**Possible strong electron-lattice interaction and giant magneto-elastic effects in Fe-pnictides**

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Introduction. – Recently, superconductivity (SC) with high critical temperature $T_c$ was discovered in several families of Fe-pnictides. In the electron (e)-doped (1111) system LaFeAsO$_{1-x}$F$_x$ one has $T_c \approx 26$ K (and 43 K at high pressure) [1]. The record values are $T_c \approx 55$ K in SmFeAsO$_{1-x}$F$_x$ [2] and $T_c \approx 56$ K in Sr$_{1-x}$Sm$_x$FeAsF [3], etc. In the hole (h)-doped (122) system Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$ one has $T_c = 38$ K [4]. Other families are reported, such as MFeAs with M = Li, Na and $T_c = 18$ K, and the binary systems Fe(Se,Te) with $T_c < 12$ K. A common phase diagram has emerged with: i) the structural transition appears around $T_{str} = (140–200)$; ii) the SDW-type magnetic ordering occurs at $T_{sdw} < T_{str}$, while superconductivity appears when the SDW ordering vanishes. The latter can be done either by e- or h-doping or by applying high pressure.

The important question is — what is the pairing mechanism in Fe-pnictides? The vicinity of these systems to the antiferromagnetic phase was inspiration for spin fluctuation (SF) pairing models with repulsive interaction in the $s$-wave channel. This line of thinking was encouraged by the small electron-phonon coupling $\lambda_{ep}$ obtained in the LDA band structure calculations for LaO$_{1-x}$F$_x$FeAs [5], with $(\lambda_{ep}^{LD}) \sim 0.2$ and $T_{c, ep}^{LD} \sim 1$ K. However, this repulsive interaction in the singlet channel might be effective only if the coupling constant for the scattering of pairs from the hole to the electron band — the $hh \leftrightarrow ee$ scattering, is much larger than the intra-band (repulsive) couplings, i.e. $|\lambda_{hh}^{ep}| \gg |\lambda_{he}^{ep}|$, $|\lambda_{ee}^{ep}|$. In that case the $s_{\pm}$ superconductivity is realized, where the gaps on the $h$ and $e$ Fermi surfaces exhibit opposite signs, sign($\Delta_h$) = −sign($\Delta_e$) [6]. An indirect experimental support for $s_\pm$ pairing would be existence of an very pronounced resonance peak in the dynamical spin

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**Abstract** — The possibility for an appreciable many-body contribution to the electron-phonon interaction (EPI) in Fe-pnictides is discussed in the model where EPI is due to the electronic polarization of As-ions. The polarization induced $V_{ep}$ potential is large for vibrations of the As-ions and depends strongly on the As-Fe distance $d$, i.e. $V_{ep} \sim d^{-4}$. The EPI coupling constant $g_{ep}^{pol}$ is much larger than the one obtained in the LDA band structure calculations, with $g_{ep}^{pol} \sim 16$ eV $/\AA$ and $g_{ep}^{pol} \sim 1.6$ eV $/\AA$ and the bare pairing EPI coupling constant $\lambda_{ep, A}^{pol} \sim 1$. This contributes significantly to the intra-band $s$-wave pairing and an appreciable positive As-isotope effect in the superconducting critical temperature is expected. In the Fe-breathing mode the linear (in the Fe-displacements) EPI coupling vanishes, while the non-linear (quadratic) one is very strong. The part of the EPI coupling, which is due to the “potential” energy (the Hubbard $U$ changes), is responsible for the giant magneto-elastic effects in MFe$_2$As$_2$, M = Ca, Sr, Ba since it gives much larger contribution to the magnetic pressure than the band structure effects do. This mechanism is contrary to the LDA prediction where the magneto-elastic effects are due to the “kinetic” energy effects, i.e. the changes in the density of states by the magneto-elastic effects. The proposed EPI is expected to be operative (and strong) in other Fe-based superconductors with electronically polarizable ions such as Se, Te, S etc., and in high-temperature superconductors due to the polarizability of the $O^{2-}$-ions.
sensitivity [7] \( \Im \chi(\omega, q) \) at \( \omega/2\Delta_0 \sim 0.6 \) and at the SDW wave vector \( q \). The experimental situation is at present unclear since in LaO\(_{0.87}\)Fe\(_{1.13}\)As [8] this peak is not observed, while in [9] it is observed but not very pronounced. However, several recent NMR measurements of the \( T_1\)-relaxation rate in LaO\(_{1-x}\)Fe\(_x\)As, if confirmed, disfavor the SF scenario. First, in [10] it is reported that the \( T_1\)-relaxation rates on the nuclei \(^{139}\)La, \(^{57}\)Fe, \(^{75}\)As in LaO\(_{1-x}\)Fe\(_x\)As scale with one another, in spite of different form factors in the \( q \)-space. This means a lack of any pronounced \( q \)-structure in \( \Im \chi(\omega, q) \), thus disfavoring the SF pairing mechanism which assume that \( \Im \chi(\omega, q) \) is strongly peaked at \( Q = (1/2,1/2) \). Second, by increasing doping \( x \) in LaFeAsO\(_{1-x}\)F\(_x\) \((0.04 \leq x \leq 0.14)\) the \( T_1\)-relaxation rate of \(^{75}\)As decreases by almost two orders of magnitude, while \( T_1\) is practically unchanged [11], thus again disfavoring the SF scenario. However, these experiments do not exclude the first order direct Coulomb interaction as the inter-band pairing mechanism. In order to increase \( T_1\) in a multi-band system the intra-band pairing should contribute positively to \( T_1\). This may happen if the intra-band pairing potentials are: a) attractive giving rise to a conventional \( s\)-wave pairing, or b) repulsive and anisotropic giving rise to an unconventional pairing. In the latter case the system is very sensitive to the presence of nonmagnetic impurities. The \( s_\pm\) pairing is also sensitive to nonmagnetic impurities although in some occasions they are less detrimental than for unconventional pairing. For instance, in the unitary limit \( s_\pm\) is unaffected while in the Born limit these impurities are pair-breaking for it [12,13]. The analysis of the resistivity \( \rho(T)\) [13] and the upper critical field \( H_{c2}(T)\) [14] gives evidence for appreciable impurity effects in single crystals of the Fe-pnictides, which disfavor any gapless unconventional pairing [13]. The same analysis hints that the attractive intra-band pairings, with \( \lambda_{hh}, \lambda_{ee} > 0\), are important in the Fe-pnictides which can be only due to EPI or to an excitonic mechanism [13].

The above results imply a reconsideration of the role of EPI in the Fe-pnictides. This is supported by the recent neutron scattering experiments where the structural properties of the Fe-pnictides are sensitive to the magnetic order by showing giant magneto-elastic effects. For instance, in CaFe\(_2\)As\(_2\) there is a first-order phase transition from the orthorhombic to the tetragonal structure under the pressure \( P_c \geq 0.35\) GPa, while at the same time the magnetic order vanishes [15]. Concerning the role of EPI in these materials there were recently two controversial reports: the first one on a positive and large Fe-isotope effect in \( T_c\), and surprisingly also in \( T_{\text{sdw}}\), for the substitution \(^{56}\)Fe \( \rightarrow ^{54}\)Fe in SmFeAsO\(_{1-x}\)F\(_x\) and Ba\(_3\)\(-\)K\(_x\)Fe\(_2\)As\(_2\) with \( \alpha_{\text{Fe}}^{(T_c)} \approx 0.33\)–0.4 and \( \alpha_{\text{Fe}}^{(T_{\text{sdw}})} \approx 0.35\)–0.4 [16]. The second one [17] reports, contrary to the first one, on a negative Fe-isotope effect with \( \alpha_{\text{Fe}}^{(T_c)} = -0.18\).

These results point to a rather strong involvement of EPI in magnetic, elastic and in superconducting properties of Fe-pnictides and to the importance of many-body effects. In the following we discuss a possibility for a many-body EPI channel in the Fe-pnictides, which is due to the large electronic polarizability of the As-ions—we call it EPI\(_{\text{pol}}\). The importance of the electronic polarizability of the ligands in the screening of the core electrons in the excitonic spectra of halides and oxides was first recognized and studied by the Sawatzky group in [18] and later on applied on the Mott-Hubbard model for the screening of the (on-site) atomic Coulomb repulsion by the fast electronic polarization processes [19]—we call it the SPS model (the Sawatzky polarization screening model). The SPS model was recently applied to the Fe-pnictides [20] where the relatively small Hubbard repulsion on Fe-ions was explained by the screening via the huge electronic polarizability of the As-ions. Here we argue that if the SPS model is realized in the Fe-pnictides then it gives rise inevitably to: i) the large EPI\(_{\text{pol}}\) potential \( V_{ep}\) for vibrations of the As-ions (especially in the As-\( A_1g^*\) modes); ii) the strong dependence of \( V_{ep}\) on the As-Fe distance \( d_{\text{As-Fe}}\) with \( V_{ep} \approx d_{\text{As-Fe}}^{-4}\). As the consequence, the EPI\(_{\text{pol}}\) coupling \( g_{ep} := (\partial V_{ep}/\partial d_{\text{As-Fe}})\) is much larger than the the LDA values since \( g_{ep} \sim (20\) eV/Å) \( > g_{ep} \sim (1\) eV/Å), thus giving an appreciable contribution to the bare EPI\(_{\text{pol}}\) coupling constant \( \lambda_{ep}^0 \approx 1\). The latter may significantly contribute to the intra-band \( s\)-wave pairing, thus disfavoring any gapless unconventional intra-band pairing. In the case of EPI\(_{\text{pol}}\) an appreciable positive As-isotope effect in \( T_c\) is expected. Furthermore, EPI\(_{\text{pol}}\) may be responsible for the giant magneto-elastic effects in MFe\(_2\)As\(_2\), \( M = \) Ca, Sr, Ba. In that sense we construct the thermodynamic potential \( G(S_Q, \varepsilon, P)\) as a function of the strain \( \varepsilon\), the SDW magnetic order parameter \( S_Q\) and the pressure \( P\) by taking into account the effects of EPI\(_{\text{pol}}\). Based on this, we argue that the giant magneto-elastic effects in MFe\(_2\)As\(_2\), \( M = \) Ca, Sr, Ba are dominated by EPI\(_{\text{pol}}\), since it gives much larger contribution to the magnetic pressure than that predicted by LDA [21–23].

**EPI due to the As electronic polarizability.**—The electronic part of the Hamiltonian in the SPS model applied to the Fe-pnictides contains several many-body effects, i.e., \( \hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_2 + \hat{H}_{\text{core}} \). Here, \( \hat{H}_0\) is the kinetic energy of the conduction electrons, \( \hat{H}_1\) their long-range Coulomb interaction, while the Hubbard term \( \hat{H}_2\) describes the screened (on-site) atomic repulsion \( U_{\text{ion}}\) on the Fe-ions. \( \hat{H}_{\text{core}}\) describes the (very) polarizable electronic cores of the As-ions. Fluctuations of charges on the Fe-ions create an electric field on the As-ions which induces the polarization \( \mathbf{P}_A\) of their cores, thus lowering the energy of the system—see fig. 1. By eliminating the core degrees of freedom the part \( \hat{H}_2^{(\text{LDA})} + \hat{H}_{\text{core}}\) can be approximated by the Hamiltonian \( \hat{H}^{(\text{pol})} = \hat{H}_{\text{pol}}^{(0)} + \hat{H}_{\text{pol}}^{(1)} + \hat{H}_{\text{pol}}^{(2)}\) —see more in [18–20]. This is pure many-body effect and almost not captured by the LDA band
structure calculations. Applied to the Fe-pnictides it gives

$$\hat{H}_0^{(pol)} = -\sum_{R_{Fe}} V_F(R_{Fe}) \vec{n}_{R_{Fe}} / 2,$$

which renormalizes the local energy on the Fe-ions.

What is important for the magnetic and magneto-elastic properties is that this polarization process renormalizes also the Hubbard on-site repulsion giving $\hat{H}_H^{(pol)}$

$$\hat{H}_H^{(pol)} = \sum_{R_{Fe}} U^{(se)}(R_{Fe}) \vec{n}_{R_{Fe}} \cdot \vec{n}_{R_{Fe}},$$

with the screened Hubbard repulsion $U^{(se)}(R_{Fe}) = U_{at} - V_F(R_{Fe})$; $\vec{R}_{Fe}$ enumerates the Fe-ions. The screening term $V_F(R_{Fe})$, which is due to the electronic polarizability of the As-ions, is given in the point charge approximation by [20]

$$V_F \approx \sum_{R_{As}, n, n'} \frac{\alpha_{As} e^2}{|\vec{R}_{Fe} - \vec{R}_{As}|^4},$$

where $\vec{R}_{As}$ enumerates the As-ions which are nearest neighbors $(n.n.)$ of a given Fe-ion and $\alpha_{As}$ is the electronic polarizability of the As-ion. The physical picture behind the term $V_F(\approx 2e_Fp)$ is the following: the charge fluctuations on the neighboring Fe-ions cause local electric fields $E_{loc,As}$ on the As-ions, where $E_{loc,As}$ polarizes the As electronic clouds by exciting s-p transitions as shown schematically in Fig. 1. The induced dipole moments lower the energy by an amount $E_p \approx \alpha_{As} \sum_{R_{As}} E_{loc,As}^2$. Due to large $\alpha_{As}$, with $\alpha_{As} \sim (10-12) \text{Å}^3$ one obtains $V_F \sim 10 \text{eV}$ [20]. Since $U_{at} < 15 \text{eV}$ it gives $U^{(se)} \lesssim 3 \text{eV}$. Since $U^{(se)}$ is comparable to the band-width W this means that the Fe-pnictides are in a moderately correlated regime.

The meaning of $U^{(se)} = U_{at} - V_F$ and $V_F$ can be understood by the following analysis [18-20]. The Hubbard repulsion $U$ in solids is the difference between the ionization energy $I$ and the electron affinity $A$, i.e. $U^{(se)} = I - A$. In solids the atomic ionization energy is lowered by $E_p$ while the atomic electron affinity is increased by $E_p$, i.e. $U^{(sc)} = I - A = (I_{at} - E_p) - (A_{at} + E_p) = U_{at} - V_F$. The strong renormalization of $U_{at}$ to $U^{(sc)}$ is confirmed in the analysis of the optical data [24], due to the large background dielectric constant $\varepsilon_{\infty} \approx 12$ which gives $\alpha_{As} \sim (10-12) \text{Å}^3$ and $U^{(sc)} \approx (1-2) \text{eV}$. (There is also an additional non-local Coulomb term $\hat{H}_2^{(pol)}$ due to the As polarization, which depends on $V_F(R_{Fe})$ and will be not studied here.)

In [20] a possible excitonic mechanism of superconductivity was analyzed in the SPS model, while the giant EPI effects were not studied at all. In the presence of vibrations of the As- and Fe-ions the change of $\hat{H}_i^{(pol)}$ gives rise to an additional many-body EPI$_{pol}$ channel with a possible huge EPI coupling potential $V_{ep}$ where the EPI$_{pol}$ Hamiltonian $\hat{H}_{ep}^{(pol)} = \hat{H}_{0, ep}^{(pol)} + \hat{H}_{H, ep}^{(pol)}$ reads

$$\hat{H}_{ep}^{(pol)} = V_{ep} \sum_{R_{Fe}} \sum_{n} n_{R_{Fe}} \cdot (\mu_{R_{As}} - \mu_{R_{Fe}}),$$

where $n_{R_{Fe}} = \{R_{Fe}^- + R_{Fe}^0 - R_{As}^- - R_{As}^0\} / V_F$ and $n_{R_{As}} = \{R_{As}^\uparrow + R_{As}^\downarrow\}$. Here $\mu_{R_{As}}$, $\mu_{R_{Fe}}$ are the displacement operators of the Fe- and As-ions, respectively. For the harmonic EPI interaction one has

$$\hat{V}_{ep} = \frac{1}{2Z} \sum_{n} n_{R_{Fe}} \cdot (\mu_{R_{As}} - \mu_{R_{Fe}}),$$

where $\alpha_{As} = (R_{Fe}^2 - R_{As}^2) / d_{Fe-As}$. It is convenient to rewrite the Hubbard Hamiltonian $\hat{H}_H^{(pol)}$ in the rotational invariant form (note $2\vec{R}_{Fe}\uparrow \vec{n}_{R_{Fe}} \uparrow = \vec{n}_{R_{Fe}} \uparrow - 4\vec{S}_{R_{Fe}} / 3$)

$$\hat{H}_{ep}^{(pol)} = V_{ep} \sum_{R_{Fe}} \sum_{n} \hat{V}_{ep} \cdot (\vec{n}_{R_{Fe}} \cdot \vec{\lambda} \hat{S}_{R_{Fe}}^2),$$

where $\lambda = 2/3$ and the spin-like operator $\hat{S} = \hat{e}^2 \sigma_{\alpha \beta} \hat{c} / 2$. The EPI$_{pol}$ potential $V_{ep}$ in eq. (6) is large due to: i) the large value of $V_F$; ii) the rapid change of $V_F$ with the Fe- and As-distance $d_{Fe-As} \approx 2.4 \text{Å}$, thus giving a very large induced electron-phonon coupling $g_{ep}^{(pol)} = V_{ep} / d_{Fe-As} \approx 4V_F / d_{Fe-As} \approx 16 \text{eV}/\text{Å}$. For comparison, the average LDA coupling constant (coming mainly from the screened lattice potential) is much smaller, i.e. $g_{ep}^{(LDA)} < 1 \text{eV}/\text{Å}$ [5]. As is said before, the above model can be generalized to the multi-orbital case. In that case there is a summation over the orbital index in eqs. (4), (6) and there are terms due to the inter-orbital interaction. For instance, eq. (6) reads $\hat{H}_{ep}^{(pol)} = V_{ep} \times \sum_{R_{Fe} \neq R_{As}} \hat{V}_{ep} \cdot (\vec{n}_{R_{Fe}} \cdot \vec{\lambda} \hat{S}_{R_{Fe}}^2 + \sum_{i \neq j} \hat{n}_{i R_{Fe}} \hat{n}_{j R_{Fe}} / 2) + \hat{H}_{loc}$, where $i, j$ enumerates the orbital indices while all non-local terms mentioned above are stipulated in $\hat{H}_{loc}$. In the following we argue that the giant magneto-elastic effects in the Fe-pnictides are dominated by the EPI$_{pol}$ effects.

**Magneto-elastic coupling effects.** – If the SPS model is realized in the Fe-pnictides then the part of EPI$_{pol}$ —the second term in eqs. (4), (6), is involved in the giant magneto-elastic effects. It will be shown below.
that it gives the largest contribution to them with the following manifestations. First, in the presence of the SDW magnetic order \((S_Q \neq 0)\) the Fe-pnictides show a tendency to increase significantly the \(c\)-lattice parameter (along the \(c\)-axis) in comparison to the non-magnetic \((S_Q = 0)\) “collapsed” tetragonal \((cT)\) phase, i.e. \(c(S_Q \neq 0) > c(S_Q = 0)\). Second, recent experiments on \(\text{MFe}_2\text{As}_2\), \(\text{M} = \text{Ca}, \text{Sr}, \text{Ba}\) under pressure \((P)\) show the orthorhombic-tetragonal (the \(cT\)-phase) transition. In \(\text{CaFe}_2\text{As}_2\) at \(P \approx P_c \approx 0.4\) GPa there is a transition from the orthorhombic phase with the finite SDW order \(S_Q \neq 0\) to the non-magnetic \(cT\)-phase \((S_Q = 0)\) in which the superconductivity appears at \(T_c = 12\) K [15]. This gives evidence for strong and unusual coupling of the lattice with the magnetic order. It is worth to mention that the experimental change of volume \((\Delta V/V) \approx 3\%\) is explained by the LDA calculations by assuming much larger critical pressure \(P_c\) than in experiments [23], i.e. \(P_c^{(\text{LDA})} \approx 5\) GPa \(\gg P_c^{(\text{exp})} \approx 0.4\) GPa. The LDA magnetic pressure is given by \(P_c^{(\text{LDA})} \approx -\partial E_c^{(\text{LDA})}/\partial \epsilon_c\) and its small value causes that \(P_c^{(\text{LDA})} \gg P_c^{(\text{exp})}\), thus pointing to some missing many-body effects with much larger magnetic pressure \((P_m)\) — see eq. (7) and the analysis below it. In the following we show, that EPI\(_{\text{pol}}\) gives very large contribution to \(P_m\) — we call it the potential magnetic pressure \(P_m^{(\text{p})}\), thus lowering the value of \(P_c\).

The magneto-elastic properties of the tetragonal-orthorhombic Fe-pnictides are complicated since they depend on six elastic constants, on several other magneto-elastic constants and on the magnetic free-energy. However, for our purpose to show that \(P_m^{(\text{p})} \gg P_c^{(\text{LDA})}\) a simplified phenomenological mean-field approach is satisfactory. For the further analysis the important experimental fact is the decrease of the Fe-As distance \(d_{\text{Fe-As}}\) by 1\% in the first-order phase transition, i.e. \(\epsilon_d = (\delta d_{\text{Fe-As}}/d_{\text{Fe-As}}) = 0.01\). The latter lowers the “potential” energy \(U^{(\text{pol})}\) significantly which leads to the giant magneto-elastic effects. To estimate the effects we use the experimental fact that at the critical pressure \(P_c\) the volume is changed by \(3\%–4\%\) [15], while \(\epsilon_d\) is only a part of the total strain \(\epsilon = (\Delta V/V) = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}\), i.e. \(\epsilon_d \approx \epsilon/r\) with \(r \sim 3\%–4\%\). According to eqs. (4)–(6) one has \(U^{(\text{pol})}(\delta d) = U^{(\text{pol})} + V_{\text{ep}}\epsilon_d \approx U + V_{\text{ep}}\epsilon/r\) (note \(V_{\text{ep}} \approx 4V_p, V_p \approx 10\) eV), i.e. the “potential” energy is significantly decreased under the pressure (for \(\epsilon < 0\)). The weak SDW magnetic order (with \(S_Q = 0\)) can be qualitatively analyzed in the Hartree-Fock (or Stoner-like) approximation with the bare spin susceptibility \(\chi_0(Q) = N(0)f(Q)\), where \(N(0)\) is the density of states at the Fermi level and \(f(Q)\) describes the momentum dependence of the bare spin susceptibility. For \(U^{(\text{pol})}(P < P_c)/\chi_0(Q) > 1\) it gives finite value for \(S_Q\). The phenomenological Gibbs energy \(G(S_Q, \epsilon, P)\) includes: i) the complicated elastic properties of the lattice approximately via the effective compressibility, ii) the SDW magnetism, iii) the magnetostriction and iv) the effects of the applied pressure \(P\)

\[
G(S_Q, \epsilon, P) \approx \frac{\epsilon^2}{2k_{\text{eff}}} + P\epsilon - \frac{a(\epsilon)}{2}S_Q^2 + \frac{b}{4}S_Q^2 + \frac{c}{6}S_Q^6, \tag{7}
\]

where \(a(\epsilon) = U^{(\text{pol})}(\epsilon) - \chi_0^{-1}(Q, \epsilon, T)\). The first term in \(G\) is an effective lattice elastic energy with the effective compressibility \(k_{\text{eff}}\), while the second one is due to the work by the pressure \(P\). The magnetic part of \(G\) contains higher-order terms in \(S_Q^4\) which are proportional to \(b\) and \(c\) since the transition may be of the first order if \(b < 0\), or if \(b > 0\) for \(b = - \kappa_{\text{eff}}(\gamma_k + \gamma_p)^2/2 < 0\) (see below), where \(\kappa_{\text{eff}}\) is the renormalized fourth-order coefficient in \(G\). Note, that here we consider only effects of the homogenous strain on the magnetic transition in weak ferromagnets \((S_Q^2 \ll 1)\) in the mean-field approximation, which can take place even very far from the critical temperature \(T_{\text{sdw}}\).

In the following we omit the temperature effects due to the strain fluctuations which are pronounced very near \(T_{\text{sdw}}\) —the Larkin-Pikin mechanism [25]. The latter may also lead to the first-order transition due to the interaction of the magnetic order [25] with the share-strain fluctuations which is studied in [26]. For small strain \(\epsilon \ll 1\) one has

\[
a(\epsilon) \approx a_0 + (\gamma_k + \gamma_p)\epsilon, \tag{8}
\]

where \(a_0 = [U^{(\text{pol})} - \chi_0^{-1}(Q, 0, 0)]\). The “kinetic” energy contribution to the magnetic pressure is proportional to \(\gamma_k = 3\chi_0^{-1}(Q, 0)\) d\(n\chi_0^{(Q, \epsilon)}/d\epsilon\), while the “potential” energy contribution to \(\gamma_p = V_{\text{ep}}/r\). After the minimization of \(G(S_Q, \epsilon, P)\) (with respect to \(S_Q\) and \(\epsilon\)) and for \(b < 0\) the first-order phase transition is realized at the critical pressure \(P_c\)

\[
P_c = \frac{1}{(\gamma_k + \gamma_p)k_{\text{eff}}} \left(a_0 + \frac{3b\kappa_{\text{ren}}}{16c}\right). \tag{9}
\]

The SDW order parameter jumps from \(S_Q \neq 0\) to \(S_Q = 0\) at \(P = P_c\) and \(S_Q = 0\) at \(P = P_c\). In the case of the weak first-order phase transition one has \(b_{\text{ren}} = 4\epsilon\) which gives \(P_c \approx a_0/(\gamma_k + \gamma_p)\kappa_{\text{eff}}\), as well as for the second-order phase transition with \(b > 0\) (where \(S_Q = 0\) for \(P = P_c\)). Note, the the “kinetic” energy term \(\gamma_k\) in eq. (9) is contained in the LDA band structure calculations [21–23], where it is solely responsible for the magneto-elastic effects. However, the “potential” term \(\gamma_p\) which is due to the many-body EPI\(_{\text{pol}}\) effects is absent in the LDA calculations. This is the main reason that LDA gives too large value for \(P_c\), i.e. \(P_c^{(\text{LDA})} \sim 15P_c^{(\text{exp})}\) [23], which implies that \(\gamma_p \gg \gamma_k \approx \gamma_{LDA}\) is realized. Indeed, in most itinerant magnets one has \(\gamma_k < 2N^{-1}(0)\) and one expects similar value in the Fe-pnictides. Since \(V_{\text{ep}}(\sim 40\) eV) is very large one has \((\gamma_p/\gamma_k) \sim 10\). The latter result implies much smaller critical pressure \(P_c \ll P_c^{(\text{LDA})}\) than the LDA predicts. This means that the giant magneto-elastic effects in the Fe-pnictides are dominated by the many-body “potential” energy effects which are contained in EPI\(_{\text{pol}}\). The experimental situation concerning the type of
the phase transition (first- or second-order) in MFe$_2$As$_2$, M = Ca, Sr, Ba is still not resolved. Namely, for Ca, Sr the case $b_r < 0$ is realized while in Ba both cases $b_r > 0$ and $b_r < 0$ might be realized [15]. In spite of our limited phenomenological approach some semi-quantitative estimations are possible. For instance, one expects $\kappa_{\text{eff}} < 2 \times 10^{-2} \text{ (GPa)}^{-1}$ [27] which gives $P_{\text{Fe As}} < 10^{-2}$ and $a_0/\gamma_p < 10^{-2}$. The latter condition is a constraint for the microscopic models for the SDW order parameter and the EPI$_{\text{pol}}$ coupling.

Possible contribution of EPIL$_{\text{pol}}$ to pairing. – At present there is a confusion regarding the role of EPI in the superconducting pairing of the Fe-pnictides. In spite of numerous experiments which give appreciable evidence against gapless unconventional pairing and that the antiferromagnetic spin fluctuations are moderate in superconducting samples, the proponents of the spin fluctuation mechanism rely their belief on the small EPI calculated in the LDA calculations with $\lambda_{\text{ep}} \approx 0.2$ and $T_c \sim 1 \text{K}$ [5]. However, like in the case of high-temperature superconductors (HTSC), heavy fermions and organic superconductors, etc. the LDA calculations fail whenever many body effects play important role. For instance, in case of HTSC numerous tunnelling, transport and neutron scattering measurements point to a strong EPI, while various LDA calculations furnished diversity of values for $\lambda_{\text{ep}}$, from 0.2 — 1 — see discussion in [28]. The situation is similar in Fe-pnictides where LDA cannot explain quantitatively even the magnetic and structural properties, let alone the EPI effects and superconductivity. Here, we give some qualitative estimate of the polarization-induced EPI which is described by \( \hat{H}_{\text{pol}}^{(\text{ep})} \) in eq. (6) and not contained in LDA.

The strongest EPI$_{\text{pol}}$ coupling is for the $A_{1g}$-modes (there are at least two such modes) where the As-ions vibrate along the $c$-axis as shown in fig. 2. These modes contribute mainly to the intra-band pairing. At present we can only estimate the intra-band ($i = c, h$) bare coupling constants \( \lambda_{\text{ep}, A_{1g}}^{i} \) of the $A_{1g}$-mode, \( N_i(0)g_{A_{1g}}^2/\omega_{A_{1g}} \) with \( g_{A_{1g}}^2 \approx V_{\text{ep}}^2 \cos^2 \theta (\hat{u}^2_{A_{1g}})/d_{\text{Fe-As}}^2 \). Here, \( \omega_{A_{1g}} \) is the energy of the $A_{1g}$-mode, \( N_i(0) \) is the (intra-band) density of states, \( \langle \hat{u}^2_{A_{1g}} \rangle \) is the average of the quadratic As-displacement, \( \theta \) is the angle between \( n_4 \) and the $c$-axis. In the approximation of one-phonon processes one has $\langle \hat{u}^2_{A_{1g}} \rangle \approx \hbar^2/2M_{A_{1g}}\omega_{A_{1g}}$, where $M_{A_{1g}}$ is the atomic mass of the As-ion. For $\omega_{A_{1g}} \approx 25 \text{meV}$ [29] and $N_i(0) \approx 0.5 \text{states/eV} \cdot \text{spin}$ (note that $N_i(0) \sim N_h(0) \sim N(0)$) one obtains $\lambda_{\text{ep}, A_{1g}}^{i} \approx 0.7$.

The estimated $\lambda_{\text{ep}, A_{1g}}^{i}$ is rather large giving a hope that the real (renormalized) coupling $\lambda_{\text{ep}, A_{1g}}^{i} < \lambda_{\text{ep}, A_{1g}}^{i/2}$ might be also appreciable. In order to calculate $\lambda_{\text{ep}, A_{1g}}^{i}$ one should correctly take into account the matrix elements of $g_{A_{1g}}$ in the band-basis, screening effects, etc. Even if $\lambda_{\text{ep}, A_{1g}}^{i} \approx 0.3$ this would give an appreciable total intra-band coupling constant $\lambda_{\text{ep}, A_{1g}} = 2 \sum_i \lambda_{\text{ep}, A_{1g}}^{i} \sim 1$ thus contributing significantly to the effective pairing constant $\lambda_{\text{eff}}$ — see [13].

In [30] was proposed that the Fe-breathing mode may give appreciable EPI due to the change of the Fe-Fe hopping energy in this mode. However, the latter effects are not considered here. In that respect, we point out that the linear (in the displacement $u_{\text{Fe}}$) contribution of the Fe-breathing mode to EPI$_{\text{pol}}$ vanishes due to the symmetry reasons — see fig. 2, but this mode gives very large nonlinear EPI$_{\text{pol}}$ coupling (with $\phi_{\text{RFe}} \sim u^2_{\text{Fe}}$) due to the large value of $\partial^3 V_{\text{ep}}/\partial d^2_{\text{Fe-As}}$ — see eq. (3). The large nonlinear EPI$_{\text{pol}}$ coupling is the strongest in the Fe-breathing mode and its effect on superconductivity and magneto-elastic properties might be also important.

Conclusions. – We have analyzed a possibility for an appreciable many-body contribution to the electron-phonon interaction (EPI) in the Fe-pnictides, which is due to the electronic polarization of the As-ions in the presence of charge fluctuations on the Fe-ions which is proposed in [20]. In that case the polarization induced EPI$_{\text{pol}}$ potential $V_{\text{ep}} \sim 40\text{ eV}$ is especially large for vibrations of the As-ions and depends strongly on the As-Fe distance $d_{\text{As-Fe}}$, i.e. $V_{\text{ep}} \sim d_{\text{As-Fe}}^{-4}$. The corresponding EPI$_{\text{pol}}$ coupling $g^2_{\text{ep}} = \partial^3 V_{\text{ep}}/\partial d^2_{\text{As-Fe}}$ is much larger than the one obtained in the LDA band structure calculations, i.e. $g^2_{\text{ep}} \gg g_{\text{pol}}^{(\text{LDA})}$ with $g_{\text{pol}}^{(\text{LDA})} \sim 16 \text{eV}/\text{Å} > 1 \text{eV}/\text{Å}$. The latter may significantly contribute to the intra-band $s$-wave pairing with the bare coupling constant $\lambda_{\text{ep}, A_{1g}} \sim 1$, thus disfavoring any gapless unconventional intra-band superconductivity. As the result an appreciable positive As-isotope effect in the superconducting critical temperature is expected. The EPI$_{\text{pol}}$ channel gives very strong nonlinear coupling in the Fe-breathing mode, which might be important for superconductivity and additional magneto-elastic effect.
The electron-lattice coupling $E_{\text{PI pol}}$ gives much larger contribution to the magnetic pressure than the LDA calculations predict, thus giving rise to the giant magneto-elastic effects in the transition from the magnetic to the non-magnetic state under pressure in MFe$_2$As$_2$, M = Ca, Sr, Ba. The critical pressure $P_c$ for the magnetic and structural phase transition is dominated by the “potential” energy contribution $E_{\text{PI pol}}$ in the magnetic pressure, while the LDA “kinetic” energy effects are much smaller. $E_{\text{PI pol}}$ is expected to be important in other Fe-based superconductors which contain highly electronically polarizable ions such as Se, Te, S etc. It might be operative also for some oxygen modes in high-temperature superconductors due to the appreciable electronic polarizability of the O$^{2-}$-ions.

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