Diverse Exotic Orders and Fermiology in Fe-based Superconductors: A Unified Mechanism for $B_{1g}/B_{2g}$ Nematicity in FeSe/(Cs,Rb)Fe$_2$As$_2$ and Smectic Order in BaFe$_2$As$_2$

Seiichiro Onari$^{1,*}$ and Hiroshi Kontani$^{1}$

$^1$Department of Physics, Nagoya University, Furo-cho, Nagoya 464-8602, Japan.

Correspondence*:
Seiichiro Onari
onari@s.phys.nagoya-u.ac.jp

ABSTRACT

A rich variety of nematic/smectic orders in Fe-based superconductors is an important unsolved problem in strongly correlated electron systems. A unified understanding of these orders has been investigated for the last decade. In this article, we explain the $B_{1g}$ symmetry nematic transition in FeSe$_{1-x}$Te$_x$, the $B_{2g}$ symmetry nematicity in AFe$_2$As$_2$ (A=Cs, Rb), and the smectic state in BaFe$_2$As$_2$ based on the same framework. We investigate the quantum interference mechanism between spin fluctuations by developing the density wave equation. The observed rich variety of nematic/smectic orders is naturally understood in this mechanism. The nematic/smectic orders depend on the characteristic shape and topology of the Fermi surface (FS) of each compound. (i) In FeSe$_{1-x}$Te$_x$ ($n_d = 6.0$), each FS is very small and the $d_{xy}$-orbital hole pocket is below the Fermi level. In this case, the small spin fluctuations on three $d_{xz}$, $d_{yz}$, and $d_{xy}$ orbitals cooperatively lead to the $B_{1g}$ nematic ($q = 0$) order without magnetization. The experimental Lifshitz transition below the nematic transition temperature ($T_S$) is naturally reproduced. (ii) In BaFe$_2$As$_2$ ($n_d = 6.0$), the $d_{xy}$-orbital hole pocket emerges around M point, and each FS is relatively large. The strong spin fluctuations due to the $d_{xy}$-orbital nesting give rise to the $B_{1g}$ nematic ($q = 0$) order and the smectic [$q = (0, \pi)$] order, and the latter transition temperature ($T^* \sim 170$K) exceeds the former one ($T_S \sim 140$K). (iii) In heavily hole-doped AFe$_2$As$_2$ ($n_d = 5.5$), the large $d_{xy}$-orbital hole pocket and the four tiny Dirac pockets appear due to the hole-doping. The $B_{2g}$ nematic bond order emerges on the $d_{xy}$-orbital hole pocket due to the same interference mechanism. The present paramagnon interference mechanism provides a unified explanation of why the variety of nematic/smectic orders in Fe-based superconductors is so rich, based on the well-established fermiology of Fe-based superconductors.

Keywords: Nematic state, Smectic state, Orbital order, Bond order, Quantum critical point, Fe-based superconductors

1 INTRODUCTION

The emergence of electron nematic ($q = 0$) state is one of the most important unsolved problems in Fe-based superconductors [1]. In LaFeAsO and Ba122 compounds, the antiferro (AF) magnetic state
appears at the Néel temperature $T_N$, which is lower than the nematic transition temperature $T_S$. Since the superconducting phase with high transition temperature ($T_c$) appears near the nematic phase and the AF magnetic phase, it is expected that the nematic fluctuations and the spin fluctuations are related to the mechanism of the high-$T_c$ superconductivity. However, the questions appear before discussing the superconductivity: (i) What is the order parameter of the nematic state? (ii) What is the driving force of the nematic state? (iii) Why do the diverse nematic states emerge in various compounds.

It is known that the nematic order cannot be derived from the mean-field theory since the spin-channel order always dominates over the nematic order unless unphysical parameters (such as the negative Hund’s coupling) are assumed. Previously, in order to explain the nematic state [2], the vestigial order (spin nematic) scenario [3, 4, 5, 6, 7, 8, 9] and the orbital order scenario [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22] have been proposed.

To investigate the nematic state, the FeSe family is an ideal platform since the AF magnetic state is absent [23, 24, 25, 26]. This family is also attractive from the aspect of superconductivity since the highest $T_c$ $\geq$ 65K in Fe-based superconductors has been reported in electron-doped FeSe [27, 28, 29, 30, 31]. In FeSe, the orbital polarization between $d_{xz}$ and $d_{yz}$ orbitals in the nematic state has been observed by the angle-resolved-photoemission spectroscopy (ARPES) [32, 33, 34, 35, 36]. To be more precise, the orbital polarization energy $E_{xz} - E_{yz}$ has $k$ dependence and changes the sign between $\Gamma$ point and $X(Y)$ point. This sign reversal orbital polarization has been explained by the orbital order scenario [16, 17, 19, 20] based on the paramagnon interference mechanism and by the renormalization group (RG) theory [37, 38].

In both theories, the vertex correction (VC) of the Coulomb interaction, which corresponds to the higher-order many-body effect, plays the essential role. Since the AF magnetic correlation is weak in FeSe, it is difficult to explain the nematic state by the vestigial order (spin nematic) scenario [3, 4, 5, 6, 7, 8, 9] and the orbital order scenario [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22] have been proposed.

The rich variety of the nematicity in the FeSe family remains a significant open problem. In FeSe$_{1-x}$S$_x$, $T_S$ disappears at $x \sim 0.17$, where the emergence of the nematic quantum critical point (QCP) has been suggested by experiments [45, 46, 47, 48]. Recently, whole $x$ dependent phase diagram for FeSe$_{1-x}$Te$_x$ ($x \lesssim 0.6$) has reported [49, 50, 51]. In the phase diagram shown in Fig. 1A, $T_S$ decreases with Te doping $x$, and $T_S$ disappears at $x \sim 0.5$. $T_c$ becomes maximum $\sim 15$K at $x \sim 0.6$, which indicates that the nematic fluctuations enlarge superconducting pairing interaction near the nematic QCP. Thus, it is essential to clarify the mechanism of $x$ dependence of $T_S$ to understand the mechanism of superconductivity in the FeSe family.

In addition, a significant open issue in the nematicity is the emergence of another type of nematicity in various Ba122 compounds below $T = T^*$, which is higher than $T_S$ by tens of Kelvin, as shown in Fig. 1B. An actual bulk nematic transition at $T = T^*$ has been reported in many experimental studies, such as a magnetic torque study [52], an X-ray study [53], an optical measurement study [54], and a laser photoemission electron microscope (PEEM) study [55]. Since the orthorhombicity $(a-b)/(a+b) \ll 0.1$% below $T^*$ is tiny, an extrinsic origin such as the inhomogeneity of the nematic transition temperature $T_S$ due to local uniaxial pressure and randomness was proposed [4, 56, 57, 58, 59, 60]. On the other hand, $T^*$ seems not to be sensitive to the sample quality and the local strain, and the domain structure of nematicity observed above $T_S$ is homogeneous [54, 55]. It is noteworthy that the bulk orbital polarization starts to emerge at $T = T^* (> T_S)$ in Ba122 compounds, according to the recent PEEM study [55]. In this paper,
we will explain the multistage smectic/nematic transitions: the smectic order \((q \neq 0)\) at \(T = T^*\) and the nematic order \((q = 0)\) at \(T_S\). In this scenario, \(T^*\) is given by the intrinsic smectic order free from the randomness.

In contrast to the \(B_{1g}\) nematicity in typical Fe-based superconductors, the emergence of 45° rotated \(B_{2g}\) nematicity in heavily hole-doped AFe\(_2\)As\(_2\) (A=Cs, Rb) has been reported in Refs. \([61, 62, 63, 64]\), while Refs. \([65, 66]\) have reported the absence of the nematic order. As shown in Fig. 1C, the dominant \(B_{1g}\) nematicity changes to the \(B_{2g}\) nematicity with doping \(x\) in Ba\(_{1-x}\)Rb\(_x\)Fe\(_2\)As\(_2\). As for the mechanism of the \(B_{2g}\) nematicity, vestigial nematic order by using the double-stripe magnetic configuration was suggested \([67]\). However, no SDW transition has been observed \([64, 68]\) in AFe\(_2\)As\(_2\), and the spin fluctuations are weak around \(T_S\) in RbFe\(_2\)As\(_2\) \([69]\). In this paper, we reveal the emergence of \(B_{2g}\)-symmetry bond order in AFe\(_2\)As\(_2\).

As described above, the variety of nematicity in Fe-based superconductors is very rich. In order to understand the mechanism of nematic/smectic state and superconductivity, it is important to explain these nematic/smectic states in the same theoretical framework.

In this paper, we study the \(B_{1g}\) nematicity in FeSe\(_{1-x}\)Te\(_x\) \((n_d = 6.0)\), the tiny nematicity below \(T^*\) in BaFe\(_2\)As\(_2\) \((n_d = 6.0)\), and the \(B_{2g}\) nematicity in AFe\(_2\)As\(_2\) (A=Cs, Rb) \((n_d = 5.5)\) by developing the density wave (DW) equation theory. In this theory, the paramagnon interference mechanism due to the Aslamazov–Larkin (AL) type VCs shown in Fig. 1D is taken into account. We also take account of the self-energy effect shown in Fig. 1E. In this mechanism, the rich variety of nematicity is naturally understood. The obtained nematicity depends on the shape and topology of FSs, as shown in Figs. 2A, 2B, 2C. (i) In FeSe\(_{1-x}\)Te\(_x\), all FSs are very small, and \(d_{xy}\)-orbital hole pocket is absent. The small spin fluctuations on the three \(d_{xz}, d_{yz}\), and \(d_{xy}\) orbitals cooperatively lead to the \(B_{1g}\) nematic order, where the orbital order for \(d_{xz}\) and \(d_{yz}\) orbitals coexists with the bond order for the \(d_{xy}\) orbital. The experimental Lifshitz transition below \(T_S\) is naturally explained by the nematic order. (ii) In BaFe\(_2\)As\(_2\), the \(d_{xy}\) hole pocket emerges, and each FS is relatively large. The smectic order at \(T = T^*(> T_S)\) and the nematic order at \(T = T_S\) emerge due to the strong \(d_{xy}\)-orbital nesting. The smectic order explains the tiny nematicity below \(T^*\), and the multistage transitions are explained by the smectic and nematic orders. (iii) In heavily hole-doped AFe\(_2\)As\(_2\), the large \(d_{xy}\)-orbital hole pocket and the four tiny Dirac pockets appear. The \(B_{2g}\) nematic bond order emerges due to the \(d_{xy}\)-orbital paramagnon interference mechanism, where the nesting between the Dirac pockets and the large \(d_{xy}\)-orbital hole pocket plays an important role. By considering the fermiology of each compound, these various nematic/smectic states are explained by the same theoretical framework base on the paramagnon interference mechanism.

In the present study, we intensively study the effect of the self-energy on the nematic/smectic orders. It has been dropped in many previous studies, in spite of the fact that the self-energy is necessary to satisfy the criteria of Baym-Kadanoff’s conserving approximation \([70, 71]\). We revealed that (a) the nematic/smectic order is stabilized by the AL-type VCs, while (b) \(T_S\) is reduced to become realistic \((\sim 100 K)\) by introducing the self-energy. These results validate the idea of the "nematic/smectic state due to the paramagnon interference mechanism" proposed in our previous studies \([14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44]\). In addition, (c) the phase diagram of FeSe\(_{1-x}\)Te\(_x\) \([49, 50, 51]\) is understood by using a fixed Coulomb interaction thanks to the self-energy. (In the absence of the self-energy, add-hoc doping \(x\) dependence of the Coulomb interaction has to be introduced.) The main merits (a)-(c) in the present study strongly indicate that the nematic/smectic states originate from the paramagnon interference mechanism \([14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44]\).
Onari et al.  
Exotic orders in Fe-based superconductors

\[ Q = Q' + Q'' \]

Figure 1. (A) Schematic \( x-T \) phase diagram of FeSe_{1-x}Te\_x, where \( T_S \) decreases with \( x \), and \( T_c \) becomes maximum near the nematic QCP. (B) Schematic \( x-T \) phase diagram of BaFe\_2(As\_1-xP\_x)\_2, where the tiny nematicity appears for \( T_S < T < T' \). We explain that “tiny nematicity” above \( T_S \) originates from smectic bond order in later section. (C) Schematic \( x-T \) phase diagram of Ba_{1-x}Rb\_xFe\_2As\_2, \( B_{2g} \) nematic order appears for heavily hole doped region \( x > 0.5 \). (D) Feynman diagram of the paramagnon interference mechanism for the orbital/bond order. (E) Feynman diagram of the self-energy \( \Sigma(k) \).

\[ \Sigma(k) = \sum_{k'} V^2(k-k') G(k') \]

Figure 2. FSs of (A) FeSe (\( n_d = 6.0 \)), (B) BaFe\_2As\_2 (\( n_d = 6.0 \)), and (C) AFe\_2As\_2 (A=Cs, Rb) (\( n_d = 5.5 \)). The colors green, red and blue correspond to orbitals 2, 3, and 4, respectively. A variety of nematic/smectic states originates from the characteristic structure of FSs.

2 MULTIORBITAL MODELS AND FORMULATION

2.1 Multiorbital models

Here, we introduce the multiorbital models based on the first-principles calculations. We analyze the following two-dimensional \( d-p \) Hubbard model with a unique parameter \( r \), which controls the strength of the Coulomb interaction [16]:

\[ H_x = H_x^0 + r H^{ij}, \]
where $H^0_\text{F}$ is the first-principles model, and $H^U$ is the Coulomb interaction for $d$-orbitals. We neglect the Coulomb interaction for $p$-orbitals. We denote the five Fe $d$-orbitals $d_{3z^2-r^2}$, $d_{x^2}$, $d_{yz}$, $d_{xy}$, $d_{x^2-y^2}$ as $l = 1, 2, 3, 4, 5$, and three Se(As) $p$-orbitals $p_x$, $p_y$, $p_z$ as $l = 6, 7, 8$. To obtain the model, we first use the WIEN2k [72] and Wannier90 [73] codes. Next, to reproduce the experimentally observed FSs, we introduce the $k$-dependent shifts for orbital $l$, $\delta E_l$, by modifying the intra-orbital hopping parameters, as explained in Ref. [74]. In FeSe$_{1-x}$Te$_x$ model, we shift the $d_{xy}$-orbital band and the $d_{x^2-y^2}$-orbital band at $[\Gamma, M, X]$ points by [0eV, $-0.27$eV, $+0.40$eV] and $[-0.24$eV, 0eV, $+0.13$eV], respectively. In BaFe$_2$As$_2$ model, the shifts are absent. In CsFe$_2$As$_2$ model, we shift the $d_{xy}$-orbital band and the $d_{x^2-y^2}$-orbital band at $[\Gamma, M, X]$ points by [0eV, $+0.40$eV, 0eV] and $[-0.40$eV, 0eV, $+0.10$eV], respectively.

We employ the $d$-orbital Coulomb interaction introduced by the constraint random phase approximation (RPA) method in Ref. [74]. The Coulomb interactions for the spin and charge channels are generally given as

$$U^\sigma_{l_1,l_2,l_3,l_4} = \begin{cases} 
U_{l_1,l_1}, & l_1 = l_2 = l_3 = l_4 \\
U'_{l_1,l_2}, & l_1 = l_3 \neq l_2 = l_4 \\
J_{l_1,l_3}, & l_1 = l_2 \neq l_3 = l_4 \\
J_{l_1,l_2}, & l_1 = l_4 \neq l_2 = l_3 \\
0, & \text{otherwise.}
\end{cases}$$

(2)

$$U^c_{l_1,l_2,l_3,l_4} = \begin{cases} 
-U_{l_1,l_1}, & l_1 = l_2 = l_3 = l_4 \\
U'_{l_1,l_2} - 2J_{l_1,l_3}, & l_1 = l_3 \neq l_2 = l_4 \\
-2U'_{l_1,l_3} + J_{l_1,l_4}, & l_1 = l_2 \neq l_3 = l_4 \\
-J_{l_1,l_2}, & l_1 = l_4 \neq l_2 = l_3 \\
0, & \text{otherwise.}
\end{cases}$$

(3)

Hamiltonian of the Coulomb interaction is given as

$$H^U = -\sum_{kk'q,\sigma}\sum_{l_1,l_2,l_3,l_4} \frac{(U^c + U^s\sigma\sigma')}{4} l_1,l_2,l_3,l_4 \chi^{l_1^\dagger l_2^\dagger l_3^\dagger l_4^\dagger}_{k+q,\sigma k',\sigma'} \chi^{l_4}_{k',\sigma'},$$

(4)

where $\sigma, \sigma' = \pm 1$ denote spin.

By using the multiorbital Coulomb interaction, the spin (charge) susceptibility $\hat{\chi}^{s(c)}(q)$ for $q = (q, \omega_m = 2m\pi T)$ is given by

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

(5)

where the irreducible susceptibility is

$$\chi^{0}_{l,l';m,m'}(q) = -\frac{T}{N} \sum_k G_{l,m}(k + q)G_{m',l'}(k).$$

(6)
\( \hat{G}(k) \) is the multiorbital Green function with the self-energy \( \hat{\Sigma} \) and given as \( \hat{G}(k) = [(i\epsilon_n + \mu)\hat{1} - \hat{h}^0(k) - \hat{\Sigma}(k)]^{-1} \) for = \([k, \epsilon_n = (2n + 1)\pi T] \). Here, \( \hat{h}^0(k) \) is the matrix expression of \( H^0 \), and \( \mu \) is the chemical potential. The spin (charge) Stoner factor \( \alpha_{s(c)} \) is defined as the maximum eigenvalue of \( \hat{\chi}^s(0, q) \). Since \( \hat{\chi}^s(0)(q) \propto (1 - \alpha_{s(c)})^{-1} \) holds, spin (charge) fluctuations develop with increasing \( \alpha_{s(c)} \), and \( \alpha_{s(c)} = 1 \) corresponds to spin- (charge)-channel ordered state.

### 2.2 FLEX approximation

Here, we introduce the multiorbital fluctuation exchange (FLEX) approximation [15, 75]. The FLEX approximation satisfies the conserving-approximation formalism of Baym and Kadanoff [70, 71]. In the FLEX approximation, the self-energy is given as

\[
\hat{\Sigma}(k) = \frac{T}{N} \sum_{k'} \hat{V}^\Sigma(k - k') \hat{G}(k'),
\]

which is shown by the Feynman diagram in Fig. 3E. The effective interaction \( \hat{V}^\Sigma \) for the self-energy in the FLEX approximation is given as

\[
\hat{V}^\Sigma(q) = \frac{3}{2} \hat{U}^s \hat{\chi}^s(q) \hat{U}^s + \frac{1}{2} \hat{U}^c \hat{\chi}^c(q) \hat{U}^c + \frac{3}{2} \hat{U}^c + \frac{1}{2} \hat{U}^c
\]

\[
- \hat{U}^{\uparrow \downarrow} \hat{\chi}^0(q) \hat{U}^{\uparrow \downarrow} - \frac{1}{2} \hat{U}^{\uparrow \uparrow} \hat{\chi}^0(q) \hat{U}^{\uparrow \uparrow},
\]

where \( \hat{U}^{\uparrow \downarrow} \equiv \hat{U}^c - \hat{U}^s \) and \( \hat{U}^{\uparrow \uparrow} \equiv \hat{U}^c + \hat{U}^s / 2 \) are denoted. We set \( \mu = 0 \). \( \hat{\chi}^{s(c)}(q), \hat{\Sigma}(k), \) and \( \hat{G}(k) \) are calculated self-consistently. In multiband systems, the FSs are modified from the original FSs due to the self-energy correction. To escape from this difficulty, we subtract the Hermite term [\( \hat{\Sigma}(k, +i0) + \hat{\Sigma}(k, -i0) \)]/2 from the original self-energy, which corresponds to the elimination of double-counting terms between LDA and FLEX.

### 2.3 DW equation

We derive the strongest charge-channel density-wave (DW) instability without assuming the order parameter and wavevector. For this purpose, we use the DW equation method developed in Refs. [16, 19, 76]. We obtain the optimized non-local form factor \( \hat{f}^q(k) \) with the momentum and orbital dependences by solving the following linearized DW equation shown in Fig. 3A:

\[
\lambda_q f_{l,l'}^q(k) = \frac{T}{N} \sum_{k',m,m'} K_{l,l',m,m'}^q(k, k') f_{m,m'}^q(k'),
\]

\[
K_{l,l',m,m'}^q(k, k') = \sum_{m_1, m_2} I_{l,l',m_1,m_1}^q(k, k') g_{m_1,m_2}^q(k, k'),
\]

where \( \lambda_q \) is the eigenvalue of the form factor \( \hat{f}^q(k) \), \( g_{l,l',m,m'}^q(k, k') \equiv -G_{l,m}(k + q) G_{m',l'}(k) \), and \( I_{l,l'}^q(k, k') \) is the charge-channel irreducible four-point vertex shown in Fig. 3B. The four-point vertex interaction
\( \hat{I}^q(k, k') \) in the DW equation \([10, 16, 19]\) is given by

\[
\hat{I}^q_{l, l', m, m'}(k, k') = \sum_{b = s, c} \left[ -\frac{\alpha_b}{2} \hat{V}^b_{l, m; l', m'}(k - k') + \frac{T}{N} \sum_{p,l_1,l_2,m_1,m_2} \frac{\alpha_b}{2} \hat{V}^b_{l_1, l_2; m, m_2}(p + q) \hat{V}^b_{m_1, l_2, m'; l_1, m_1}(p) \times G_{l_1, m_1}(k - p) G_{l_2, m_2}(k' - p) + \frac{T}{N} \sum_{p,l_1,l_2,m_1,m_2} \frac{\alpha_b}{2} \hat{V}^b_{l_1, l_2; m_2, m_1}(p + q) \hat{V}^b_{m_2, m_1; l_2, m_1}(p) \times G_{l_1, m_1}(k - p) G_{l_2, m_2}(k' + p + q) \right],
\]

where \( \alpha_s = 3, \alpha_c = 1, \) and \( \hat{V}^s(c)(q) = \hat{U}^s(c) + \hat{U}^s(c) \hat{\chi}^s(c)(q) \hat{U}^s(c) \).

In Eq. (11), the first line corresponds to the Maki-Thompson (MT) term, and the second and third lines give the AL terms, respectively. Feynman diagrams of the MT terms and AL terms are shown in Fig. 3B.

**Figure 3.** Feynman diagrams of (A) the DW equation and (B) the charge-channel irreducible four point vertex. Each wavy line represents a spin-fluctuation-mediated interaction.

The AL terms are enhanced by the paramagnon interference \( \hat{\chi}^s(Q) \times \hat{\chi}^s(Q') \) shown in Fig 1D. Thus, \( q = Q + Q' = 0 \) nematic order is naturally induced by the paramagnon interference at the same nesting vector \( (Q' = -Q) \). In the MT term, the first-order term with respect to \( \hat{U}^s(c) \) gives the Hartree–Fock (HF) term in the mean-field theory. The charge-channel DW with wavevector \( q \) is established when the largest \( \lambda_q = 1 \). Thus, the smaller \( \lambda_q \) corresponds to the lower \( T_S \). The DW susceptibility is proportional to \( 1/(1 - \lambda_q) \) as explained in Ref. [20]. Therefore, \( \lambda_q \) represents the strength of the DW instability.

### 3 RESULTS AND DISCUSSIONS

#### 3.1 Results of FeSe\(_{1-x}\)Te\(_x\)

In this section, we show that (i) the \( B_{1g} \) nematic orbital+bond order originates from the paramagnon interference, and (ii) the effect of self-energy is essential to reproduce the \( x \) dependence of \( T_S \) shown in Fig. 1A in FeSe\(_{1-x}\)Te\(_x\). The effect of the self-energy on the nematic/smectic order caused by the VCs is systematically studied in the present manuscript. Thanks to the self-energy, \( T_S \) is reduced to become realistic (\( \sim 100K \)), while the symmetry of the nematic/smectic order is unchanged. Thus, the idea of
electronic nematicity due to "the paramagnon-interference mechanism" proposed in Refs. [14, 15, 16, 17, 18, 19, 20, 21, 40, 41, 42, 43, 44] has been confirmed by the present study. Hereafter, we fix $r = 0.35$, $T = 15\text{meV}$ in calculations with the self-energy and $r = 0.15$, $T = 15\text{meV}$ in calculations without the self-energy, unless otherwise noted.

Figures 4A and 4B show $x$ dependent FSs and band structures, respectively. The FSs are small compared to other Fe-based superconductors. $d_{xy}$ orbital level $E_{xy}^M$ at M point increases with increasing $x$, as shown in Fig. 4C. This behavior is consistent with ARPES measurements [77, 78]. On the other hand, $d_{xy}$ orbital level $E_{xy}^\Gamma$ at $\Gamma$ point decreases with increasing $x$. $E_{xy}^\Gamma$ becomes lower than the $d_{xz(yz)}$ orbital level for $x \gtrsim 0.3$, and the topology of band changes. The change of topology has been observed between $\Gamma$ and $Z$ points in ARPES measurements of FeSe$_{0.5}$Te$_{0.5}$ [79, 80]. Figure 4D shows the density of state (DOS) of orbitals 3 and 4 for $x = 0, 0.5$. DOS near the Fermi level for $x = 0.5$ is larger than that for $x = 0$ since the bandwidth decreases, and $E_{xy}^M$ comes close to the Fermi level with increasing $x$. In addition, the dispersion of orbitals 2 and 3 at $\Gamma$ point becomes flat as $E_{xy}^\Gamma$ decreases with increasing $x$, which also enlarges the DOS for orbitals 2 and 3 near the Fermi level.

**Figure 4.** (A) FSs and (B) band structures of FeSe$_{1-x}$Te$_x$ for $x = 0$ and 0.5. (C) $x$ dependences of $E_{xy}^\Gamma$ and $E_{xy}^M$. (D) DOS of orbitals 3 and 4 for $x = 0, 0.5$. 

This is a provisional file, not the final typeset article
In order to discuss the self-energy effect, we calculate the mass enhancement factors. Figure 5 shows the obtained $x$ dependence of the mass enhancement factors $z^{-1}_l(\pi, 0)$ for orbital $l = 3, 4$, which are given by $z^{-1}_l(k) = 1 - \text{Im}\Sigma_{l,l}(k, \pi T)/\pi T$ in the FLEX approximation. The value of $z^{-1}_l(\pi, 0)$ increases with increasing $x$ since the electron correlation increases due to the reduction of bandwidth and the increase of DOS shown in Fig. 4D. Particularly, $z^{-1}_l(\pi, 0)$ is enhanced by the $d_{xy}$ orbital electron correlation between the electron pockets and the band around M point since $E^M_{xy}$ comes close to the Fermi level, as shown in Fig. 4C. The behaviors of $z^{-1}_l$ are similar to those given by the dynamical mean-field theory [81] and experiment [82].

![Figure 5](image)

**Figure 5.** $x$ dependences of mass enhancement factor $z^{-1}_l(\pi, 0)$ for orbitals $l = 3$ and $4$.

Figure 6 shows $x$ dependences of $\chi^s_{3,3;3,3}(\pi, 0)$ and $\chi^s_{4,4;4,4}(\pi, 0)$ in the FLEX approximation and the RPA. $\chi^s_{3,3;3,3}(\pi, 0)$ is almost independent of doping $x$, which means that change of topology or number of FS around $\Gamma$ composed of $d_{xz}$ and $d_{yz}$ orbitals does not strongly affect the spin fluctuation for $d_{xz(yz)}$ orbital. On the other hand, $\chi^s_{4,4;4,4}(\pi, 0)$ in the RPA without the self-energy is strongly enhanced with increasing $x$ since the electron correlation for $d_{xy}$ orbital between electron pockets and the band around M point is significant for the enhancement of $\chi^s_{4,4;4,4}(\pi, 0)$. The strong enhancement of $\chi^s_{4,4;4,4}(\pi, 0)$ is suppressed by the self-energy in the FLEX approximation. This suppression is necessary to reproduce the $x$ dependence of $T_S$ in the phase diagram.

Hereafter, we discuss the DW instability given by the DW equation (9). Figure 7A shows $x$ dependences of $\lambda_0$ for the $B_{1g}$ nematic state with and without the self-energy. $\lambda_0$ without the self-energy rapidly increases with doping $x$ due to the paramagnon interference shown in Fig. 1D. $\lambda_0$ is enlarged by the interference between $\chi^s_{4,4;4,4}$ strongly enhanced in the RPA, as shown in Fig. 6. Since this result means $T_S$ increases with $x$, the phase diagram in Fig. 1A cannot be explained when the self-energy is absent. However, $\lambda_0$ including the self-energy decreases with doping $x$ since the enhancement of $\chi^s_{4,4;4,4}$ in the FLEX approximation is moderate and the self-energy suppresses the $\hat{G}$ and $\hat{I}$ in the DW equation (10). The value of $\lambda_0$ increases with decreasing $T$, as shown in Fig. 7B. $T = T_S$ is given when $\lambda_0 = 1$ is satisfied. Thus, $T_S$ at $x = 0$ is higher than that at $x = 0.5$, and $T_S$ at $x = 0.65$ cannot be obtained for $T > 6\text{meV}$. The $x$ dependence of $T_S$ obtained by the paramagnon interference mechanism is consistent with the phase diagram in Fig. 1A [49]. We see that $T$ dependences of the strength of nematic fluctuations $1/(1 - \lambda_0)$ satisfy the Curie–Weiss law at low temperatures, as shown in Fig. 7C. We note that the $B_{1g}$ nematic state is realized due to the small FSs even for the weak spin fluctuations [16, 17].
Here, we analytically explain that $T_S$ is reduced by the self-energy by focusing on the mass renormalization factor $z$. As discussed in Ref. [17], $\alpha_s(\epsilon)$ is independent of $z$ under the scaling $T \rightarrow zT$ and $r \rightarrow r/z$. Under this scaling, the eigenvalue of the DW equation is unchanged [17]. Thus, $T_S$ obtained by the DW equation without the self-energy is reduced to $zT_S$ due to the self-energy. As a result, realistic $T_S$ is obtained by taking the self-energy into account.

Figure 6. $x$ dependences of $\chi^s_{3,3;3,3}(\pi,0)$ in the FLEX approximation. Those in the RPA are shown in the inset.

Figure 7. (A) $x$ dependences of $\lambda_0$ in the DW equation with and without the self-energy at $T = 15$ meV. (B) $T$ dependences of $\lambda_0$ with the self-energy for $x = 0, 0.5, 0.65$. (C) $T$ dependences of $1/(1 - \lambda_0)$ with the self-energy for $x = 0, 0.5$.

Figure 8A shows $q$ dependences of $\lambda_q$ with the self-energy at $x = 0, 0.5$. $\lambda_q$ has peak at $q = 0$, which means that the ferro nematic order is favored. Figure 8B shows $k$ dependences of the static form factors $f^0_{33}(k)$ and $f^0_{44}(k)$, where $f^q(k)$ is given by the analytic continuation of $f^q(k)$. $f^0_{33}(k_x, k_y) = -f^0_{22}(k_y, k_x)$ represents $B_{1g}$ orbital order between orbitals 2 and 3. From the $k$ dependence of $f^0_{33(22)}(k)$, the sign-reversing orbital order is confirmed along $k_x(k_y)$ axis. As shown in Fig. 8C, $k$ dependence of $f^0_{44}(k) \propto \cos(k_x) - \cos(k_y)$ causes the $B_{1g}$ nearest-neighbor bond order, which is the modulation of correlated hopping. Based on the paramagnon interference mechanism, we find that the small spin fluctuations on the three $d_{xz}$, $d_{yz}$, and $d_{xy}$ orbitals cooperatively cause the $B_{1g}$ nematic orbital+bond...
order. The FSs and the band structure under the nematic order with the maximum value of the form factor \( f_{\text{max}}^0 = 80 \text{meV} \) are shown in Figs. 8D and 8E. \( f_{\text{max}}^0 = 80 \text{meV} \) with the mass enhancement factor \( z^{-1} = 2 \sim 4 \) is consistent with ARPES measurements [35, 36]. The Lifshitz transition, where the FS around Y point is missing, has been reported in recent experiments [83, 84, 85, 86]. The Lifshitz transition is naturally explained by the increase of \( d_{xy} \) level around Y point induced by \( f^0(k) \). We note that the obtained coexistence of the bond order on the \( d_{xy} \) orbital and the orbital order on the \( (d_{xz}, d_{yz}) \) orbitals has already been shown in the supplementary material of Refs. [19, 20]. In Fig. 8D, we derived the Lifshitz transition by setting \( f_{\text{max}}^0 = 80 \text{meV} \) by hand. It is noteworthy that the same result is recently obtained by solving the full DW equation in Ref. [87]. The full DW equation enables us to study the electronic states below \( T_S \) without introducing additional fitting parameters.

![Figure 8](image)

**Figure 8.** (A) \( q \) dependences of \( \lambda_q \) with the self-energy for \( x = 0, 0.5 \). (B) \( k \) dependences of \( f_{3,3}^0(k) \) and \( f_{4,4}^0(k) \) for \( x = 0 \), where green lines denote FSs. \( f_{3,3}^0(k) \) changes sign along \( k_x \) axis (yellow dashed line). (C) \( B_{1g} \) nearest-neighbor bond order corresponding to \( f_{4,4}^0(k) \). (D) FSs and (E) band structure under the nematic order with \( f_{\text{max}}^0 = 80 \text{meV} \) for \( x = 0 \).

Here, we confirm that the \( d_{xy} \) orbital levels at \( \Gamma \) and M points are important for the \( x \) dependence of \( \lambda_0 \). We employ the simple model, where only the shift of \( E_{\Gamma xy} \) or \( E_{M xy} \) is introduced for the \( x = 0 \) model. Figure 9A shows \( E_{\Gamma xy} \) dependences of \( z_{\Gamma}^{-1}(\pi, 0) \) and \( \lambda_0 \), respectively. \( z_{\Gamma}^{-1}(\pi, 0) \) is almost independent of the value of \( E_{\Gamma xy} \). \( \lambda_0 \) decreases with decreasing \( E_{\Gamma xy} \), which is consistent with the result in Fig. 7A. The
topology of band structure changes at \( \Gamma \) point with decreasing \( E_{xy}^\Gamma \), which plays important role to decrease \( \lambda_0 \). Figure 9B shows \( E_{xy}^M \) dependences of \( z_l^{-1}(\pi, 0) \) and \( \lambda_0 \), respectively. The behaviors of \( z_4^{-1}(\pi, 0) \) and \( \lambda_0 \) are similar to the results in Figs. 5 and 7A. The \( x \) dependences of \( z_l^{-1}(\pi, 0) \) and \( \lambda_0 \) are explained by the electron correlation between the electron pockets and the \( d_{xy} \) band around M point. \( \lambda_0 \) is suppressed by the self-energy for the \( d_{xy} \) orbital. The suppression becomes strong with increasing \( E_{xy}^M \) due to the feedback effect of the self-energy. To summarize, the \( B_{1g} \) nematic orbital+bond order is explained by the paramagnon interference mechanism in FeSe\( _{1-x} \)Te\( _x \), and \( x \) dependence of \( T_S \) is well reproduced by the self-energy effect for the \( d_{xy} \) orbital.

**Figure 9.** (A) \( E_{xy}^\Gamma \) dependences of \( z_l^{-1}(\pi, 0) \) for \( l = 3, 4 \), and \( \lambda_0 \) given by introducing only \( E_{xy}^\Gamma \) shift for the \( x = 0 \) model. (B) \( E_{xy}^M \) dependences of \( z_l^{-1}(\pi, 0) \) for \( l = 3, 4 \), and \( \lambda_0 \) given by introducing only \( E_{xy}^M \) shift for the \( x = 0 \) model.

### 3.2 Results of BaFe\(_2\)As\(_2\)

In this section, we discuss the multi nematicity in BaFe\(_2\)As\(_2\) [20]. The effect of the self-energy on the nematic/smectic orders caused by the VCs is studied in the present manuscript. Transition temperatures are reduced to become realistic due to the self-energy, while the symmetries of the nematic/smectic orders are unchanged. We reveal the origin of tiny nematicity below \( T = T^* \) and explain the multistage transitions at \( T = T^* \) and \( T_S \) in the phase diagram shown in Fig. 1B. As shown in Fig. 2B, the size of hole FS around M point composed of \( d_{xy} \) orbital is similar to that of electron FSs around X and Y points, which causes the good intra- and inter-orbital nestings. As explained later, the inter-orbital nesting is important to realize the smectic state at \( T = T^* \).

Figure 10A shows the \( q \)-dependence of \( \lambda_q \) with and without the self-energy. \( q = (0, \pi) \) smectic bond order is dominant over the \( q = 0 \) nematic orbital+bond order because of the relation \( \lambda_{(0,\pi)} > \lambda_0 \), which is robust in the presence of moderate spin fluctuations \( \alpha_s \gtrsim 0.85 \). Thus, the nematic orbital+bond transition temperature \( T_S \) is lower than \( T^* \), where the smectic bond order appears. Figure 10B shows the dominant component of the static form factor, \( f_{3,4}^{(0,\pi)}(k) \), for \( q = (0, \pi) \). Focusing on the X and M points, \( f_{3,4}^{(0,\pi)}(k) \) is proportional to \(-\cos(k_y)\), which corresponds to the inter-orbital smectic bond order, where the \( y \)-direction hoppings between orbitals 3 and 4 are modulated by the correlated hopping \( \delta t_{3,4}(y; y \pm 1) = \delta t_{4,3}(y; y \pm 1) = \delta t_1(-1)^y \). Note that \( \delta t_{1,m}(y; y') \) is real and equal to \( \delta t_{m,1}(y'; y) \).

As shown in Fig. 10D, the origin of the smectic bond order \( f_{3,4}^{(0,\pi)} \) is the quantum interference between the spin fluctuations \( \chi^x(Q) \) for \( Q \approx (0, \pi) \) and \( \chi^s(0) \) due to the AL terms. In this case, \( q = (0, \pi)(= Q + Q') \).
is given by $Q' = 0$. $\chi^s(Q)$ is enhanced when the FS appears around M point since the nesting between FSs around X and M points becomes good, while the moderate $\chi^s(0)$ is caused by the forward scattering. We find that $f_{3,4}^{(0,\pi)}$ is significantly enlarged by inter-orbital nesting between the $d_{xy}$-orbital FS around M point and $d_{yz}$-orbital FS around X point. In addition to the quantum interference due to the AL terms, the MT terms strengthen the sign change of $f_{3,4}^{(0,\pi)}(k)$ between X and M points, as reported previously [16, 19, 37]. Thus, the smectic bond order originates from the cooperation between the AL and MT terms due to the good inter-orbital nesting between FSs around X and M points. In contrast, the $B_{1g}$ nematic orbital+bond order shown in Figs. 10C and 10D originates from the interference between $\chi^s(Q)$ and $\chi^s(-Q)$. This nematic orbital+bond order is similar to that in FeSe and FeSe$_{1-x}$Te$_x$.

Here, we examine the DOS under the smectic bond order to verify the present theory. For $T < T^* = 32.4$meV without the self-energy, we introduce the mean-field-like $T$-dependent form factor $\hat{f}^q(T) = f_{\text{max}}^q \tanh \left( 1.74 \sqrt{T^*/T - 1} \right) \hat{f}^q$, where $\hat{f}^q$ is the obtained form factor for $q = (0, \pi)$ normalized as $\max_k |\hat{f}^q(k)| = 1$. We put $f_{\text{max}}^q = 60$meV. Figure 11A shows the DOS at $T = T^*$ and 28meV($< T^*$). For $T < T^*$, a pseudogap appears due to the smectic bond order, which is consistent with the experiments [88, 89]. Since the smectic bond order is an antiferroic order, the folded band structure emerges below $T^*$, which is also consistent with the experiment [90].
Next, we focus on another mystery, the $T$-linear behavior of tiny nematicity $\psi$ in Ba122 [52] below $T^*$. In order to solve this mystery, we calculate the $T$ dependence of uniform nematicity $\psi = (n_2 - n_3)/(n_2 + n_3)$ in Fig. 11B, where both $f(0,\pi)(T)$ for $T < T^*$ and the ferro nematic orbital+bond order $f^0(T)$ for $T < T_S (=27.8\text{meV})$ are introduced. For $T < T_S$, we assume $f^0(T) = f^{\text{max}} \tanh \left(1.74 \sqrt{T_S/T - 1}\right) f^0$, where $f^0$ is the obtained form factor normalized as $\max_k |f^0(k)| = 1$. We employ $f^{\text{max}} = 60\text{meV}$, which corresponds to the $d_{xz/yz}$ orbital energy split $\sim 60\text{meV}$ in the ARPES measurements [91] by considering the mass enhancement factor $z_l^{-1} \sim 2$ for $l = 2, 3$. The $T$-linear behavior $\psi \propto (T^* - T)$ for $T_S < T < T^*$ is a consequence of the relation $\psi \propto [f(0,\pi)(T)]^2$ because the $f(0,\pi)$ term cannot contribute to any $q = 0$ linear response. Note that the form factor $f^0(\pi,0)$ for $q = (\pi,0)$ gives $\psi < 0$. Thus, the $T$-linear behavior of $\psi$ below $T^*$ is also naturally explained by the smectic bond order. On the other hand, $\psi \propto \sqrt{T_S - T}$ for $T < T_S$ is induced by the nematic orbital+bond order. To summarize, the multistage transitions at $T = T^*$ and $T_S$, and the $T$-linear $\psi$ below $T^*$, are naturally explained by the smectic bond order and nematic orbital+bond order. The hole pocket around M point is necessary to realize the smectic bond order by the paramagnon interference mechanism.

We stress that the present mechanism of the bulk nematicity for $T_S < T < T^*$ is intrinsic and free from the strength of the disorder and local strain in the system. The present smectic order originates from the AL-VC and the FS nesting between the $d_{xy}$ orbital hole pocket and the electron pockets [20]. We stress that the present theory explains the absence of the smectic order in bulk FeSe [55] because the $d_{xy}$-orbital hole-pocket, which is necessary for the smectic order formation, is below the Fermi level in FeSe.

Here, we explain the details of the recent microscopy measurements in P-doped Ba122 [54, 55], that support the present intrinsic scenario. These are bulk and real-space measurements. In the PEEM measurement [55], very uniform bulk nematic domains have been observed for $T_S < T < T^*$. The width of each nematic domain is about 500nm. The structure of the nematic domains is unchanged for $T < T_S$. In addition, once the nematic domain completely disappears by increasing $T$, it never appears at the same location if the temperature is lowered again. These results are consistent with the present intrinsic smectic order scenario for $T_S < T < T^*$ in P-doped Ba122. In the photomodulation measurement [54], uniform nematic domains have also been observed. The observed nematicity becomes small near the nematic domain boundary, irrespective of the fact that the large local strain anisotropy is observed at the domain boundary. The observed anticorrelation between the nematicity and the local strain anisotropy may conflict with the assumption of the extrinsic scenario of the nematicity above $T_S$.

In contrast, the extrinsic scenario has been proposed by other groups [4, 56, 57, 58, 59, 60]. In the extrinsic mechanism, the nematicity for $T > T_S$ in Co-doped Ba122, which exhibits large residual resistivity ($>100\mu\Omega\text{cm}$), has been explained by the inhomogeneity of $T_S$ induced by the disorder and local strain. However, it is not easy to explain the nematicity above $T_S$ in clean P-doped (non-doped) Ba122 on the same footing in the extrinsic scenario.

We note that the multistage smectic/nematic transitions observed in NaFeAs [92] are also explained by the present intrinsic mechanism. [20].

### 3.3 Results of Ba$_{1-x}$Cs$_x$Fe$_2$As$_2$

In this section, we discuss the $B_{2g}$ nematicity in heavily hole-doped compound AFe$_2$As$_2$ (A=Cs, Rb) [19]. The effect of the self-energy on the nematic order caused by the VCs is studied in the present manuscript. Thanks to the self-energy, $T_S$ is reduced to become realistic, while the symmetry of the nematic order is unchanged. The direction of $B_{2g}$ nematicity is rotated by $45^\circ$ from that of the conventional
Figure 11. (A) DOS at \( T = T^* = 32.4 \text{meV} \) and that at \( T = 28 \text{meV} < T^* \) including the smectic bond order. (B) \( T \) dependence of nematicity \( \psi = (n_2 - n_3)/(n_2 + n_3) \) including both smectic-bond order for \( T < T^* \) and ferro-orbital/bond order for \( T < T_S \).

\( B_{1g} \) nematicity. Figure 12A shows FSs of CsFe\(_2\)As\(_2\): The hole FS around M point composed of \( d_{xy} \)-orbital is large, while the Dirac pockets near X and Y points are small. In this system, the \( d_{xy} \)-orbital spin fluctuations are dominant.

Figure 12A shows \( q \) dependence of largest eigenvalue \( \lambda_q \) with the self-energy for \( r = 0.96 \) at \( T = 5 \text{meV} \) and that without the self-energy for \( r = 0.30 \) at \( T = 20 \text{meV} \). \( \lambda_q \) becomes maximum at \( q = 0 \) and the dominant form factor \( I_{4,4}^0(k) \propto \sin(k_x) \sin(k_y) \) at \( q = 0 \) is shown in Fig. 12B. As shown in Fig. 12C, this form factor corresponds to the \( B_{2g} \) next-nearest-neighbor bond order for \( d_{xy} \) orbital, which is consistent with experimentally observed \( B_{2g} \) nematicity \([61, 62, 63, 64]\). By analyzing the irreducible four-point vertex \( I_{4,4}^0(k, k') \) in the DW Eq. (10), we find that the attractive (repulsive) interactions originate from the AL (MT) terms, as shown in Fig. 12D. The obtained \( q = 0 \) \( B_{2g} \) bond order is derived from these interactions. Since the AL terms are enhanced by the quantum interference between the spin fluctuations with \( Q \) and \( Q' = -Q \), as shown in Fig. 13D, \( q = 0 \) nematic bond order is realized. The value of \( \lambda_0 \) is strongly enhanced by the attractive interactions for \( d_{xy} \) orbital due to the AL terms. In this system, the nesting vector is short \( Q \sim (0.5\pi, 0) \), as shown in Fig. 12B. Due to repulsive interaction by the MT terms, \( I_{4,4}^0(k) \) changes sign between \( k \) points on the FSs connected by \( Q \), as shown in Fig. 12D. To summarize, the AL terms strongly enlarge \( \lambda_0 \) due to the paramagnon interference mechanism, and the MT terms favor the \( B_{2g} \) symmetry. Cooperation of the AL and MT terms is important to realize the \( B_{2g} \) bond order.

We comment on the recent experiments on RbFe\(_2\)As\(_2\). The specific heat jump at \( T_S = 40 \text{K} \) (\( \Delta C/T_S \)) is very small \([64]\). However, it is naturally understood based on the recent theoretical scaling relation \( \Delta C/T_S \propto T_S^{\frac{b}{3}} \) with \( b \sim 3 \) derived in Ref. [87]. Although the smallness of \( B_{2g} \) nematic susceptibility in RbFe\(_2\)As\(_2\) was recently reported in Refs. [65, 66], the field-angle dependent specific heat measurement has shown the finite \( B_{2g} \) nematicity above \( T_c \) \([93]\). Further experimental and theoretical studies are necessary to clarify the nematicity in AFe\(_2\)As\(_2\) (A=Cs, Rb).

Finally, we discuss \( x \) dependence of nematicity in Ba\(_{1-x}\)Rb\(_x\)Fe\(_2\)As\(_2\) (A=Cs, Rb). The schematic phase diagram in Ba\(_{1-x}\)Rb\(_x\)Fe\(_2\)As\(_2\) given by the experiment \([64]\) is shown in Fig. 13C. We introduce model Hamiltonian for Ba\(_{1-x}\)Cs\(_x\)Fe\(_2\)As\(_2\), by interpolating between BaFe\(_2\)As\(_2\) model and CsFe\(_2\)As\(_2\) model with the ratio \( 1 - x : x \). Figure 13A shows \( x \) dependences of \( \lambda_q=0 \) without the self-energy for the \( B_{2g} \) and the \( B_{1g} \) symmetries by fixing \( T = 30 \text{meV} \) and \( r = 0.30 \). Below \( x = x_c \sim 0.5 \), \( B_{1g} \) nematic orbital order is dominant as discussed in the previous section, while \( B_{2g} \) nematic bond order dominates over the \( B_{1g} \) nematic orbital order for \( x > x_c \). As shown in Fig. 13B, the Lifshitz transition occurs at \( x \sim x_c \), where
Figure 12. (A) $q$ dependence of $\lambda_q$ with the self-energy in CsFe$_2$As$_2$, and that without the self-energy in the inset. (B) $k$ dependence of $B_{2g}$ form factor $f_{4,4}^0(k) \propto \sin(k_x) \sin(k_y)$, where the green lines and black arrow denote FSs and nesting vector $Q \sim (0.5\pi, 0)$, respectively. (C) The $B_{2g}$ next-nearest-neighbor bond order corresponding to the $f_{4,4}^0(k)$. (D) $B_{2g}$ form factor $\propto \sin(k_x) \sin(k_y)$ driven by the attractive interactions (red arrows) A and B, and the repulsive interaction (blue arrow) C in the DW equation, where green lines denote nodes in the $B_{2g}$ form factor.

The electron pockets split into the four tiny Dirac pockets. Thus, the $B_{2g}$ nematic bond order appears when the nesting vector $Q$ between the electron pockets and hole pocket around M point becomes short $Q \sim (0.5\pi, 0)$. By taking account of the Lifshitz transition at $x \sim x_c$, the schematic phase diagram in Fig. 1C is also well reproduced by the orbital/bond order due to the paramagnon interference mechanism. We note that the $q = (0, \pi)$ smectic order is dominant over the $q = 0$ $B_{1g}$ nematic order at $x = 0$, as shown in previous section.

Figure 13. (A) $x$ dependences of $\lambda_{q=0}$ without the self-energy for $B_{1g}$ and $B_{2g}$ symmetries in Ba$_{1-x}$Cs$_x$Fe$_2$As$_2$. (B) FSs for $x = 0.4$ and $x = 0.6$. Dominant nematic order changes at $x = x_c \sim 0.5$ near the Lifshitz transition, where the electron FSs split into the four tiny Dirac pockets.
4 CONCLUSION

We discussed the rich variety of nematic/smectic states in Fe-based superconductors in the same theoretical framework based on the paramagnon interference mechanism. In this mechanism, the charge-channel order is induced by the quantum interference between the spin fluctuations, as shown in Fig. 1D. The form factor and wavevector of the DW instability are derived from the DW equation based on the paramagnon interference mechanism. Recently, a rigorous formalism of the DW equation has been constructed based on the Luttinger–Ward (LW) theory in Ref. [87]. According to Ref. [87], the solution of the DW equation gives the minimum of the grand potential in the LW theory. Thus, the nematic/smectic order discussed in the present manuscript is thermodynamically stable in the framework of the conserving approximation.

By considering the characteristic fermiology of each compound, the paramagnon interference mechanism explains the rich variety of the nematic/smectic states. In Figs. 14A, 14B, 14C, we summarized the nematic/smectic orders revealed by the mechanism in the present study. (i) In FeSe$_{1-x}$Te$_x$, each FS is very small and the $d_{xy}$-orbital hole pocket is absent. In this case, the small spin fluctuations on the three orbitals cooperatively lead to the $B_{1g}$ orbital order for $d_{xz}$ and $d_{yz}$ orbitals coexisting with the $d_{xy}$-orbital bond order, as shown in Fig. 14A. The nematic orbital+bond order causes the Lifshitz transition, where the FS around Y point disappears, consistently with the recent experiments. The $x$ dependence of $T_S$ in the phase diagram is reproduced by introducing the self-energy. (ii) In BaFe$_2$As$_2$, the $d_{xy}$-orbital hole pocket emerges. Since each electron and hole pocket is relatively large and similar in size, the strong $d_{xy}$-orbital spin fluctuations due to good nesting give rise to the smectic order shown in Fig. 14B and the $B_{1g}$ nematic order. The smectic order explains the tiny $T$-linear nematicity below $T = T^* (> T_S)$. We predict the multistage transitions with the smectic order at $T = T^*$ and nematic order at $T_S$. (iii) In heavily hole-doped AFe$_2$As$_2$ (A=Cs, Rb), the tiny Dirac pockets around X(Y) point and the large $d_{xy}$-orbital hole pocket appear due to the hole-doping. The $B_{2g}$ bond order for the $d_{xy}$ orbital shown in Fig. 14C emerges due to the $d_{xy}$-orbital paramagnon interference mechanism. The $B_{2g}$ bond order is triggered by the Lifshitz transition of the electron FSs by the hole-doping.

The limitation of this theory is that the calculated VCs are reduced to the infinite series of the MT and AL terms. To verify the validity of the present theory, we performed the functional renormalization group (fRG) analysis for the single-orbital Hubbard model for cuprates [41] and the two-orbital Hubbard model for ruthenates [94], and obtained the bond-order (orbital order) in the former (latter) model. These results are consistent with experiments, and they are also obtained by the DW equation analysis. In the fRG theory, a huge number of higher-order VCs are generated in an unbiased way by solving the RG equation. Thus, the significance of the MT and AL terms in the present theory has been confirmed by the different and excellent theoretical framework.

It is an important future problem to clarify the mechanism of superconductivity and non-Fermi-liquid behaviors of transport phenomena in the FeSe family by considering the nematic fluctuations enlarged near the nematic QCP. This issue will be discussed in future publications [95].

AUTHOR CONTRIBUTIONS

S.O. performed all calculations with contributions from H.K. S.O. and H.K wrote the paper.
Figure 14. (A) Schematic picture of the $B_{1g}$ nematic orbital+bond order in FeSe$_{1-x}$Te$_x$ and BaFe$_2$As$_2$, where the orbital order for $d_{xz}$ and $d_{yz}$ orbitals coexists with the bond order for $d_{xy}$ orbital. (B) Schematic picture of the smectic bond order for $d_{yz}$ and $d_{xy}$ orbitals in BaFe$_2$As$_2$. (C) Schematic picture of the $B_{2g}$ nematic bond order for $d_{xy}$ orbital in AFe$_2$As$_2$ (A=Cs, Rb).

FUNDING

This work was supported by Grants-in-Aid for Scientific Research from MEXT, Japan (No. JP19H05825, No. JP18H01175, and No. JP17K05543), and Nagoya University Research Fund.

ACKNOWLEDGMENTS

We acknowledge Y. Yamakawa, R. Tazai, and S. Matsubara for their collaboration in the theoretical studies. We are grateful to Y. Matsuda, T. Hanaguri, T. Shibauchi, S. Kasahara, T. Shimojima, and Y. Mizukami for useful discussions about experiments.

REFERENCES

[1] Hosono H, Kuroki K. Iron-based superconductors: Current status of materials and pairing mechanism. *Physica C* **514** (2015) 399. doi:10.1016/j.physc.2015.02.020.

[2] Hirschfeld PJ, Korshunov MM, Mazin II. Gap symmetry and structure of Fe-based superconductors. *Rep. Prog. Phys.* **74** (2011) 124508. doi:10.1088/0034-4885/74/12/124508.

[3] Fernandes RM, VanBebber LH, Bhattacharya S, Chandra P, Keppens V, Mandrus D, et al. Effects of Nematic Fluctuations on the Elastic Properties of Iron Arsenide Superconductors. *Phys. Rev. Lett.* **105** (2010) 157003. doi:10.1103/PhysRevLett.105.157003.

[4] Fernandes RM, Abrahams E, Schmalian J. Anisotropic In-Plane Resistivity in the Nematic Phase of the Iron Pnictides. *Phys. Rev. Lett.* **107** (2011) 217002. doi:10.1103/PhysRevLett.107.217002.

[5] Wang F, Kivelson SA, Lee DH. Nematicity and quantum paramagnetism in FeSe. *Nat. Phys.* **11** (2015) 959. doi:10.1038/nphys3456.

[6] Yu R, Si Q. Antiferroquadrupolar and Ising-Nematic Orders of a Frustrated Bilinear-Biquadratic Heisenberg Model and Implications for the Magnetism of FeSe. *Phys. Rev. Lett.* **115** (2015) 116401. doi:10.1103/PhysRevLett.115.116401.

[7] Glasbrenner JK, Mazin II, Jeschke HO, Hirschfeld PJ, Valenti R. Effect of magnetic frustration on nematicity and superconductivity in Fe chalcogenides. *Nat. Phys.* **11** (2015) 953. doi:10.1038/nphys3434.
Onari et al.

Exotic orders in Fe-based superconductors

[8] Fang C, Yao H, Tsai WF, Hu JP, Kivelson SA. Theory of electron nematic order in LaFeAsO. *Phys. Rev. B.* **77** (2008) 224509. doi:10.1103/PhysRevB.77.224509.

[9] Fernandes RM, Chubukov AV. Low-energy microscopic models for iron-based superconductors. *Rep. Prog. Phys.* **80** (2017) 014503. doi:10.1088/1361-6633/80/1/014503.

[10] Kruger F, Kumar S, Zaanan J, van den Brink J. Spin-orbital frustrations and anomalous metallic state in iron-pnictide superconductors. *Phys. Rev. B.* **79** (2009) 054504. doi:10.1103/PhysRevB.79.054504.

[11] Lv W, Wu J, Phillips P. Orbital ordering induces structural phase transition and the resistivity anomaly in iron pnictides. *Phys. Rev. B.* **80** (2009) 224506. doi:10.1103/PhysRevB.89.224506.

[12] Lee CC, Yin WG, Ku W. Ferro-Orbital Order and Strong Magnetic Anisotropy in the Parent Compounds of Iron-Pnictide Superconductors. *Phys. Rev. Lett.* **103** (2009) 267001. doi:10.1103/PhysRevLett.103.267001.

[13] Kontani H, Onari S. Orbital-Fluctuation-Mediated Superconductivity in Iron Pnictides: Analysis of the Five-Orbital Hubbard-Holstein Model. *Phys. Rev. Lett.* **104** (2010) 157001. doi:10.1103/PhysRevLett.104.157001.

[14] Onari S, Kontani H. Self-consistent Vertex Correction Analysis for Iron-based Superconductors: Mechanism of Coulomb Interaction-Driven Orbital Fluctuations. *Phys. Rev. Lett.* **109** (2012) 137001. doi:10.1103/PhysRevLett.109.137001.

[15] Onari S, Yamakawa Y, Kontani H. High-$T_c$ Superconductivity near the Anion Height Instability in Fe-Based Superconductors: Analysis of LaFeAsO$_{1-x}$H$_x$. *Phys. Rev. Lett.* **112** (2014) 187001. doi:10.1103/PhysRevLett.112.187001.

[16] Onari S, Yamakawa Y, Kontani H. Sign-Reversing Orbital Polarization in the Nematic Phase of FeSe due to the $C_2$ Symmetry Breaking in the Self-Energy. *Phys. Rev. Lett.* **116** (2016) 227001. doi:10.1103/PhysRevLett.116.227001.

[17] Yamakawa Y, Onari S, Kontani H. Nematicity and Magnetism in FeSe and Other Families of Fe-Based superconductors. *Phys. Rev. X* **6** (2016) 021032. doi:10.1103/PhysRevX.6.021032.

[18] Yamakawa Y, Kontani H. Nematicity, magnetism, and superconductivity in FeSe under pressure: Unified explanation based on the self-consistent vertex correction theory. *Phys. Rev. B.* **96** (2017) 144509. doi:10.1103/PhysRevB.96.144509.

[19] Onari S, Kontani H. Origin of diverse nematic orders in Fe-based superconductors: 45° rotated nematicity in AFe$_2$As$_2$(A=Cs,Rb). *Phys. Rev. B.* **100** (2019) 020507(R). doi:10.1103/PhysRevB.100.020507.

[20] Onari S, Kontani H. Hidden antiferromagnetic order in Fe-based superconductor BaFe$_2$As$_2$ and NaFeAs above $T_S$. *Phys. Rev. Research* **2** (2020) 042005(R). doi:10.1103/PhysRevResearch.2.042005.

[21] Jiang K, Hu J, Ding H, Wang Z. Interatomic Coulomb interaction and electron nematic bond order in FeSe. *Phys. Rev. B.* **93** (2016) 115138. doi:10.1103/PhysRevB.93.115138.

[22] Fanfarillo L, Giovannetti G, Capone M, Bascones E. Nematicity at the Hund’s metal crossover in iron superconductors. *Phys. Rev. B.* **95** (2017) 144511. doi:10.1103/PhysRevB.95.144511.

[23] Hsu FC, Luo JY, Yeh KW, Chen TK, Huang TW, Lee YC, et al. Superconductivity in the PbO-type structure $\alpha$-FeSe. *Proc. Natl. Acad. Sci. U.S.A.* **105** (2008) 14262. doi:10.1073/pnas.0807325105.

[24] Bohmer AE, Kreisel A. Nematicity, magnetism and superconductivity in FeSe. *J. Phys.: Condens. Matter* **30** (2018) 023001. doi:10.1088/1361-648X/aa9caaa.

[25] Kreisel A, Hirschfeld PJ, Andersen BM. On the Remarkable Superconductivity of FeSe and Its Close Cousins. *Symmetry* **12** (2020) 1402. doi:10.3390/sym12091402.
[26] Shibauchi T, Hanaguri T, Matsuda Y. Exotic Superconducting States in FeSe-based Materials. *J. Phys. Soc. Jpn.* 89 (2020) 102002. doi:10.1143/JPSJ.89.102002.

[27] Wang QY, Li Z, Zhang WH, Zhang ZC, Zhang JS, Li W, et al. Interface-Induced High-Temperature Superconductivity in Single Unit-Cell FeSe Films on SrTiO$_3$. *Chin. Phys. Lett.* 29 (2012) 037402. doi:10.1088/0256-307X/29/3/037402.

[28] Ge JF, Liu ZL, Liu C, Gao CL, Qian D, Xue QK, et al. Superconductivity above 100 K in single-layer FeSe films on doped SrTiO$_3$. *Nat. Mater.* 14 (2015) 285. doi:10.1038/nmat4153.

[29] Fan Q, Zhang WH, Liu X, Yan YJ, Ren MQ, Peng R, et al. Plain s-wave superconductivity in single-layer FeSe on SrTiO$_3$ probed by scanning tunnelling microscopy. *Nat. Phys.* 11 (2015) 946. doi:10.1038/nphys3450.

[30] Zhang Y, Lee JJ, Moore RG, Li W, Yi M, Hashimoto M, et al. Superconducting gap anisotropy in monolayer FeSe thin film. *Phys. Rev. Lett.* 117 (2016) 117001. doi:10.1103/PhysRevLett.117.117001.

[31] Miyata Y, Nakayama K, Sugawara K, Sato T, Takahashi T. High-temperature superconductivity in potassium-coated multilayer FeSe thin films. *Nat. Mater.* 14 (2015) 775. doi:10.1038/nmat4302.

[32] Shimojima T, Suzuki Y, Sonobe T, Nakamura A, Sakano M, Omachi J, et al. Lifting of $xz/yz$ orbital degeneracy at the structural transition in detwinned FeSe. *Phys. Rev. B* 90 (2014) 121111(R). doi:10.1103/PhysRevB.90.121111.

[33] Nakayama K, Miyata Y, Phan GN, Sato T, Tanabe Y, Urata T, et al. Reconstruction of Band Structure Induced by Electronic Nematicity in an FeSe Superconductor. *Phys. Rev. Lett.* 113 (2014) 237001. doi:10.1103/PhysRevLett.113.237001.

[34] Suzuki Y, Shimojima T, Sonobe T, Nakamura A, Sakano M, Tsuji H, et al. Momentum-dependent sign inversion of orbital order in superconducting FeSe. *Phys. Rev. B* 92 (2015) 205117. doi:10.1103/PhysRevB.92.205117.

[35] Zhang Y, Yi M, Liu ZK, Li W, Lee JJ, Moore RG, et al. Distinctive orbital anisotropy observed in the nematic state of a FeSe thin film. *Phys. Rev. B* 94 (2016) 115153. doi:10.1103/PhysRevB.94.115153.

[36] Yi M, Pfau H, Zhang Y, He Y, Wu H, Chen T, et al. Nematic Energy Scale and the Missing Electron Pocket in FeSe. *Phys. Rev. X* 9 (2019) 041049. doi:10.1103/PhysRevX.9.041049.

[37] Xing RQ, Classen L, Chubukov AV. Orbital order in FeSe: The case for vertex renormalization. *Phys. Rev. B.* 98 (2018) 041108(R). doi:10.1103/PhysRevB.98.041108.

[38] Chubukov AV, Khodas M, Fernandes RM. Magnetism, Superconductivity, and Spontaneous Orbital Order in Iron-Based Superconductors: Which Comes First and Why? *Phys. Rev. X* 6 (2016) 041045. doi:10.1103/PhysRevX.6.041045.

[39] Kawaguchi K, Yamakawa Y, Tsuchizuz M, Kontani H. Competing Unconventional Charge-Density-Wave States in Cuprate Superconductors: Spin-Fluctuation-Driven Mechanism. *J. Phys. Soc. Jpn.* 86 (2017) 063707. doi:10.1143/JPSJ.86.063707.

[40] Yamakawa Y, Kontani H. Spin-Fluctuation-Driven Nematic Charge-Density Wave in Cuprate Superconductors: Impact of Aslamazov-Larkin Vertex Corrections. *Phys. Rev. Lett.* 114 (2015) 257001. doi:10.1103/PhysRevLett.114.257001.

[41] Tsuchizuz M, Kawaguchi K, Yamakawa Y, Kontani H. Multistage electronic nematic transitions in cuprate superconductors: A functional-renormalization-group analysis. *Phys. Rev. B.* 97 (2018) 165131. doi:10.1103/PhysRevB.97.165131.

[42] Onari S, Kontani H. SU(4) Valley + Spin Fluctuation Interference Mechanism for Nematic Order in Magic-Angle Twisted Bilayer Graphene: The Impact of Vertex Corrections. *Phys. Rev. Lett.* 128 (2022) 066401. doi:10.1103/PhysRevLett.128.066401.

---

*This is a provisional file, not the final typeset article*
[43] Hirata T, Yamakawa Y, Onari S, Kontani H. Unconventional orbital charge density wave mechanism in the transition metal dichalcogenide 1T-TaS$_2$. *Phys. Rev. Research* 3 (2021) L032053. doi:10.1103/PhysRevResearch.3.L032053.

[44] Tazai R, Yamakawa Y, Onari S, Kontani H. Mechanism of exotic density-wave and beyond-Migdal unconventional superconductivity in kagome metal A$\nu_3$Sb$_5$ (A = K, Rb, Cs). *Sci. Adv.* 8 (2022) eabl4108. doi:10.1126/sciadv.abl4108.

[45] Licciardello S, Buhot J, Lu J, Ayres J, Kasahara S, Matsuda Y, et al. Electrical resistivity across a nematic quantum critical point. *Nature* 567 (2019) 213. doi:10.1038/s41586-019-0923-y.

[46] Coldea AI, Blake SF, Kasahara S, Haghighirad AA, Watson MD, Knafo W, et al. Evolution of the low-temperature Fermi surface of superconducting FeSe$_{1-x}$S$_x$ across a nematic phase transition. *npj Quantum Materials* 4 (2019) 2. doi:10.1038/s41535-018-0141-0.

[47] Huang WK, Hosoi S, Čulo M, Kasahara S, Sato Y, Matsuura K, et al. Magnetization switching driven by current-induced torque from weakly spin-orbit coupled Zr. *Phys. Rev. Research* 2 (2020) 033367. doi:10.1103/PhysRevResearch.2.033367.

[48] Huang WK, Hosoi S, Čulo M, Kasahara S, Sato Y, Matsuura K, et al. Non-Fermi liquid transport in the vicinity of the nematic quantum critical point of superconducting FeSe$_{1-x}$S$_x$. *Phys. Rev. Research* 2 (2020) 033367. doi:10.1103/PhysRevResearch.2.033367.

[49] Mukasa K, Matsuura K, Qiu M, Saito M, Sugimura Y, Ishida K, et al. High-pressure phase diagrams of FeSe$_{1-x}$Te$_x$: correlation between suppressed nematicity and enhanced superconductivity. *Nat. Commun.* 12 (2021) 381. doi:10.1038/s41467-020-20621-2.

[50] Mukasa K, Ishida K, Imajo S, Qiu MW, Saito M, Matsuura K, et al. Enhanced superconducting pairing strength near a nonmagnetic nematic quantum critical point. *ArXiv* (2022) 2202.11657. doi:10.48550/arXiv.2202.2202.11657.

[51] Ishida K, Onishi Y, Tsujii M, Mukasa K, Qiu M, Saito M, et al. Pure nematic quantum critical point accompanied by a superconducting dome. *ArXiv* (2022) 2202.11674.

[52] Kasahara S, Shi HJ, Hashimoto K, Tonegawa S, Mizukami Y, Shibauchi T, et al. Electronic nematicity above the structural and superconducting transition in BaFe$_2$(As$_{1-x}$P$_x$)$_2$. *Nature* 486 (2012) 382. doi:10.1038/nature11178.

[53] Kim YK, Jung WS, Han GR, Choi KY, Chen CC, Devereaux TP, et al. Existence of Orbital Order and its Fluctuation in Superconducting Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ Single Crystals Revealed by X-ray Absorption Spectroscopy. *Phys. Rev. Lett.* 111 (2013) 217001. doi:10.1103/PhysRevLett.111.217001.

[54] Thewalt E, Hayes IM, Hinton JP, Little A, Patankar S, Wu L, et al. Imaging Anomalous Nematic Order and Strain in Optimally Doped BaFe$_2$(As,P)$_2$. *Phys. Rev. Lett.* 121 (2018) 027001. doi:10.1103/PhysRevLett.121.027001.

[55] Shimojima T, Motosugi Y, Taniuchi T, Bareille C, Onari S, Kontani H, et al. Discovery of mesoscopic nematic wave in iron-based superconductors. *Science* 373 (2021) 1122. doi:10.1126/science.abd6701.

[56] Chu JH, Analytis JG, Greve KD, McMahon PL, Islam Z, Yamamoto Y, et al. In-Plane Resistivity Anisotropy in an Underdoped Iron Arsenide Superconductor. *Science* 329 (2010) 824. doi:10.1126/science.1190482.

[57] Ren X, Duan L, Hu Y, Li J, Zhang R, Luo H, et al. Nematic Crossover in BaFe$_2$As$_2$ under Uniaxial Stress. *Phys. Rev. Lett.* 115 (2015) 197002. doi:10.1103/PhysRevLett.115.197002.
[58] Man H, Zhang R, Park JT, Lu X, Kulda J, Ivanov A, et al. Direct observation of spin excitation anisotropy in the paramagnetic orthorhombic state of BaFe$_{2-x}$Ni$_x$As$_2$. *Phys. Rev. B* **97** (2018) 060507(R). doi:10.1103/PhysRevB.97.060507.

[59] Wiecki P, Zhou R, Julien MH, Bohmer AE, Schmalian J. Edwards-Anderson parameter and local Ising nematicity in FeSe revealed via NMR spectral broadening. *Phys. Rev. B* **104** (2021) 125134. doi:10.1103/PhysRevB.104.125134.

[60] Lahiri A, Klein A, Fernandes RM. Defect-induced electronic smectic state at the surface of nematic materials. *ArXiv* (2021) 2111.00541. doi:10.48550/arXiv.2111.00541.

[61] Li J, Zhao D, Wu YP, Li SJ, Song DW, Zheng LX, et al. Reemerging electronic nematicity in heavily hole-doped Fe-based superconductors. *ArXiv* (2021) 1611.04694. doi:10.48550/arXiv.1611.04694.

[62] Liu X, Tao R, Ren M, Chen W, Yao Q, Wolf T, et al. Evidence of nematic order and nodal superconducting gap along [110] direction in RbFe$_2$As$_2$. *Nat. Commun.* **10** (2019) 1039. doi:10.1038/s41467-019-08962-z.

[63] Moroni M, Prando G, Aswartham S, Morozov I, Bukowski Z, Buchner B, et al. Charge and nematic orders in AFe$_2$As$_2$ (A=Rb,Cs) superconductors. *Phys. Rev. B* **99** (2019) 235147. doi:10.1103/PhysRevB.99.235147.

[64] Ishida K, Tsujii M, Hosoi S, Mizukami Y, Ishida S, Iyo A, et al. Novel electronic nematicity in heavily hole-doped iron pnictide superconductors. *Proc. Natl. Acad. Sci. U.S.A.* **117** (2020) 6424. doi:10.1073/pnas.1909172117.

[65] Wiecki P, Haghighirad AA, Weber F, Merz M, Heid R, Bohmer AE. Dominant In-Plane Symmetric Elastoresistance in CsFe$_2$As$_2$. *Phys. Rev. Lett.* **125** (2020) 187001. doi:10.1103/PhysRevLett.125.187001.

[66] Wiecki P, Frachet M, Haghighirad AA, Wolf T, Meingast C, Heid R, et al. Emerging symmetric strain response and weakening nematic fluctuations in strongly hole-doped iron-based superconductors. *Nat. Commun.* **12** (2021) 4824. doi:10.1038/s41467-021-25121-5.

[67] Borisov V, Fernandes RM, Valenti R. Evolution from $B_{2g}$ Nematics to $B_{1g}$ Nematics in Heavily Hole-Doped Iron-Based Superconductors. *Phys. Rev. Lett.* **123** (2019) 146402. doi:10.1103/PhysRevLett.123.146402.

[68] Wu YP, Zhao D, Wang AF, Wang NZ, Xiang ZJ, Luo XG, et al. Emergent Kondo Lattice Behavior in Iron-Based Superconductors AFe$_2$As$_2$ (A=K, Rb, Cs). *Phys. Rev. Lett.* **116** (2016) 147001. doi:10.1103/PhysRevLett.116.147001.

[69] Civardi E, Moroni M, Babij M, Bukowski Z, Carretta P. Superconductivity Emerging from an Electronic Phase Separation in the Charge Ordered Phase of RbFe$_2$As$_2$. *Phys. Rev. Lett.* **117** (2016) 217001. doi:10.1103/PhysRevLett.117.217001.

[70] Baym G, Kadanoff P. Conservation Laws and Correlation Functions. *Phys. Rev.* **124** (1961) 287. doi:10.1103/PhysRev.124.287.

[71] Allen S, Tremblay AMS, Vilk YM. *Theoretical Methods for Strongly Correlated Electrons* (New-York: Springer-Verlag) (2004).

[72] Blaha P, Schwarz K, Tran F, Laskowski R, Madsen GKH, Marks LD. WIEN2k: An APW+lo program for calculating the properties of solids. *J. Chem. Phys.* **152** (2020) 074101. doi:10.1063/1.5143061.

[73] Mostofi AA, Yates JR, Pizzi G, Lee YS, Souza I, Vanderbilt D, et al. An updated version of wannier90: A tool for obtaining maximally-localised Wannier functions. *Comput. Phys. Commun.* **185** (2014) 2309. doi:10.1016/j.cpc.2014.05.003.
Onari et al.  Exotic orders in Fe-based superconductors

[74] Miyake T, Nakamura K, Arita R, Imada M. Comparison of Ab initio Low-Energy Models for LaFePO, LaFeAsO, BaFe$_2$As$_2$, LiFeAs, FeSe, and FeTe: Electron Correlation and Covalency. *J. Phys. Soc. Jpn.* **79** (2010) 044705. doi:10.1143/JPSJ.79.044705.

[75] Bickers NE, White SR. Conserving approximations for strongly fluctuating electron systems. II. numerical results and parquet extension. *Phys. Rev. B* **43** (1991) 8044. doi:10.1103/PhysRevB.43.8044.

[76] Kontani H, Yamakawa Y, Tazai R, Onari S. Odd-parity spin-loop-current order mediated by transverse spin fluctuations in cuprates and related electron systems. *Phys. Rev. Research* **3** (2021) 013127. doi:10.1103/PhysRevResearch.3.013127.

[77] Nakayama K, Tsubono R, Phan GN, Nabeshima F, Shikama N, Ishikawa T, et al. Orbital mixing at the onset of high-temperature superconductivity in FeSe$_{1-x}$Te$_x$/CaF$_2$. *Phys. Rev. Research* **3** (2021) L012007. doi:10.1103/PhysRevResearch.3.L012007.

[78] Zhang P, Wang Z, Wu X, Yaji K, Ishida Y, Kohama Y, et al. Multiple topological states in iron-based superconductors. *Nat. Phys.* **15** (2019) 41. doi:10.1038/s41567-018-0280-z.

[79] ZWang, Zhang P, Xu G, Zeng LK, Miao H, Xu X, et al. Topological nature of the FeSe$_{0.5}$Te$_{0.5}$ superconductor. *Phys. Rev. B.* **92** (2015) 115119. doi:10.1103/PhysRevB.92.115119.

[80] Lohani H, Hazra T, Ribak A, Nitzav Y, Fu H, Yan B, et al. Band inversion and topology of the bulk electronic structure in FeSe$_{0.45}$Te$_{0.55}$. *Phys. Rev. B.* **101** (2020) 245146. doi:10.1103/PhysRevB.101.245146.

[81] Yin ZP, Haule K, Kotliar G. Kinetic frustration and the nature of the magnetic and paramagnetic states in iron pnictides and iron chalcogenides. *Nat. Mater.* **10** (2011) 932. doi:10.1038/nmat3120.

[82] Yamasaki A, Matsui Y, Imada S, Takase K, Azuma H, Muro T, et al. Electron correlation in the FeSe superconductor studied by bulk-sensitive photoemission spectroscopy. *Phys. Rev. B.* **82** (2010) 184511. doi:10.1103/PhysRevB.82.184511.

[83] Watson MD, Haghhighirad AA, Rhodes LC, Hoesch M, Kim TK. Electronic anisotropies revealed by detwinned angle-resolved photo-emission spectroscopy measurements of fese. *New J. Phys.* **19** (2017) 103021. doi:10.1088/1367-2630/aa8a04.

[84] Yi M, Pfau H, Zhang Y, He Y, Wu H, Chen T, et al. Nematic Energy Scale and the Missing Electron Pocket in FeSe. *Phys. Rev. X* **9** (2019) 041049. doi:10.1103/PhysRevX.9.041049.

[85] Huh SS, Seo JJ, Kim BS, Cho SH, Jung JK, Kim S, et al. Absence of Y-pocket in 1-Fe brillouin zone and reversed orbital occupation imbalance in FeSe. *Commun. Phys.* **3** (2020) 52. doi:10.1038/s42005-020-0319-1.

[86] Rhodes LC, Boker J, Muller MA, Eschrig M, Eremin IM. Non-local $d_{xy}$ nematicity and the missing electron pocket in FeSe. *npj Quantum Materials* **6** (2021) 45. doi:10.1038/s41535-021-00341-6.

[87] Tazai R, Matsubara S, Yamakawa Y, Onari S, Kontani H. A Rigorous Formalism of Unconventional Symmetry Breaking in Fermi Liquid Theory and Its Application to Nematicity in FeSe. *ArXiv* (2022) 2205.02280. doi:10.48550/arXiv.2205.02280.

[88] Moon SJ, Schafgans AA, Kasahara S, Shibauchi T, Terashima T, Matsuda Y, et al. Infrared Measurement of the Pseudogap of P-Doped and Co-Doped High-Temperature BaFe$_2$As$_2$ Superconductors. *Phys. Rev. Lett.* **109** (2012) 027006. doi:10.1103/PhysRevLett.109.027006.

[89] Shimojima T, Sonobe T, Malaeb W, Shinada K, Chainani A, Shin S, et al. Pseudogap formation above the superconducting dome in iron pnictides. *Phys. Rev. B.* **89** (2014) 045101. doi:10.1103/PhysRevB.89.045101.
[90] Shimojima T, Malaeb W, Nakamura A, Kondo T, Kihou K, Lee CH, et al. Antiferroic electronic structure in the nonmagnetic superconducting state of the iron-based superconductors. Sci. Adv. 3 (2017) e1700466. doi:10.1126/sciadv.1700466.

[91] Yi M, Lu DH, Chu JH, Analytis JG, Sorini AP, Kemper AF, et al. Symmetry-breaking orbital anisotropy observed for detwinned Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ above the spin density wave transition. Proc. Natl. Acad. Sci. U.S.A. 108 (2011) 6878. doi:10.1073/pnas.1015572108.

[92] Zhou R, Xing LY, Wang XC, Jin CQ, Zheng G. Orbital order and spin nematicity in the tetragonal phase of the electron-doped iron pnictides NaFe$_{1-x}$Co$_x$As. Phys. Rev. B. 93 (2016) 060502(R). doi:10.1103/PhysRevB.93.060502.

[93] Mizukami Y, Tanaka O, Ishida K, Tsujii M, Mitsui T, Kitao S, et al. Thermodynamic Signatures of Diagonal Nematicity in RbFe$_2$As$_2$ Superconductor. ArXiv (2021) 2108.13081. doi:10.48550/arXiv.2108.13081.

[94] Tsuchiizu M, Ohno Y, Onari S, Kontani H. Orbital Nematic Instability in the Two-Orbital Hubbard Model: Renormalization-Group + Constrained RPA Analysis. Phys. Rev. Lett. 111 (2013) 057003. doi:10.1103/PhysRevLett.111.057003.

[95] Yamakawa Y, Onari S, Kontani H. Unpublished (2022).