Self-consistent Vertex Correction Analysis for Iron-based Superconductors: Mechanism of Coulomb Interaction-Driven Orbital Fluctuations

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We study the mechanism of orbital or spin fluctuations due to multiorbital Coulomb interaction in iron-based superconductors, going beyond the random-phase approximation. For this purpose, we develop a self-consistent vertex correction (VC) method, and find that multiple orbital fluctuations in addition to spin fluctuations are mutually emphasized by the "multimode interference effect" described by the VC. Then, both antiferro-orbital and ferro-orbital (= nematic) fluctuations simultaneously develop for $J/U \sim 0.1$, both of which contribute to the s-wave superconductivity. Especially, the ferro-orbital fluctuations give the orthorhombic structure transition as well as the softening of shear modulus C_{66}.

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Since the discovery of iron-based superconductors, the mechanism of high-T_c superconductivity has been studied very actively. Theoretically, both the spin fluctuation-mediated $s_{\pm}$-wave state [with sign reversal of the gap between hole pocket (h pocket) and electron pocket (e pocket)] [1–5] and the orbital fluctuation-mediated s_{++}-wave state (without sign reversal) [6,7] has been proposed. The latter scenario is supported by the robustness of T_c against impurities in many iron pnictides [8–12]. The possibility of an impurity-induced crossover from $s_{\pm}$ to s_{++} states had been discussed theoretically [3,6]. In addition, the orbital-independent gap observed in $BaFe_2(As, P)_2$ and $(K, Ba)Fe_2As_2$ by laser angle-resolved photoemission spectroscopy measurement [13,14], and the "resonancelike" hump structure in the neutron inelastic scattering [15] are consistent with the orbital fluctuation scenario.

The nature of orbital fluctuations has been intensively studied after the discovery of large softening of the shear modulus C_{66} [16–18] and renormalization of phonon velocity [19] observed well above the orthorhombic structure transition temperature T_S. Consistently, a sizable orbital polarization is observed in the orthorhombic phase [20,21]. Moreover, the "electronic nematic state" with large in-plane anisotropy of resistivity or magnetization well above T_S and T_c [22,23] also indicates the occurrence of (impurity-induced local) orbital order [24].

The origin of orbital order or fluctuation has been actively discussed, mainly based on the multiorbital Hubbard model with intraorbital (interorbital) interaction U (U') and the exchange interaction $J = (U - U')/2 > 0$ [6,25]. In this Letter, we focused our attention to a good interorbital nesting of the Fermi surfaces shown in Fig. 1(a): Although moderate orbital fluctuations are induced by U' in the random-phase approximation (RPA), the spin susceptibility due to the intraorbital nesting, $\chi^s(\boldsymbol{q})$, is the most divergent for $J > 0$ (i.e., $U > U'$). Because $J/U \approx 0.12$–0.15 according to the first-principle study [26], the RPA fails to explain experimental "nonmagnetic" structure transition. This situation is unchanged even when the self-energy correction is considered in the fluctuation-exchange (FLEX) approximation [27].

To explain the strong development of orbital fluctuations, we had introduced a quadrupole interaction [6]:

$$H_{\text{quad}} = -g\sum_i (\hat{O}^i_{xz}\hat{O}^i_{xz} + \hat{O}^i_{yz}\hat{O}^i_{yz}), \tag{1}$$

where g is the coupling constant and $\hat{O}_\gamma$ is the charge quadrupole operator: $\gamma = xz,\ yz,\ xy,\ x^2\text{-}y^2,\ 3z^2\text{-}r^2$.

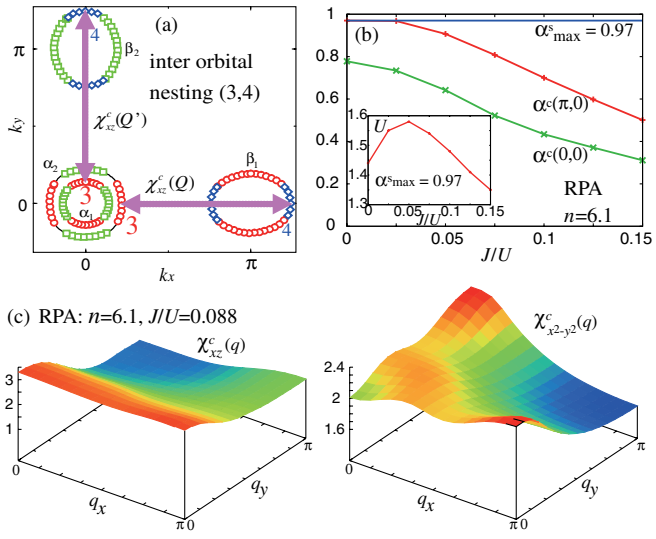

FIG. 1 (color online). (a) Fermi surfaces of iron pnictides. The colors correspond to $2 = xz$ (green square), $3 = yz$ (red circle), and $4 = xy$ (blue diamond), respectively. (b) $\alpha^c_{\boldsymbol{Q}}$, $\alpha^c_{\boldsymbol{0}}$, and U as function of J/U in RPA under the condition $\alpha^s_{\max} = 0.97$. (c) $\chi^c_{xz}(\boldsymbol{q})$ and $\chi^c_{x^2\text{-}y^2}(\boldsymbol{q})$ given by the RPA for $(J/U, U) = (0.088, 1.53)$.

[Hereafter, x, y axes (X, Y axes) are along the nearest Fe-Fe (Fe-As) direction.] This term is actually caused by the electron-phonon (e-ph) coupling due to in-plane Fe-ion oscillations [6,14,27]. Because $\hat{O}_{xz(yz)}$ induces the interorbital scattering, strong antiferro-orbital (AF orbital) fluctuations develop for $g \gtrsim 0.2$ eV owing to a good interorbital nesting. We also studied the vertex correction (VC) beyond the RPA [28], and obtained strong enhancement of ferro-quadrupole ($\hat{O}_{x^2\text{-}y^2} \propto \hat{n}_{xz} - \hat{n}_{yz}$) susceptibility $\chi^c_{x^2\text{-}y^2}(\mathbf{0})$, which causes the orthorhombic structure transition and the softening of C_{66} [28]. This "nematic fluctuation" is derived from the interference of two AF orbitons due to the symmetry relation $\hat{O}_{x^2\text{-}y^2}(\mathbf{0}) \sim \hat{O}_{XZ}(\boldsymbol{Q}) \times \hat{O}_{YZ}(-\boldsymbol{Q})$, where $\hat{O}_{XZ(YZ)} = [\hat{O}_{xz} + (-)\hat{O}_{yz}]/\sqrt{2}$. Then, it was natural to expect that such multiorbiton interference effect, which is given by the VC while dropped in the RPA, induces large "Coulomb interaction"driven orbital fluctuations.

In this Letter, we study the orbital and spin fluctuations in iron-based superconductors by considering the multiorbital Coulomb interaction with $U = U' + 2J$ and $J/U \sim O(0.1)$. We develop the self-consistent VC (SC-VC) method, and find that both ferro-$O_{x^2\text{-}y^2}$ and AF-$O_{xz/yz}$ fluctuations strongly develop even for $J/U \sim 0.1$, due to the interorbital nesting and the positive interference between multifluctuation (orbiton + magnon) modes. This result leads to a conclusion that RPA underestimates the orbital fluctuations in multiorbital systems. This study offers a unified explanation for both the superconductivity and the structure transition in many compounds.

Here, we study the five-orbital Hubbard model introduced in Ref. [1]. We denote d orbitals $m = 3z^2\text{-}r^2$, xz, yz, xy, and $x^2\text{-}y^2$ as 1, 2, 3, 4, and 5, respectively. The Fermi surfaces are mainly composed of orbitals 2, 3, and 4 [28]. Then, the susceptibility for the charge (spin) channel is given by the following 25×25 matrix form in the orbital basis:

$$\hat{\chi}^{c(s)}(q) = \hat{\chi}^{\mathrm{irr},c(s)}(q)[1 - \hat{\Gamma}^{c(s)}\hat{\chi}^{\mathrm{irr},c(s)}(q)]^{-1}, \quad (2)$$

where $q = (\boldsymbol{q}, \omega_l = 2\pi lT)$ and $\hat{\Gamma}^{c(s)}$ represents the Coulomb interaction for the charge (spin) channel composed of U, U', and J given in Refs. [6,14]. The irreducible susceptibility in Eq. (2) is given as

$$\hat{\chi}^{\mathrm{irr},c(s)}(q) = \hat{\chi}^{0}(q) + \hat{X}^{c(s)}(q), \quad (3)$$

where $\chi^0_{ll',mm'}(q) = -T\sum_p G_{lm}(p+q)G_{m'l'}(p)$ is the bare bubble, and the second term is the VC (or orbiton or magnon self-energy) that is neglected in both RPA and FLEX approximation. In the present discussion, it is convenient to consider the quadrupole susceptibilities:

$$\chi^c_{\gamma,\gamma'}(q) \equiv \sum_{ll',mm'} O^{l,l'}_{\gamma}\chi^c_{ll',mm'}(q)O^{m',m}_{\gamma'} = \mathrm{Tr}\{\hat{O}_\gamma\hat{\chi}^c(q)\hat{O}_{\gamma'}\}. \quad (4)$$

Nonzero matrix elements of the quadrupole operators for the orbitals 2–4 are $O^{3,4}_{xz} = O^{2,4}_{yz} = O^{2,2}_{x^2\text{-}y^2} = -O^{3,3}_{x^2\text{-}y^2} = 1$ [28]. Because of the symmetry, the off-diagonal susceptibilities ($\gamma \neq \gamma'$) are zero or very small for $\boldsymbol{q} = 0$ and the nesting vector $\boldsymbol{Q} \approx (\pi, 0)$ or $\boldsymbol{Q}' \approx (0, \pi)$ [28]. We do not discuss the angular momentum (dipole) susceptibility, $\chi^c_\mu(\boldsymbol{q}) \sim \langle \hat{l}_\mu(\boldsymbol{q})\hat{l}_\mu(-\boldsymbol{q})\rangle$, as it is found to be suppressed by the VC. Note that $\hat{O}_{\mu\nu} \propto \hat{l}_\mu\hat{l}_\nu + \hat{l}_\nu\hat{l}_\mu$.

To measure the distance from the criticality, we introduce the charge (spin) Stoner factor $\alpha^{c(s)}_{\boldsymbol{q}}$, which is the largest eigenvalue of $\hat{\Gamma}^{c(s)}\hat{\chi}^{\mathrm{irr},c(s)}(\boldsymbol{q})$ at $\omega_l = 0$: The charge (spin) susceptibility diverges when $\alpha^{c(s)}_{\max} \equiv \max_{\boldsymbol{q}}\{\alpha^{c(s)}_{\boldsymbol{q}}\} = 1$. In a special case $J = 0$, the relation $\alpha^s_{\max} = \alpha^c_{\max}$ holds at the momentum $\boldsymbol{Q}$ in the RPA; see Fig. 1(b). That is, both spin and orbital susceptibilities are equally enhanced at $J = 0$, which is unchanged by the self-energy correction in the FLEX approximation [27]. For $J > 0$, the spin fluctuations are always dominant ($\alpha^s_{\max} > \alpha^c_{\max}$) in the RPA or FLEX. However, because of large $\hat{X}^c(q)$, the opposite relation $\alpha^s_{\max} \lesssim \alpha^c_{\max}$ can be realized even for $J/U \lesssim 0.1$ in the SC-VC method.

First, we perform the RPA calculation for $n = 6.1$ and $T = 0.05$, using 32×32 $\boldsymbol{k}$ meshes: The unit of energy is electron volt (eV) hereafter. Figure 1(c) shows the diagonal quadrupole susceptibilities for $J/U = 0.088$: $\chi^c_\gamma(q) \equiv \chi^c_{\gamma\gamma}(q)$. (The spin susceptibility is shown in Ref. [1].) The Stoner factors are $\alpha^s_{\max} = 0.97$, $\alpha^c_{\boldsymbol{Q}} = 0.76$, and $\alpha^c_0 = 0.47$; see Fig. 1(b). In the RPA calculation, $\chi^c_{xz}(\boldsymbol{Q})$ [$\chi^c_{yz}(\boldsymbol{Q}')$] is weakly enlarged by the interorbital (3, 4) [(2, 4)] nesting, while $\chi^c_{x^2\text{-}y^2}(\boldsymbol{q})$ is relatively small and AF-like. Thus, the RPA calculation cannot explain the structure transition that requires the divergence of $\chi^c_{x^2-y^2}(\mathbf{0})$.

Next, we study the role of VC due to the Maki-Thompson (MT) and Aslamazov-Larkin (AL) terms in Fig. 2(a), which becomes important near the critical point [29,30]. Here, $\hat{X}^{c(s)}(q) \equiv \hat{X}^{\uparrow,\uparrow}(q) + (-)\hat{X}^{\uparrow,\downarrow}(q)$, and wavy lines represent $\chi^{s,c}$. The AL term (AL1 + AL2) for the charge sector, $X^{\mathrm{AL},c}_{ll',mm'}(q)$, is given as

$$\frac{T}{2}\sum_k\sum_{a\sim h}\Lambda_{ll',ab,ef}(q;k)\{V^c_{ab,cd}(k+q)V^c_{ef,gh}(-k) + 3V^s_{ab,cd}(k+q)V^s_{ef,gh}(-k)\}\Lambda'_{mm',cd,gh}(q;k), \quad (5)$$

where $\hat{V}^{s,c}(q) \equiv \hat{\Gamma}^{s,c} + \hat{\Gamma}^{s,c}\hat{\chi}^{s,c}(q)\hat{\Gamma}^{s,c}$, $\hat{\Lambda}(q;k)$ is the three-point vertex made of three Green functions in Fig. 2(a) [28], and $\Lambda'_{mm',cd,gh}(q;k) \equiv \Lambda_{ch,mg,dm'}(q;k) + \Lambda_{gd,mc,hm'}(q;-k-q)$. We include all U^2 terms, which are important for reliable results. The expressions of other VCs will be published in the future.

Both MT and AL terms correspond to the first-order mode-coupling corrections to the RPA susceptibility:

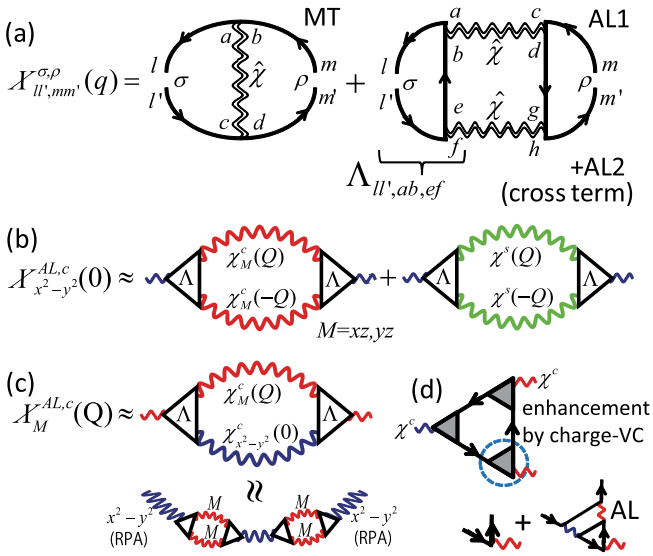

FIG. 2 (color online). (a) The MT and AL terms: The wavy and solid lines are susceptibilities and electron Green functions, respectively. $\Lambda_{ll',ab,ef}$ is the three-point vertex. (b) Dominant AL terms for $\chi^c_{x^2-y^2}(\mathbf{0})$; the first (second) term represents the two-orbiton (two-magnon) process. (c) Dominant AL terms for $\chi^c_M(\boldsymbol{Q})$ ($M = xz,\ yz$); higher-order terms with bubbles made of $\chi^c_M(\pm\boldsymbol{Q})$ (= multifluctuation process) are relevant. (d) Enhancement of $\Lambda_{ll',ab,ef}$ due to charge VCs.

The intrabubble (interbubble) correction gives the MT (AL) term [29]. In single-orbital models, the VC due to MT + AL terms had been studied by the self-consistent renormalization theory [29] or FLEX approximation with VC [30], and successful results had been obtained. In the former (latter) theory, the susceptibility is calculated in the self-consistent (self-inconsistent) way. Here, we find a significant role of the AL term inherent in the multiorbital Hubbard model.

In the present SC-VC method, we perform a self-consistent calculation of the VCs as well as charge/spin susceptibilities, which are given by Eqs. (2) and (3) and (5). Then, $\hat{\chi}^c(q)$ is strongly enhanced by $X^{\mathrm{AL},c}$ in Eq. (5), which is relevant when either $\hat{\chi}^c$ or $\hat{\chi}^s$ is large. On the other hand, we have numerically verified that $\hat{X}^s \sim T\sum \Lambda V^s V^c \Lambda$ is less important, although it can be relevant only when both $\hat{\chi}^c$ and $\hat{\chi}^s$ are large. Hereafter, we drop $\hat{X}^s(q)$ to simplify the argument. Figure 3(a) shows $\chi^c_\gamma(\boldsymbol{q})$ given by the SC-VC method for $n = 6.1$, $J/U = 0.088$, and $U = 1.53$, in which the Stoner factors are $\alpha^s_{\max} = \alpha^c_0 = 0.97$ and $\alpha^c_{\boldsymbol{Q}} = 0.86$. Compared with RPA, both $\chi^c_{x^2-y^2}(\boldsymbol{q})$ and $\chi^c_{xz}(\boldsymbol{q})$ are strongly enhanced by the charge AL term, $\hat{X}^{\mathrm{AL},c}$, because the results are essentially unchanged even if MT term is dropped. In the SC-VC method, the enhancements of other charge multipole susceptibilities are small. Especially, both the density and the dipole susceptibilities, $\sum_{l,m}\hat{\chi}^c_{ll,mm}(\boldsymbol{q})$ and $\chi^c_\mu(q)$ ($\mu = x,\ y,\ z$) respectively, are suppressed.

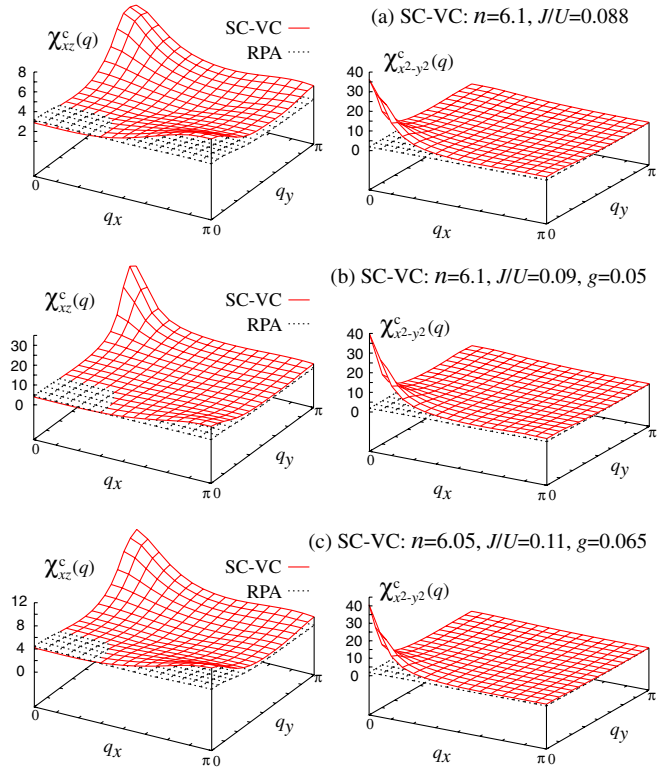

FIG. 3 (color online). $\chi^c_{xz}(\boldsymbol{q})$ and $\chi^c_{x^2-y^2}(\boldsymbol{q})$ given by the SC-VC method. The relation $\alpha^s_{\max} = \alpha^c_0 = 0.97$ is satisfied in all cases: (a) $n = 6.1$ and $J/U = 0.88$ ($\alpha^c_{\boldsymbol{Q}} = 0.86$), (b) $n = 6.1$, $J/U = 0.9$, and $g = 0.05$ ($\alpha^c_{\boldsymbol{Q}} = 0.96$), and (c) $n = 6.05$, $J/U = 0.11$, and $g = 0.065$ ($\alpha^c_{\boldsymbol{Q}} = 0.87$).

Here, we discuss the importance of the AL term: At $\boldsymbol{q} \approx \mathbf{0}$ or $\boldsymbol{Q}$, $\chi^c_\gamma(\boldsymbol{q})$ is enlarged by the diagonal VC with respect to γ, $X^{\mathrm{AL},c}_\gamma(\boldsymbol{q}) \equiv \mathrm{Tr}\{\hat{O}_\gamma \hat{X}^{\mathrm{AL},c}(\boldsymbol{q})\hat{O}_\gamma\}/\mathrm{Tr}\{\hat{O}^2_\gamma\}$, as the off-diagonal terms are absent or small [28]. The charge AL term in Eq. (5) is given by the products of two χ^c's (two-orbiton process) and two χ^s's (two-magnon process), shown in Fig. 2(b). The former process was discussed in Ref. [28], and the latter has a similarity to the spin nematic theory in Ref. [16] based on a frustrated spin model. Now, we consider the orbital selection rule for the two-orbiton process: Because of the relation $\mathrm{Tr}\{\hat{O}_{x^2-y^2}\hat{O}^2_M\} \neq 0$ for $M = xz,\ yz$ and a rough relation $\Lambda_{ll',ab,cd} \sim \Lambda_{ll',l'b,bl}\delta_{l',a}\delta_{b,c}\delta_{d,l}$ [28], the two-orbiton process for $\gamma = x^2$-y^2 is mainly given by $\chi^c_M(\boldsymbol{Q})^2$. According to Eq. (5) and Ref. [28], $X^{\mathrm{AL},c}_{x^2-y^2}(0) \sim \Lambda^2 U^4 T\sum_q \{\chi(q)\}^2$ grows in proportion to $T\chi(\boldsymbol{Q})$ [$\log\{\chi(\boldsymbol{Q})\}^2$] at high [low] temperatures. In the case of Fig. 3(a), the two-magnon process is more important for $\chi^c_{x^2-y^2}(0)$ because of the relation $\alpha^s_{\boldsymbol{Q}} > \alpha^c_{\boldsymbol{Q}}$. We checked that the two-magnon process is mainly caused by $\chi^s_{22,22}(\boldsymbol{Q})^2 - \chi^s_{22,33}(\boldsymbol{Q})^2 > 0$.

In the same way, $X^c_M(\boldsymbol{Q}) \sim \Lambda^2 U^4 T\sum_q \chi^c_M(q+Q)\chi^c_{x^2-y^2}(q)$ is enlarged by the two-orbiton process due to $\chi^c_M(\boldsymbol{Q})$ and $\chi^c_{x^2y^2}(\mathbf{0})$ as shown in Fig. 2(c). [In this case, two-magnon

process is less important as $\chi^s(0)$ is small.] The obtained $\chi^c_{xz}(\boldsymbol{q})$ has peaks at $\boldsymbol{q} = \boldsymbol{Q}$ and $\boldsymbol{Q}'$ because the interorbital scattering is emphasized by $X^c_{xz}(\boldsymbol{Q}) \propto \chi^c_{x^2-y^2}(\boldsymbol{0}) \gg 1$. Thus, both $\chi^c_{xz}(\boldsymbol{Q})$ and $\chi^c_{x^2-y^2}(\boldsymbol{0})$ are strongly enlarged in the SC-VC method, because of the "positive feedback" brought by these two AL terms: Figure 2(c) shows an example of the higher-order terms that are automatically generated in the SC-VC method. Such "multifluctuation processes" inherent in the self-consistent method magnify the RPA results.

Thus, strong ferro- and AF-orbital fluctuations are caused by AL terms. Both fluctuations work as the pairing interaction for the s_{++} state, while the ferro fluctuations are also favorable for the $s_{\pm}$ state. For $J/U < (J/U)_c \equiv 0.088$, the relation $\alpha^s_{\max} < \alpha^c_0 = 0.97$ is realized and $\alpha^c_{\boldsymbol{Q}}$ increases towards unity. In this case, orbital order occurs before the spin order as increasing U with J/U is fixed, since the VC (due to two-orbiton process) can efficiently enlarge orbital susceptibilities because of large $\alpha^c_{\max}$(RPA). This situation would be consistent with wider nonmagnetic orthorhombic phase in Nd(Fe,Co)As and many 1111 compounds.

Because the present SC-VC method is very time consuming, we applied some simplifications: In the self-inconsistent calculation, we have verified that $\mathrm{Tr}\{\hat{O}_\gamma \hat{X}(q) \hat{O}_{\gamma'}\}$ with $\gamma \neq \gamma'$ is zero or very small, especially at $\boldsymbol{q} = \boldsymbol{0}$ and $\boldsymbol{Q}$ for the reason of symmetry. As we are interested in the enhancement of $\chi^c_\gamma(\boldsymbol{q})$ at $\boldsymbol{q} = 0$ and $\boldsymbol{Q}$, and the dominant interferences between $\gamma = xz$, yz, $x^2 - y^2$, we calculated $X_{ll',mm'}(q)$ only for $\{(l, l'), (m, m')\} \in xz$, yz, x^2-y^2. [$(l, l') \in \gamma$ means that $O^{l,l'}_\gamma \neq 0$.] That is, $\{(l, l'), (m, m')\} = \{(1, 2), (3, 4), (2, 5)\}$, $\{(1, 3), (2, 4), (3, 5)\}$, and $\{(1, 5), (2, 2), (3, 3)\}$.

We stress that both $(J/U)_c$ and AF-orbital fluctuations increase by considering the following two factors: The first one is the charge VC at each point of the three-point vertex in Fig. 2(d), as a consequence of the Ward identity between $\hat{\Lambda}$ and $\hat{\chi}^{\mathrm{irr}}$. The enhancement factor at each point is estimated as $1 + X^c_\gamma/\chi^0_\gamma = 1.3$–$2.5$ for $\gamma = xz$ and x^2-y^2 in the present calculation near the critical point. This effect will increase $(J/U)_c$ sensitively. The second factor is the e-ph interaction: We introduce the quadrupole interaction in Eq. (1) due to Fe-ion oscillations [6,14,27]. As shown in Fig. 3(b), very strong AF-orbital fluctuations are obtained for $J/U = 0.09$ and $g = 0.05$: $\alpha^s_{\max} = \alpha^c_0 = 0.97$ and $\alpha^c_{\boldsymbol{Q}} = 0.96$. The corresponding dimensionless coupling is just $\lambda = gN(0) \sim 0.035$ [6,27]. We also study the case $n = 6.05$ and $g = 0.065$, and find that the relation $\alpha^s_{\max} = \alpha^c_{\max} = 0.97$ is realized at $(J/U)_c = 0.11$, as shown in Fig. 3(c). For these reasons, strong ferro- and AF-orbital fluctuations would be realized by the cooperation of the Coulomb and weak e -ph interactions.

Finally, we make some comments: The present multifluctuation mechanism is not described by the dynamical-mean-field theory, because the irreducible VC is treated as local. Also, the local density approximation, in which the VC is neglected, does not reproduce the nonmagnetic orthorhombic phase. Although Yanagi *et al.* studied $U' > U$ model [7] based on the RPA calculation, the model was first studied in Ref. [31], $\chi^c_{3z^2-r^2}(\boldsymbol{0})$ develops while $\chi^c_{x^2-y^2}(\boldsymbol{0})$ remains small, which is inconsistent with the structure transition. Our important future issue is to include the electron self-energy correction into the SC-VC method, which is important to discuss the filling and T dependences of orbital and spin fluctuations, and to obtain more reliable $(J/U)_c$.

In summary, we developed the SC-VC method, and obtained the Coulomb interaction-driven nematic and AF-orbital fluctuations due to the multimode (orbitons + magnons) interference effect [28] that is overlooked in the RPA calculation. For $J/U \lesssim (J/U)_c$, the structure transition ($\alpha^c_0 \approx 1$) occurs before the magnetic transition ($\alpha^s_{\boldsymbol{Q}} \approx 1$), which is consistent with the experiments. When $\alpha^s_{\max} \sim \alpha^c_{\max}$, both s_{++} and $s_{\pm}$ states could be realized, depending on model parameters such as the impurity concentration [3,6]. In a sense of the renormalization group scheme, the quadrupole interaction in Eq. (1) is induced by the Coulomb interaction beyond the RPA. We expect that orbital fluctuation-mediated superconductivity and structure transition are realized in many iron-based superconductors due to the cooperation of the Coulomb and e-ph interactions.

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