Possible pairing states of the Fe-based superconductors

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We consider the minimal two-band model for the Fe-based superconducting compounds provided a great impetus to the research of superconductivity (SC). Since the first report on the superconducting transition at 7K with the doped LaOFeP by Kamihara et al., various substitutions (mainly, P by As and La by Ce, Gd, Sm, Pr) for this mother compound increase the superconducting temperature $T_c$ over 50K with Sm(OF)FeAs. Intensive investigations by many experimentalists and theorists have already revealed main metallic and superconducting properties of this group of materials.

From band calculations, it is agreed on that the 3d electrons of Fe atoms are the main contributors to the conduction bands crossing the Fermi surface (FS). Besides the degree of degeneracy, the key feature of conduction bands is that it consist of hole band(s) around $\Gamma$ point and electron band(s) around $M$ point [in the notation of the folded Brillouin-zone (BZ) scheme].

Regarding the pairing symmetry, there are already many experiments: (1) Knight shift below $T_c$ shows a clear drop indicating a spin singlet pairing; (2) tunneling spectroscopy showed the zero-bias conductance peak (ZBCP) - signature of a sign changing gap, but the interpretation of the shape of density of states (DOS) $N(\omega)$ is diverse; (3) nuclear spin-lattice relaxation rate $1/T_1\gamma^2$ unambiguously showed no coherent peak and $T^3$ dependence below $T_c$, hence strongly suggesting a d-wave type gap; and (4) specific-heat coefficient $C(T)/T$ below $T_c$ (Ref.12) - although the measurement is not yet reaching low enough temperature - appears $T$ linear indicating SC gap with lines of node. All these experiments appear to be consistent with a d-wave type gap. However, recent penetration depth measurements with PrFeAsO, Sm(OF)FeAs and Nd(OF)FeAs (Ref.13) strongly suggest a fully opened gap at low temperatures indicating a s-wave type pairing symmetry.

Regarding the paring glues, the phonon interaction appears unlikely mainly because the electron-phonon coupling is estimated to be very weak ($\lambda < 0.2$). On the other hand, this series of materials, without doping, commonly has a spin density wave (SDW) transition at around $\sim 150$ K. When the superconductivity appears with doping, the SDW correlation is expected to remain, albeit the long range order disappears.

Recent neutron-scattering experiments with La(OF)FeAs and Ce(OF)FeAs (Ref.13) directly measured the antiferromagnetic (AFM)-type correlation of the Fe d-electron spin moment. The overall phase diagram with doping for Ce(OF)FeAs reveals a close correlation with an antiferromagnetism and superconductivity, suggesting the important role of magnetic fluctuations as a pairing glue. It also shows that the generic phase diagram of these compounds shares the universal features with the high-$T_c$ cuprates, Pu-115 superconductor, and various heavy fermion superconductors; namely, the SC occurs in the neighborhood of the magnetic long range order when this magnetic order is suppressed. In particular, the magnetic order is an AFM type. This universal phase diagram is very tantalizing because it appears to cover a wide class of unconventional SC materials with a range of $T_c$ from a few mK to 100 K and suggests that the AFM fluctuation is a common thread and its characteristic energy roughly scales with the SC $T_c$.

For the Fe-based SC materials, several theoretical models were already proposed and most of them started with the orbital basis of the Fe 3d-electrons including Hubbard $U$ interaction(s) and Hund coupling(s). Some of these studies found that the ±s-wave gap as a dominant instability. A d-wave gap also often appears as a second instability. In this paper, we took a phenomenological approach to investigate possible pairing states in the Fe-pnictide superconductors. The non-interacting part of Hamiltonian is constructed by choosing a minimal set of topologically distinct two bands and the interaction part of Hamiltonian is assumed from the experimental input, simulating a short range AFM correlation. By solving the coupled BCS gap equations, we found the two SC gap solutions: a sign-changing s-wave gap and a double d-wave gap. For the both
SC states, we carried out the calculations of the SC properties such as the DOS, temperature dependencies of the spin-lattice relaxation rate $1/T_1$, Knight shift, and penetration depth. We particularly take into account of the interband coherence factors, unique to the two band model, in these calculations. The results are discussed in comparison with the currently available experimental data.

II. MODEL

We propose a minimal phenomenological two band model for the Fe-based superconductors. For the non-interacting part of Hamiltonian, we observe that several band structure calculations3,13,15,16,17,18 of the Fe-pnictide compounds reached the consensus that the FS of the doped compounds consists of two hole pockets and two electron pockets. To keep the essential physics, but avoiding unnecessary complexity, we choose only two topologically distinct bands: one hole band around Γ point (0,0) and one electron band around M point ($\pm \pi$, $\pm \pi$).

The main phenomenological assumption of our model is the interacting part of Hamiltonian. This pairing interaction $V(\mathbf{q})$ is chosen to simulate a short range AFM spin fluctuations peaking at the ordering wave vector $Q = (\pm \pi, \pm \pi)$. This assumption is directly motivated by the experimental observations of the AFM correlation in the Fe-pnictide compounds by neutron-scattering measurements15,21. The elastic neutron-scattering experiments for LaFeO$_{1-x}$FeAs and Ce(Fe$_1$O$_{1-x}$)FeAs by Dai and co-workers15 showed the long-range AFM order of the Fe3d-electron spins for the doping range of $x = 0 - 0.05$. When this long-range AFM order disappears beyond the doping around $x=0.05$, SC appears up to the doping range $x \sim 0.2$ (this is only the limit of the measured data). This overall phase diagram appears to be generic for the Fe-pnictides, and clearly shows that the AFM correlation is the dominant magnetic correlation in this group of materials.

More importantly, this AFM correlation is expected to continue to exist in the doping range where the SC phase occurs albeit becoming a short-rang one. This speculations is supported by more recent inelastic neutron-scattering experiment in the doped (BaK)Fe$_2$As$_2$ compound ($T_c=38$K) by Christianson et al.21. In this experiment, a clear magnetic-resonance peak is observed at the expected position of the AFM correlation, i.e., at $(\pi, \pi)$ momentum. With this series of experiments it is clear that the AFM correlation is the dominant magnetic correlation in the Fe-pnictides among other competing magnetic correlations such as weak ferromagnetism22, checkerboard AFM6,8, and AFM stripe phases5,19, which were theoretically proposed. Finally, the coupling matrix element is assumed to be a constant for simplicity. The Hamiltonian is written as

$$H = \sum_{k\sigma} \epsilon_h(k) h_{\sigma}^{\dagger} h_{\sigma} + \sum_{k\sigma} \epsilon_e(k) e_{\sigma}^{\dagger} e_{\sigma}$$

$$+ \sum_{kk'\uparrow\downarrow} V(k,k') h_{\downarrow}^{\dagger} h_{\uparrow}^{\dagger} e_{\uparrow}^{\dagger} e_{\downarrow} + \sum_{kk'\uparrow\downarrow} V(k,k') h_{\uparrow}^{\dagger} h_{\downarrow}^{\dagger} e_{\downarrow}^{\dagger} e_{\uparrow}$$

$$+ \sum_{kk'\uparrow\downarrow} V(k,k') h_{\downarrow}^{\dagger} h_{\uparrow}^{\dagger} e_{\downarrow}^{\dagger} e_{\uparrow}$$

$$+ \sum_{kk'\uparrow\downarrow} V(k,k') h_{\uparrow}^{\dagger} h_{\downarrow}^{\dagger} e_{\uparrow}^{\dagger} e_{\downarrow}$$

(1)

where $h_{\sigma}^{\dagger}$ and $e_{\sigma}^{\dagger}$ are the electron creation operators on the hole and the electron bands, respectively. $\epsilon_h,e(k)$ are the dispersions of the hole band and electron bands, respectively, defined as $\epsilon_h(k) = t_1^{\rm h}(\cos k_x + \cos k_y) + t_2^{\rm h} \cos k_x \cos k_y + \frac{V}{2}$ and $\epsilon_e(k) = t_1^{\rm e}(\cos k_x + \cos k_y) + t_2^{\rm e} \cos \frac{k_x}{2} \cos \frac{k_y}{2} + \epsilon'$. In this paper, we choose the band parameters as $(0.30,0.24,-0.6)$ for hole band and $(1.14,0.74,1.70)$ for electron band with the notation $(t_1,t_2,\epsilon)$18.

The pairing interaction $V(k,k')$ is phenomenologically defined below. It is all repulsive in momentum space and it represents a short range AFM spin fluctuations as explained above.

$$V(k,k') = V_M \frac{k^2}{|\mathbf{k} - \mathbf{k'}|^2 + \kappa^2}$$

(2)

where $\bar{k}$ and $\bar{k'}$ are the two-dimensional momenta on the two dimensional BZ and the parameter $\kappa$ controls the magnetic correlation length as $\xi_{AFM} = 2\pi\kappa/(\kappa$ (is the unit-cell distance). This interaction mediates the strongest repulsion when two momenta $\bar{k}$ and $\bar{k'}$ are spanned by the ordering wave vector $\bar{Q}$. This condition is better fulfilled when the two momenta $\bar{k}$ and $\bar{k'}$ reside each other on different bands in the model band structure (see Fig.1). As a result, the sign-changing s-wave gap can form on each band as already suggested by several papers15,17,18,19. However, this opposite sign gap on the hole and electron bands is not limited with the $\pm s$-wave state ([Fig.1 (a)]). Another possibility, which conforms to the lattice symmetry, is that each band develops a d-wave gap but with $\pi$ phase shift between two bands [Fig.1 (b)]. We call this type of gap as double d-wave gap.
We need to mention that our model did not include the screened Coulomb interaction (neither did the other theoretical investigations\textsuperscript{5,17,18,19}), which certainly exists in the Fe-pnictide superconductors as well as all metals in general. The screened Coulomb interaction is traditionally treated as "Coulomb pseudo potential" $\mu^*$ in the conventional phonondriven SC. However, the reliable estimate for its strength is practically impossible because even a small difference in $\mu^*$ would cause a large change in $T_c$. In the Fe-pnictides, if we are to determine $T_c$ theoretically, a quantitative estimate of $\mu^*$ is necessary. We did not include it in our model interaction, first, because we do not know how to reliably estimate it in these compounds and, second, because the primary purpose of the present paper is not the prediction of the precise $T_c$. Still we could investigate its generic effects on the different pairing symmetries such as $\pm s$-wave and double $d$-wave gaps; for example, how large value of $\mu^*$ is necessary to kill the $\pm s$-wave pairing for a given strength of the AFM interaction. We think that this kind of analysis will dilute the focus of the present paper and therefore should be a separate investigation. We briefly remark, however, on the general effects of the screened Coulomb interaction. The screened Coulomb interaction becomes a short-range interaction in real space and therefore weakly momentum dependent in momentum space. This type of interaction is almost harmless for the $d$-wave type pairing but extremely detrimental for the $s$-wave type pairing. The pairing solutions in this paper should be considered with this point in mind.

Now we solve the Hamiltonian Eq.(1) using the BCS approximation and the two band electrons need two SC order parameters (OPs)

$$\Delta_h(k) = \sum_{k'} V(h,k') \langle h_{k',h_{-k'}} \rangle, \quad (3)$$

$$\Delta_e(k) = \sum_{k'} V(e,k') \langle e_{k',e_{-k'}} \rangle. \quad (4)$$

After decoupling the interaction terms of Eq.(1) using the above OPs, the self-consistent mean field conditions lead to the following two coupled gap equations.

$$\Delta_h(k) = - \sum_{k'} [V_{hh}(h,k') \Delta_h(k') \chi_h(k') + V_{he}(h,k') \Delta_e(k') \chi_e(k')], \quad (5)$$

$$\Delta_e(k) = - \sum_{k'} [V_{eh}(e,k') \Delta_h(k') \chi_h(k') + V_{ee}(e,k') \Delta_e(k') \chi_e(k')]. \quad (6)$$

where $V_{hh}(h,k')$, $V_{he}(h,k')$, etc. are the same interaction defined in Eq.(2) but the subscripts are written to clarify the meaning of $V_{hh}(h,k') = V(h, k'_h)$, $V_{he}(h,k') = V(h, k'_e)$, etc., and $k'_h$ and $k'_e$ specify the momentum $k$ located on the hole and electron bands, respectively. The pair susceptibilities are defined as

$$\chi_{h,e}(k) = N(0)_{h,e} \int_0^{\omega_{AFM}} d\xi \frac{\tanh(\xi/2T)}{E_{h,e}(k)} \quad (7)$$

where $E_{h,e}(k) = \sqrt{k^2 + \Delta_h^2(k)}$, and $N(0)_{h,e}$ are the quasiparticle excitations and the DOS of the hole and electron bands, respectively, and $\omega_{AFM}$ is the cutoff energy of the pairing potential $V(q)$.

When we solve the above gap equations Eq(5) and Eq.(6), we numerically restricted the momenta $k_{h,e}$ and $k'_h,e$ around the FSs of the hole and electron bands within $\omega_{AFM}$ energy range. Therefore, the FS shapes and the local DOS $N(0)_{h,e}$ of the realistic bands are faithfully taken into account in our gap solutions. Also no restriction on the functional forms of the gaps $\Delta_{h,e}(k)$ was imposed except the general symmetry depicted in Fig.1, so that the $k$-dependence of the gap functions $\Delta_{h,e}(k)$ will follow the characteristics of the bands and pairing interaction.

### III. GAP SOLUTIONS

As explained in Sec. II, the main pairing process with the AFM spin-fluctuation mediated interaction $V(q)$ is the interband pair hopping between the hole and the electron bands, in which a pair of electrons $(k, -k)$ on the hole band scatters to a pair of electrons $(k', -k')$ on the electron band and vice versa. This process is particularly dominant when the size of the FS of each band is much smaller than the size of $\tilde{Q}$ vector. Considering only this interband pair process [keeping only $V_{he}$ and $V_{eh}$ terms in Eqs.(5) and (6)], we observe the fact that the pair potential $\Delta_h(k)$ for the hole band electrons is provided by the pairs of electrons in the electron band and vice versa. The physical consequence of it is that the relative sizes of the gaps and DOSs on each band are reversed; namely, if $N_h(0) > N_e(0)$, then $|\Delta_h(k)| < |\Delta_e(k)|$ holds in general. This relation holds both for the $\pm s$-wave and for the double $d$-wave gap solutions and affects all superconducting properties such as tunneling DOS, Knight shift, $1/T_1$, and penetration depth.

For all numerical calculations in this paper, we choose the parameters $\kappa = 0.2\pi$ ($\tilde{Q}_{AFM} \approx 10\tilde{a}$), $\omega_{AFM} = 20\text{meV}$, and $V_M = 10\text{eV}$ (average interaction $<V(q)> = 1.115\text{eV}$). Our choice of band parameters produces $N_h(0) = 0.74/\text{eV}$ and $N_e(0) = 0.285/\text{eV}$ so that $N_h(0)/N_e(0) \approx 2.6$. We think that these numbers represent the Fe-based SC materials but should not be taken too seriously; in particular the pairing strength $V_M = 10\text{eV}$ is chosen freely for demonstration.

#### A. $\pm s$-wave gap

This solution for the Fe-based SC is already proposed by several authors\textsuperscript{5,17,18,19}. Here we demonstrate that this solution is indeed realized with a simple phenomenological interaction, which mimics an AFM spin fluctuations, on the minimal two band model representing the Fe-based SC compounds.

As we described above, the reversed relation between the magnitude of the DOSs and the size of gaps holds more rigorously for the $s$-wave case and we suggest an approximate relation $\Delta_h^{\text{max}} N_h \approx \Delta_e^{\text{max}} N_e$ (see the Appendix for more detailed discussions). This relation is a generic feature of the model.
Therefore, given a substantial difference of DOS between the hole and electron bands (several band calculations indicate that this is true for the Fe-based SC materials), at least two distinctively different sizes of the SC gaps should be observed in various experiments. In particular, because the band with a larger DOS would dominate the physical properties but actually holds a smaller gap, this feature will modify various SC properties of the Fe-based SC in unorthodox manner, such as $\Delta/T_c$ value, temperature dependencies of various SC properties below $T_c$, and the responses to impurities.

In Fig.2, the solution of the $\pm$s-wave gap and the corresponding DOS are shown. As mentioned, $N_h(0) = 2.6N_e(0)$ for our bands. Accordingly the size of gaps of the hole band and the electron band is reversed as $\Delta^\text{max}_h \approx 10\text{meV}$ and $\Delta^\text{max}_e \approx 25\text{meV}$. The strongly momentum dependent pairing interaction and the realistic bands naturally induce an anisotropic modulation of the s-wave gaps with $C_4$ symmetry; the modulation is stronger for the larger gap on the smaller DOS band (electron band around $M$ point). Compared to the case of the double d-wave solution, the average size of the $\pm$s-wave gap is larger by a factor of $\sim 5$ with the same pairing potential. Therefore, unless some other interactions are added, the ground state of our model is the $\pm$s-wave SC state. This conclusion is already obtained by other authors with different models and approaches. The separate and total DOSs plotted in Fig.2(b) show the main features of the $\pm$s-wave gap: two peak structure, the large DOS with a small gap and the small DOS with a large gap. The overall shape of the total DOS is not very much revealing compared to the current tunneling DOS measurements. However, it is too early to make a decisive conclusion with our calculations without including Andreev scattering. Also the ZBCP, the hallmark of a d-wave gap and observed in experiments with the Fe-based superconductors, can equally be obtained with the $\pm$s-wave gap state.

We consider nuclear spin-lattice relaxation rate $1/T_1$ for the $\pm$s-wave gap. Several groups have reported that $1/T_1$ shows no coherence peak and the $T^3$ power law below $T_c$, strongly suggesting an unconventional gap with lines of node such as a d-wave gap. s-wave gap is known to have a constructive coherent factors for $1/T_1$ to induce the coherence peak over a temperature range below $T_c$. However, as Mazin et al. envisaged, the sign-changing gaps between two bands provide a destructive coherent factor for the interband scattering which will largely cancel the intraband coherent factors. As a result the coherent peak of $1/T_1$ for the $\pm$s-wave gap SC will be substantially reduced. The explicit formula that we used for the calculations is the following:

$$
\frac{1}{T_1} \sim -T \int_0^\infty \frac{df_{FD}(\omega)}{d\omega} \left\{ N_h^2(0) \left\langle \frac{Re \frac{\omega}{\sqrt{\omega^2 - \Delta_h^2(k)}}}{k} \right\rangle^2 + 2N_h(0)N_e(0) \left\langle \frac{Re \frac{\omega}{\sqrt{\omega^2 - \Delta_h^2(k)}}}{k} \right\rangle \left\langle \frac{Re \frac{\omega}{\sqrt{\omega^2 - \Delta_e^2(k')}}}{k'} \right\rangle + N_e^2(0) \left\langle \frac{Re \frac{\omega}{\sqrt{\omega^2 - \Delta_e^2(k)}}}{k} \right\rangle^2 \right. \\
+ \left. \left[ N_h^2(0) \left\langle \frac{Re \frac{\Delta_h}{\sqrt{\omega^2 - \Delta_h^2(k)}}}{k} \right\rangle \right]^2 + 2N_h(0)N_e(0) \left\langle \frac{Re \frac{\Delta_h}{\sqrt{\omega^2 - \Delta_h^2(k)}}}{k} \right\rangle \left\langle \frac{Re \frac{\Delta_e}{\sqrt{\omega^2 - \Delta_e^2(k')}}}{k'} \right\rangle + N_e^2(0) \left\langle \frac{Re \frac{\Delta_e}{\sqrt{\omega^2 - \Delta_e^2(k)}}}{k} \right\rangle^2 \right\}. \tag{8}
$$

For the temperature dependence of the gaps $\Delta_{h,e}(k,T)$, we use a phenomenological formula, $\Delta_{h,e}(k,T) = \Delta_{h,e}(k,T = 0) \tanh(\beta \sqrt{T_c/T - 1})$. By choosing the values of $\Delta^\text{max}_{h,e}/T_c$, we can partially take into account of the strong coupling superconductivity effect. $\beta$ is not a sensitive parameter for final results; we take $\beta = 1.74$ in this paper.

Fig.3(a) shows the contributions to the $1/T_1$ relaxation rate from each terms of Eq.(8): the hole band, the electron band, and the interband terms. It shows that the cancellation of the coherence factors is not perfect in general unless the cond-
Nevertheless, due to the large cancellation by the interband coherence factor, the height of the coherence peak is very much reduced [compare the total $1/T_1$ and the hole band only $1/T_1$ in Fig.3(a)]. Small amount of impurities can easily wash out this reduced coherence peak as shown in Fig.3(b); the damping rate $\Gamma = 0.05 \Delta_h^{\text{max}}$ is enough to completely kill the coherence peak. The subtle part is to fit the $\sim T^3$ power law below $T_c$. It requires to tune $R = \Delta_h^{\text{max}}/T_c$ ratio. In Fig.3, $R = 1.5$ (automatically, it makes $\Delta_h^{\text{max}}/T_c \approx 3.75$ which is quite a large value) is used for the best fit. Fig.3(c) shows that this pseudo-$T^3$ behavior is not extended to the very low-temperature region as in the d-wave case because this $T^3$ behavior in the $\pm$s-wave gap is not an intrinsic property of the lines of nodes. At low temperatures, there appears the exponential drop inevitably due to the full gaps, and then it finally reaches the impurity-induced $T$-linear region because we added some amount of impurities to kill the coherent peak. All these details put rather stringent conditions to confirm the $\pm$s-wave gap state with experiments.

Now we consider the Knight shift which is the measure of uniform susceptibility in SC phase. Because it is a $q \to 0$ probe, there is no interband contribution and the total Knight shift is just sum of the contributions from each band as follows:

$\chi_c(T) = \chi_{c, \text{el}}(T) + \chi_{c, \text{h}}(T)$

with $\chi_{c, \text{el}}(T) = \chi_{c, \text{el}}^{\text{max}}/T_c$ and $\chi_{c, \text{h}}(T) = \chi_{c, \text{h}}^{\text{max}}/T_c$.
interband screening current. The vex shape of Knight shift which was reported by Matano et al. can be rewritten in more convenient form as

\[ \chi(T) = -\int_0^\infty \frac{\partial F_D(\omega)}{\partial \omega} \left[ N_h(0) \langle R \frac{\omega}{\omega^2 - \Delta_n^2(k)} \rangle_k + N_e(0) \langle R \frac{\omega}{\omega^2 - \Delta_c^2(k)} \rangle_k \right] \]

The overall magnitude. Therefore, we take \( \alpha_0 = 0.0 \) for the calculations of the penetration depth in the \( \pm s \) case. However, this effect can induce an important modifications in the d-wave case, which will be discussed in Sec.IIIB.

Fig.5 shows the normalized superfluidity density \( \lambda^2(0)/\lambda^2(T) \) and separate contributions from the hole and electron bands. The exponentially flat region appears at low temperatures due to the full gap opening, which is consistent with recent experiments. Relatively narrower region of the flat part (for \( T < 0.2T_c \)) compared to the ordinary s-wave gap is another feature due to the smaller gap with the larger DOS of the \( \pm s \) gap SC. A subtler part here is that the high temperature region (0.3 \( T_c \) < \( T < T_c \)). With \( \Delta_n^{\text{max}}/T_c = 1.5 \) (the same value used for the 1/\( T_1 \) fit), this part becomes too convex [Fig.5(A)] in comparison to the experiments. A smaller gap-Tc ratio can make it concave as shown in Fig.5(B) (with \( \Delta_n^{\text{max}}/T_c = 0.5 \); this concave feature was recently observed by Martin et al.).

In summary, the \( \pm s \) gap state provides the most consistent descriptions for the penetration depth experiments. However, it explains 1/\( T_1 \) only for a limited temperature range, even with a fine tuning of \( \Delta_n/\alpha \), ratio and impurities. Knight shift of any shape can be fit with two band parameter (this is also true with the double d-wave gap). The tunneling DOS does not provide a decisive conclusion.

B. Double d-wave gap

In Fig.6, the gap solution and the corresponding DOS of the double d-wave gap are shown. As mentioned, our model bands have \( N_h(0) = 2.6N_e(0) \), and consequently gap in the hole band \( \Delta_n^{\text{max}} \approx 2 \text{meV} \) is smaller than the one of the electron band \( \Delta_e^{\text{max}} \approx 4 \text{meV} \). The sizes of the maximum gaps are \( \sim 5 \) times smaller than the \( \pm s \) gap solutions. Therefore, the double d-wave gap solution is not the best SC state for our phenomenological model with an antiferromagnetic pairing interaction. This result is in agreement with other theoretical studies. This conclusion may change with the correlation length of the AFM fluctuations, the sizes of the FS of the hole and electron bands, etc. But we numerically found that \( \pm s \) gap solution is favored compared to the double d-wave gap solution for most cases. As discussed in Sec.II, however, the screened Coulomb interaction may change this conclusion. The detailed studies about this issue will be discussed in a separate paper.

To complete the comparisons, we calculated the same SC properties of the double d-wave gap state. The separate and total DOSs shown in Fig.6(b) demonstrates the main features of the double d-wave gap: the large DOS band with a small and the penetration depth at zero temperature, respectively. Apparently if \( \frac{\Delta_n}{\lambda_0} \approx 0 \) is small compared to 1, the non-local effect becomes negligible. A typical value of \( \alpha_0 \) for YBCO was estimated about 0.01, for example. For the Fe-based superconductors, we believe that \( \alpha_0 \) is not much larger than the values of the high-\( T_c \) cuprates. Also for a s-wave case, the non-local effect does not change much of the temperature dependence of 1/\( \lambda^2(T) \) except the overall magnitude. Therefore, we take \( \alpha_0 = 0.0 \) for the calculations of the penetration depth in the \( \pm s \) wave case.
ably good fits, showing a more tolerance than the case.

FIG. 6: (Color online) (a) Double d-wave gap solutions $\Delta_+(k)$ and $\Delta_-(k)$. (b) Normalized DOS of the hole band $N_h(\alpha)$ (red dotted line), electron band $N_e(\alpha)$ (blue dotted line), and the total $N_{tot}(\alpha)$ (black squares).

gap and the small DOS band with a large gap. This result shows a similar feature of the tunneling DOS measurement by Wang et al. except the ZBCP, which does not show up in our simple DOS calculation but should appear when the tunneling conductivity is properly calculated with Andreev scattering process.

We consider the nuclear spin-lattice relaxation rate $1/T_1$. As in the case of ±s-wave gap, there are three contributions for the total $1/T_1$ relaxation rate: hole band, electron band, and interband scattering terms. The formula is the same as Eq.(8) but the last three terms should be dropped because the FS average of $\Delta_{h,e}(k)$ vanishes in this case. We use the same form of temperature dependent gap function as $\Delta_{h,e}(k,T) = \Delta_{h,e}(k,T=0)\operatorname{tanh}(1.74\sqrt{T_c/T-1})$. In Fig.7, $R = \Delta_h^{\text{max}}/T_c = 1.75$ is used for the best $T^3$ fit below $T_c$. However, in the double d-wave gap, $R = 1.5 - 2.5$ provide reasonably good fits, showing a more tolerance than the ±s-wave gap state.

Fig.7(a) shows the separate contributions from each channel together with the total contribution. As in the ±s-wave case, $1/T_{1,h}$ provides the largest contribution and $1/T_{1,e}$ provides the smallest contribution. There is also the interband term $1/T_{1,\text{inter}}$. In contrast to the ±s-wave case, all three terms display a similar temperature dependence and no coherence peaks. Fig.7(b) shows the same $1/T_{1}\text{total}$ (black squares) in log-log plot. The overall features of $1/T_1$ are the ones of the typical d-wave SC state: no coherence peak near $T_c$ and $\sim T^3$ below $T_c$, and consistent with the current NMR experiments. At very low temperatures, $T^3$-linear behavior starts to appear due to a small damping for the numerical calculations ($T = 0.005\Delta_h^{\text{max}}$). For comparison, we also show $1/T_{1}\text{total}$ (open green circles) with $\Delta_h^{\text{max}}/T_c = 1.0$, a smaller gap-$T_c$ ratio; it exhibits a substantial convex part below $T_c$ and then starts displaying the universal $T^3$ behavior before entering the impurity dominating region.

In Fig.8, we show the result of the uniform spin susceptibility which is measured as Knight shift. Fig.8(a) shows the results with $\Delta_h^{\text{max}}/T_c = 1.75$. The hole band contribution is dominant as in $1/T_1$ and the electron band contribution show the steeper drop just below $T_c$ because of the larger gap-$T_c$ ratio $\Delta_e^{\text{max}}/T_c \approx 3.5$. The overall behavior of the total $\chi_s(T)$ below $T_c$ shows a typical d-wave behavior such as $T$-linear at low temperatures. Fig.8(b) shows the results with $\Delta_h^{\text{max}}/T_c = 1.0$. A smaller gap-$T_c$ ratio makes the Knight shift convex as in the ±s-wave case and observed by Matano et al.
specular boundary condition, the temperature dependence of in Sec.II, most of experiments, up to now, report a flat temperature. Therefore, we consider a non-local effect of the electromagnetic response of the double d-wave gap superconductor as a possible cause to modify the typical temperature dependence. In order to include the effect of the non-local electrodynamics, we use the fully q-dependent kernel $K_{h,e}(q,T)$ [Eq.(10)] and put it into the integral formula for $\lambda(T)$ with the specular boundary condition,

$$\lambda_{\text{spec}}(T) = \frac{2}{\pi} \int_0^\infty \frac{d\tilde{q}}{\tilde{q}^2 + N_h(0)\tilde{K}_h(q,T) + N_e(0)\tilde{K}_e(q,T)} \tag{11}$$

where $\tilde{K}_{h,e}(q,T)$ are the normalized kernels as $\tilde{K}_{h,e}(0,0) = 1$ and $\tilde{q} = q\alpha_0$ is a dimensionless momentum. The results with a diffusive boundary condition are qualitatively the same; therefore, they will not be discussed. For the non-local parameter $\alpha_0$, we think it to be much smaller than 1 for the Fe-based superconductors, but here we take it as a free parameter and see how large value is needed to fit experimental data.

Fig.9 and Fig.10 show the normalized total superfluidity density $\lambda^2(0)/\lambda^2(T)$ of double d-wave gap and its separate contributions from the hole and electron bands for the double d-wave gap state. Fig 9 used $\Delta_h^{\text{max}}/T_c=1.75$ and $\Delta_h^{\text{max}}/T_c=1.0$. In each figure, panel (A) is a local limit ($\alpha = 0.0$) and the panel (B) is a non-local limit ($\alpha = 0.5$). The local cases display the typical d-wave behavior at low temperatures, i.e., the linear decrease in $T$ from $T_c = 0$. The extreme non-local cases ($\alpha_0 = \frac{\hat{q}}{\hat{q}_0} = 0.0$ and $\alpha_0 = 0.5$) introduce a substantial round-off ($\sim T^2$) region at low temperatures, which is, however, not an exponentially flat behavior as the recent experiments claim. Further, even a rough fitting requires an unreasonably large non-local parameter $\alpha_0$.

In summary, the double d-wave gap state can provide consistent descriptions for tunneling DOS, $1/T_1$, and Knight shift. However, there is an intrinsic difficulty to explain the flat behavior of the penetration depth at low temperatures. Also, in our model with an AFM mediated pairing interaction only, the double d-wave gap solution is energetically less favored than the $\pm s$-wave gap solution.

**IV. CONCLUSION**

We demonstrated that a minimal model with a phenomenological pairing interaction of the AFM spin fluctuations can allow both the $\pm s$-wave gap and the double d-wave gap solutions with the realistic bands of the Fe-based SC compounds. With the same parameters, the $\pm s$-wave gap solution is energetically more favorable by a factor of $\sim 5$ times, so that it has a better chance to be realized in the Fe-based SC compounds.
In both cases, we found that the approximate relation $\Delta_{\text{max}}N_{h} \approx \Delta_{\text{max}}N_{e}$ holds because it is a generic feature of the two gap SC when an interband pair scattering is the dominant pairing interaction. This relation appears for all SC properties in a subtle way, which modifies the value of $\Delta(0)/T_c$ and other SC properties in an unorthodox way. Numerically solving the coupled gap equations for the two bands, we found the detailed structure of the gap functions $\Delta_{\text{s}c}(k)$, which showed an anisotropy ($\sim 20\%$) of the $\pm s$-wave gaps. We also calculated the key SC properties, for both gap states, such as tunneling DOS, $1/T_{1}$, Knight shift, and penetration depth and discussed them in comparison with experiments. When we calculated these quantities, we paid a special attention to the interband coherence factor which is a unique feature of multi-gap SC. This interband coherence factor particularly produced an important modification to the $1/T_{1}$ relaxation rate of the $\pm s$-wave gap state.

The $\pm s$-wave gap state provides the most consistent descriptions for the penetration depth experiments: the flat low-temperature behavior.\textsuperscript{13} Besides the low-temperature behavior, the high-temperature ($0.3 T_c < T < T_c$) behavior – due to a large difference of the gap sizes $\Delta_{h}$ and $\Delta_{e}$ and their corresponding DOS $N_{h,e}$ – can be either concave or convex. However, $1/T_{1}$ experiments can only be fitted for a limited temperature range, even with a fine tuning of $\Delta_{h,e}/T_c$ ratio and impurities. The $\pm s$-wave gap state is not inconsistent with the Knight shift and the tunneling DOS data, but overall does not provide any decisive merit in comparison with the double $d$-wave gap.

The double $d$-wave gap state, although it is energetically less favorable in our model unless additional interactions are added, provides the best fit to the $1/T_{1}$ experiments. However, it has a difficulty to explain the penetration depth experiments for the low temperature flat behavior. It requires an unreasonably large non-local effect to fit the low temperature part; it is still not exponentially flat but only $\sim T^2$. If this low temperature part of $\lambda(T)$ is, indeed, confirmed to be exponentially flat, the double $d$-wave gap state should be ruled out. Tunneling DOS and Knight shift can be fit with the double $d$-wave gap state as much as with the $\pm s$-wave gap state.

In conclusion, quantitative calculations, carried out in this paper, with the two most promising SC gap states can serve as guidelines for sorting out the possible pairing states of the Fe-based SC in comparison with the current and future experiments. For that, very low temperature measurements and systematic studies with the amount of impurities will provide decisive information to determine the correct gap symmetry.

Note added – Recently, we have known that similar studies of $1/T_1$ for the $\pm s$-wave state were carried out by two groups\textsuperscript{25} where only the interband scattering process was analyzed and by another recent paper\textsuperscript{26} where both the interband and intraband processes were considered as in our paper.

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APPENDIX A: RELATION BETWEEN $\Delta_{h}/\Delta_{e}$ AND $N_{h}/N_{e}$

In the main text, we claimed the approximate relation $N_{h}\Delta_{h} \approx N_{e}\Delta_{e}$ as a generic feature of the two-band model with a dominant interband interaction. This kind of relation will have direct and important implications to the experimental observations. However it is pointed out by Mazin\textsuperscript{22} that this is not a rigorous identity in general. In this appendix, we clarify the degree of the validity of this relation.

Here we consider the $\pm s$-wave gap state only. Assuming constant gaps, $\Delta_{h}(k) = \Delta_{h}$ and $\Delta_{e}(k) = -\Delta_{e}$, and only the interband interaction, the coupled gap equations (5) and (6) are simplified as

\begin{equation}
\lambda(T) = \frac{\Delta_{h}}{\sqrt{N_{h}/N_{e}}} - \frac{\Delta_{e}}{\sqrt{N_{e}/N_{h}}}
\end{equation}
\[ \Delta_h = V_{hh} \Delta_c(T, \Delta_c, \omega_{AFM}) \quad (A.1) \]
\[ \Delta_c = V_{ch} \Delta_h(T, \Delta_h, \omega_{AFM}) \quad (A.2) \]

where \( \chi_h \) and \( \chi_c \) are defined with Eq.(7).

First, when \( T = T_c \), the above equations can be written as
\[ \Delta_h = V_{hh} N_c \Delta_c \times \text{const} \quad (A.3) \]
\[ \Delta_c = V_{ch} N_h \Delta_h \times \text{const} \quad (A.4) \]

where \( \text{const} = \int_0^{\omega_{AFM}} d \xi \frac{1}{\xi} \approx \log 1.14 \omega_{AFM} / T_c \). Because of \( V_{hh} = V_{ch} \), we immediately obtain the following relation from the above equations.
\[ \frac{\Delta_c}{\Delta_h} = \sqrt{\frac{N_h}{N_c}} ; \ \text{when} \ T = T_c. \quad (A.5) \]

Next, when \( T = 0 \), Eqs. (A.1) and (A.2) are written as
\[ \Delta_h = V_{hh} N_c \Delta_c \log(\frac{\omega_{AFM}}{\Delta_c} + \sqrt{\frac{\omega_{AFM}^2 + \Delta_c^2}{\Delta_c}}) \quad (A.6) \]
\[ \Delta_c = V_{ch} N_h \Delta_h \log(\frac{\omega_{AFM}}{\Delta_h} + \sqrt{\frac{\omega_{AFM}^2 + \Delta_h^2}{\Delta_h}}) \quad (A.7) \]

In general, these equations do not yield a simple algebraic relation between \( \Delta_c/\Delta_h \) and \( N_h/N_c \), but we can obtain the simple relations for the limiting cases. First, for the extreme weak coupling limit, i.e., when \( \Delta_h \ll \omega_{AFM} \), the two logarithmic terms become asymptotically equal as \( \log(2\omega_{AFM}/\Delta_c) \approx \log(2\omega_{AFM}/\Delta_h) \), and we obtain the same relation as the \( T = T_c \) case Eq.(A.5). On the other hand, for strong-coupling limit, i.e., when \( \Delta_h \gg \omega_{AFM} \) (which is certainly an unphysical limit), \( \log((\omega_{AFM} + \sqrt{\omega_{AFM}^2 + \Delta_{h,c}^2})/\Delta_{h,c}) \approx \omega_{AFM}/\Delta_{h,c} \) and we obtain the relation,
\[ \frac{\Delta_c}{\Delta_h} = \frac{N_h}{N_c} ; \ \text{when} \ T = 0 \ \text{and} \ \Delta_{h,c} \gg \omega_{AFM}. \quad (A.8) \]

Having found the results of the two limiting cases, we can guess that the gap ratio \( \Delta_c/\Delta_h \) should be in between these two limiting ratios. For example, we can attempt an expansion with \( x = \log [N_h/N_c] \) starting from the weak-coupling limit, and we obtain, in the first order of \( x \),
\[ \frac{\Delta_c}{\Delta_h} \approx \sqrt{\frac{N_h}{N_c}} (1 + \frac{\log [N_h/N_c]}{4} \lambda + \ldots) \quad (A.9) \]

where \( \lambda = \sqrt{V_{hh} V_{ch} N_h N_c} \) is a dimensionless coupling constant. For practical use, we numerically solve Eqs. (A.1) and Eq.(A.2) and plot the ratio \( \Delta_c/\Delta_h \) as a function of \( \lambda \) in Fig.A.1. The ratio \( \Delta_c/\Delta_h \) becomes a universal curve when it is normalized by the distance between \( \sqrt{\frac{N_h}{N_c}} \) and \( \frac{N_h}{N_c} \). The result indeed shows that when \( \lambda \approx 1 \), it is in between two limiting ratios, \( \sqrt{\frac{N_h}{N_c}} \) and \( \frac{N_h}{N_c} \) as we expected from the above analysis.

In reality, there exist two complications. First, the intraband couplings \( V_{hh} \) and \( V_{ch} \) need to be included. A little analysis of Eqs. (5) and (6) as well as of numerical results reveals that this effect always enhances the gap ratio toward the limit \( N_h/N_c \). Another complication arises from the fact that there are more than two bands in real materials\(^3,4,5,6,7\). Applying the results of the above analysis, we can suggest the following approximate relations. First, we classify the bands of the real materials into two groups: the hole bands around \( \Gamma \) point and the electron bands around \( M \) point, respectively. Then in the strong-coupling limit,
\[ \sum_i \Delta_{h,i} N_{h,i} \approx \sum_i \Delta_{c,i} N_{c,i}, \quad (A.10) \]

and in the extreme weak-coupling limit,
\[ \sum_i \Delta_{h,i} \sqrt{N_{h,i}} \approx \sum_i \Delta_{c,i} \sqrt{N_{c,i}}. \quad (A.11) \]

Considering several uncertainties in reality, Eq.(A.10) can serve as a practical rule of the thumb.
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