Orbital fluctuation theory in iron-based superconductors: $s_{++}$-wave superconductivity, structure transition, and impurity-induced nematic order

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The main features in iron-based superconductors would be (i) the orthorhombic transition accompanied by remarkable softening of shear modulus, (ii) high-$T_c$ superconductivity close to the orthorhombic phase, and (iii) nematic transition in the tetragonal phase. In this paper, we present a unified explanation for them, based on the orbital fluctuation theory, considering both the $c$-ph and the Coulomb interaction. It is found that a small $c$-phonon coupling constant ($\lambda \sim 0.2$) is enough to produce large orbital (=charge quadrupole $O_{xx/yz}$) fluctuations, which causes the $s$-wave superconductivity without sign reversal ($s_{++}$-wave state). The derived orbital fluctuations also cause the instability toward the structure transition due to the bound state formation of two orbitons with opposite momenta, which is called the “two-orbition process”. Moreover, impurity-induced non-local orbital order with $C_2$-symmetry is obtained when the orbital fluctuations are strong. This “impurity-induced nematic state” explains the in-plane anisotropy of resistivity in detwinned samples. We stress that (i)-(iii) are reproducible only when orbital fluctuations with respect to $O_{xz}$ and $O_{yz}$ charge quadrupoles are the most divergent. This fact ensures the reliability of the present model Hamiltonian and calculation.

Keywords: iron-based superconductors, orbital fluctuation, superconductivity, structure transition, shear modulus softening

I. INTRODUCTION

Iron-based high-$T_c$ superconductors had been discovered by Kamihara et al. in 2008$^1$, and the highest superconducting (SC) transition temperature $T_c$ at present reaches 56K. The SC state occurs when the crystal structure is tetragonal, which is realized by chemical doping (or applying the pressure) on mother compounds, through the structure transition from orthorhombic to tetragonal. In the phase diagram, the SC phase is next to the non-SC and metallic orthorhombic phase, and the structure transition at $T = T_s$ is second-order in Ba(Fe,Co)$_2$As$_2$$_2$. Very large softening of shear modulus $C_s$ suggests the existence of strong orbital (quadrupole) fluctuations$^3$-5. Moreover, the spin-density-wave (SDW) state with $Q \approx (\pi, 0)$ occurs in the orthorhombic phase, that is, $T_N$ is close to but always lower than $T_s$. These experimental facts suggest a close relation between the mechanism of superconductivity and structure/orbital/SDW transition.

Although the lattice deformation in the orthorhombic phase is very small ($(a - b)/(a + b) < 0.003$), in-plane resistivity shows sizable anisotropy in the orthorhombic phase. This fact means that the structure transition is driven by electron-electron (or electron-optical-phonon) interaction, not by the cooperative Jahn-Teller effect due to electron-acoustic-phonon interaction. Very interestingly, large in-plane anisotropy starts to occur in the tetragonal phase at $T^*$, which is about 10K-100K higher than $T_s$ in detwinned Ba(Fe,Co)$_2$As$_2$$_2$. The discovery of this “nematic electronic state” free from lattice deformation had attracted great attention. The nematic transition also occurs in the tetragonal phase of BaFe$_2$(As$_{1-x}$P$_x$)$_2$, confirmed by the in-plane anisotropy of susceptibility$^7$ using neutron inelastic scattering. The origin of the spin fluctuations is the intra-orbital nesting and the Coulomb interaction. However, the robustness of $T_c$ against randomness in iron pnictides indicates the absence of sign-reversal in the SC state had been predicted$^8$-12. The origin of the spin fluctuations is the intra-orbital nesting and the Coulomb interaction. However, the robustness of $T_c$ against randomness in iron pnictides indicates the absence of sign-reversal in the SC gap$^{13-16}$. Later, orbital-fluctuation-mediated $s$-wave state without sign reversal ($s_{++}$-wave) had been proposed$^{17-19}$. The orbital fluctuations mainly originate from the inter-orbital nesting and the electron-phonon ($c$-ph) interactions due to non-$A_{1g}$ optical phonons.

One of the main merits of the orbital fluctuation scenario is the robustness of the $s_{++}$-wave state against impurities or randomness, consistently many experiments$^{14-16}$. Moreover, orbital-fluctuation-mediated $s_{++}$-wave state scenario is consistent with the large SC gap on the $z^2$-orbital band in Ba$_2$122 systems$^{18}$, observed by bulk-sensitive laser ARPES measurement$^{20}$. Note that the “resonance-like” hump structure in the neutron inelastic scattering$^6$ is frequently explained as the spin-resonance due to the sign reversal in the SC gap$^{21,22}$. However, experimental hump structure is well reproduced in terms of the $s_{++}$-wave SC state, rather
than the \( s_\pm \)-wave SC state, by taking the suppression in the inelastic scattering \( \gamma(\omega) \) for \( |\omega| \lesssim 3\Delta \) in the SC state (dissipationless mechanism)\textsuperscript{23,24}.

In this paper, we present recent developments of the orbital fluctuation theory presented in Refs.\textsuperscript{17–19,25,26}. We present a unified explanation for the following main characters in iron-based superconductors: (i) orthorhombic transition accompanied by remarkable \( C_S \) softening\textsuperscript{8–10}, and (ii) emergence of high-\( T_\text{c} \) superconductivity strong against randomness next to the orthorhombic phase. We also discuss (iii) “nematic transition” in the tetragonal phase\textsuperscript{9} in terms of the impurity-induced non-local orbital order. It is noteworthy that (i)-(iii) can be explained only when orbital fluctuations with respect to \( O_{xz} \) and \( O_{yz} \) charge quadrupoles are the most divergent. This fact assures the reliability of the present theory and model Hamiltonian.

II. ORBITAL FLUCTUATIONS AND \( s_{++} \)-WAVE SUPERCONDUCTIVITY

A. Antiferro-orbital fluctuations due to inter-orbital nesting

Here, we study the five-orbital tight-binding model introduced in Refs.\textsuperscript{8,27}, which reproduces the experimental multiband structure very well. We also include both the Coulomb interaction (\( U, U' \), and \( J \)) and the quadrupole-quadrupole interaction induced by optical phonons. In this paper, we introduce the \( xy \)-coordinate, in which \( x \) - and \( y \)-axes are along Fe-Fe direction.

Because of the symmetry of \( \text{A}_{4l} \) tetrahedron, Fe-ion optical phonon induces the following quadrupole-quadrupole interaction:\textsuperscript{18}

\[
H_{\text{quad}} = -g(\omega_i) \sum_i \sum_\Gamma \hat{O}_{\Gamma i}^\dagger \hat{O}_\Gamma \tag{1}
\]

where \( \hat{O}_{\Gamma i} \) is the quadrupole operator for channel \( \Gamma \) at site \( i \) introduced in (I). \( g(\omega_i) = g(0) \cdot \omega_i^2/(\omega_i^2 + \omega_D^2) \) is the quadrupole coupling induced by the optical phonons, \( \omega_D = 200 \sim 300 \text{K} \) is the phonon frequency and \( \omega_l = 2\pi T_l \) is the boson Matsubara frequency. Note that \( \hat{O}_{\mu\nu} \propto \hat{l}_\mu \hat{l}_\nu + \hat{\ell}_\mu \hat{\ell}_\nu \), where \( \ell \) is the angular momentum. Here, we set \( \langle xz|\hat{O}_{yz}|xy \rangle = \langle yz|\hat{O}_{xy}|xz \rangle = \langle xy|\hat{O}_{yz}|yz \rangle = 1 \) by multiplying a constant. Recently, it was found that Eq. (1) is also caused by the multiorbital Coulomb interaction, by including the multiorbital exchange process\textsuperscript{9} that is absent in the random-phase approximation (RPA) [S. Onari and H. Kontani, arXiv:1203.28741].

In iron pnictides, antiferro-quadrupole (AFQ) fluctuations with respect to \( \Gamma = xx/yz \) are induced by the quadrupole interaction and the inter-orbital nesting. The quadrupole susceptibility is \( \chi^Q_\Gamma(q, \tau) = \int_0^B d\tau e^{i\omega \tau} T_{\tau} \hat{O}_\Gamma(q, \tau) \hat{O}_\Gamma(q, 0) \).

When \( g = 0 \), five quadrupole susceptibilities \( \chi^Q_\Gamma(q) \) (\( \Gamma = xx, yz, xy, z^2, x^2 - y^2 \)) induced by Coulomb interaction are small and almost comparable, with peaks at \( q = (0, pi) \) or \( (pi, 0) \). By introducing small quadrupole interaction \( g \), quadrupole susceptibilities with \( \Gamma = xx, yz, xy \) are largely enhanced. The most divergent susceptibilities are \( \chi^Q_{xz}(q) \) at \( q = (0, pi) \) and \( \chi^Q_{yz}(q) \) at \( q = (pi, 0) \): They are approximately expressed as

\[
\chi^Q_{\Gamma}(q) = \frac{e\xi^2}{1 + \xi^2 (Q_\Gamma - q)^2 - i\omega/\omega_0} \tag{2}
\]

for \( \Gamma = xx \) and \( yz \), where \( Q_{xz} = (pi, 0) \) and \( Q_{yz} = (0, pi) \). In two-dimensional systems, orbital fluctuation parameters behave as\textsuperscript{29}

\[
\xi^2 = l(T - T_{\text{AFQ}})^{-1}, \quad \omega_0 = l'(T - T_{\text{AFQ}}) \tag{3}
\]

The Weiss temperature \( T_{\text{AFQ}} \) becomes zero at orbital quantum-critical-point (QCP). In eq. (3), the unit of the length is \( a_{\text{Fe-Fe}} \approx 3\text{Angstrom} \).

In later sections, we will explain that the development of \( \chi^Q_{xz}(y)Q_{xz/yz}(y) \) gives rise to not only the \( s_{+-} \)-wave state, but also the structure transition as well as impurity-induced nematic transition in the tetragonal phase. Although superconductivity can be caused by other orbital fluctuations (such as \( \Gamma = xy, z^2 - y^2 \), or \( z^2 \)), both structure and nematic transitions are uniquely explained only when \( \Gamma = xx \) and \( yz \) are the most divergent. Therefore, the present orbital fluctuation model is considered to be reliable.

B. Phase diagram for \( s_{+-} \) and \( s_{++} \)-wave states

Figure 1 (a) shows the phase diagram obtained by the RPA (mean-field approximation) for the electron filling \( n = 6.1 \), where \( g(0) \) is the quadrupole interaction and \( U \) is the intra-orbital Coulomb interaction; we set the Hund’s coupling term \( U' = U/10 \) and the inter-orbital term \( U' = U - 2J \). \( a_c \) (\( a_s \)) is the charge (spin) Stoner factor; \( a_c = 1 \) (\( a_s = 1 \)) corresponds to the orbital (spin) ordered state. For \( U = 1.3\text{eV} \), orbital order appears when \( g(0) \approx 0.1\text{eV} \), meaning that about 50\% of orbital fluctuations originate from the Coulomb interaction. By solving the SC gap equation, we obtain the \( s_{++} \)-wave state when the orbital fluctuations dominate the spin fluctuations\textsuperscript{17}.

In Fig. 1 (b), we show the \( U-g \) phase diagram obtained by the FLEX approximation. The dashed-dotted line represents the condition \( a_c = 0.98 \) at \( T = 0.015 \), corresponding to \( g = 0.25 \sim 0.3 \). Therefore, substantial orbital fluctuations emerge for \( \lambda = gN(0) \lesssim 0.2 \) even if the self-energy correction is taken into account. On the other hand, \( a_s = 0.95 \) (0.92) for \( U = 1.8 \) and \( g = 0 \) (0.3) in the FLEX approximation, although \( U_{\text{ct}} = 1.25 \).
for $\alpha_s = 1$ in the RPA. Thus, the renormalization in $\alpha_s$ is rather larger than that in $\alpha_c$. The region of the $s_{++}$-wave state is widely expanded in the presence of dilute impurities. In the present model, both $\chi^Q_{zz}$ and $\chi^Q_{xy}$ are strongly developed. Since all $t_{2g}$-orbitals on the Fermi surfaces are involved in these fluctuations, we obtained a fully-gapped $s_{++}$-wave state as shown in Fig. 1 (c), consistently with many high-$T_c$ pnictides. When the spin fluctuations are comparable to orbital fluctuations, on the other hand, competition of these fluctuations induce the nodal structure in the SC gap, as shown in (e).

In summary, we discussed both the spin-fluctuation mediated $s_{\pm}$-wave state and orbital-fluctuation mediated $s_{++}$-wave state in iron-based superconductors. We have shown that the latter is realized by inter-orbital nesting in the presence of small quadrupole interaction $g$ in eq. (1). Figure 1 (b) show the $U$-$g$ phase diagram obtained by the FLEX approximation. Since both $s_{\pm}$- and $s_{++}$-states belong to the same $A_{1g}$ symmetry, a smooth crossover from $s_{\pm}$-state to $s_{++}$-state is realized as increasing $g$ or impurity concentration $n_{\text{imp}}$. During the crossover, nodal $s$-wave state is realized, at which the obtained $T_c$ is rather suppressed but finite. (Mathematically, it is impossible to distinguish between nodal $s_{++}$- and nodal $s_{\pm}$-states.) Experimentally, nodal line structure appears in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, in which both spin and orbital fluctuations are considered to be developed$^{30}$. Recently, we have verified that the realization condition for the nodal structure is much moderate if we study a realistic “three dimensional” model$^{31}$.

### C. heavily hole-doped system: KFe$_2$As$_2$

Here, we study the superconducting state in newly discovered heavily h-doped superconductor K$_3$Fe$_2$Se$_2$ ($T_c \sim 30$K) based on the ten-orbital model$^{25}$. Since the hole-pockets are absent, the $s_{\pm}$-wave state is unlikely. However, when the Coulomb interaction is large enough, spin-fluctuation mediated $d$-wave state would appear due to the nesting between electron-pockets$^{32}$. However, the symmetry of the body-centered tetragonal structure in K$_3$Fe$_2$Se$_2$ requires the existence of nodes in the $d$-wave gap$^{25}$, although fully-gapped $d$-wave state is realized in the case of simple tetragonal structure. In the presence of moderate quadrupole interaction $g$, on the other hand, we find that orbital fluctuations give rise to the fully-gapped $s_{++}$-wave state.

In Fig. 2 (a), we show the $\alpha_s$-dependence of the eigenvalue of the gap equation, $\lambda_E$, for the $s_{++}$-wave state with $U = 0$, and the $\alpha_s$-dependence of $\lambda_E$ for the $d$-wave state with $g = 0$. In calculating the $s_{++}$-wave state, we use rather larger phonon energy; $\omega_D = 0.15$ eV, considering that the calculating temperature is about ten times larger than the real $T_c$. The SC gap functions for $s_{++}$-wave state are shown in Fig. 2 (b). The SC gap would become more anisotropic in case of $U > 0$.

Therefore, similar to iron-pnictide superconductors, spin-fluctuation-mediated $s_{++}$-wave state is realized by small $e$-$ph$ interaction $\lambda = gN(0) \sim 0.2$. The obtained $\lambda_E$ for the $s_{++}$-wave state is larger than that for the spin-fluctuation-mediated $d$-wave state. We stress that nodal lines appear on the large e-pockets in the $d$-wave state, due to the hybridization between two e-pockets that is inherent in 122 systems, which is inconsistent with the
specific heat measurements\textsuperscript{33} that report the isotropic SC gap. We propose that the study of impurity effect on SC gap. We propose that the study of impurity effect at $\alpha$-wave deformation in the orthorhombic phase is very small in relation to these two phenomena. Since the lattice deformation due to the Coulomb interaction gives rise to the AFQ fluctuations for the channels $xz$, $yz$ and $xy$, while $\chi_{xz,yz}^Q(0)$ remains small. Therefore, $C_S$ softening cannot be explained within the RPA. However, the mode-mode coupling process with respect to $\chi_{xz}^Q(q)$ gives the development of ferro-quadrupole fluctuations; $\chi_{xy}^Q(0) \sim T \sum_q \chi_{xz}^Q(q)^2$. This process is called the “two-orbition term” in Ref.\textsuperscript{26} since the condensation of composite bosons with zero momentum, $O_{xz}(q)O_{xz}(-q)$, induces the tetragonal structure transition, because of the relation $O_{xz,yz} \sim O_{xz}^2 - O_{yz}^2$. The two-orbition term has close similarity to the Aslamazov-Larkin theory of excess conductivity given by superconducting fluctuations.

By taking the two-orbition term, the irreducible susceptibility is given as

$$\chi^{\text{irr}}_{xz,yz}(q) = \chi_{xz,yz}(0) + \chi_{TO}(q)$$

where $\chi_{xz,yz}(0)$ is the bare bubble term, and its temperature dependence is weak. Within the classical approximation, the two-orbition term is $\chi_{TO}(q) = \Lambda^2 \sum_k \chi_{xz}^Q(q + k)\chi_{xz}^Q(-k)$, where $\Lambda$ is the three-point vertex\textsuperscript{26}. The exact expression is given in eq. (61) in Ref.\textsuperscript{26}:

$$\chi_{TO}(0) = X \xi^2 \left[ \frac{\omega_n}{\pi} \left( n_{\max} + \frac{\omega_n}{2\pi T} + 1 \right) - \psi \left( \frac{\omega_n}{2\pi T} + 1 \right) \right] + T$$

where $\psi(x)$ is di-Gamma function, and $X \equiv \frac{(2g)^4\epsilon^2}{4\pi} \Lambda^2$. ($\epsilon$ was introduced in eq. (2).) Since $\chi_{TO}(q) \propto T \xi^2$ for

III. ORTHORHOMBIC STRUCTURE TRANSITION AND SOFTENING OF SHEAR MODULUS $C_S$

A. Two-orbition mechanism

In many Fe-based superconductors, the SC state occurs next to the structure transition, suggesting a close relation between these two phenomena. Since the lattice deformation in the orthorhombic phase is very small ($(a-b)/(a+b) \approx 0.003$), we can safely rule out the cooperative Jahn-Teller effect due to electron-acoustic-phonon. Hereafter, we promise that $a = x$ axis and $b = y$ axis. Below, we discuss the structure transition due to ferro quadrupole-quadrupole interaction.

For this purpose, we introduce the strain-quadrupole coupling:

$$H_S = \eta_S \sum_i \epsilon_S \phi_S,$$

where $\epsilon_S$ is the strain for the orthorhombic deformation ($\epsilon_S \propto a-b$), $\phi_S$ is a quadrupole operator that belong to the same representation of $\epsilon_S$, and $\eta_S$ is the coupling constant. Fernandes et al.\textsuperscript{34} considered the “spin quadrupole operator” $\hat{\phi}_S = s_1 \cdot s_2$, where $s_1$ represents the spin operator at sublattice $l = 1, 2$. (In their theory, stripe-type commensurate magnetic correlation is assumed.) In this case, $\phi_S$ is a non-local operator. On the other hand, the present authors studied the “charge quadrupole operator” $\phi_S = \hat{O}_{x^2-y^2}$, which is a local operator. In the presence of the strain-quadrupole coupling, the shear modulus $C_S$ is given as

$$C_S^{-1} = C_{S,0}^{-1}(1 + g_S \chi_S(0,0))$$

where $C_{S,0}$ is the lattice shear modulus, and $g_S = \eta_S^2 C_{S,0}^{-1}$.

Experimentally, $C_S$ follows the Curie-Weiss relation in the under-doped systems with $T_S > 0$:

$$C_S \frac{C_{S,0}}{C_{S,0}} = \frac{T - T_S}{T - \theta}$$

On the other hand, $C_S$ deviates from the Curie-Weiss law in the over-doped systems without structure transition.

From now on, we consider the charge quadrupole susceptibility for $\phi = \hat{O}_{x^2-y^2}$, $\chi^Q_S(\mathbf{q}, \omega)$ is the total quadrupole susceptibility, given by the Fourier transformation of $\chi_S(\mathbf{q}, \tau) = \langle T\tau \hat{\phi}_S(\mathbf{q}, \tau) \hat{\phi}^\dagger_S(0) \rangle$.

$$\chi_S(\mathbf{q}, \tau) \equiv \langle T\tau \hat{\phi}_S(\mathbf{q}, \tau) \hat{\phi}^\dagger_S(0) \rangle$$

FIG. 2: (a) $\alpha_{zz}$ - $(\alpha_{zz})$ dependence of $\lambda_{E}$ for $d$-wave ($s_{++}$-wave) state at $T = 0.03$ eV. (b) SC gap functions for $s_{++}$-wave state.
where \( q \to 0 \), the two-orbiton term shows strong \( T \)-dependence. When \( U = 0 \), the total quadrupole susceptibility is given as

\[
\chi_{Q}^{\text{irr}}(q) = \chi_{Q}^{\text{irr}}(q)/\left(1 - gS\chi_{Q}^{\text{irr}}(q)\right)
\]

(10)

where \( gS \) is the quadrupole-quadrupole interaction due to acoustic phonon. As a result, the elastic constant \( C \) in Ref. is given by eqs. (6), (8) and (10), together with eq. (61) in Ref.\(^{26}\).

\[
\frac{C}{C_{0}} \rightarrow q^{2} \chi_{Q}^{\text{irr}}(q)
\]

The phase diagram and SC transition temperature

In Fig. 3, we plot \( C_{0}/C_{S,0} \) based on the two-orbiton theory. We put orbital fluctuation parameters as \( l = 1200K \), \( l' = 1400K \), and \( T_{\text{AFQ}} = 92K \sim -120K \). These values are consistent with theoretical calculation based on the FLEX approximation\(^{19}\). As for the spin fluctuation parameters in cuprates, \( l = 0.2eV \) (0.1eV) for La\(_{1-x}\)Sr\(_{x}\)CuO\(_{2}\) (YaBa\(_{2}\)Cu\(_{3}\)O\(_{7}\)). We also set \( gS = 0.183eV \), \( aS = \chi_{Q}^{(2)}(0) = 2.88eV^{-1} \), and \( X = \chi_{T}(0)/\xi^{2}T = 5.47 \sim 7.11 \).

In the FLEX approximation\(^{19}\), \( T_{\text{AFQ}} \) changes from positive to negative by carrier doping, while other parameters (such as \( l \) and \( l' \)) are insensitive to the doping. We can fit the recent experimental data by Yoshizawa et al.\(^{4}\) for Ba(Fe\(_{1-x}\)Co\(_{x}\))\(_{2}\)As\(_{2}\) with \( x = 0 \sim 16\% \), by changing \( T_{\text{AFQ}} \) from 90K to \(-120K \), together with \( X = 5.47 \to 7.11 \). The fitting data shown in Fig. 3 reproduce the experimental data of Ref.\(^{4}\) almost perfectly. This fact is a strong evidence for the success of orbital fluctuation theory in iron pnictide superconductors.

B. Phase diagram and SC transition temperature

We show the phase diagram for Ba(Fe\(_{2}\)Co\(_{1-x}\))\(_{2}\)As\(_{2}\) in Fig. 4. \( T_{c} \) and \( T_{S} \) shows the experimental values, and \( T_{\text{AFQ}} \) is obtained by the fitting using the two-orbiton theory. While \( T_{\text{AFQ}} \) should almost coincide to \( T_{S} \) at \( T_{S} = 0 \) theoretically, the obtained \( T_{AFQ} \) slightly exceeds \( T_{S} \) for \( x = 7 \sim 8\% \), because of the lack of experimental data at low temperatures. In fact, \( \xi^{2} \) is expected to deviate from the Curie-Weiss behavior at low temperatures, as predicted by the SCR theory. In Fig. 4, \( \theta \) is obtained experimentally by using the relation \( (1 - C_{S}/C_{S,0})^{-1} \propto T - \theta \) when \( C_{S}/C_{S,0} \) follows the Curie-Weiss relation in eq. (7).

![Phase diagram for Ba(Fe\(_{2}\)Co\(_{1-x}\))\(_{2}\)As\(_{2}\) obtained by the orbital fluctuation theory.](image)

Based on the obtained orbital fluctuation parameters, we calculate the SC transition temperature. Here, we consider the orbital-fluctuation mediated \( s_{+} \)-wave state due to inter-pocket nesting. The linearized gap equation is given as

\[
\lambda_{E} \Delta_{\alpha}(k, \epsilon_{n}) = \frac{\pi T}{(2\pi)^{2}} \sum_{\beta, p} \sum_{m} \int \frac{dp}{v_{p}} V_{\alpha, \beta}(k_{n}, p_{m}) \Delta_{\beta}(p, \epsilon_{m}) \left| \epsilon_{m} \right|
\]

(11)

where \( \lambda_{E} \) is the eigenvalue; \( \lambda_{E} = 1 \) is satisfied at \( T = T_{c} \). \( \alpha, \beta \) represent Fermi surfaces (FSs), \( k(p) \) is the momentum on the FS \( \alpha \) (FS \( \beta \), and \( V_{\alpha, \beta}(k_{n}, p_{m}) \) is the interaction between \( \alpha \) and \( \beta \). Here, we consider the attractive interaction due to orbital fluctuation; \( V_{\alpha, \beta} \propto \chi_{Q}^{(2)}(q^{2}) \). For simplicity, we assume that both the Fermi velocity and SC gap are isotropic. Then, the momentum integration along the FS in eq. (11) can be performed as \( \int_{\beta} \frac{dp}{v_{p}} V_{\alpha, \beta}(k_{n}, p_{m}) = C\xi/(1 + |\epsilon_{n} - \epsilon_{m}|/\omega_{0}) \).
where $C$ is a constant. If we assume $\Delta^\alpha = \Delta^\beta$, we obtain the following simplified gap equation:

$$\lambda E \Delta(\epsilon_n) = T \sum_\beta \sum_m \frac{C \xi - \mu^*}{1 + |\epsilon_n - \epsilon_m|/\omega_0} \Delta(\epsilon_m)$$

(12)

where $\mu^*$ is the Morel-Anderson pseudo potential; we put $\mu^* = 0.1$. We put $C = 0.075$ to obtain $T_c = 25K$ when $T_{AFQ} = 0$. In Fig. 4, we show the SC transition temperatures obtained by eq. (12) by solid squares, which are similar to experimental values. This fact means that the orbital fluctuation parameters derived from $C_S$ are reasonable.

Next, we discuss the non-Fermi-liquid behavior of the resistivity caused by the AF orbital fluctuations. In Fig. 5, circles show the resistivity of single crystal Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ reported in Ref.35. According to spin/orbital fluctuation theory29, the resistivity in two dimension is given as

$$\rho = AT^2\xi^2 + \rho_0$$

(13)

where $\xi$ is the correlation length of AF fluctuations, $\rho_0$ is the residual resistivity, and $A$ is a constant. Using this equation together with $\xi^2 = l/(T - T_{AFQ})$ derived from $C_S$, we can reproduce experimental data below 200K very well, as shown in Fig. 5. Here, we put $A = 0.49$ for all $x$, and $(T_{AFQ}, \rho_0) = (-8, 80)$ for $x = 8\%$, $(0, 72)$ for $x = 10\%$, $(-50, 70)$ for $x = 12\%$, and $(-90, 67)$ for $x = 14\%$, respectively. ($T_{AFQ}$'s are obtained from Fig. 4.) In the present theory, Fe-ion optical phonons together with the Coulomb interaction induce the AF-orbital fluctuations, which give rise to the $s_{++}$-wave state and non-Fermi-liquid-like transport phenomena. Moreover, two AF-orbitons with zero total momentum induce the ferro-orbital fluctuations, which are the origin of the orthorhombic structure transition. Therefore, the present orbital fluctuation theory can explain both the structure transition and the superconductivity.

C. Difficulties in other orbital fluctuation theories

Here, we discuss various difficulties in other orbital fluctuation models proposed for iron-based superconductors36,37. To explain the orthorhombic structure transition, the ferro-$O_{x^2-y^2}$ fluctuations should be the most divergent. The $U' > U$ model in Ref.36 cannot explain the structure transition since the most divergent fluctuation is $O_{x^2}$-type.

Next, we consider the "$O_{x^2-y^2}$-fluctuation model", in which all quadrupoles other than $O_{x^2-y^2}$ do not fluctuate. Then, electrons with $xy$-orbital character, which occupies one-third of the total DOS at Fermi level, are not involved in the $O_{x^2-y^2}$-fluctuations, since $\langle xy|O_{x^2-y^2}|m = 0 \rangle$ for any $d$-orbital $m$. This fact means that "gapless SC state with large residual DOS" is realized in the $O_{x^2-y^2}$-fluctuation model. Figure 6 shows the gap structure given by the (a) "$O_{xz/yz}$-fluctuation model" in Ref.17 and (b) "$O_{x^2-y^2}$-fluctuation model" in Ref.37. In the latter model, the quadrupole interaction $H' = -g(\omega) \sum_i O_{x^2-y^2} \cdot \hat{O}_{x^2-y^2}$ is introduced, considering the As-ion acoustic phonons. In (a), fully-gapped $s_{++}$-wave state is realized. In (b), in contrast, the SC gap on the $xy$-orbital hole-pocket around $(\pi, \pi)$ in the unfolded BZ is almost gapless, and the SC gap on e-pockets is highly anisotropic. Therefore, $O_{x^2-y^2}$ fluctuation model cannot explain the fully-gapped nodal gap structure observed in almost all iron-based superconductors.

We also comment on the "$T$-linear resistivity" observed in various iron-based superconductors. In the ferro-$O_{x^2-y^2}$ fluctuation model, the portion of Fermi surfaces with $xy$-orbital would become the cold-spot with $\gamma \propto T^2$. Thus, a conventional Fermi liquid behavior $\rho \propto T^2$ would be obtained in the ferro-$O_{x^2-y^2}$ fluctuation model, inconsistently with experiments.

Therefore, orbital fluctuations theories in Refs.36,37 have serious difficulty in explaining the "fully-gapped" $s_{++}$-wave state as well as non-Fermi liquid transport phenomena in iron-based superconductors.

D. Effective Action

In Ref.26, we have calculated the shear modulus $C_S$ using the Green function method. Since the derivation was rather complex, we rederive the same expression in a more simple manner by introducing the Hubbard-Stratonovich field, in analogy to the analysis in Ref.34. By performing the Hubbard-Stratonovich transformation, we introduce the following effective action $S = S_0 + S_{int} + S_{strain}$ for the charge quadrupole field $\phi_T$.
In (a), the eigenvalue of the gap equation (11), $\lambda_T$, is larger with smaller interaction $g$. In (b), the eigenvalue of the gap equation (11), $\lambda_E$, is larger with smaller interaction $g$.

$$
\begin{align*}
\Gamma &= XZ, YZ \\
S_0[\phi_T] &= \frac{1}{2} \sum_{\Gamma} \int_{\Gamma} \left\{ \chi_{XZY}(q) \right\}^{-1} \phi_T(q), \quad (14) \\
S_{\text{int}}[\phi_T] &= -\frac{g_S}{2} \sum_j \left\{ \phi_{XZ}(x) \phi_{YZ}(x) \right\}^2 \quad (15) \\
S_{\text{strain}}[\phi_T] &= \eta_S \sum_x \epsilon_S(x) \phi_{XZ}(x) \phi_{YZ}(x) \quad (16)
\end{align*}
$$

where $f_x \cdots = \int_0^{1/T} d\tau \int d^2x \cdots$, $S_0$ represents the most divergent AF quadrupole susceptibility $\chi_{XZY}(q)$, $S_{\text{int}}$ is the quadrupole-quadrupole interaction due to acoustic phonons, and $S_{\text{strain}}$ is the strain-quadrupole coupling. In this subsection, we introduce the $XY$-coordinate that is $-45$ degree rotated from the $xy$-coordinate along $z$-axis. Apparently, $\phi_{XZ} = (\phi_{xz} - \phi_{yz})/\sqrt{2}$, $\phi_{YZ} = (\phi_{xz} + \phi_{yz})/\sqrt{2}$, and $\chi_{x^2-y^2} = O_{XY}$. In Eqs. (15) and (16), $g_S \equiv g_S \cdot \Lambda^2$ and $\eta_S \equiv \eta_S \cdot \Lambda$, where $\Lambda$ is the three-point vertex with respect to $(O_{XY}, O_{XZ}, O_{YZ})$ that had been analyzed in Ref. 20.

Now, the quadrupole susceptibility $\chi_{x^2-y^2}$ is given by the second derivative of the partition function with respect to $\eta_S(x)$. If we put $g_S = 0$, the quadrupole susceptibility is given as $\Lambda^2 \chi_{XZ}(x) \chi_{YZ}(-x)$. By performing the Fourier transformation and taking the interaction $g_S$ into account, the total quadrupole susceptibility is obtained as

$$
\begin{align*}
\chi_{x^2−y^2}^Q(q) &= \Lambda^2 \frac{\chi_{irr}^Q(q)}{1 - g_S^2 \chi_{irr}^Q(q)}, \quad (17) \\
\chi_{irr}^Q(q) &= \int_k \chi_{XZ}(k + q) \chi_{YZ}(q) \\
&\quad + \Lambda^{-2} \chi_{x^2−y^2}(q) \quad (18)
\end{align*}
$$

where $f_x \cdots = T \sum_n \int \frac{dk}{\sqrt{\omega}} \cdots$. Here, we have dropped both the vertex and self-energy corrections. Apart from the factor $\Lambda^2$, the first term the irreducible susceptibility (18) is equivalent to $\chi_{TO}$ in eq. (9), or $\chi_{0 \text{, nem}}$ in Ref. 34. We also added the bare susceptibility $\chi_{x^2−y^2}$ as the second term in eq. (18). Due to the two-orbiton term, $\chi_{irr}^Q(0)$ is strongly enhanced near AFQ-QCP in proportion to $\xi^2$. When $\gamma_S$ is finite, $\chi_{x^2−y^2}(0)$ diverges even if $\xi$ is finite, and therefore the orthorhombic structure transition takes place in iron-based superconductors.

Note that the present action in eqs. (14)-(16) are mathematically equivalent to eqs. (3) and (4) in the spin-quadrupole theory in Ref. 34, by replacing $\phi_T (\Gamma = XZ, YZ)$ with $\phi_i (i = 1, 2)$, and $\chi_{XZ}^Q(q)$ with $\chi(x)$. Thus, the derived $T$-dependences of $C_S$ are essentially the same. However, the coupling between strain and spin-quadrupole, $\eta_S$, would be too small to fit experimental data: We will discuss this issue below.

### E. Comparison with spin quadrupole theory

As discussed in Sec. III, the orthorhombic structure transition is cause by the divergence of the $\Phi$ susceptibility with $\hat{x}^2 - \hat{y}^2$ symmetry. In this paper, we discussed the $\Phi$ fluctuation induced by the AF quadrupole fluctuations, due to the two-orbiton process. That is, antiferro-orbital fluctuations with respect to $O_{XZ}$ and $O_{YZ}$ (=orbitons) induce the $s_+$ wave superconducting state, and the bound-state formation of two-orbitons with zero momentum, $O_{XZ}(q) O_{YZ}(-q) \sim O_{XY}(0)$, give rise to the development of $\chi_{XY}^Q(0) = \chi_{x^2−y^2}^Q(0)$.

In this subsection, we discuss the “spin-nematic theory” for the structure transition discussed in Refs. 34,38, and explain a close relation to the two-orbiton mechanism. Their theories can be interpreted as the “two-magnon process” in our language. They had studied the non-local spin quadrupole operator $\hat{S}_S = m_1 \cdot m_2$ as explained in Sec. III A, and shown that the Ising-like order $\hat{S}_S \neq 0$ In both theories, the Ising-like order $(\langle \hat{S}_S \rangle \not= 0)$ occurs prior to the vector order $(\langle m_1 \rangle, \langle O_{XZ}, O_{YZ} \rangle \not= 0)$, since the latter is easily suppressed by thermal and quantum fluctuations. When the boson is orbiton (magnon), the realized superconductivity is the $s_+$ ($\pm$) wave state.

According to the fitting done in Sec. III, we have to assume $g_S \sim O(0.1) eV$ to reproduce $E_{JT} \equiv T_S - \theta \sim O(10)K$; the corresponding dimensionless $\epsilon$-ph coupling is...
had been also observed by ARPES measurements. The "nematic electronic state" free from lattice deformation was found in many pnictides. For example, in nearly antiferromagnetic metals, antiferromagnetic correlation is drastically enhanced near the nonmagnetic impurity site, and the local magnetic moment emerges around the impurity. Such phenomena are indeed observed in under-doped cuprates. As for the iron-based superconductors, the system would be close to antiferro-orbital QCP. Therefore, it is natural to expect the occurrence of "impurity-induced non-local orbital order" in pnictides.

In this section, we study the single impurity problem with potential $I$ in ten-orbital tight-binding model for pnictides, using the mean-field approximation in real space. Since we concentrate on the impurity-induced orbital-ordered state, we take only the quadrupole-quadrupole interaction in eq. (1) into account: We consider that the coupling constant $g$ in eq. (1) originates from both the $e$-$p$ hybridization as well as the multiorbital Coulomb interaction, as discussed in Sec. II. We obtain the following mean-field self-consistently for $g < g_c$, where $g_c = 0.221$ is the critical value for the bulk orbital order \cite{47}:

$$M_{i,m} \equiv \langle c_{i,l\sigma}^\dagger c_{i,m\sigma} \rangle_{l,g} - \langle c_{i,l\sigma}^\dagger c_{i,m\sigma} \rangle_{l,0}$$

where $i$ is the Fe site, and $l, m$ represent the $d$-orbital. Note that $M_{i,m}$ is impurity-induced mean-field for $g < g_c$ since it vanishes when $I = 0$. Then, the mean-field potential is given as

$$S_{l,m} = 2 \sum_{l',m'} \Gamma^c_{l,m,l',m'} M_{l',m'}$$

and the mean-field Hamiltonian is $\hat{H}_{\text{MF}} = \hat{H}_0 + \sum_i \hat{S}_i + \text{const.}$ $\Gamma^c$ is the bare four-vertex for the charge sector. We solve eqs. (19)-(20) self-consistently.

Since the present mean-field has 15 components at each site, it is convenient to consider the following quadrupole order:

$$O_{l,m} = 2 \sum_{l,m} \delta_{l,m} M_{l,m}$$

where $\Gamma = xz, yz, xy, z^2$, and $x^2 - y^2$. $O_{l,m}$ is the matrix element of the charge quadrupole operator given in Ref.\cite{18}. We note that the hexadecapole ($l = 4$) order is negligible in the present study.
In Fig. 7, we show the obtained DOS in real space for the cluster of 800 Fe sites with a single impurity site. First, we consider the case \( I = -2 \text{eV} \) in (a)-(c). For \( g = 0.200 \) (a), the impurity induced mean-field is absent. The small modulation of the LDOS around the impurity is caused by the Friedel oscillation. For \( g \geq 0.206 \), impurity induced non-local orbital order is induced. The symmetry of the corresponding LDOS is \( C_{2v} \), as shown in (b) for \( g = 0.210 \). The suppression of the DOS is caused by the non-local orbital order, consistently with a recent optical conductivity measurement. The LDOS are further suppressed with increasing \( g \), and the symmetry is lowered to \( C_2 \) for \( g > 0.212 \). In (c), we show the numerical result for \( g = 0.216 \) with \( C_{2v} \)-symmetry. Similar impurity-induced LDOS with \( C_{2v(V)} \)-symmetry is also obtained for a positive impurity potential. In contrast, we obtain the orbital order with \( C_4 \) symmetry for \( I = +1 \text{eV} \).

![FIG. 7: Obtained LDOS given by the mean-field theory in the presence of impurity potential at \((0,0)\). (a) \((I,g) = (-2,0.200)\): without orbital order. (b) \((I,g) = (-2,0.208)\): orbital order with \( C_{2v} \)-symmetry. (c) \((I,g) = (-2,0.216)\): orbital order with \( C_2 \)-symmetry. (d) \((I,g) = (+1,0.216)\): orbital order with \( C_{4v} \)-symmetry.](image)

The dominant impurity-induced quadrupole orders are antiferro \( O_{xz}, O_{yz} \) and \( O_{xy} \), reflecting the quadrupole-quadrupole interaction in eq. (1). The indispensable ingredient for \( C_2 \)-order is the quadrupole interaction for \( \Gamma = xz/yz \) channels. We have verified that the quadrupole interaction for \( \Gamma = x^2 - y^2 \) channel, which is caused by acoustic phonon, cannot realize the \( C_2 \)-order.

By symmetry, the obtained \( C_2 \)-order can be aligned by the strain-induced quadrupole potential, which is given in eq. (5) with \( \phi_S = O_{x^2 - y^2} \). The effective quadrupole potential is \( \Delta E = \eta_\delta \epsilon_S \cdot \chi^Q_{2 - y^2} (0) / \chi^Q_{2 - y^2} (0) \), which is strongly enhanced near \( T_S \) due to the two-orbital process as discussed in Sec. IIIA. This would be the reason why the nematic ordered state is easily detwinned by small uniaxial pressure near \( T_S \). In fact, detwinning by uniaxial pressure is possible only when the structure transition is the second-order, in which case the factor \( \chi^Q_{2 - y^2} (0) / \chi^Q_{2 - y^2} (0) \) develops divergently. In over-doped systems, detwinning by pressure would be difficult since \( \chi^Q_{2 - y^2} (0) / \chi^Q_{2 - y^2} (0) \) is no more large.

### B. in-plane anisotropy of resistivity

According to ARPES measurements in detwinned systems, \( \Delta E < 0 \) for \( x = a \)-axis is longer than \( y = b \)-axis, i.e., \( n_x > n_y \). Then, experimentally observed \((\pi,0)\) SDW order should be induced theoretically. In this case, the \( C_2 \) order aligns along the \( x = a \)-axis in the present numerical results in Figs. 7 (c) and (d). We have calculated the in-plane resistivity \( \rho_{ab} \) and \( \rho_{ab} \) in the presence of dilute \( C_2 \) orders along \( a \)-axis using the \( T \)-matrix approximation, which gives the exact result when the impurity concentration is dilute and localization is negligible. We find that \( \rho_{ab} \) is smaller than \( \rho_{ab} \) by \(~40\%) consistently with experimental reports. In Fig. 8 (a), we show the alignment of impurity-induced \( C_2 \) objects under uniaxial pressure. The anisotropy of resistivity in the nematic phase given by the \( T \)-matrix approximation is shown in Fig. 8 (b).

Here, we explain how to calculate the resistivity in the presence of aligned non-local orbital orders (nematic phase). The \( T \)-matrix is given by solving the following equation in the orbital-diagonal basis:

\[
\hat{T}_{r,r'}(\omega) = (\hat{I} + \hat{S})_r \delta_{r,r'} + \sum_{r''} (\hat{I} + \hat{S})_r \tilde{G}^{(0)}_{r',r''}(\omega) \hat{T}^R_{r''r'}(\omega)
\]

where \( \hat{S} \) is the mean-field potential, and \( \tilde{G}^{(0)}(\omega) \) is the Green function in real space without impurities. \( \hat{T} = \hat{T}_{\alpha} \delta_{\alpha} \) is the impurity potential. Note that \( \hat{T}_r \) is diagonal with respect to the position since our interaction Hamiltonian is local.

The preset \( T \)-matrix is non-local because of \( \hat{T}_r \) for \( r \neq r' \). After the Fourier transformation, the self-energy due to multiple scattering in the \( T \)-matrix approximation is \( \Sigma(k,\omega) = n_{\text{imp}} \hat{T}^{kk}(\omega) \), and the full Green function is \( \tilde{G}(k,\omega) = (\omega + \mu - H^0_k - \Sigma^R(k,\omega))^{-1} \). Then, the in-plane conductivity is given by

\[
\sigma_{\nu} = \frac{e^2}{\pi} \sum_{k,\alpha} v_{\nu,k}^a \tilde{G}_\alpha(k,\omega) G_\alpha(k,i\delta)'^2
\]

where \( \nu = x, y \), and \( \alpha \) represents the \( \alpha \)th band. \( v_{\nu,k} \) is the group velocity of the \( \alpha \)th band, and \( G_\alpha(k,\omega) \) is the full Green function in the band-diagonal basis. \( J_{k,\nu} \) is
the total current including the current vertex correction, which is given by solving the following Bethe-Salpeter equation:

\[ J_{\mathbf{k},\mathbf{k}'}^{\alpha} = \delta_{\mathbf{k},\mathbf{k}'} + \sum_{\mathbf{p},\mathbf{p}'\beta} J_{\mathbf{k},\mathbf{p}}^{\alpha\beta} G_{\mathbf{p}' \mathbf{p}}(\mathbf{p}, i\delta)^2 J_{\mathbf{p},\mathbf{k}'}^{\beta\alpha} \]  

(24)

where \( J_{\mathbf{k},\mathbf{k}'} \) is the irreducible vertex. As shown in Fig. 8(b), we obtain \( \rho_s / \rho_n \sim 2 \) in the nematic phase: The anisotropy is enhanced by including the current vertex correction.

Note that the averaged residual resistivity \( (\rho_s + \rho_b)/2 \) per 1\% impurity with \( I = +1\text{eV} \) or \( -2\text{eV} \) reaches \( \sim 50\mu\Omega\text{cm} \), which is comparable to the residual resistivity by 1\% Co impurities in Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\): 50 \( \sim 100\mu\Omega\text{cm} \).\(^{14,46}\)

C. Comparison between theory and experiments

In a pure two-dimension system, a single nonlocal orbital order in the mean-field approximation might disappear by thermal and quantum fluctuations. In real systems, however, orbital order would be stabilized by the correlation between impurities for \( n_{\text{imp}} \gtrsim 1\% \). Since the AF fluctuations increase as \( T \) decreases in real systems, we can interpret that \( g \) monotonically increases as \( T \) decreases in the present mean-field approximation. Therefore, we expect that impurity-induced non-local orbital order is stabilized below the nematic transition temperature \( T^* \), at which \( g(T) \) would be close to \( g_c \).

Although orbital order is absent above \( T^* \), strong orbital fluctuations should appear near the impurity site, in analogy to the impurity-induced strong magnetic fluctuations realized in under-doped cuprates.\(^{49}\) Therefore, inelastic scattering given by impurity-induced strong fluctuations causes large “residual resistivity” even above the impurity-induced Neel temperature.\(^{49}\) By the same reason, residual resistivity in under-doped pnictides would be large even above \( T^* \). The order parameters for the impurity induced nematic order are antiferro-\( O_{xz}/yz/zy \), while the order parameter for the structure transition is ferro-\( O_{x^2-y^2} \). Because of the difference in order parameters, \( T_S \) would be rather insensitive to the presence of impurities.

The nematic transition also occurs in the tetragonal phase of BaFe\(_2\)(As\(_{1-x}\)P\(_x\))\(_2\), which was confirmed by the in-plane anisotropy in the magnetization \( (\chi_{x} \neq \chi_{y}) \) using the torque measurement under magnetic field.\(^{7}\) In BaFe\(_2\)(As\(_{1-x}\)P\(_x\))\(_2\), \( P \) sites would works as impurities, which give finite potential on the neighboring for Fe sites. In this case, we had verified that non-local orbital order with \( C_{2z} \) or \( C_{1h} \)-symmetry appears around the impurity site in the mean-field approximation. In contrast, nematic order had not be observed in (K,Ba)Fe\(_2\)As\(_2\), maybe because impurities outside of FeAs plane would be too weak to induce orbital order.

In this paper, we consider that the charge quadrupole order occurs at \( T_S \), and the nematic order at \( T^* \) (\( > T_S \)) originates from the impurity-induced orbital order. However, difference scenario had been proposed by the authors in Ref.\(^7\): They consider that the quadrupole order occurs at \( T^* \), and \( T_S \) is just a meta-transition without symmetry breaking. In their phenomenological Landau model, very small orthorhombicity \( (a-b)/(a+b) \) occurs below \( T^* \), and it increases drastically below \( T_S \) as a meta-transition, consistently with experiments.

V. DISCUSSION

In the present paper, we have studied the realistic five-orbital model for iron pnictides. It was found that the \( O_{x^2-y^2} \)-AFQ fluctuations develop owing to the quadrupole-quadrupole interaction due to \( \epsilon \)-ph and Coulomb interactions. This fluctuations not only cause the \( s_{++} \)-wave
superconductivity, but also the orthorhombic structure transition due to two-orbital process. Using the two-orbital term, we can fit the recent experimental data of $C_S$ in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ for wide range of doping, only by choosing $T_{AFQ}$ while other parameters are almost fixed. This fact is a strong evidence for the success of orbital fluctuation theory in iron pnictide superconductors.

However, we consider the impurity effect on the $s_{++}$-wave state: In the weakly correlated metals, impurity effect on the $s_{++}$-wave state is very small, known as the Anderson theorem. In strongly correlated metals, in contrast, impurity-induced change in the many-body electronic states could violate the Anderson theorem. In Sec. IV, we have shown that the impurity-induced orbital order causes remarkable reduction in the DOS, accompanied by the suppression of orbital fluctuations. For this reason, orbital-fluctuation-induced $s_{++}$-wave state should be suppressed by impurities in the nematic state. In Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, the suppression in $T_c$ per 1% Zn-impurity, which gives a strong impurity potential, is $-\Delta T_c/\% \sim 3K^{16}$, while $-\Delta T_c/\% \sim 20K$ is expected in the $s_{++}$-wave state when the mass-enhancement is $m'/m_b \sim 3^{13}$. Such small impurity-induced suppression of $T_c$ in Ref.16 would be naturally explained by the impurity-induced orbital order.

In summary, the present orbital fluctuation theory can explain the (i) superconductivity, (ii) orthorhombic transition accompanied by large softening of $C_S$, and (iii) impurity-induced nematic order. To explain (i)-(iii), we have to assume that $\chi^{Q}_{zz(yz)}$ is the most divergent quadrupole susceptibility, which is actually satisfied in the present model Hamiltonian. We have derived the orbital fluctuation parameters from $C_S$, and succeeded in explaining $T_c$ and $\rho(T)$ using the derived parameters. These results are strong evidence for the realization of the orbital-fluctuation-mediated $s_{++}$-wave superconductivity in iron pnictides.

In Fig. 9, we summarize the phase-diagram of iron-pnictides given by the present orbital fluctuation theory. We stress that $T_{AFQ}$, which is determined experimentally from $C_S$, is positive in the under-doped case ($T_S > 0$) while it is negative in the over-doped case. Especially, $T_S \approx 0$ for $T_{AFQ} = 0$, consistently with experiments$^{4,5}$. This result indicates that QCPs for AFQ and FQ orders almost coincide at the endpoint of the orthorhombic phase. Therefore, AFQ-QCP is not hidden inside of the orthorhombic phase, favorably to the orbital-fluctuation-mediated $s_{++}$-wave SC state$^{17-19}$. Below $T^*$, impurity-induced orbital order with $C_{2(\nu)}$-symmetry starts to occur. Each orbital order can be aligned by applying tiny uniaxial pressure, resulting in the large in-plane anisotropy in the resistivity.

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