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Review Article

Spin-Lattice Coupling and Superconductivity in Fe Pnictides

T. Egami,[1,2,3] B. V. Fine,[4] D. Parshall,[2] A. Subedi,[2] and D. J. Singh[3]

[1] *Department of Materials Science and Engineering, Joint Institute for Neutron Sciences, University of Tennessee, Knoxville, TN 37996, USA*
[2] *Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA*
[3] *Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*
[4] *Institute for Theoretical Physics, University of Heidelberg, Heidelberg 69120, Germany*

Correspondence should be addressed to T. Egami, egami@utk.edu

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We consider strong spin-lattice and spin-phonon coupling in iron pnictides and discuss its implications on superconductivity. Strong magneto-volume effect in iron compounds has long been known as the Invar effect. Fe pnictides also exhibit this effect, reflected in particular on the dependence of the magnetic moment on the atomic volume of Fe defined by the positions of the nearest neighbor atoms. Through the phenomenological Landau theory, developed on the basis of the calculations by the density functional theory (DFT) and the experimental results, we quantify the strength of the spin-lattice interaction as it relates to the Stoner criterion for the onset of magnetism. We suggest that the coupling between electrons and phonons through the spin channel may be sufficiently strong to be an important part of the superconductivity mechanism in Fe pnictides.

1. Introduction

Recent discovery of superconductivity in Fe pnictides [1] with the critical temperature T_C up to 55 K [2] caused enormous excitement in the field, for various reasons. First, this is the first noncuprate family of superconductors with T_C above 40 K. Second, superconductivity appears when the antiferromagnetic (AFM) order is suppressed by doping [3], just as in the cuprates. Third, unlike the cuprates, strong electron correlations are not observed by spectroscopy [4], suggesting that the Mott physics may not be a necessary ingredient for the mechanism of high-temperature superconductivity. Finally, there is a large family of similar compounds that show superconductivity, making experimental research less restricted by chemical or materials issues. The field is making surprisingly fast development, partly because of the accumulated experience of working on the cuprates. It is possible that the origin of thesuperconductivity in this family of compounds may be easier to identify than for the cuprates, and the success of solving this problem hopefully will facilitate understanding of the cuprate problem.

Even though the AFM order is suppressed by doping, spins are active in the doped Fe pnictide superconductors. Again, just as in the cuprates strong magnetic excitations, including the so-called resonance peak, are observed by inelastic neutron scattering [5–8]. Core level spectroscopy is consistent with the local Fe moment of about $1\,\mu_B$ [4]. Interestingly, the density functional theory (DFT) calculations always predict the magnetic ground state (AFM or incommensurate order) for the experimental lattice constants [9–12]. The phonon dispersions observed by inelastic X-ray scattering are consistent with the DFT calculations only when the magnetic ground state is assumed [13]. Only in the collapsed phase of $CaFe_2As_2$, in which the c-axis lattice constant is reduced by as much as 10% compared to the magnetic state, does the material become truly spin-degenerate [14]. All these observations strongly suggest that the superconducting samples are locally and dynamically spin-polarized, and show strong dynamic Fe spin fluctuations. Although we do not have precise knowledge of their spin dynamics, judged from the absence of strong quasielastic scattering in neutron scattering with energy resolution of 1 meV, the time-scale of fluctuation must not be slower than 1 ps. This result supports the view that spins are involved in the mechanism of superconductivity, for instance though the spin-fluctuation mechanism [15–17].

However, there are many puzzling, important questions that need to be answered before addressing the question of the mechanism: the first puzzle is the effect of doping. In the cuprates, doping is necessary for introducing mobile charge carriers, since the parent compounds are Mott-Hubbard insulators. In Fe pnictides, on the other hand, the parent compounds are already metallic, and doping does not appear to change the charge carrier density very much [9]. Rather, the main effect of doping is to suppress the AFM ground state. In the pnictide parent compounds strongly two-dimensional spin fluctuations are observed above T_N [18], just as in the superconducting Fe pnictides [6, 8]. However, whereas the LaFeAsO (1111) type compounds are strongly two-dimensional [10], $BaFe_2As_2$ (122) type compounds are much more three-dimensional [19]. The second curious behavior is that the observed magnetic moment on the AFM phase varies from a compound to compound, but is always significantly smaller than predicted by the DFT calculations [10–12]. Third, there is an interesting interplay between both the lattice and magnetism [20], and the lattice and superconductivity [21, 22]. In this article, we focus on the third point, that of the lattice effect. For the purpose of highlighting the essence of the effect, we use simple approximations, namely the Landau theory and the Stoner theory, using the results of the LDA calculations as a guide. We argue that through the spin-lattice coupling effect the lattice may play a much larger role than generally acknowledged in determining the properties of Fe pnictides, possibly including even the superconductivity.

2. Magneto-Volume Effect in Fe Pnictides

2.1. Dependence of Fe Moment on the Structure. It has long been known that the magnetic moment of transition metals depends on volume [23]. Because of the Pauli exclusion principle, the electron kinetic energy of the spin-polarized state is higher for parallel spins if the volume is the same, and volume expansion relaxes the kinetic energy. In some iron alloys, thermal volume expansion due to lattice anharmonicity cancels the decrease in volume associated in the decrease in spin-splitting, resulting in zero thermal expansion, widely known as the Invar behavior. The negative or zero thermal expansion is indeed observed for PrFeAsO [24]. The collapsed phase of $CaFe_2As_2$ is a dramatic case of such a magneto-volume effect. This compound shows AFM order below 140 K, but with the pressure of 0.4 GPa it undergoes the first-order phase transition into a nonmagnetic phase with the reduction in volume of 5% [14].

In Fe pnictides, layers of Fe atoms are sandwiched by layers of pnictide such as As or P [1]. Thus if the layer-layer distance of pnictide is changed, the magnetic moment of Fe is strongly affected. This coupling of the Fe moment to the pnictide position in the lattice was recognized early by the DFT calculations [9, 20]. Figure 1 shows the calculated dependence of the Fe moment in $Ba(Fe_{0.92}Co_{0.08})_2As_2$ on the separation between the As layer and the Fe layer (z). The calculations were done within virtual crystal approximation (VCA) and local density approximation (LDA) with general

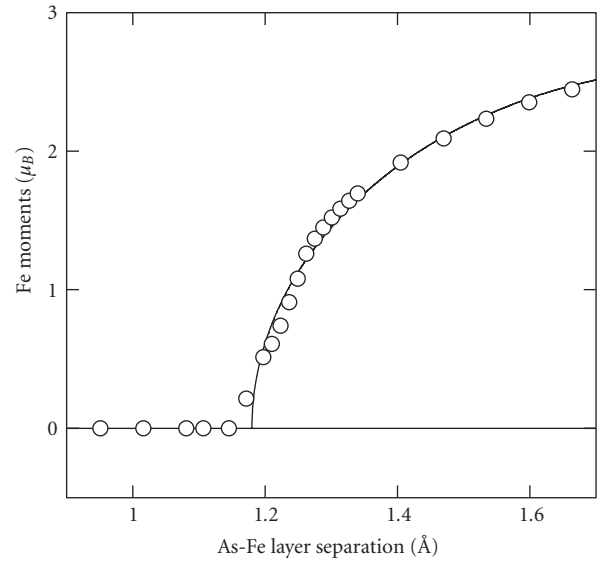

Figure 1: The magnetic moment, M, as a function of the Fe-As layer separation, z, calculated for $Ba(Fe_{0.92}Co_{0.08})_2As_2$. The solid curve is a fit by (3).

potential linearized augmented plane-wave (LAPW) method [25], including local orbitals [26]. LAPW sphere radii of 2.2 a_0, 2.0 a_0, and 2.0 a_0, where a_0 is Bohr radius, were used for Ba, Fe, and As, respectively. To account for Co doping, an electron number of 26.08 was used for Fe. We used the experimentally reported tetragonal lattice parameters (a = 3.9625 Å, c = 13.0168 Å) [27]. In the calculated result, clearly there is a quantum critical point (QCP) for magnetism near $z_c = 1.20$ Å as shown in Figure 1. The local exchange interaction is strong enough to spin-split the band by overcoming the kinetic energy cost only for $z > z_c$. We obtain similar results from the calculation on undoped $BaFe_2As_2$. Compared also with other data [12, 20], the relation between z and Fe moment M appears to be rather insensitive to compositions, and the relation shown in Figure 1 appears to be a nearly universal property of the FeAs triple layer. This must be because the in-plane lattice constant, thus the Fe-Fe distance, is very similar within ±1% among many Fe pnictide compounds. Thus the parameter z, the As-Fe layer separation, is a good common measure of the magneto-volume effect. For instance, in the collapsed phase of $CaFe_2As_2$ the value of z is 1.23 Å [14], close to the value of z_c in Figure 1.

2.2. Landau Theory. Let us develop a Landau-type theory to describe the dependence of the local magnetic moment, M, on the As-Fe layer separation, z. We may write the magnetic free energy as

$$F_M = AM^2 + BM^4 + F_{s-l}, \tag{1}$$

where F_{s-l} is the spin-lattice interaction energy expanded by $z - z_c$,

$$F_{s-l} = \left[\alpha(z - z_c) + \beta(z - z_c)^2\right]M^2, \tag{2}$$

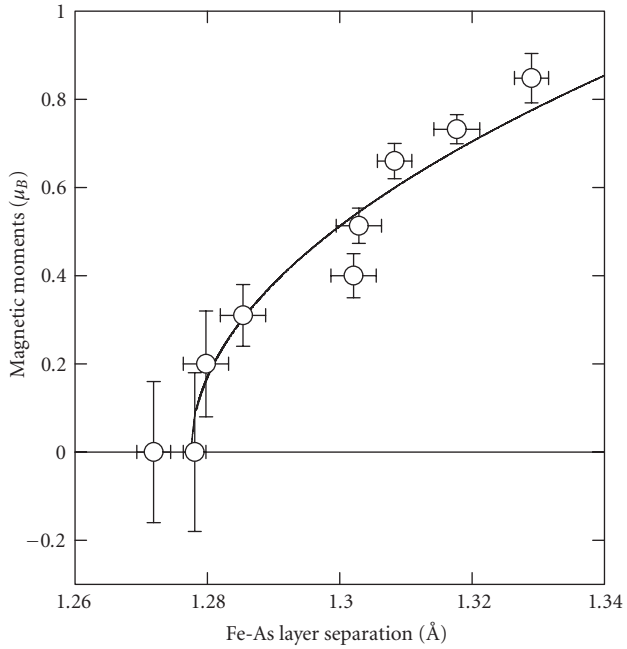

Figure 2: Dependence of the experimentally determined magnetic moment on the Fe-As layer separation for CeFe(As,P)O (open circles) [28], and the fit by (3) (solid curve).

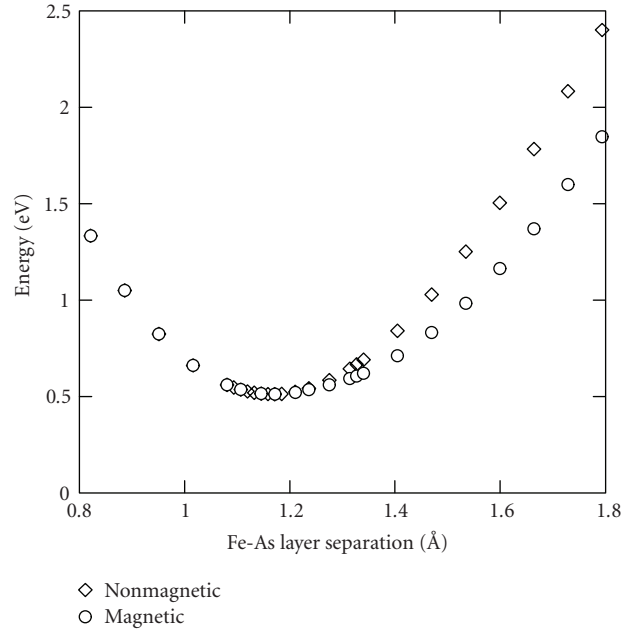

Figure 3: Electron energy as a function of the Fe-As layer separation is calculated by LDA for $Ba(Fe_{0.92}Co_{0.08})_2As_2$, with spin polarization; the elastic constant is reduced by 29% compared to the state without spin polarization, accounting for the phonon softening by 15% due to spin polarization.

where $\alpha < 0$. F_{s-l} is negative only for $z > z_c$. We retain only the terms with even powers of M because of the symmetry. We set $A = 0$ so that z_c is the critical point. By minimizing F_M with respect to M we obtain,

$$M^2 = \frac{|\alpha|}{2B}\left[(z - z_c) + \frac{\beta}{\alpha}(z - z_c)^2\right]. \tag{3}$$

The dashed line in Figure 1 gives the fit of this equation to the calculated moment. From this fit we obtain $z_c = 1.20$ Å, $\alpha/2B = 19.16\ \mu_B^2/$Å, and $\alpha/\beta = -1.40$ Å. In $CaFe_2As_2$, the QCP is hidden because the nature of the transition is strongly first order. In the vicinity of z_c, the moment is proportional to $(z - z_c)^{1/2}$.

Recently, the magnetic moment was experimentally determined for the series of compounds, $CeFe(As_{1-x}P_x)O$ [28]. Because As and P are isovalent, the replacement of As by P does not dope carriers to the system, but merely change the Fe(As/P) layer separation. Indeed (3) fits the results nicely as shown in Figure 2 [29]. Since the range of z is relatively, small β was neglected. The fit to the data gave $z_c = 1.278$ Å, $\alpha/2B = 11.67$ (μ_B/Å). Theoretical calculations for the CeFe(As,P)O system are in progress. Note that in the calculation presented in Figure 1, the lattice is assumed to be static. In reality, however, the zero-point phonons are present, with the amplitude of the order of 0.1 Å. This should shift the critical point upward, in better agreement with the data in Figure 2.

2.3. Phonon Softening. We now add the lattice elastic energy in order to consider the phonon softening due to the magneto-volume effect. The phonon to be considered here is the As Raman mode, in which As layers move against each other along the c-axis, either toward or away from the Fe layer. The magneto-elastic free energy is

$$\begin{aligned} F_S(z) &= \left[\alpha(z - z_c) + \beta(z - z_c)^2\right]M^2 + K(z - z_1)^2 \\ &= -\frac{\alpha^2(z - z_c)^2}{2B}\left[1 + \frac{\beta}{\alpha}(z - z_c)\right]^2 + K(z - z_1)^2. \end{aligned} \tag{4}$$

By minimizing F_S with respect to z we obtain the As position, z_M,

$$\begin{aligned} \left.\frac{\partial F_S}{\partial z}\right|_{z=z_M} &= -\frac{\alpha^2(z_M - z_c)}{B}\left[1 + \frac{2\beta}{\alpha}(z_M - z_c)\right]\left(1 + \frac{\beta}{\alpha}(z_M - z_c)\right) \\ &\quad + 2K(z_M - z_1) = 0. \end{aligned} \tag{5}$$

Then by taking the second derivative we obtain the elastic stiffness renormalized by the spin-lattice interaction,

$$K' = K\left\{1 - \frac{\alpha^2}{2KB}\left[1 + \frac{6\beta}{\alpha}(z_M - z_c) + 6\left(\frac{\beta}{\alpha}\right)^2(z_M - z_c)^2\right]\right\}. \tag{6}$$

As shown in Figure 3, allowing spin polarization softens the As Raman phonon frequency by 15% at $z_M = 1.36$ Å. This effect was noted earlier [12], and agrees with the experimental observations [13]. Note that the energy minimum of the DFT calculation systematically underestimates the lattice constant. Thus we obtain, $\alpha = -0.193$ eV/Å μ_B^2,

$\beta = 0.137\,\text{eV/Å}^2\mu_B^2$, and $z_1 = 1.32\,$Å. The value of z_1 is in good agreement with the LDA calculation (1.32 Å after correcting for the systematic underestimation), proving the internal consistency. Thus this theory elucidates how the magneto-volume interaction, (2) can induce magnetization as a function of the As-Fe layer separation, and softening of the As Raman phonon mode.

3. Generalized Stoner Condition

We now turn our attention to the Fe band splitting. We start with the classical Stoner theory of itinerant ferromagnetism [30], and generalize it to an antiferromagnet [31–33]. Even though more complex and accurate DFT calculations can be made, this is a useful exercise for simplicity and clarity of logic. In the Stoner theory the electron energy is given by

$$E = \int_0^{\varepsilon_{F\uparrow}} \varepsilon N_\uparrow(\varepsilon_\uparrow) d\varepsilon_\uparrow + \int_0^{\varepsilon_{F\downarrow}} \varepsilon N_\downarrow(\varepsilon_\downarrow) d\varepsilon_\downarrow + I n_\uparrow n_\downarrow, \quad (7)$$

where $N_\uparrow(\varepsilon)$ is the electron density of states for up spins, $n_\uparrow$ is the density of electrons with up spin, and $\varepsilon_\uparrow$ is the energy of an electron with up spin. Magnetization is given by $M = n_\uparrow - n_\downarrow$. If we start with the nonmagnetic state and introduce a small spin splitting by shifting the up spin by $d\varepsilon_\uparrow$, the energy changes

$$dE = 2N(\varepsilon_F)[1 - IN(\varepsilon_F)] d\varepsilon_\uparrow{}^2, \quad (8)$$

which gives the Stoner criterion,

$$IN(\varepsilon_F) \geq 1. \quad (9)$$

Near the Stoner QCP,

$$M = dn_\uparrow - dn_\downarrow = 2dn_\uparrow = 2N(\varepsilon_F) d\varepsilon_\uparrow, \quad (10)$$

thus

$$dE = \frac{1 - IN(\varepsilon_F)}{2N(\varepsilon_F)} M^2, \quad (11)$$

and in (1),

$$A = \frac{1 - IN(\varepsilon_F)}{2N(\varepsilon_F)}. \quad (12)$$

Thus $A = 0$ at the QCP.

In the case of an antiferromagnet, the same argument can be constructed for the staggered spin-split bands, except that the exchange energy term I includes the kinetic energy cost for modulating the spin split band by $K = \pi/a$ [32, 33]. Therefore, we can interpret z_c as the generalized Stoner QCP. In general for a spin density wave (SDW) ordering with Q, within the random phase approximation (RPA), the magnetic moment above the SDW ordering temperature is given by

$$M(Q) = \frac{\chi_0(Q)}{1 - I\chi_0(Q)} h_Q, \quad (13)$$

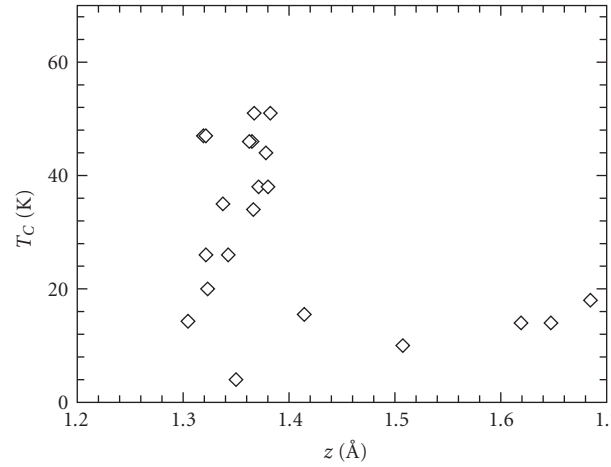

Figure 4: Superconducting critical temprture T_C, as a function of the As-Fe layer separation, z.

where $M(Q)$ is the SDW amplitude, $\chi_0(Q)$ is the generalized bare susceptibility, and h_Q is the SDW mean-field [31]. Thus the generalized Stoner condition is given by [31–33]

$$I\chi_0(Q) \geq 1. \quad (14)$$

Note that $\chi_0(Q = 0) = N(\varepsilon_F)$, which recovers the Stoner condition for ferromagnetism. Now the effect of lattice strain is to modify the generalized Stoner condition. For instance, reducing the As-Fe separation increases the bandwidth, thus decreases the generalized susceptibility. This brings the system closer to the Stoner QCP, and reduces the magnetic moment. Because the Fe pnictides are close to the Stoner QCP, even a small lattice strain, including phonons, can have very significant effects. Similarly, the in-plane Fe phonon mode that is relevant to the tetragonal-orthorhombic structural phase transition could also be important to the magnetism of Fe pnictides. The strong anisotropy of the spin exchange in the Fe plane [34] is indicative of the strong spin-lattice coupling in the Fe plane.

4. Relation to Superconductivity

One of the most intriguing lattice effects on the superconductivity of Fe pnictides is the dependence of the critical temperature, T_C, on the geometry of the $FeAs_4$ tetrahedron [21, 22]. Data show that T_C is strongly related to the As-Fe-As angle. Because the As-Fe-As angle is directly related to the Fe-As layer separation, z, in Figure 4, we plotted T_C as a function of z, using the published results of crystallographic analysis. The results are shown also in Table 1, with references for the data. Clearly the behavior above $z_a = 1.4\,$Å is different from that below z_a. Above z_a T_C is not much dependent on z, whereas there is strong dependence below. It is possible that the systems with $z > z_a$ are regular BCS superconductors, and the enhancement is present only for $z < z_a$. Below z_a, there is recognizable correlation between T_C and z, except for a few outliers. This correlation supports the idea that z is a universal parameter for the properties of FeAs

Table 1: The values of z, T_C for various Fe pnictides. Na-111 means NaFeAs, K-Ba122 means $K_{1-x}Ba_xFe_2As_2$, and so forth.

Compound	z (Å)	T_C (K)	Ref.
Na111	1.41	15.5	[35]
K-Ba122	1.37	38	[36]
F-La1111	1.34	26	[37]
F-Nd1111	1.37	46	[38]
F-Ce1111	1.34	35	[39]
F-Pr1111	1.32	47	[40]
F-La1111	1.32	20	[41]
Pr1111	1.32	47	[40]
O-Sm1111	1.37	34	[42]
V-Nd1111	1.38	51	[43]
Co-La1111	1.34	14.3	[44]
$Fe(Se_{0.416}Te_{0.584})$	1.65	14	[45]
$Fe(Se_{0.493}Te_{0.507})$	1.62	14	[45]
Li111	1.51	10	[46]
Li111	1.68	18	[47]
F-Sm1111	1.36	46	[48]
F-Tb1111	1.38	44	[49]
V-Nd1111	1.37	51	[43]
Co-SrFeAsF	1.35	4	[50]
K-Ba122	1.38	38	[36]

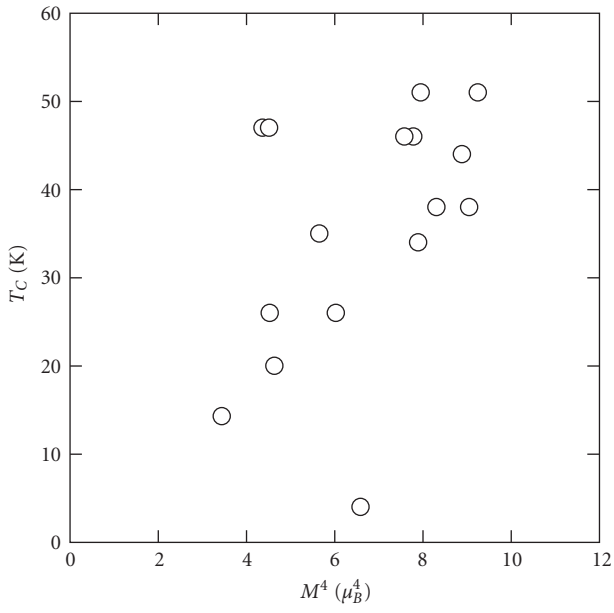

Figure 5: Superconducting critical temperature, T_C, against M^4 calculated by the LDA.

compounds, including the superconductivity, regardless of the composition.

It is interesting to note that, from (2) and (3), $F_{s-p} = -2BM^4$. Thus we plotted T_C against M^4 calculated by (3), not the experimental values of M, in Figure 5. Again a linear correlation appears to be present, although the correlation is far from perfect. On the other hand, the relation, $T_C \propto M^2$, is observed if we plot T_C against the moment experimentally determined for the CeFe(As, P)O system shown in Figure 2 [29]. An obvious implication of these correlations is that indeed magnetism is deeply involved in superconductivity, even though there is no static magnetic order in most of the superconducting samples. However, the involvement of spins in the mechanism may not be limited to the spin-fluctuation mechanism. The spin-lattice coupling could be involved in the superconductivity mechanism through the electron-phonon (e-p) coupling in the spin-channel.

For instance, the phonon can modify the electron hopping integral t_{ij} [51]. In the presence of antiferromagnetic correlation, the phonon-induced charge transfer from one spin sublattice to the other can be given by

$$H = \sum_{q,k,s} \Delta t_{q,k} \left[\left(a_q^+ f_{k,s}^+ g_{k+q,s} + a_q f_{k,s}^+ g_{k-q,s} \right) + H.c. \right], \quad (15)$$

where s refers to spin ($\downarrow$ or $\uparrow$), $\Delta t_{q,k}$ is the derivative of t with respect to phonon displacement, a_q is a phonon annihilation operator, and f_k and g_k are electron annihilation operators for the spin $\uparrow$ sublattice and the spin $\downarrow$ sublattice. The $\uparrow$ spin is a minority spin for the spin $\downarrow$ sublattice, so (15) results in the spin transfer between the majority band and the minority band. Note that this coupling is different from the usual spin-phonon coupling through the modification of the exchange integral J by phonons, and ultimately we will have to consider both [52]. Even though the conventional charge-channel e-p coupling (Fröhlich coupling) is weak for the Fe pnictides [53], the e-p coupling through the spin-channel, such as the one in (15), may be strong enough to make a difference. Other possibility includes the mechanism proposed by Kulic and Haghighirad [54] in which the on-site Hubbard repulsion, U, is modified by the dipolar moment of pnictide ions.

Possible importance of the spin-phonon coupling in the cuprates was discussed earlier [55–57]. Whereas many people speculate that the spin-fluctuation is the common mechanism for the cuprates as well as for Fe pnictides, it is possible that the spin-channel e-p coupling is the common thread for high-temperature superconductors, although much remain to be researched before we reach any definite conclusion.

5. Conclusions

The conventional electron-phonon (e-p) coupling through the charge channel is quite small for the Fe pnictide compounds [53]. This led many to conclude that lattice and phonons are irrelevant to the superconductivity of the Fe pnictides. Consequently, the spin-fluctuation mechanism is regarded to be the leading mechanism to explain their high T_C [15]. However, the lattice is intimately involved in the magnetism of this compound through the magneto-volume effect, as shown in this paper. This coupling has been known for a long time as Invar effect. The lattice controls the Stoner condition, and thus the onset of spin-splitting. Because the lattice is so intimately involved in magnetism, it is furthermore possible that the e-p coupling through the spin-channel is relevant, for instance involving the As Raman

phonon mode or the in-plane Fe mode. The lattice effect may be much more important than generally assumed to the properties of Fe pnictides, including superconductivity.

Acknowledgments

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