Orbital-transverse density-wave instabilities in iron-based superconductors

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Abstract – Besides the conventional spin-density-wave (SDW) state, an orbital-transverse density-wave (OTDW) state is shown to exist generally in multi-orbital systems. We demonstrate that the orbital character of Fermi surface nesting plays an important role in density responses. The relationship between antiferromagnetism and structural phase transition in LaFe\(_2\)AsO (1111) and BaFe\(_2\)As\(_2\) (122) compounds of iron-based superconductors may be understood in terms of the interplay between the SDW and OTDW with a five-orbital Hamiltonian.

Introduction. – Over the last two years, research on iron-based superconductors has been an exciting topic that has intensely attracted experimental \([1–5]\) and theoretical \([6–11]\) investigations. Although it has been well established experimentally that this family of compounds exhibits several phase transitions including the structural phase transition \([12–14]\), the antiferromagnetic (AF) phase transition \([13–15]\), and the superconducting phase transition, the mechanism of these phase transitions remains highly controversial. However, there has been a consensus on the basic Fermi surface (FS) topology — hole pockets centered at \((0,0)\) and electron pockets centered at \((\pi,0)\) (The unfolded Brillouin zone is used in this paper) \([16–18]\). From a viewpoint of itinerant antiferromagnetism, the hole and electron pockets are assumed to be nested nearly perfectly in the parent compound. The spin-density-wave (SDW) state is stabilized due to the existence of the on-site Coulomb repulsions. Upon doping, the long-range AF order is destroyed and short-range AF spin fluctuations are developed, which is responsible for the high-temperature superconductivity \([19,20]\).

The multi-orbital nature of iron-based superconductors is believed to play a prominent role in the superconductivity, which signifies the importance of extracting the distinct physics that emerges from multi-orbital effects in this new family of materials. In this paper, we reveal that a new kind of unconventional orbital-transverse density-wave state exists generally in multi-orbital systems with certain orbital configuration of FS nesting. This type of density wave stems from the rotation asymmetry of Hamiltonian in the orbital space, which is reflected in the multi-orbital FS nesting geometry, and has an intriguing impact on the electron charge- and spin-density responses. In connection to the iron-based superconductors, our calculations show that the orbital-transverse density wave is a competing order with conventional SDW.

Multi-orbital Hamiltonian. – A multi-orbital Hamiltonian incorporating the on-site intra- and inter-orbital Coulomb interaction reads

\[
H = H_0 + \frac{1}{2} U \sum_{i\alpha\sigma} n_{i\alpha\sigma} n_{i\alpha\bar{\sigma}} + \frac{1}{2} U' \sum_{i\alpha\neq\beta} n_{i\alpha} n_{i\beta},
\]

where \(H_0 = \sum_{i\alpha j\beta} t_{i\alpha j\beta} c_{i\alpha\sigma}^\dagger c_{j\beta\sigma}\), \(t_{i\alpha j\beta}\) is the hopping term between orbital \(\alpha\) of site \(i\) and orbital \(\beta\) of site \(j\), and \(n_{i\alpha\sigma}\) the electron number operator, \(U\) and \(U'\) are the on-site intra- and inter-orbital Coulomb repulsions, respectively. For simplicity, \(U\) is assumed to be equal to \(U'\) in the present study and the terms of Hund’s rule coupling are ignored. In order to illustrate various types of density responses of the multi-orbital system more clearly, we start...
from a simple two-orbital model in the square lattice with a hole pocket lying at (0, 0) and an electron pocket lying at (π, 0). The dispersion and chemical potential ensure that the electron pocket and hole pocket are circular and nested perfectly. This fermiology is compatible with many possible orbital configurations, which have different orbital weights of the FS. In fig. 1 we show three prototypes of them. As will be seen below, their density response behaviors are quite different.

Definition of density quantities. – The introduction of orbital degrees of freedom enables us to define extra physical quantities of density whose translational symmetry could be broken when the system is phase transferred into the density-wave ground state. Similar to the spin-1/2 degrees of freedom, we represent the two-orbital degrees of freedom by a 1/2 pseudospin. The density operators in such a spin-orbital space can be written as D(r_i) = φ(G) 0 \phi^\dagger, with \Gamma = \sigma \otimes \sigma and \phi^\dagger = [c_{i1\uparrow}^\dagger, c_{i1\downarrow}^\dagger, c_{i2\uparrow}^\dagger, c_{i2\downarrow}^\dagger] the 4-component spinor (\tau^0 = \sigma^0 = \mathbb{I} and \tau^1-3 = \sigma^1-3 the Pauli matrices, where \tau is defined in the orbital space and \sigma is defined in the spin space). To study the instability in the particle-hole channels, the sixteen particle-hole operators \phi^\dagger (\tau^{0-3} \otimes \sigma^{0-3}) \phi can be reduced into six different density channels (three of spin and three of charge) due to the SU(2) symmetry of Hamiltonian (1) in the spin space, which are listed in table 1.

Table 1: Density waves with two orbital degrees of freedom.

| Ordering densities | Orientation in orbital space | Density operator | Response function | Divergent block |
|--------------------|-----------------------------|------------------|------------------|-----------------|
| total spin         | n/a                         | D_{0,3}(r_i): ρ_{i1\uparrow} - ρ_{i1\downarrow} + ρ_{i2\downarrow} - ρ_{i2\uparrow} | \frac{1}{2}(\chi_1^{111} + \chi_2^{222} + \chi_1^{112} + \chi_2^{221}) | \hat{x}^2 |
| total charge       | n/a                         | D_{0,0}(r_i): ρ_{i1\uparrow} + ρ_{i1\downarrow} + ρ_{i2\downarrow} + ρ_{i2\uparrow} | \frac{1}{2}(\chi_1^{111} + \chi_2^{222} + \chi_1^{112} + \chi_2^{221}) | \hat{x}^2 |
| orbital-polarized spin | longitudinal transverse | D_{3,3}(r_i): ρ_{i1\uparrow} - ρ_{i1\downarrow} - (ρ_{i2\uparrow} - ρ_{i2\downarrow}) | \frac{1}{2}(\chi_1^{111} + \chi_2^{222} - \chi_1^{112} - \chi_2^{221}) | \hat{x}^1 |
| orbital-polarized charge | longitudinal transverse | D_{3,0}(r_i): ρ_{i1\uparrow} + ρ_{i1\downarrow} - (ρ_{i2\uparrow} + ρ_{i2\downarrow}) | \frac{1}{2}(\chi_1^{111} + \chi_2^{222} - \chi_1^{112} - \chi_2^{221}) | \hat{x}^1 |

Fig. 1: (Color online) Schematic plot of the Fermi surfaces with different orbital configurations. Blue and red indicate dominant weights of orbital 1 and 2, respectively. (a) Inter-orbital FS nesting. (b) Intra-orbital FS nesting.

Fig. 2: Schematic plot of density waves with wave vector Q = (π, 0), (a)–(f) correspond to the density-wave states with density operators D_{0,3}, D_{3,3}, D_{3,0}, D_{3,0}, D_{3,0}, and D_{3,0}. Black (blank) circle represents orbital 1 (2). Dark grey and grey circles represent two orthogonal mixtures of orbitals 1 and 2, e.g., \chi_3(1) + |2) for dark grey and \chi_3(1) − |2) for grey. The arrow indicates spin density and the vertical line indicates the charge density. i, i+1, ... denote the lattice sites and each site represents a reduced unit cell. Only modulated direction is shown.

Instability criterions. – The particle-hole instabilities in the presence of Coulomb interactions may be
examined within the random-phase approximation (RPA). The interaction matrices for the magnetic ($\hat{U}^s$) and charge ($\hat{U}^c$) channels reads

$$\hat{U}^s = \begin{pmatrix} U & 0 & 0 & 0 \\ 0 & U & 0 & 0 \\ 0 & 0 & U' & 0 \\ 0 & 0 & 0 & U' \end{pmatrix},$$

and

$$\hat{U}^c = \begin{pmatrix} U & 2U' & 0 & 0 \\ 2U' & U & 0 & 0 \\ 0 & 0 & -U' & 0 \\ 0 & 0 & 0 & -U' \end{pmatrix}.$$.  

Defining the orbital indices of the bare susceptibility as $\chi^0_{\alpha,\mu\nu}(q) = -\frac{2}{N} \sum_k G^\alpha_{\mu\nu}(k+q)G^\nu_{\gamma\beta}(k)$, we get the RPA spin and charge susceptibility matrices

$$\hat{\chi}^s(q) = \left[ I - \chi^0(q)\hat{U}^s \right]^{-1}\chi^0(q),$$

$$\hat{\chi}^c(q) = \left[ I + \chi^0(q)\hat{U}^c \right]^{-1}\chi^0(q).$$

The response functions listed in table 1 are given by

$$\tilde{\chi}_{A,B}(q, i\omega) = \frac{1}{2} \int_0^\beta d\tau e^{i\omega\tau} \langle T_\tau T_{\tau+\beta} \rangle_{A,B(-q,0)},$$

$$\tilde{\chi}_{-,A,B}(q, i\omega) = \frac{1}{2} \int_0^\beta d\tau e^{i\omega\tau} \langle T_\tau T_{\tau+\beta} \rangle_{A,B(-q,0)},$$

where $A$ and $B$ are numbers and $D_{A,B} = \phi^\dagger(\tau_{A} \otimes \sigma_{B})\phi$. A direct calculation gives the response functions of density operators defined in table 1

$$\tilde{\chi}_{0,3} = \frac{1}{2} (\chi^0_{1111} + \chi^0_{2222} + \chi^0_{1122} + \chi^0_{2211}),$$

$$\tilde{\chi}_{0,0} = \frac{1}{2} (\chi^0_{1111} + \chi^0_{2222} + \chi^0_{1122} + \chi^0_{2211}),$$

$$\tilde{\chi}_{3,3} = \frac{1}{2} (\chi^0_{1111} + \chi^0_{2222} - \chi^0_{1122} - \chi^0_{2211}),$$

$$\tilde{\chi}_{-,3} = \chi^0_{2121},$$

$$\tilde{\chi}_{3,0} = \frac{1}{2} (\chi^0_{1111} + \chi^0_{2222} - \chi^0_{1122} - \chi^0_{2211}),$$

$$\tilde{\chi}_{-,0} = \chi^0_{2121}.$$

To a good approximation, especially at $Q = (\pi,0)$, the bare susceptibility matrix in the two-orbital case can be regarded as a block matrix $\chi^0 = \text{diag}(\hat{\chi}^1, \hat{\chi}^2)$, where

$$\hat{\chi}^1 = \begin{pmatrix} \chi^0_{1111} & \chi^0_{1122} \\ \chi^0_{1122} & \chi^0_{2211} \end{pmatrix}, \quad \hat{\chi}^2 = \begin{pmatrix} \chi^0_{1212} & \chi^0_{1221} \\ \chi^0_{2112} & \chi^0_{2212} \end{pmatrix}.$$

As a result, the RPA spin and charge susceptibility matrices are also blocked,

$$\hat{\chi}^{s,c}(c) = \begin{pmatrix} \hat{\chi}^{s,c}(c_1) & 0 \\ 0 & \hat{\chi}^{s,c}(c_2) \end{pmatrix},$$

where

$$\hat{\chi}^{s_1} = \frac{\hat{M}_1}{d_1}, \quad \hat{\chi}^{s_2} = \frac{\hat{M}_2}{d_2}, \quad \hat{\chi}^{c_1} = \frac{\hat{M}_3}{d_3}, \quad \hat{\chi}^{c_2} = \frac{\hat{M}_4}{d_4}. $$

Here $M_n$ are some $2 \times 2$ matrices and

$$d_1 = \det[\chi^{s_1}] = (1 - U\chi^0_{1111})(1 - U\chi^0_{2222}) - U^2\chi^0_{1122}\chi^0_{2211},$$

$$d_2 = \det[\chi^{s_2}] = (1 - U\chi^0_{1122})(1 - U\chi^0_{2211}) - U^2\chi^0_{1122}\chi^0_{2211},$$

$$d_3 = \det[\chi^{c_1}] = 1 + U\chi^0_{1111} + U\chi^0_{2222} + 2U\chi^0_{1122} + 2\chi^0_{2211},$$

$$d_4 = d_2,$$

are the denominators that come from the inversion of matrices $\hat{I} - \chi^0(q)\hat{U}^s$ and $\hat{I} + \chi^0(q)\hat{U}^c$ in eq. (8). Deviated from the single band RPA, there are two instability criterions for the spin channel, which are indicated by $d_1 \to 0$ and $d_2 \to 0$, respectively. When approaching the critical temperature, either the upper block $\hat{\chi}^{s_1}$ or the lower block $\hat{\chi}^{s_2}$ may diverge. Comparing the response functions listed in table 1 and eq. (8), we can see that the divergence of the upper block or the lower block corresponds to a transition to one or the other totally different magnetic phase, i.e., the former indicates an SDW transition while the latter indicates an orbital-transverse-polarized spin-density-wave transition. The same conclusion holds for the charge susceptibility matrix. We will refer the orbital-transverse density-wave ground state as OTDW in this paper hereafter.

Now we turn to the real-space distribution of these density waves. From definition it is clear that the orbital-longitudinal operators represent the density differences between orbitals 1 and 2. On the other hand, the real-space distribution of the orbital-transverse density wave can be revealed by performing a rotation in the orbital space:

$$\psi_i = \hat{R}\psi_i' = [c_i^{+\uparrow}, c_i^{+\downarrow}, c_i^{-\uparrow}, c_i^{-\downarrow}],$$

where

$$c_i^{+\pm} = \frac{1}{\sqrt{2}}(c_{i\sigma}^{+\uparrow} \pm c_{i\sigma}^{+\downarrow}).$$

The charge- and spin-density differences between the two orbitals $\left| + \right>$ and $\left| - \right>$ can be represented by

$$D^{s}_{3,3}(r_i) = \psi_i'(\tau_3 \otimes \sigma_3)\psi_i = S_{+,-} - S_{-,+},$$

$$D^{s}_{3,0}(r_i) = \psi_i'(\tau_3 \otimes \sigma_0)\psi_i = \rho_{+,-} - \rho_{-,+}$$

$$= c_{i\uparrow}c_{i\downarrow} - c_{i\downarrow}c_{i\uparrow} + H.c.,$$

where $S_{+,-}$ and $\rho_{+,-}$ represent the spin and charge density of orbital $\left| \pm \right>$ at $i$ site, respectively. Similarly, the response functions for density operators $D^{s,c}_{A,B}$ are

$$\tilde{\chi}^{s}_{3,3} = \frac{1}{2}(\chi^0_{1212} + \chi^0_{2121} + \chi^0_{1221} + \chi^0_{2212}),$$

$$\tilde{\chi}^{s}_{3,0} = \frac{1}{2}(\chi^0_{1212} + \chi^0_{2121} + \chi^0_{1221} + \chi^0_{2212}).$$

Therefore, in OTDW state, the translational symmetry of the local density difference between the two orthogonal mixtures of orbitals 1 and 2 is broken.
Nesting-induced OTDW: a weak-coupling analysis. – Roughly speaking, the density response of a Hubbard-like Hamiltonian is mainly determined by two factors: one is the band structure, and the other is the Coulomb interactions. We now look into the influence of different band structures shown in fig. 1 on the density responses. The bare susceptibility of a general multi-orbital system is given by

$$\chi_{\alpha\beta\mu\nu}(q,0) = \frac{1}{N} \sum_{k,m,n} a_{\alpha m}(k + q) a_{\beta m}^*(k) a_{\nu n}^*(k) a_{\mu n}(k + q)$$

$$\times \frac{f[\epsilon_n(k + q)] - f[\epsilon_m(k)]}{\epsilon_m(k) - \epsilon_n(k + q) + i\eta}, \quad (12)$$

where $\alpha$, $\beta$, $\mu$ and $\nu$ are the orbital indices, $m$ and $n$ are the band indices, and $a_{\alpha m}^*(k) = (a, k|m, k)$ is the orbital weight. For the case indicated in fig. 1 (a1), the matrix elements of bare susceptibility are simplified to

$$\chi_{\mu\nu\mu\nu}(q,0) = \frac{1}{N} \sum_{k,\mu,\nu} \frac{f[\epsilon_{\mu}(k + q)] - f[\epsilon_{\nu}(k)]}{\epsilon_{\mu}(k) - \epsilon_{\nu}(k + q) + i\eta}, \quad (13)$$

The susceptibilities $\chi_{\mu\nu\mu\nu}(\mu \neq \nu)$ vanish since there is no hybridization between the two orbitals. Straightforwardly, $\chi_{1212}(Q)$ and $\chi_{1212}(Q)$ are divergent due to FS nesting, while $\chi_{1111}$ and $\chi_{2222}$ keep finite as they take no advantage from the nesting between electron and hole pockets. Bear in mind that although the cases of figs. 1(a1) and (a2) have different orbital configurations, their FS nestings are both from the inter-orbital contribution. Hence the above conclusion holds also for the band structure shown in (a2). For the case fig. 1(b), from eq. (12) the divergent components of bare susceptibilities are $\chi_{1111}$ and $\chi_{2222}$.

The above considerations focus on the band structure, but do not take into account the electron-electron interactions explicitly. Given the interaction vertices in eq. (2) and the instability criterions in eq. (9), three spin-density waves ($D_{0,3}$, $D_{3,3}$, and $D_{-(+),3}$), and one charge-density wave ($D_{-(+),0}$) could be established in Hamiltonian (1). The $D_{0,0}$ and $D_{3,0}$ charge-density waves are prohibited due to repulsive on-site Coulomb interactions (note that $d_3$ is always greater than zero when $U \chi_{1111/2222}^0 < 1$ and the hybridization is negligible). $D_{0,3}$ and $D_{3,3}$ density waves occur simultaneously since they both come from the divergence of the upper block of $\hat{\chi}^0(Q)$, which indicates the real-space distribution of spin density to be compatible with figs. 2(a) and (b). A typical pattern of spin density that is either $D_{0,3}$ or $D_{3,3}$ density wave is shown in fig. 3, where the staggered spin density is orbital-polarized and dominantly appears in one orbital. On the other hand, the phase transition in $D_{-(+),0}(3)$ channel comes from the divergence of the lower block of $\hat{\chi}^{0,3}(Q)$ which is coupled to the inter-orbital repulsion, with order parameter $\langle c^\dagger_{\mu\nu}(k + Q)c_{\nu\sigma}(k) \rangle$.

Fig. 3: Intra-orbital-nesting–induced spin-density-wave state that is realized in the iron-based superconductors, where the translational symmetries of $(D_{0,3})$ and $(D_{3,3})$ are broken simultaneously. All the symbols are the same as that in fig. 2.

In the present model, instabilities in $D_{-(+),3}$ and $D_{-(+),0}$ channels are degenerated due to $U = U'$, while the actually established state depends on the additional interaction terms that break the degeneracy, e.g., the former is favored by Hund’s rule coupling while the latter is favored by the presence of electron-phonon interactions.

We now conclude that for configurations shown in figs. 1(a1) and (a2), the divergent susceptibility matrix is $\chi_{22}(Q)$ or $\chi_{22}(Q)$, indicating that the system undergoes an OTDW transition. There is no long-range order of the total local spin density, as is shown in figs. 2(c) and (f). For the configuration of fig. 1(b), the divergent susceptibility matrix is $\chi_{11}(Q)$, corresponding to a spin-density-wave transition whose real-space distribution is shown in fig. 3.

OTDW and the iron-based superconductors. – Mixing the intra- and inter-orbital nesting in the fermiology, the multi-orbital band structure of iron-based superconductors provides an intermediate example between prototypes of figs. 1(a) and (b). To be more concrete, we here employ a realistic five-orbital Hamiltonian with on-site intra- and inter-orbital Coulomb repulsions. The involved orbitals are $d_{xz}$, $d_{yz}$, $d_{x^2−y^2}$, $d_{xy}$, and $d_{3z^2−r^2}$ (defined in the reduced unit cell) which are labeled with 1, 2, 3, 4, and 5, respectively. Then the orbital indices in Hamiltonian 1 run from 1 to 5. We adopt the hopping parameters given by Graser et al. [21] fitted from first principle calculated band structure by Cao et al. [22]. The density-wave instabilities defined in table 1 can be realized in the space spanned by the two most relevant orbitals. In our calculations, $d_{xz}/d_{yz}$ (orbital 1/2) and $d_{xy}$ (orbital 4) are the two orbitals with largest intra- and inter-orbital susceptibilities. The instabilities of OTDW and SDW are found to be nearly degenerated, consequently the competition between them is sensitive to the detailed band structure. We consider this to be a key point to understand the essential difference between RFeAsO (1111) and AF2As2 (122) compounds (R = rare earth and A = Sr, Ca, Ba and K), which will be discussed in the following paragraphs.

The AF and structural transitions in the iron-based superconductors exhibit different properties in different systems: the static AF order develops after the structure distortion in 1111 compounds [13], while in the 122 compounds, the two transitions occur at the same temperature [14,23]. The structure distortion has been
theoretically proposed to be driven magnetically [24–26] or electrically [27,28]. Here we present an alternative view. Note that all the density waves we discuss are nesting-driven and occur at the same wave vector \( Q = (\pi, 0) \). The order parameters of these density waves and the tetragonal-to-orthorhombic distortion break the same symmetry. Therefore, we propose that either SDW (as was proposed by Yildirim [24]) or OTDW could induce a structure distortion. When the transition temperature of SDW \( T_{d1} \) is higher than that of OTDW \( T_{d2} \), the AF transition is orbital-polarized as shown in fig. 3 and is accompanied with a structure distortion which is magnetically driven, thus the critical temperature of structure distortion \( T_S \) and AF transition \( T_{AF} \) equal to \( T_{d1} \). The temperature gap between \( T_S \) and \( T_{AF} \) appears when \( T_{d2} > T_{d1} \), which indicates \( T_S = T_{d2} > T_{AF} = T_{d1} \).

We make two remarks here. First, \( D_{-(-1),0} \) and \( D_{-(-1),3} \) density waves are two candidates for OTDW-induced lattice distortion. As an orbital-ordered state of charge, \( D_{-(-1),0} \) density wave could induce a structure distortion electrically by Jahn-Teller effect. The coupling between \( D_{-(-1),3} \) density wave and lattice distortion is, if it exists, magnetic relevant and more subtle. It is out of scope of the present work to determine which of the two density waves is actually established in the real materials of iron-based superconductors. Since the two states are degenerated in our model, we just generally relate the structure distortion with OTDWs. It is also noteworthy that starting from a two-band model, the \( D_{-(-1),0} \) density wave is considered by Podolsky et al. as a competing order of SDW [29]. Second, in this scenario, from high temperature to low temperature, the system undergoes two phase transitions. However, only one structure distortion is identified in experimental measurements. Since the lattice distortion is weak and driven by breaking of \( C_4 \) lattice rotation symmetry, if the system is already in the orthorhombic structure phase, another density-wave phase transition with wave vector \((\pi, 0)\) would not break an extra lattice symmetry.

It is known from band calculations of 1111 compounds that along \( \Gamma-Z \) direction lies a \( d_{xy} \)-like two-dimensional (2D) FS (denoted as \( \varepsilon \)-FS hereafter) [30]. While for 122 compounds, a 2D FS with \( d_{xy} \) character is found to be absent in density functional calculations when the puctogen height is relaxed using total-energy minimization [31] and also in angle-resolved photoemission spectroscopy (ARPES) measurements [32]. In our model calculation we find the existence of \( \varepsilon \)-FS enhances the inter-orbital susceptibility \( \chi_{1111}^d \) substantially, while without \( \varepsilon \)-FS, the susceptibility \( \chi_{1111}^d \) is in general, at least slightly, stronger than that of \( \chi_{1111}^s \). The enhancement of \( \chi_{1111}^d \) by the appearance of a \( d_{xy} \)-like FS is expected because of the strengthened inter-orbital nesting between \( \varepsilon \)-FS and the \( dxz/dyz \)-dominant FS sections around M. In fig. 4 we show dominant components (1111 and 1414) of spin susceptibility matrix with (upper) and without (lower) the appearance of the \( \varepsilon \)-FS. To produce the \( \varepsilon \)-FS, the on-site energy of orbital \( d_{xy} \) is adjusted from 0.3 to 0.38, and \( \mu \) is adjusted from 0 to 0.006 to keep the band filling at \( n = 6 \) in the upper panel, where the divergent susceptibility is \( \chi_{1414}^d \) at \( T = 0.019 \) and \( U = 1.38 \). In the lower panel, \( \chi_{1414}^d \) is suppressed by the annihilation of the \( \varepsilon \)-FS, and the divergent channel changes to \( \chi_{1111}^s \). With the definition of pseudo-transition-temperatures \( T_{d1} \) and \( T_{d2} \), \( \chi^d(Q, T_{d1}^*(d2)) = 10^2 \chi^0(Q, T_{d1}^*(d2)) \), our numerical results show that the transition temperature \( T_{d2}^* = 0.019 \) is higher than \( T_{d2}^* = 0.012 \) in the presence of \( \varepsilon \)-FS, which leads to a higher transition temperature of OTDW than that of SDW, thus the separation between \( T_S \) and \( T_N \) appears, as is observed in 1111 compounds. Without \( \varepsilon \)-FS, we get \( T_{d1}^* = 0.017 \) with \( d_{xy} \)-dominant FS sections around M. In the \( \varepsilon \)-FS in splitting \( T_{d1} \) and \( T_{d2}^* = 0.0068 \) which indicates same \( T_S \) and \( T_N \) in our scenario, as is observed in 122 compounds. In this sense, the essential difference in the structure distortion between 1111 and 122 systems may be attributed to the existence of \( \varepsilon \)-FS in 1111 parent compounds. Meanwhile, we want to emphasize that depending on the detailed band structure, there are other possible realizations of OTDW, such as the inter-orbital nesting between \( d_{xz} \) and \( d_{yz} \) orbitals. The importance of the \( \varepsilon \)-FS in splitting \( T_S \) and \( T_N \) awaits for further experimental verification.

In the end we briefly comment on the experimental detection of OTDW. A direct consequence of our theory is that the OTDW gap opens on the sections of Fermi surface with inter-orbital nesting, while the SDW gap opens on the sections with intra-orbital nesting. In the small temperature window between \( T_S \) and \( T_N \), it is in principle possible to observe the OTDW gap on corresponding FS sections by ARPES measurements. The partially gapped
behavior of OTDW and SDW also can be used to distinguish between the density wave and the orbital ordering proposals [28,33] for the structural transition of iron pnictides.

Summary. – We make several remarks as a summary. 1) The transverse nature of OTDW implies that the ordered orbital component is a mixture of the two involved orbitals, for instance, a mixture of $d_{xz}/d_{yz}$ and $d_{xy}$ orbitals. 2) In our model calculations, the instabilities of OTDWs occur in the space spanned by $d_{xz}$ (or $d_{yz}$) and $d_{xy}$ orbitals. However, depending on the band structure, other possibilities exist. 3) The OTDW might be related with the “hidden” order claimed by some experiments [34]. 4) One intriguing feature stemming from the itinerant multi-orbital model is that the established SDW should be orbital-polarized (as is shown in fig. 3).

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REFERENCES

[1] Kamihara Y., Watanabe T., Hirano M. and Hosono H., J. Am. Chem. Soc., 130 (2008) 3296.

[2] Chen X. H., Wu T., Wu G., Liu R. H., Chen H. and Fang D. P., Nature, 453 (2008) 761.

[3] Ren Z.-A., Yang J., Li W., Shi X.-L., Li Z.-C., Che G.-C., Dong X.-L., Sun L.-L., Zhou F. and Zhao Z.-X., EPL, 82 (2008) 57002.

[4] Chen G. F., Li Z., Wu D., Li G., Hu W. Z., Dong J., Zheng P., Luo J. L. and Wang N. L., Phys. Rev. Lett., 100 (2008) 247002.

[5] Rotter M., Tegel M. and Johrendt D., Phys. Rev. Lett., 101 (2008) 107006.

[6] Han Q., Chen Y. and Wang Z. D., EPL, 82 (2008) 37007.

[7] Daghofer M., Moreo A., Riera J. A., Arrigoni E., Scalapino D. J. and Dagotto E., Phys. Rev. Lett., 101 (2008) 237004.

[8] Chen W.-Q., Yang K.-Y., Zhou Y. and Zhang F.-C., Phys. Rev. Lett., 102 (2009) 047006.

[9] Cveticovic V. and Tesanovic Z., Phys. Rev. B, 80 (2009) 024512.

[10] Chubukov A. V., Efremov D. V. and Eremin I., Phys. Rev. B, 78 (2008) 134512.

[11] Yu S.-L., Kang J. and Li J.-X., Phys. Rev. B, 79 (2009) 064517.

[12] Zhao J., Huang Q., de la Cruz C., Shiliang L., Lynn W. J., Chen Y., Green M. A., Chen G. F., Li G., Li Z., Luo J. L., Wang N. L. and Dai F., Nat. Mater., 7 (2008) 953.

[13] McGuire M. A., Christianson A. D., Sefat A. S., Sales B. C., Lumsden M. D., Jin R., Payzant E. A., Mandrus D., Luan Y., Keppens V., Varadarajan V., Brill J. W., Hermann R. P., Sougrati M. T., Grandjean F. and Long G. J., Phys. Rev. B, 78 (2008) 094517.

[14] Krellner C., Caroca-Canales N., Jesche A., Rosner H., Ormeci A. and Geibel C., Phys. Rev. B, 78 (2008) 100504.

[15] Dong J., Zhang H. J., Xu G., Li Z., Li G., Hu W. Z., Wu D., Chen G. F., Dai X., Luo J. L., Fang Z. and Wang N. L., EPL, 83 (2008) 27006.

[16] Ding H., Richard P., Nakayama K., Sugawara K., Arakane T., Sekiba Y., Takayama A., Souma S., Sato T., Takahashi T., Wang Z., Dai X., Fang Z., Chen G. F., Luo J. L. and Wang N. L., EPL, 83 (2008) 47001.

[17] Sato T., Nakayama K., Sekiba Y., Richard P., Xu Y.-M., Souma S., Takahashi T., Chen G. F., Luo J. L., Wang N. L. and Ding H., Phys. Rev. Lett., 103 (2009) 047002.

[18] Liu C., Samolyuk G. D., Lee Y., Ni N., Kondo T., Santander-Syro A. F., Bud’ko S. L., McChesney J. L., Rotenberg E., Valla T., Fedorov A. V., Canfield P. C., Harmon B. N. and Kaminski A., Phys. Rev. Lett., 101 (2008) 177005.

[19] Yao Z.-J., Li J.-X. and Wang Z. D., New J. Phys., 11 (2009) 025009.

[20] Wang F., Zhao H., Yan Y., Vishwanath A. and Lee D.-H., Phys. Rev. Lett., 102 (2009) 047005.

[21] Graser S., Maier T. A., Hirschfeld P. J. and Scalapino D. J., New J. Phys., 11 (2009) 025016.

[22] Cao C., Hirschfeld P. J. and Cheng H., Phys. Rev. B, 77 (2008) 220506.

[23] Zhao J., Ratichew L., Lynn J. W. II, Chen G. F., Luo J. L., Wang N. L., Hu J. and Dai P., Phys. Rev. B, 78 (2008) 140504.

[24] Yildirim T., Phys. Rev. Lett., 101 (2008) 057010.

[25] Fang C., Yao H., Tsai W.-F., Hu J. and Kivelson S. A., Phys. Rev. B, 77 (2008) 224509.

[26] Xu C., Muller M. and Sachdev S., Phys. Rev. B, 78 (2008) 020512.

[27] Turner A. M., Wang F. and Vishwanath A., Phys. Rev. B, 80 (2009) 224504.

[28] Lv W., Wu J. and Phillips P., Phys. Rev. B, 80 (2009) 224506.

[29] Podolsky D., Kee H. and Kim Y. B., EPL, 88 (2009) 17004 (note that in this reference, the density-wave order parameters are defined with the band electron operators, which is in turn unequal to the density-wave states defined in table 1).

[30] Vildosola V., Pourovskii L., Arita R., Biermann S. and Georges A., Phys. Rev. B, 78 (2008) 094518.

[31] Singh D. J., Phys. Rev. B, 78 (2008) 094511.

[32] Zhang Y., Chen F., He C., Zhou B., Xie B. P., Fang C., Tsai W. F., Chen H. X., Hayashi H., Jiang J., Iwasa H., Shimada K., Natamase H., Taniguchi M., Hu J. P. and Feng D. L., eprint arXiv:0904.4022 (2009).

[33] Lee C.-C., Yin W.-G. and Ku W., Phys. Rev. Lett., 103 (2009) 267001.

[34] Zabolotnyy V. B., Inosov D. S., Evtushinsky D. V., Kozitsch A., Kordyuk A. A., Sun G. L., Park J. T., Haug D., Hinkov V., Boris A. V., Lin C. T., Kneuper M., Yaresko A. N., Buchner B., Varykhalov A., Follath R. and Borisenko S. V., Nature, 457 (2009) 569.