy of the SDW order parameter. This result will most likely be true if the higher-order terms in the expansion of the energy in a power series of t/t' are included.

In this talk, the formation mechanism of spin density waves in iron-based pnictides were analyzed based on the results of paper [16]. We have considered a model of itinerant electrons with two hole Fermi surfaces centered around the Γ point of the Brillouin iron zone and with two electron pockets near $(0, \pi)$ and $(\pi, 0)$ points.

In general, the SDW order parameter in this model is a combination of two components with respective wave vectors $\mathbf{Q}_2(0,\pi)$ and $\mathbf{Q}_1(\pi,0)$. However, only one of these components is observed in neutron scattering experiments. As shown in the talk, indeed only one of the components, $(0, \pi)$ or $(\pi, 0)$, is stabilized if only one of the hole bands is assumed to mix with the electron bands when SDW states form. The other hole band remains gapless, which is precisely what explains the metallicity of pnictides with SDWs. For perfect nesting, the SDW order parameter in this three-band model is strongly degenerate. This degeneracy is lifted in favor of either $(0,\pi)$ ordering or $(\pi,0)$ ordering by including interactions and elliptical electron pockets. The calculated Fermi contours, ARPES spectral intensity, and the band dispersion near the Fermi level are consistent with the experimental data.

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Superconducting state in iron-based materials and spin-fluctuation pairing theory

M M Korshunov

Beyond the pairs of opposites of which the world consists, other, new insights begin. Herman Hesse, "Inside and Outside," in Stories of Five Decades (London: Jonathan Cape, 1974)

Quite recently, the scientific community was shaken up by a new discovery. In the field of high- T_c superconductivity, where cuprates had overwhelmingly predominated for the previous two decades, a new player—iron compounds—has appeared [1]. Although the superconducting transition temperature (T_c) in iron-based compounds has not exceeded the liquid-nitrogen temperature, already in late 2008, i.e., less than a year after the discovery of this new class of super-

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