Effect of electron-phonon interactions on orbital fluctuations in iron-based superconductors

Yusuke Nomura\textsuperscript{1}, Kazuma Nakamura\textsuperscript{2}, and Ryotaro Arita\textsuperscript{1,3}
\textsuperscript{1}Department of Applied Physics, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113-8656, Japan
\textsuperscript{2}Quantum Physics Section, Kyushu Institute of Technology, 1-1 Sensui-cho, Tobata, Kitakyushu, Fukuoka, 804-8550, Japan and
\textsuperscript{3}JST-PRESTO, Kawaguchi, Saitama, 332-0012, Japan
(Dated: May 15, 2013)

To investigate the possibility whether electron-phonon coupling can enhance orbital fluctuations in iron-based superconductors, we develop an \textit{ab initio} method to construct the effective low-energy models including the phonon-related terms. With the derived effective electron-phonon interactions and phonon frequencies, we estimate the static part ($\omega = 0$) of the phonon-mediated effective on-site intra- or inter-orbital electron-electron attractions as $\sim -0.4$ eV and exchange or pair-hopping terms as $\sim -0.02$ eV. We analyze the model with the derived interactions together with the electronic repulsions within the random phase approximation. We find that the enhancement of the orbital fluctuations due to the electron-phonon interactions is small, making the spin fluctuations dominant. As a result, the superconducting state with the sign reversal in gap functions ($s_{\pm}$-wave) is realized.

PACS numbers: 74.70.Xa, 74.25.Kc, 63.20.dk, 74.20.Rp

\textit{-Introduction.} The mechanism of superconductivity in iron-based superconductors has attracted much attention owing to its high critical temperature ($T_c$) \cite{1}. The pairing symmetry of the Cooper pair is a central issue and in active debate. The $s_{\pm}$ symmetry with a sign reversal in the gap functions mediated by spin fluctuations is a possible candidate \cite{2-11}. On the other hand, a possibility of the $s_{++}$-wave state without the sign reversal is also pursued \cite{12-14}. \textit{Ab initio} estimated total electron-phonon (el-ph) coupling constant $\lambda$ is known to be too small as $\sim 0.2$ to reproduce the experimental $T_c$ \cite{15}, so the $s_{++}$-wave state here is not realized by conventional phonon-mediated mechanism. Instead, the el-ph interactions can enhance the orbital fluctuations in the Fe-3$d$ orbitals, and, as a result, contribute to the superconductivity \cite{12, 13}. \textit{Ab initio} estimations of hopping parameters and effective Coulomb interactions are widely done with several approximations \cite{16-21}, while, in this issue, we also need to evaluate effective electron-electron (el-el) interactions mediated by phonons. To pursue the realistic mechanism and handle the complexity in the iron-based superconductors, such estimates and related methodological developments are highly needed.

In this Letter, we present an \textit{ab initio} effective low-energy model including phonon terms for the iron-based superconductor, LaFeAsO. The effective el-ph interactions and phonon frequencies in the model are estimated using the density-functional perturbation theory (DFPT) \cite{22} with a constraint that screening processes in the Fe-3$d$ bands are excluded. From the derived parameters, we estimated the phonon-mediated on-site el-el attractions. The resulting values for the static part are $\sim -0.4$ eV for the intra- and inter-orbital terms and $\sim -0.02$ eV for the exchange and pair-hopping ones. This result is in contrast to the past classical estimates in Refs. \cite{12, 13}, where the intra-orbital and exchange terms are comparable as $\sim -0.4$ eV.

We analyzed the model including electronic repulsions as well as the derived phonon-mediated interactions within the random phase approximation (RPA). Due to the small phonon-mediated on-site exchange and pair-hopping interactions, the enhancement of the orbital fluctuations is small, and thus the $s_{\pm}$-wave state mediated by spin fluctuations is realized. Therefore, the introduction of the el-ph interactions with the \textit{ab initio} energy scale does not lead to the $s_{++}$-wave state, leaving the possibility that the el-el vertex corrections is the driving force \cite{23}.

\textit{-Downfolding.} We now describe the basic idea of the derivation of the phonon-related terms in the effective model. In the present approach, we first divide the one-particle Hilbert space into two parts. One is the target subspace ($t$-subspace) consisting of electronic bands near the Fermi level. In the case of LaFeAsO, the $t$-subspace corresponds to Fe-3$d$ bands, which are the target-band degrees of freedom of the effective model. The other is the rest of the Hilbert space, which is referred to as $r$-subspace. With these definitions, the total RPA polarization $\chi$ can be divided into $\chi_t$ and $\chi_r$ with $\chi_t$ being the polarization within the $t$-subspace and $\chi_r = \chi - \chi_t$ is the rest of the polarization.

The screened el-ph interaction for the effective model is calculated by

\[ g^{(t)} = [1 - v \chi_r]^{-1} g^{(b)}, \]  

where $v$ and $g^{(b)}$ are the bare Coulomb and el-ph interaction, respectively \cite{24}. Note that, in this treatment, we use $\chi_r$, excluding a screening due to $\chi_t$. This is because the $t$-subspace screening is accounted when the model is solved. Therefore, in the derivation step of the effective
model, we have to exclude the t-subspace screening to avoid its double counting [25]. In the sense of the partially screened quantity, we attach the superscript “p” to the el-ph interaction $g$ in Eq. (1).

The same idea is applied to the derivation of the phonon frequencies in the effective model. The partially dressed phonon Green’s function $D^{(p)}$ is given by

$$
[D^{(p)}]^{-1} = [D^{(b)}]^{-1} - \Sigma_r,
$$

where $D^{(b)}$ is the bare phonon Green’s function. $\Sigma_r$ is defined as $\Sigma_r = \Sigma - \Sigma_i$ with $\Sigma$ and $\Sigma_i$ being the total phonon self-energy and the phonon self-energy due to the interactions between the t-subspace electrons and the phonons, respectively. The pole of $D^{(p)}$ gives the effective phonon frequency $\omega_r^{(p)}$ in the model.

Practically, we calculate $g^{(p)}$ and $\omega^{(p)}$ using the DFPT [22] in the constraint on the electron density response to the perturbation. In the usual DFPT, the density response is represented by the sum of the variations of the Kohn-Sham wave functions, but, in our treatment, we do not include contributions from the t-subspace wave functions to the sum. With such an exclusion, we perform DFPT calculations to obtain $g^{(p)}$ and $\omega^{(p)}$ not including the t-subspace screening and self-energy effects. Without the constraint, fully-screened quantities are calculated, to which we attach the superscript “f”. Detailed descriptions of our method, which we call constrained DFPT (cDFPT), are given elsewhere [26].

Now we write down the phonon-related terms in the effective model. The effective el-ph interactions are

$$
\mathcal{H}_{\text{el-ph}} = \frac{1}{\sqrt{N_k}} \sum_{\mathbf{q}'} \sum_{\mathbf{k}j\sigma} g^{(p)\nu}_{ij\sigma}(\mathbf{k}, \mathbf{q}) c_{\mathbf{k}q\nu}^\dagger c_{\mathbf{k}q\nu} + h.c.,
$$

where $b_{\mathbf{q}\nu}$ ($b_{\mathbf{q}\nu}^\dagger$) is the annihilation (creation) operator of the phonon with the wave vector $\mathbf{q}$ and the branch $\nu$. $c_{\mathbf{k}q\nu}^\dagger (c_{\mathbf{k}q\nu})$ annihilates (creates) the $i$-th Wannier orbital’s electron with the wave vector $\mathbf{k}$ and the spin $\sigma$. $N_k$ is the number of $\mathbf{k}$ points. The phonon one-body part is given as

$$
\mathcal{H}_{\text{ph}} = \sum_{\mathbf{q}\nu} \omega^{(p)}_{\mathbf{q}\nu} b_{\mathbf{q}\nu}^\dagger b_{\mathbf{q}\nu}.
$$

The momentum-space-averaged phonon-mediated effective el-el interaction $V^{(p)}_{ij,i'j'}$ [Fig. 1(a)] is given by

$$
V^{(p)}_{ij,i'j'}(\omega_t) = \frac{1}{N_\mathbf{k}} \sum_{\mathbf{q}\nu} \left( \frac{1}{N_\mathbf{k}} \sum_{\mathbf{k}} g^{(p)\nu}_{ij}(\mathbf{k}, \mathbf{q}) \right) D^{(p)}_{\mathbf{q}\nu}(\omega_t) \times \left( \frac{1}{N_\mathbf{k}} \sum_{\mathbf{k}'} \left( g^{(p)\nu}_{i'j'}(\mathbf{k}', \mathbf{q}) \right)^* \right),
$$

with $\omega_t = 2\pi IT$ being the boson Matsubara frequency. Note that $V^{(p)}_{ij,i'j'}$ corresponds to the on-site quantity because of the momentum-space averaging.

This $V^{(p)}_{ij,i'j'}$ is distinguished from the momentum-space-averaged phonon-mediated effective pairing interaction $V^{(p)}_{ij,i'j'}$ [Fig. 1(b)] as

$$
V^{(p)}_{ij,i'j'}(\omega_t) = \frac{1}{N_\mathbf{q}_\mathbf{k}} \sum_{\mathbf{q}\nu} \sum_{\mathbf{k}} \left( g^{(p)\nu}_{ij}(\mathbf{k}, \mathbf{q}) \right) D^{(p)}_{\mathbf{q}\nu}(\omega_t) \times \left( g^{(p)\nu}_{i'j'}(\mathbf{k}, \mathbf{q}) \right)^*.
$$

FIG. 1: Feynman diagrams for phonon-mediated effective (a) el-el [Eq. (5)] and (b) pairing [Eq. (6)] interactions. Solid lines with arrows are electron propagators, wavy lines are phonon Green’s functions, and dots represent el-ph couplings.

-Results. We performed density-functional calculations with QUANTUM ESPRESSO package [27]. The generalized-gradient approximation (GGA) with the Perdew-Burke-Ernzerhof parameterization [28] and the Troullier-Martins norm-conserving pseudopotentials [29] in the Kleinman-Bylander representation [30] are adopted. The cutoff energy for the wave functions is set to 95 Ry, and we employ $8 \times 8 \times 6$ $\mathbf{k}$ points. The phonon frequencies and the el-ph interactions are calculated using the DFPT [22] with and without the constraint, where $4 \times 4 \times 3$ $\mathbf{q}$-mesh and a Gaussian smearing of 0.02 Ry are employed. The maximally localized Wannier function [31] is used as the basis of the model. The lattice parameter and the internal coordinates are fully optimized and we get $a = 4.0344$ Å, $c = 8.9005$ Å, $z_{\text{La}} = 0.14233$, and $z_{\text{As}} = 0.63330$.

We show in Fig. 2(a) our calculated GGA band (solid curves) of LaFeAsO with the optimized structure, and compare with the Wannier-interpolated band (dotted
TABLE I: Our calculated static phonon-mediated effective el-el $V_{i,j',j'}(\omega_l=0)$ and pairing $V_{i,j',j'}(\omega_0=0)$ interactions. Note that the values are represented with the negative sign. The upper (lower) panel shows the partially (fully) screened interactions. $V_{i,j',j'}$ is symmetric with respect to $i \leftrightarrow j$, $i' \leftrightarrow j'$, and $(ij) \leftrightarrow (i'j')$. $V_{i,j',j'}$ is symmetric with respect to $(ii') \leftrightarrow (jj')$ and $(ij) \leftrightarrow (i'j')$. Units are given in eV.

| $-V_{i,j',j'}^{(p)}(0)$ | $-V_{i,j',j'}^{(p)}(= -V_{i,j',j'}^{(p)} \times 10^2)$ | $-V_{i,j',j'}^{(p)}$ | $-V_{i,j',j'}^{(p)}(= -V_{i,j',j'}^{(p)} \times 10^2)$ |
|---|---|---|---|
| 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 |
| 1 0.47 0.41 0.38 0.44 0.23 0.23 0.21 0.03 | 0.57 0.49 0.39 0.33 0.44 | 0.09 0.09 0.22 0.12 | 0.001 0.001 0.41 0.61 |
| 2 - 0.43 0.43 0.36 0.42 | - 0.06 0.20 0.23 | - 0.52 0.28 0.27 0.46 | - 0.10 0.16 0.14 |
| 3 - - 0.43 0.36 0.42 | - 0.20 0.23 | - 0.52 0.27 0.46 | - 0.16 0.14 |
| 4 - - - 0.32 0.35 | - - 0.03 | - - 0.54 0.23 | - - 0.08 |
| 5 - - - - 0.43 | - - - | - - - 0.69 | - - - |


| $-V_{i,j',j'}^{(f)}(0)$ | $-V_{i,j',j'}^{(f)}(= -V_{i,j',j'}^{(f)} \times 10^2)$ | $-V_{i,j',j'}^{(f)}$ | $-V_{i,j',j'}^{(f)}(= -V_{i,j',j'}^{(f)} \times 10^2)$ |
|---|---|---|---|
| 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 | 1 2 3 4 5 |
| 1 0.27 0.28 0.28 0.24 0.21 | 0.25 0.25 0.24 0.01 | 1.80 0.97 0.97 -0.46 0.32 | 0.13 0.13 0.31 0.17 |
| 2 - 0.37 0.24 0.27 0.21 | - 0.03 0.14 0.18 | - 1.60 1.05 -0.89 1.07 | - 0.15 0.22 0.18 |
| 3 - - 0.37 0.24 0.27 | - - 0.14 0.18 | - 1.60 -0.89 1.07 | - 0.22 0.18 |
| 4 - - - 0.39 0.11 | - - - 0.04 | - - 3.48 -1.87 | - - - 0.12 |
| 5 - - - - 0.28 | - - - - | - - - 4.33 | - - - - |

ones) for the Fe-3d orbitals. Hereafter, $d_{xz,-yz}$, $d_{xy}$, $d_{yz}$, $d_{x^2-y^2}$, and $d_{XY}$ orbitals are represented as 1, 2, 3, 4, and 5, respectively, where the X and Y axes are parallel to the nearest Fe-As bonds and the Z axis is perpendicular to the FeAs layer. The screening and self-energy effects within the energy range from the bottom of the Fe-3d bands up to 2.32 eV are excluded to derive $y^{(p)}$ and $\omega^{(p)}$.

Figure 2(b) displays our calculated phonon dispersions with (dotted curves) and without (solid ones) the constraint on the t-subspace screening. We see a discernible difference in the frequencies for the phonon modes which couple to the t-subspace electrons. However, the difference is not large, at most ~ 20 percent.

Table I lists our calculated static on-site phonon-mediated interactions. The upper left-side two 5×5 matrices are the el-el interaction $V_{i,j',j'}^{(p)}(0)$ in Eq. (5). The intra- and inter-orbital terms $V_{i,j',j'}^{(p)}(0)$ are ~0.4 eV, while the exchange and pair-hopping terms $V_{i,j',j'}^{(p)}(0) = V_{i,j',j'}^{(p)}(0)$ are rather small as ~0.02 eV. Compared to the on-site Coulomb repulsion $U \sim$ 2 eV [20], $V_{i,j',j'}^{(p)}(0)$ ~0.4 eV are not negligible. However, it should be noted here that, while $U(\omega_l)$ is almost constant up to the typical plasmon frequency (~25 eV in the iron-based superconductors [32]), the attractions $V_{i,j',j'}^{(p)}(\omega_l)$ quickly decay as $\omega_l$ increases and vanish around $\omega_l \sim \omega_D$ with $\omega_D$ being the Debye frequency.

The three matrices in the upper right side of Table I are the effective pairing interactions $V_{i,j',j'}^{(p)}(0)$ in Eq. (6). Due to the off-site pairing interactions, the pair-hopping terms $V_{i,j',j'}^{(p)}(0)$ are substantially larger in magnitude than the on-site quantities $V_{i,j',j'}^{(p)}(0)$.

The lower part of Table I describes fully screened ones $V_{i,j',j'}^{(f)}(0)$ and $V_{i,j',j'}^{(f)}(0)$. The intra- and inter-orbital terms are efficiently screened from the t-subspace electrons, while others not. We note that the quantity $\sum_{ij} V_{i,j',j'}^{(f)}(N_i(N_0)/N_0)$ with $N_i$, $N_0$ being the partial (total) density of states at the Fermi level $\sim$ 0.18, which gives a reasonable estimate to the total el-ph coupling constant $\lambda \sim 0.2$ in this system [15].

- Effect on pairing symmetry. Here we analyze a five-band model including the electronic repulsions and phonon-mediated interactions within the RPA. The calculation details follows Refs. [12, 13]. The spin and charge susceptibilities are given by

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

where $\chi^{0}(q)$ is the irreducible susceptibility and $\Gamma^{c}_{i,j',j'} = U, U', J$, and $J'$ for $i = j = j' = j', i = i' \neq j = j', i = j \neq i' = j', i = j \neq i' = j'$, respectively [12]. $U (U')$ is the intra- (inter-) orbital Coulomb repulsion, $J$ is the Hund’s coupling, and $J'$ is the pair-hopping. The matrix $\hat{\Gamma}^{c}$ is given by $\hat{\Gamma}^{c} = -\hat{C} - 2\hat{V}^{(p)}(\omega_l)$, where $\hat{C}_{i,j',j'} = U, -U' + 2J, 2U' - J$, and $J'$ for $i = j = j' = j', i = i' \neq j = j', i = j \neq i' = j', i = j \neq i' = j'$, respectively [12].

With these susceptibilities, we solve the linearized gap equation

$$\lambda_{E}\Delta_{k}^{c}(k) = \frac{T}{N} \sum_{k',j_{j'}} W_{i,j_{j'}}^{0}(k - k')G_{j,j'}^{0}(k') \Delta_{j,j'}^{c}(k') \times G_{j_{j'},j_{j'}}^{0}(-k'),$$

where $\Delta_{k}^{c}(k)$ ($G_{j,j'}^{0}(k)$) is the gap (non-interacting Green’s) function in the orbital representation and
$W_{ij,i'j'}(q)$ is the pairing interaction kernel. For the singlet pairing, $\tilde{W}(q) = -\frac{2}{n} \tilde{G}_{ij}^{s} \tilde{G}_{ij}^{s}(q) \tilde{G}_{i'i'}^{s} \tilde{G}_{i'i'}^{s}(q) \tilde{G}_{cc} - \frac{1}{n} \tilde{G}_{cc}^{c} \tilde{G}_{cc}^{c}(q) \tilde{G}_{cc} - \frac{1}{n} \tilde{G}_{cc}^{c} \tilde{G}_{cc}^{c}(q)$ with $\tilde{G}_{cc} = -\tilde{C} - 2V^{(p)}(\omega_l)$. The eigenvalue $\Delta_E$ grows as the temperature decreases, reaching unity at the superconducting transition temperature.

We adopt two dimensional model and 64 × 64 k-point meshes and 2048 Matsubara frequencies are taken. The temperature and the filling are set to $T = 0.02$ eV and $n = 6.1$, respectively. We discuss the structure of the diagonal elements of the gap-function matrices in the band representation at the lowest Matsubara frequency and we denote them as $\phi_m(k)$ with $m$ being the band index. When the Coulomb interactions are large, the RPA treatment is known to be unstable [3]. So, we scale the original $ab$ initio electronic interactions $U$, $U'$, $J$ and $J'$ [33] by 1/2 with keeping the phonon-mediated interactions $V_{ij,i'j'}^{(p)}$, and $V_{ij,i'}^{(p)}$ at the original values in Table I.

Our calculated gap functions $\phi_2(k)$, $\phi_3(k)$, and $\phi_4(k)$ are shown in Figs. 3(a), (b), and (c), respectively. We see the sign change in the gap functions on the Fermi surfaces (FS’s), i.e., the $s_±$-wave state is realized. In our parameter setting, the phonon-mediated interactions are considerably overemphasized to the scaled electronic repulsions; nevertheless, we get the $s_±$-wave solution. Thus, the $s_±$-wave pairing based on the orbital fluctuations due to the el-ph interactions would not be realized in the $ab$ initio parameter range [34].

To clarify why the $s_±$-wave state is stable even if we introduce the el-ph interactions, we analyze simpler models. We use the following Coulomb parameters: $U = 0.8$ eV, $U' = 0.69U$, and $J = J' = 0.16U$. For the phonon-mediated interaction matrix $\tilde{V}$ [35], we consider two parameter sets. One is the same as that of Ref. [12]; the exchange terms $V_{ij,ij}$ are set to be equal to the intra-orbital ones $V_{i,i}$ such as $V_{24,24} = V_{34,34} = V_{22,22} = V_{33,33} = -V_{22,33} = V(\omega_l)$, where $V(\omega_l) = V(0)\omega_D^2/\omega_D^2 + \omega_D^2$ with $V(0) = -0.385$ eV and $\omega_D = 0.02$ eV [36]. Note that $V_{ij,i'j'}$ has the symmetry on the index interchange as $i \leftrightarrow j$, $i' \leftrightarrow j'$, and $(ij) \leftrightarrow (i'j')$. The other parameter set is based on the present $ab$ initio results; the exchange terms are appreciably weakened from the intra- and inter-orbital ones: $V_{24,24} = V_{34,34} = V(\omega_l)/20$ and $V_{22,22} = V_{33,33} = V_{22,33} = V(\omega_l)$. We found that the former parameter set gives the $s_±$-wave pairing, while the latter one leads to the $s_±$-wave pairing. In the analysis for the former case, we checked that the sign change of $V_{22,33}$ has no qualitative effect on the pairing symmetry. Therefore, it is deduced that the magnitudes of $V_{24,24}$ and $V_{34,34}$ are crucial in determining $s_±$ or $s_±$-wave states.

When the exchange and pair-hopping terms $V_{24,24} = V_{34,34} = V_{34,43} = V_{34,43}$ are large in magnitude, the scattering channels $W_{24,42}$ and $W_{34,43}$, which connect $\Delta_{44}$ and $\Delta_{22}$, and $\Delta_{44}$ and $\Delta_{33}$, respectively, are enhanced through the charge sector and both channels have the positive value [12]. These attractive pairing channels lead to the same sign in $\Delta_{22}$, $\Delta_{33}$, and $\Delta_{44}$. Since the FS’s consist of these three (2-4) orbitals, the $s_±$-wave state is realized. On the other hand, when $V_{24,24}$ and $V_{34,34}$ are small as with the $ab$ initio results, the scattering channels enhanced by the spin part become dominant and the $s_±$-wave state is realized. Thus, the el-ph interactions with the $ab$ initio energy scale alone cannot drive the orbital-fluctuation-mediated $s_±$-wave pairing. If realized, the origin is electronic (Coulombic) where the vertex corrections play a key role [23, 37].

-Conclusion. We have developed an $ab$ initio downfolding method for el-ph coupled systems and applied it to the derivation of the effective model of LaFeAsO. With the derived effective el-ph interactions $g^{(p)}$ and phonon frequencies $\omega^{(p)}$, we have estimated the phonon-mediated effective on-site el-el interactions as $V_{ij,ij}^{(p)}(0) \sim V_{ij,ij}^{(p)}(0) \sim -0.4$ eV and $V_{ij,ij}^{(p)}(0) = V_{ij,ij}^{(p)}(0) \sim -0.02$ eV. We have analyzed the derived five band model consisting of Fe-3d bands using the RPA. The $s_±$-wave pairing is not realized with the $ab$ initio el-ph interaction with the tiny exchange and pair-hopping terms, and the $s_±$-wave state mediated by spin-fluctuations is robustly realized.

-Acknowledgments. We would like to thank Hiroshi Kontani, Seiichiro Onari, Hiroaki Ikeda, Ryosuke Akashi and Hideyuki Miyahara for fruitful discussions. This work was supported by Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST program) on "Quantum Science on Strong Correlation" JST-PRESTO, Grants-in-Aid for Scientific Research (22740215, 22104010, 23110708, 23340095, 23510120, 25800200) and the Next Generation Super Computing Project and Nanoscience Program from MEXT, Japan. Y. N. is supported by Grant-in-Aid for JSPS Fellows (12J08652).
[1] G. R. Stewart, Rev. Mod. Phys. 83, 1589 (2011).
[2] I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du, Phys. Rev. Lett. 101, 057003 (2008).
[3] K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Kontani, and H. Aoki, Phys. Rev. Lett. 101, 087004 (2008).
[4] H. Ikeda, J. Phys. Soc. Jpn. 77, 123707 (2008).
[5] A. V. Chubukov, D. V. Efremov, and I. Eremin, Phys. Rev. B 78, 134512 (2008).
[6] T. Nomura, J. Phys. Soc. Jpn. 78, 034716 (2009).
[7] F. Wang, H. Zhai, Y. Ran, A. Vishwanath, and D.-H. Lee, Phys. Rev. Lett. 102, 047005 (2009).
[8] Z.-J. Yao, J.-X. Li, and Z. D. Wang, New J. Phys. 11, 025009 (2009).
[9] R. Arita and H. Ikeda, J. Phys. Soc. Jpn. 78, 113707 (2009).
[10] A. F. Kemper, T. A. Maier, S. Graser, H.-P. Cheng, P. J. Hirschfeld, and D. J. Scalapino, New J. Phys. 12, 073030 (2010).
[11] R. M. Fernandes and J. Schmalian, Phys. Rev. B 82, 014521 (2010).
[12] H. Kontani and S. Onari, Phys. Rev. Lett. 104, 157001 (2010).
[13] T. Saito, S. Onari, and H. Kontani, Phys. Rev. B 82, 144510 (2010).
[14] Y. Yanagi and Y. Yamakawa, Y. ¯Ono, Phys. Rev. B 81, 054518 (2010).
[15] L. Boeri, O. V. Dolgov, and A. A. Golubov, Phys. Rev. Lett. 101, 026403 (2008).
[16] K. Nakamura, R. Arita, and M. Imada, J. Phys. Soc. Jpn. 77, 093711 (2008).
[17] T. Miyake, L. Prouvoskii, V. Vildosola, S. Biermann, and A. Georges, J. Phys. Soc. Jpn. Suppl. C 77, 99 (2008).
[18] T. Miyake, K. Nakamura, R. Arita, and M. Imada, J. Phys. Soc. Jpn. 79, 044705 (2010).
[19] K. Nakamura, Y. Yoshimoto, Y. Nohara, and M. Imada, J. Phys. Soc. Jpn. 79 123708 (2010).
[20] T. Misawa, K. Nakamura, and M. Imada, Phys. Rev. Lett. 108, 177007 (2012).
[21] M. Hirayama, T. Miyaka, and M. Imada, arXiv:1211.0597.
[22] S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Gian- nozzi, Rev. Mod. Phys. 73, 515 (2001).
[23] S. Onari and H. Kontani, Phys. Rev. Lett. 109, 137001 (2012).
[24] In the practical calculation based on the DFPT, instead of $v$ in Eq. (1), $v + K_{xc}$ is used, where $K_{xc}$ is defined as $\delta V_{xc}/\delta \rho$ with $V_{xc}$ and $\rho$ being the exchange-correlation potential and the electron density, respectively.
[25] F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, and A. I. Lichtenstein, Phys. Rev. B 70, 195104 (2004).
[26] Y. Nomura, K. Nakamura, and R. Arita, in preparation.
[27] S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, Rev. Mod. Phys. 73, 515 (2001).
[28] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).
[29] N. Troullier and J. L. Martins, Phys. Rev. B 43, 1993 (1991).
[30] L. Kleinman and D. M. Bylander, Phys. Rev. Lett. 48, 1425 (1982).
[31] N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997); I. Souza, N. Marzari, and D. Vanderbilt, ibid. 65, 035109 (2001).
[32] P. Werner, M. Casula, T. Miyake, F. Aryasetiawan, A. J. Millis, and S. Biermann, Nature Physics 8, 331 (2012).
[33] As for the effective Coulomb interactions, we employ the values in Ref. [20].
[34] We note that the $s_{\pm}$-wave state is always realized when we change the scaling parameter for Coulomb interactions from 0.4 to 0.6.
[35] We use the common phonon-mediated interaction parameters for $\Gamma_c$ and $\Gamma'_{xc}$, i.e., $\Gamma_c = \Gamma'_{xc} = -\hat{C} - 2\hat{V}(\omega_l)$.
[36] For simplicity, the $V$ terms are introduced only for the 2, 3, and 4 orbitals which compose the FS’s, following Ref. [12].
[37] H. Miyahara, R. Arita, H. Ikeda, Phys. Rev. B 87, 045113 (2013).