Model for the inverse isotope effect of FeAs-based superconductors in the π-phase-shifted pairing state

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The isotope effects for Fe-based superconductors are considered by including the phonon and magnetic fluctuations within the two-band Eliashberg theory. We show that the recently observed inverse isotope effects of Fe, $\alpha_{\mathrm{Fe}} \approx -0.18 \pm 0.03$ [P. M. Shirage, K. Kihou, K. Miyazawa, C.-H. Lee, H. Kito, H. Eisaki, Y. Tanaka, and A. Iyo, arXiv:0903.3515 (unpublished)] as well as the large positive isotope exponent ($\alpha \approx 0.35$) can naturally arise for the magnetically induced sign revered s-wave pairing state within reasonable parameter range. Either experimental report cannot be discarded from the present analysis based on the parameter values they require. The inverse and positive isotope effects mean, respectively, the interband and intraband dominant electron-phonon interactions. We first make our points based on the analytic result from the square-well potential model and present explicit numerical calculations of the two-band Eliashberg theory.

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I. INTRODUCTION

The alluring prospect of opening a key window to understanding the mechanism of high-temperature superconductivity has attracted fierce research activities in the iron-based pnictides.[1–3] The first step toward this path is to establish the pairing symmetry and dynamics of the FeAs superconductors. Among the many ideas put forward, particularly appealing is the sign reversed pairing state.[4,5] It is the ground state of a two-band superconductivity where both pairing order parameters, Δ_1 and Δ_2, on the two bands have full gaps while acquiring the π phase shift between them. A repulsive interband interaction is turned to induce pairing by generating the sign reversal between the two order parameters. The subsequent theoretical studies supported the idea of the sign reversed full gaps. The $s_{\pm}$ or $s\pi$ pairing state seems to be able explain the experimental observations indicating the full gap as well as a gap with nodes.[6–9] The evidence for the full gaps came from the several independent angle-resolved photoemission spectroscopy (ARPES) experiments on single crystals.[10–12] The phase shift of π may account for the absence of the Hebel-Slichter peak and the low-temperature behavior of $\sim T^3$ in the spin-lattice relaxation rate $1/T_1$,[13–15] which seemed difficult to understand in terms of a full gap scenario.

As for the pairing interaction, one widespread school of thought maintains that magnetic fluctuations are intimately involved for the superconductivity. The superconductivity emerges out of the interplay between the density of charge carriers and strength of antiferromagnetic (AF) interaction such that their combined effect becomes optimum. This view seems natural from the overall phase diagram of the pnictides in the temperature and doping plane. The superconductivity emerges from the parent metallic antiferromagnetic state as the static AF order is suppressed and charge carriers are introduced through the chemical doping.[16] This view is further supported by the neutron-scattering investigations showing a resonance at a wave vector related to the AF order coincident with the onset of superconductivity.[17] Within this school of thought, combined with the theoretical estimates of the small electron-phonon coupling constant, it came rather as a surprise that a large isotope coefficient $\alpha \approx 0.34-0.37$ was observed by Liu *et al.* with a substitution of ^{56}Fe by ^{54}Fe in $SmFeAsO_{1-x}F_x$ ($x=0.15$) and $Ba_{1-x}K_xFe_2As_2$ ($x=0.4$).[18] Theoretical calculation by Boeri *et al.* reported a very weak electron-phonon coupling constant ($\lambda_{ph} \approx 0.21$),[19] which is too small to account for the observed T_c of the pnictides. Recall that α is indeed very small for the cuprate superconductors particularly near the optimal doping.[20] Perhaps even more surprising is the observation of the sizable *inverse* isotope effect of $\alpha_{\mathrm{Fe}} = -0.18 \pm 0.03$ by Shirage *et al.* in $Ba_{1-x}K_xFe_2As_2$ ($x=0.4$).[21]

In view of this controversy, it is important that the Liu *et al.* and Shirage *et al.* results be confirmed. What we study here is to check if these experimental results are compatible with the current understanding of the pnictide superconductivity. We can estimate the parameters such as the coupling constants that these experiments require. These motivate us to revisit the issue of electron-phonon coupling in the Fe pnictides. We argue that the inverse isotope effect as well as the large positive effect can arise with a reasonable parameter range within the widely held view of the magnetically mediated π phase-shifted s-wave pairing scheme. We first make our points based on the analytic result from the square-well potential model applied to the sign changing s-wave state and substantiate them by the explicit numerical calculations of the two-band Eliashberg theory.

II. IDEA AND MODEL

As sketched below in Sec. III, a straightforward application of the square-well potential model to the case where there are AF spin fluctuations and phonons yield that the critical temperature T_c and isotope exponent α are given as follows:

$$T_c = 1.14\omega_{ph} \exp\left(-\frac{1+\lambda^{+}_{\mathrm{AF}}+\lambda^{+}_{ph}}{\Lambda_{eff}-\lambda^{-}_{ph}}\right), \tag{1}$$

$$\alpha = \frac{1}{2}\left[1-\frac{1+\lambda^{+}_{\mathrm{AF}}+\lambda^{+}_{ph}}{1+\lambda^{+}_{\mathrm{AF}}}\left(\frac{\Lambda_{eff}}{\Lambda_{eff}-\lambda^{-}_{ph}}\right)^2\right], \tag{2}$$

$$\Lambda_{eff} = \frac{\lambda^{-}_{\mathrm{AF}}}{1-\frac{\lambda^{-}_{\mathrm{AF}}}{1+\lambda^{+}_{\mathrm{AF}}}\ln\left(\frac{\omega_{\mathrm{AF}}}{\omega_{ph}}\right)}, \tag{3}$$

where ω_{AF} and ω_{ph} are the AF fluctuation and phonon frequencies and $\lambda^{\pm}_{\mathrm{AF}/ph}$ is given by the sum/difference between the interband and intraband interactions as

$$\lambda^{\pm}_{\mathrm{AF}/ph} = \lambda^{(inter)}_{\mathrm{AF}/ph} \pm \lambda^{(intra)}_{\mathrm{AF}/ph}. \tag{4}$$

Note that the T_c formula of Eq. (1) is reduced to the formula in Shirage *et al.*[21] in the limit that $\lambda^{(intra)}=0$ and the quasiparticle renormalization is neglected. Also similar formulas were obtained before in different contexts.[22,23] The result of Eqs. (1) and (2), which will be backed up below by numerically solving the two-band Eliashberg theory, explicitly shows that depending on whether $\lambda^{-}_{ph} \gtrsim 0$ or $\lesssim 0$, the isotope effect can show the inverse or conventional behavior.

Two factors are behind this interesting effect: the − sign between the Λ_{eff} and λ^{-}_{ph} of Eq. (2) and the possibility of both signs of λ^{-}_{ph} of Eq. (4). The first factor comes from that the phonon and spin fluctuations enter the pairing kernel $\lambda^{(-)}_{ij}$ with the opposite sign as in Eqs. (6) and (7) and the second factor from the sign change between the two gaps as suggested by the $s_{\pm}$ model.[4,5] An inspection of α of Eq. (2) then reveals that the inverse isotope effect implies that the interband electron-phonon coupling is comparable to or stronger than the intraband coupling. Note also that $\lambda^{inter}_{ph}=\lambda^{intra}_{ph}$ gives the inverse isotope effect except when both are equal to zero. Also noteworthy is that when $\Lambda_{eff}-\lambda^{-}_{ph}\approx 0$, T_c becomes very small and a giant isotope effect will appear, $|\alpha| \gg 1/2$. It seems that both the large isotope effect and the inverse isotope effect can arise in the magnetically induced π phase-shifted pairing for the pnictides within a reasonable parameter range. Either experimental report cannot be discarded from the present analysis based on the parameter values they require.

Although this discussion demonstrates the essential physics, it neglects the more general spin and phonon interactions and involves the square-well potential model which is not a controlled approximation. We will therefore present the results of the numerical calculations to show that inclusion of these effects still supports this conclusion. We will show this by the two-band Eliashberg calculations as presented in what follows.

III. FORMALISM

The two-band Eliashberg equation with an isotropic gap in each band may be written in the Matsubara frequency as

$$Z_i(ip_n) = 1 + \frac{\pi T}{p_n}\sum_{j,m}\lambda^{(+)}_{ij}(i\omega_n)\frac{p_m}{\sqrt{p_m^2+\Delta_j(ip_m)^2}}, \tag{5}$$

$$\Delta_i(ip_n)Z_i(ip_n) = \pi T\sum_{j,m}\lambda^{(-)}_{ij}(i\omega_n)\frac{\Delta_j(ip_m)}{\sqrt{p_m^2+\Delta_j(ip_m)^2}}, \tag{6}$$

where $i,j=1,2$ are the band indices, $\omega_n=p_n-p_m$, T is the temperature, and p_n and p_m are the Matsubara frequencies. The kernel $\lambda^{(\pm)}_{ij}$ are given by

$$\lambda^{(\pm)}_{ij}(i\omega_n) = \lambda^{(ph)}_{ij}(i\omega_n) \pm \lambda^{(\mathrm{AF})}_{ij}(i\omega_n). \tag{7}$$

We take the phonon and spin fluctuations as

$$\lambda^{(\mathrm{AF}/ph)}_{ij}(i\omega_n) = \lambda^{\mathrm{AF}/ph}_{ij}\int_0^\infty d\epsilon \frac{\omega_\nu \epsilon}{\epsilon^2+\omega_n^2}F(\epsilon), \tag{8}$$

where $F(\epsilon)$ is a truncated Lorentzian centered at $\omega_\nu=\omega_{\mathrm{AF}/ph}$,

$$F(\epsilon) = \begin{cases} \frac{1}{R}\left[\frac{1}{(\epsilon-\omega_\nu)^2+\Gamma^2}-\frac{1}{\Gamma_c^2+\Gamma^2}\right], & \text{for } |\epsilon-\omega_\nu| \le \Gamma_c \\ 0, & \text{otherwise.} \end{cases} \tag{9}$$

We took $\Gamma_c=\omega_\nu$, $\Gamma=\Gamma_c/2$, and R is a normalization constant such that $\int_0^\infty d\epsilon F(\epsilon)=1$.[24] The $\Gamma_c=\omega_\nu$ was chosen such that $F(\epsilon)\sim\omega$ for small ω to simulate the overdamped AF spin fluctuations.

Equations (5) and (6) may be linearized near $T=T_c$ and may be written as the following matrix form in the basis of $\Delta_i(ip_n)$:

$$\Delta_i(ip_n) = \sum_j\sum_m M_{ij}(n,m)\Delta_j(ip_m), \tag{10}$$

where the matrix M is defined as

$$M_{ij}(n,m) = \frac{\pi T}{|p_m|}\frac{\lambda^{(-)}_{ij}(ip_n-ip_m)}{Z_i(ip_n)},$$

$$Z_i(ip_n) = 1 + \frac{\pi T}{p_n}\sum_{j,m}\lambda^{(+)}_{ij}(ip_n-ip_m)\mathrm{sgn}(p_m). \tag{11}$$

The T_c is then determined to be the temperature at which the largest eigenvalue of the matrix M becomes 1. The isotope coefficient is given by

$$\alpha = \frac{1}{2}\frac{\partial \ln T_c}{\partial \ln \omega_{ph}}. \tag{12}$$

IV. PRELIMINARY ANALYSIS

Let us first consider some preliminary analytic analyses based on the square-well potential model applied to the $s_{\pm}$ state. After neglecting the frequency dependence of $\lambda^{(\pm)}_{ij}(i\omega_n)$

and taking the standard approximation of $\Delta_i(\omega)=\Delta_{ia}$ for $0<\omega<\omega_{ph}$ and Δ_{ib} for $\omega_{ph}<\omega<\omega_{\rm AF}$ and similarly for $Z_i(\omega)$, we can rewrite Eqs. (11) and (10) as

$$Z_{ia}=1+\sum_j \lambda_{ij}^{(+)}, \tag{13}$$

$$Z_{ib}=1+\sum_j \lambda_{ij}^{\rm AF}, \tag{14}$$

$$\Delta_{ia}Z_{ia}=\sum_j [\lambda_{ij}^{(-)}F_a\Delta_{ja}-\lambda_{ij}^{\rm AF}F_b\Delta_{jb}], \tag{15}$$

$$\Delta_{ib}Z_{ib}=-\sum_j [\lambda_{ij}^{\rm AF}F_a\Delta_{ja}+\lambda_{ij}^{\rm AF}F_b\Delta_{jb}], \tag{16}$$

where the band indices take $i,j=1,2$ and

$$F_a=\int_0^{\omega_{ph}} d\xi\frac{1}{\xi}\tanh\left(\frac{\xi}{2T_c}\right)=\ln\left(\frac{1.14\omega_{ph}}{T_c}\right),$$

$$F_b=\ln\left(\frac{\omega_{\rm AF}}{\omega_{ph}}\right). \tag{17}$$

A straightforward manipulation taking advantage of the relations $\Delta_{1a}=-\Delta_{2a}$ and $\Delta_{1b}=-\Delta_{2b}$ of the $s_\pm$ state gives Eqs. (1)–(3) given above. Here, we used the definitions $\lambda_{\rm AF/ph}^{\pm}=\lambda_{12}^{\rm AF/ph}\pm\lambda_{11}^{\rm AF/ph}$ and considered the simple cases of $\lambda_{12}^{\rm AF/ph}=\lambda_{21}^{\rm AF/ph}$ and $\lambda_{11}^{\rm AF/ph}=\lambda_{22}^{\rm AF/ph}$.

Before we present the results from the numerical computations of the linearized Eliashberg equation of Eq. (10), we first consider the approximate solutions from Eqs. (1) and (2) to get ourselves oriented to the relevant parameter space. Let us first consider the inverse isotope effect in the context of the $s\pi$ pairing state. This may be realized when the interband dominates the intraband phonon interaction as discussed above. We take the simple parameterization of the interband interactions only, $\lambda_{\rm AF/ph}^{\pm}=\lambda_{\rm AF/ph}$ ($\lambda_{11}^{\rm AF/ph}=\lambda_{22}^{\rm AF/ph}=0$). From $T_c\approx 3.0$ meV and $\alpha\approx -0.2$ reported by Shirage *et al.* for $Ba_{1-x}K_xFe_2As_2$, we get $\lambda_{\rm AF}=1.53$ and $\lambda_{ph}=0.189$ for $\omega_{ph}=\omega_{\rm AF}=20$ meV, and $\lambda_{\rm AF}=0.944$ and $\lambda_{ph}=0.146$ for $\omega_{ph}=20$, $\omega_{\rm AF}=30$ meV. The obtained $\lambda_{\rm AF}>\lambda_{ph}$ is consistent with the magnetically induced pairing.

We now turn to the $\alpha>0$ case, which one of the authors considered previously.[25] This may be realized in the context of the $s\pi$ pairing state by $\lambda_{\rm AF}^{\pm}=\lambda_{\rm AF}$ and $\lambda_{ph}^{\pm}=\pm\lambda_{ph}$. From $T_c\approx 3.5$ meV and $\alpha\approx 0.35$ reported by Liu *et al.* for $SmFeAsO_{1-x}F_x$, we get $\lambda_{\rm AF}=0.836$, and $\lambda_{ph}=0.738$ by solving Eqs. (1) and (2) for $\omega_{ph}=20$ meV and $\omega_{\rm AF}=10$ meV. The solution for $\omega_{ph}=\omega_{\rm AF}=20$ meV does not satisfy $\lambda_{\rm AF}>\lambda_{ph}$ relevant for the magnetically mediated superconductivity. The inverse or positive isotope effect is naturally obtained when $\omega_{\rm AF}>\omega_{ph}$ or $<$. This was pointed out by Shimahara in a different context.[22]

In the derivation of Eqs. (1) and (2), we assumed $\omega_{\rm AF}>\omega_{ph}$; if $\omega_{\rm AF}<\omega_{ph}$, they are *not* valid. Also, they are based on the uncontrolled double-well approximation. The correctness of the results is confirmed by numerical calculations we are presenting below.

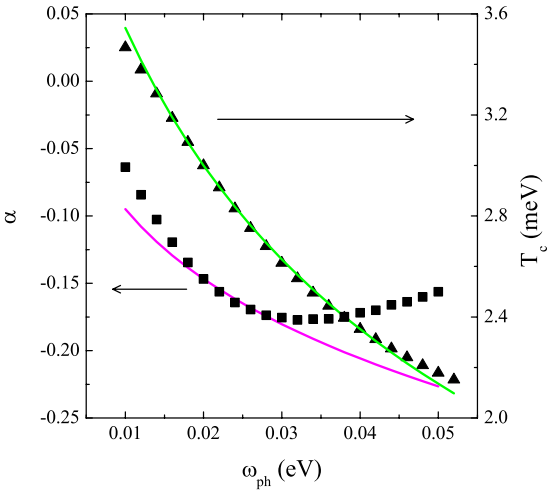

FIG. 1. (Color online) The transition temperature T_c and isotope exponent α as a function of the phonon frequency ω_{ph}. $\omega_{\rm AF}=30$ meV, $\lambda_{\rm AF}=2.26$, $\lambda_{ph}=0.5$, and all the intraband couplings are set equal to 0. Solid lines are the plots of Eqs. (1) and (2). See the text for their parameters.

V. NUMERICAL RESULTS

In Fig. 1, we show the results of numerical calculations of the inverse isotope effect. We took, guided by the above discussion, $\omega_{\rm AF}=30$ meV and adjusted the interband $\lambda_{\rm AF}$ and λ_{ph} with all intraband interactions set to 0, so that the T_c and α give the right values for $Ba_{1-x}K_xFe_2As_2$. With $\lambda_{\rm AF}=2.26$ and $\lambda_{ph}=0.5$, ω_{ph} was varied between 10 and 50 meV. The solid squares and triangles show the α and T_c, respectively. The lines are the plots from Eqs. (1) and (2). $\lambda_{\rm AF}=0.876$ and $\lambda_{ph}=0.104$ were selected such that T_c and α agree with the numerical calculations at $\omega_{ph}=20$ and $\omega_{\rm AF}=30$ meV. The interaction parameters are somewhat different between the numerical and (approximate) analytic calculations.

We then consider the positive isotope effect and present the results in Fig. 2. We took $\omega_{\rm AF}=15$ meV, interband $\lambda_{\rm AF}=1.06$, intraband $\lambda_{ph}=0.950$, and varied ω_{ph} between 10 and 50 meV as before, with other interactions set to 0. The solid triangles and squares show the α and T_c, respectively, and the lines are from the analytic expression with $\lambda_{\rm AF}=0.878$ and $\lambda_{ph}=0.491$ to agree with the numerical results at $\omega_{\rm AF}=15$ and $\omega_{ph}=20$ meV.

Although we have not fine tuned the parameters to match the observed T_c and α exactly for the $Ba_{1-x}K_xFe_2As_2$ and $SmFeAsO_{1-x}F_x$, some features are worth noting. First, the parameters for the numerical and analytical calculations to give the observed T_c and α were somewhat different. This is because $\lambda_{\rm AF}$ and λ_{ph} vary sensitively as $\omega_{\rm AF}$ is varied (but not so sensitively on ω_{ph}) in this region of parameter space as one can see easily by solving Eqs. (1) and (2). Second, it is necessary that the phonons are predominantly of interband/intraband character for the inverse/positive isotope effects. And, third, the phonon coupling constant somewhat larger than the theoretical calculation seems necessary.[19] But, this might be understood by including other effects such as the different density of states between the bands.[25]

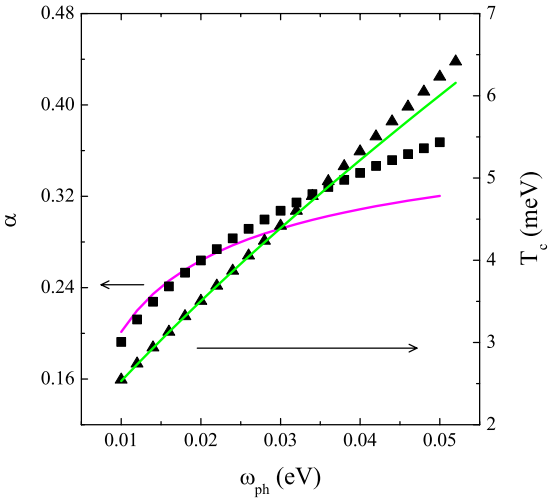

FIG. 2. (Color online) T_c and α as a function of ω_{ph}. $\omega_{\mathrm{AF}}=15$ meV, $\lambda_{\mathrm{AF}}=1.06$, $\lambda_{ph}^{(intra)}=0.950$. Solid lines are the plots of Eqs. (1) and (2). See text for their parameters.

VI. REMARKS

We have shown that both the inverse isotope effect and large isotope exponent reported in the pnictides may arise in the magnetically induced π phase-shifted pairing with reasonable parameters. Either experimental report cannot be discarded from the present analysis based on the parameter values they require. The dominant interband (intraband) phonon interaction produces the inverse (positive) isotope effect. Note that the contradicting inverse and positive isotope effects were observed in the same compound, $Ba_{1-x}K_xFe_2As_2$ ($x=0.4$), by Fe substitution. The Liu result was obtained on the sample from the solid-state reaction whereas the Shirage result from the high-pressure technique. If either result turns out to be reproducible, it will point to the interband or intraband dominant electron-phonon interaction in the pnictides. Liu *et al.* also observed that O isotope effect is quite small, $\alpha_{\mathrm{O}}\approx -0.06$. In the framework proposed here, this may be understood in terms of $\lambda_{ph}^{+}\approx\lambda_{ph}^{-}\approx 0$ for the O ions. It remains to be checked if this anticipation is correct. It will be also interesting to see if the spin-density wave isotope exponent reported by Liu *et al.* may be understood within the proposed idea here.

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