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

Seichiro Onari¹ and Hiroshi Kontani²

¹ Department of Applied Physics, Nagoya University and JST, TRIP, Furo-cho, Nagoya 464-8602, Japan.
² Department of Physics, Nagoya University and JST, TRIP, Furo-cho, Nagoya 464-8602, Japan.

(Dated: May 5, 2014)

We study the mechanism of orbital/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 (SC-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 the 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 $C_{66}$.

PACS numbers: 74.70.Xa, 74.20.-z, 74.20.Rp

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] had been proposed. The latter scenario is supported by the robustness of $T_c$ against impurities in many iron-pnictides [8–12]. Possibility of impurity-induced crossover from $s_\pm$ to $s_{++}$ states had been discussed theoretically [3, 6]. Also, orbital-independent gap observed in BaFe$_2$(As,P)$_2$ and (K,Ba)Fe$_2$As$_2$ by laser ARPES measurement [13, 14] as well as the "resonance-like" hump structure in the neutron inelastic scattering [15] are consistent with the orbital fluctuation scenario.

Nature of orbital fluctuations has been studied intensively 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].

Origin of orbital order/fluctuation had been actively discussed, mainly based on the multi-orbital Hubbard model with intra (inter) orbital interaction $U$ ($U'$) and the exchange interaction $J = (U - U')/2 > 0$ [6, 25]. We had focused attention to a good inter-orbital 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 intra-orbital nesting, $\chi'(q)$, is the most divergent for $J > 0$ (i.e., $U > U'$). Since $J/U \approx 0.12 - 0.15$ according to the first-principle study [26], the RPA fails to explain experimental "nonmagnetic" structure transition. This situation is unchanged even if 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]:

$$H_{quad} = -g \sum_i \left( \hat{O}_{xx}^i \hat{O}_{xx}^i + \hat{O}_{yz}^i \hat{O}_{yz}^i \right)$$

(1)

where $g$ is the coupling constant, and $\hat{O}_s$ is the charge quadrupole operator $\gamma = xz, yz, xy, x^2 - y^2, 3z^2 - r^2$. This term is actually caused by the electron-phonon (e-ph) coupling due to in-plane Fe-ion oscillations [6, 14, 27]. Since $\hat{O}_{xz(yz)}$ induces the inter-orbital scattering, strong antiferro (AF) orbital fluctuations develop for $g \gtrsim 0.2\text{eV}$ owing to a good inter-orbital nesting. We also studied the vertex correction (VC) beyond the RPA [28], and obtained strong enhancement of ferro-quadrupole $\langle \hat{O}_{xz(yz)} \rangle \propto \hat{n}_{xz} - \hat{n}_{yz}$ susceptibility $\chi_{xz(yz)}^c$, 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 $O_{xz-yz}(0) \sim \hat{O}_{XZ}(Q) \times \hat{O}_{YZ}(-Q)$, where $\hat{O}_{XZ(YZ)} = \hat{O}_{xz} + (-)\hat{O}_{yz}/\sqrt{2}$. Then, it was natural to expect that such multi-orbiton 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 multi-orbital 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-$O_{xz-yz}$ and AF-$O_{xz(yz)}$ fluctuations strongly develop even for $J/U \sim 0.1$, due to the inter-orbital nesting and the positive interference between multi-fluctuation (orbiton+magnon) modes. This result leads to a conclusion that RPA underestimates the orbital fluctuations in multi-orbital sys-
tems. The present study offers a unified explanation for both the superconductivity and structure transition in many compounds.

Here, we study the five-orbital Hubbard model introduced in Ref. [1]. We denote $d$-orbitals $m = 3z^2 - r^2$, $xz$, $yz$, $xy$, and $x^2 - y^2$ 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 $25 \times 25$ matrix form in the orbital basis:

$$\chi^{c(s)}(q) = \chi^{irr,c(s)}(q)(1 - \Gamma^{c(s)}\chi^{irr,c(s)}(q))^{-1},$$  \hspace{1cm} (2)

where $q = (q_x, q_y) = 2\pi i T$, and $\Gamma^{c(s)}$ 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

$$\chi^{irr,c(s)}(q) = \chi^0(q) + \tilde{\chi}^{c(s)}(q),$$  \hspace{1cm} (3)

where $\chi^0_{\ell,m\nu}(q) = -T \sum_p G_{\ell,m}(p + q)G_{m\nu'}(p)$ 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:

$$\chi^{c,\gamma\gamma}(q) = \sum_{\ell' \nu', m'\nu} O_{\gamma\delta}^{\ell'\nu'} \chi^{c,\delta\gamma}_{\ell',m'}(q)O_{\gamma\delta}^{\ell\nu}, \hspace{1cm} \text{Tr}\{\hat{O}_\gamma \hat{\chi}^{c}(q) \hat{O}_\gamma\},$$  \hspace{1cm} (4)

Non-zero matrix elements of the quadrupole operators for the orbital $2 \sim 4$ are $O^{3,4}_{-2,2} = O^{2,4}_{2,2} = -O^{3,3}_{-2,-2} = 1$ [28]. Because of the symmetry, the off-diagonal susceptibilities ($\gamma \neq \gamma'$) are zero or very small for $q = 0$ and the nesting vector $Q \approx (\pi, 0)$ or $Q' \approx (0, \pi)$ [28]. We do not discuss the angular momentum (dipole) susceptibility, $\chi^{c}(q) \sim (\hat{\ell}_{\mu}(q)\hat{\ell}_{\mu}(q))$, since it is found to be suppressed by the VC. Note that $\hat{O}_{\mu\nu} \propto \hat{\ell}_{\nu}(q)\hat{\ell}_{\mu}(q)$.

To measure the distance from the criticality, we introduce the charge (spin) Stoner factor $\alpha_a^{c(s)}$, which is the largest eigenvalue of $\Gamma^{c(s)}\chi^{irr,c(s)}(q)$ at $\omega_l = 0$.

The charge (spin) susceptibility diverges when $\alpha_{\text{max}}^{c(s)} = \max_a\{\alpha_a^{c(s)}\} = 1$. In a special case $J = 0$, the relation $\alpha_{\text{max}}^{c(s)} = \alpha_{\text{max}}^{c}$ holds at the momentum $Q$ 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 ($\alpha_{\text{max}}^{c} > \alpha_{\text{max}}^{c(s)}$) in the RPA or FLEX. However, because of large $\hat{\chi}^{c}(q)$, the opposite relation $\alpha_{\text{max}}^{c} \lesssim \alpha_{\text{max}}^{c(s)}$ 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 $32 \times 32 \times 2$ $k$-meshes: the unit of energy is eV hereafter. Figure 1 (c) shows the diagonal quadrupole susceptibilities for $J/U = 0.088$: $\chi^{c}_{x}(q) \equiv \chi^{c}_{y}(q)$. (The spin susceptibility is shown in Ref. [1].) The Stoner factors are $\alpha_{\text{max}}^{c} = 0.97$, $\alpha_{\text{Q}}^{c} = 0.76$, and $\alpha_{\text{Q}}^{c} = 0.47$; see Fig. 1 (b). In the RPA, $\chi^{c}_{xx}(Q)$ is weakly enlarged by the inter-orbital $(3, 4)$ [28] nesting, while $\chi^{c}_{x^2-y^2}(q)$ is relatively small and AF-like. Thus, the RPA cannot explain the structure transition that requires the divergence of $\chi^{c}_{x^2-y^2}(q)$.

Next, we study the role of VC due to the Maki-Thompson (MT) and Aslamazov-Larkin (AL) terms in Fig. 2 (a), which become important near the critical point [29, 30]. Here, $\hat{\chi}^{c}(q) \equiv \hat{\chi}^{c,xx}(q) + (-)\hat{\chi}^{c,yy}(q)$, and wavy lines represent $\chi^{c}$. The AL term (AL1+AL2) for the charge sector, $\xi^{c,\ell_{m\nu\mu}(q)}$, is given as

$$\frac{T}{2} \sum \Lambda_{\ell m\nu\mu}(k + q)\Lambda'_{\ell' m'\nu'\mu'}(k; k) + 3V_{ab,cd}(k) V_{ef,gh}(k)\Lambda'_{mm', cd, gh}(q; q),$$  \hspace{1cm} (5)

where $\Lambda^{c,\gamma_{\gamma}(q) \equiv \tilde{\Lambda}^{c,\gamma_{\gamma}(q) \hat{\Lambda}^{c,\gamma_{\gamma}(q)}}$ is the three-point vertex made of three Green functions in Fig. 2 (a) [28], and $\Lambda_{mm',cd, gh}(q; k) \equiv \Lambda_{g,d,mh,cd}(q; k) + \Lambda_{gd,m,cm}(q; k)$.

We include all $U^2$-terms, which are important for reliable results. The expressions of other VCAs will be published in future.

Both MT and AL terms correspond to the first-order mode-coupling corrections to the RPA susceptibility: The intra- (inter-) bubble 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 (SCR) 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.
factors are \( \chi \) to the RPA, both density and dipole susceptibilities, multipole susceptibilities are small. Especially, both the are essentially unchanged even if MT term is dropped. It could be relevant only when both \( \hat{q} \) (two-orbiton process) and two \specialchar{94}s (two-magnon process) is given by the products of two \( X \) that \( \hat{q} \) is large. On the other hand, we have verified numerically Dominant AL terms for \( \chi_{\text{M}}^{s}(Q) \) (multiorbital Hubbard model). Here, we find a significant role of the AL term inherent in the multiorbital Hubbard model.

Now, we perform the SC-VC analysis, in the way to satisfy \( \chi_{\text{M}}(q) \) in the VC are equal to the total susceptibilities in Eq. (2). Then, \( \chi_{\text{M}}(q) \) is strongly enhanced by \( X_{\text{AL},c}^{s} \) in Eq. (5), which is relevant when either \( \chi_{\text{c}}^{s} \) or \( \chi_{\text{c}}^{s} \) is large. On the other hand, we have verified numerically that \( X_{\text{c}}^{s} \sim T\sum \Delta \cdot \chi_{\text{c}}^{s} \cdot \Delta \) is less important, although it could be relevant only when both \( \chi_{\text{c}}^{s} \) and \( \chi_{\text{c}}^{s} \) are large. Hereafter, we drop \( X_{\text{c}}^{s} \) to simplify the argument. Figure 3 (a) show \( \chi_{\text{M}}^{s}(q) \) given by the SC-VC method for \( n = 6.1, J/U = 0.088 \) and \( U = 1.53 \), in which the Stoner factors are \( \alpha_{\text{max}}^{s} = \alpha_{0}^{s} = 0.97 \) and \( \alpha_{Q}^{s} = 0.86 \). Compared to the RPA, both \( \chi_{\text{c}}^{s-2} \) and \( \chi_{\text{AL},c}^{s} \) are strongly enhanced by the charge AL term, \( \hat{X}_{\text{AL},c}^{s} \), since 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 dipole susceptibilities, \( \sum_{l,m} \chi_{\text{M},m}^{s}(q) \) and \( \chi_{\text{c}}^{s}(q) \) are respectively suppressed.

Here, we discuss the importance of the AL term: At \( q \approx 0 \) or \( Q \), \( \chi_{\text{c}}^{s}(q) \) is enlarged by the diagonal vertex correction with respect to \( \gamma \), \( X_{\text{AL},c}^{s}(q) \equiv \text{Tr} \{ \hat{O}_{\gamma} \hat{X}_{\text{AL},c}^{s}(q) \hat{O}_{\gamma} \} / \text{Tr} \{ \hat{O}_{\gamma}^{2} \} \), since the off-diagonal terms are absent or small [28]. The charge AL term in Eq. (5) is given by the products of two \( \chi_{\text{c}}^{s} \) (two-orbiton process) and two \( \chi_{\text{c}}^{s} \) (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 \( \text{Tr} \{ \hat{O}_{\gamma} \hat{O}_{\gamma}^{2} \} \neq 0 \) for \( M = xz, yz \) and a rough relation \( \Lambda_{\text{MT},ab,cd}^{s} \sim \Lambda_{\text{MT},ab,cd}^{s} \delta_{a}^{b} \delta_{c}^{d} \) [28], the two-orbiton process for \( \gamma = x^{2} - y^{2} \) is mainly given by \( \chi_{\text{M}}^{s}(Q) \). According to Eq. (5) and Ref. [28], \( \chi_{\text{c}}^{2} \approx \chi_{\text{c}}^{2} \) grows in proportion to \( T \chi(Q) \left[ \log \chi(Q) \right]^{2} \) at high [low] temperatures. In the case of Fig. 3 (a), two-magnon process is more important for \( \chi_{\text{c}}^{2} \) (two-magnon process) because of the relation \( \alpha_{\gamma}^{s} > \alpha_{Q}^{s} \). We checked that the two-magnon process is mainly caused by \( \chi_{\text{c}}^{2} \).
AL terms: Figure 2 (c) shows an example of the higher-order terms that are automatically generated in the SC-VC method. Such “multi-fluctuation 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 ferrofluctuations are also favorable for the $s_{\pm}$-state. For $J/U < (J/U)_e \equiv 0.088$, the relation $\alpha^c_{e \text{max}} < \alpha^c_0 = 0.97$ is realized and $\alpha^c_0$ increases towards unity. In this case, orbital order occurs prior to the spin order as increasing $U$ with $J/U$ is fixed, since the VC (due to two-orbital process) can efficiently enlarge orbital susceptibilities because of large $\alpha^c_{\text{max}}(\text{RPA})$. This situation would be consistent with wider non-magnetic orthorhombic phase in Nd(Fe,Co)As and many 1111 compounds.

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

We stress that both $(J/U)_c$ and AF-orbital fluctuations increase by considering 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 $\Lambda$ and $\hat{\chi}^{\text{irr}}$. The enhancement factor at each point is estimated as $1 + X^\gamma_\gamma/\chi^0_\gamma \approx 1.3 \sim 2.5$ for $\gamma = xx$ 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 $g = 0.05$; $\alpha^c_{e \text{max}} = \alpha^c_0 = 0.97$ and $\alpha^c_Q = 0.96$. 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 $\alpha^c_{e \text{max}} = \alpha^c_{\text{max}} = 0.97$ 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 multi-fluctuation mechanism is not described by the dynamical-mean-field theory (DMFT), since the irreducible VC is treated as local. Also, the local density approximation (LDA), 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, that was first studied in Ref. [31], $\chi_{3z^2-r_2}(0)$ develops while $\chi_{3z^2-r_2}(0)$ remains small, inconsistently 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+magrons) interference effect [28] that is overlooked in the RPA. For $(J/U) \lesssim (J/U)_c$, the structure transition $(\alpha^c_0 \approx 1)$ occurs prior to the magnetic transition $(\alpha^c_Q \approx 1)$, consistently with experiments. When $\alpha^c_{e \text{max}} \approx \alpha^c_{\text{max}}$, both $s_{++}$- and $s_{\pm}$-states could be realized, depending on model parameters like 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.

This study has been supported by Grants-in-Aid for Scientific Research from MEXT of Japan, and by JST, TRIP. Part of numerical calculations were performed on the Yukawa Institute Computer Facility.

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