Role of striction at magnetic and structural transitions in iron pnictides

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We discuss the role of striction in the intertwined magnetic and structural phase transitions in the underdoped iron pnictides. The magnetoelastic coupling to acoustic modes is then derived and estimated in framework of the multiband spectrum for itinerant electrons with nesting features. We argue that the first-order character of the magnetoelastic phase transition originates from the lattice instabilities near the onset of spin-density wave order introducing, thus, a shear acoustic mode as another order parameter. Taking nonharmonic terms in the lattice energy into account may explain the splitting of the structural and magnetic transitions in some oxypnictides. Fluctuations of the magnetic order parameter show up in the precursory temperature dependence of the elastic moduli.

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Considerable efforts have been concentrated recently on studies of the interdependence for the antiferromagnetic (AFM) and the superconducting (SC) transitions in the new iron-based compounds.[1] Doping is known to destroy AFM and increase T_C—the temperature for the onset of SC.[2]

In this presentation, we address the peculiarities and interrelations for the magnetic (T_m) and structural ($T_{\rm str}$) transitions in the parent and underdoped iron pnictides. For concreteness, we discuss below the properties of two systems only: the quarternary REFeAsO ("1111;" RE stands for a rare earth) and the bilayered $A\mathrm{Fe}_2\mathrm{As}_2$ ("$A22$," where $A=\mathrm{Sr,Ca,Ba}$) materials. In both classes, the intertwined magnetic and the structural transitions of the weak first order are observed in a temperature interval of $\sim$100–200 K. In 1111's, the structural change precedes the magnetic ordering,[2,3] while in $A22$'s magnetic order and change in the lattice symmetry occur simultaneously in the single first-order transition.[4]

It is known that coupling to the lattice may transform a magnetically driven transition into the weak first-order transition accompanied by structural changes.[5] In Ref. 6 the problem has been rigorously solved for the elastically isotropic solid, taking fluctuations into account. Unfortunately, the method of Ref. 6 does not apply to anisotropic materials, such as iron pnictides, with the tetragonal symmetry and layered structure. The solution of Ref. 6, however, undoubtedly contains the main physics for these phenomena. Correspondingly, below we simplify the approach of Ref. 6 to model the magnetoelastic interactions (striction) and phase transitions in the parent and underdoped FeAs systems.

The magnetic order in oxypnictides is built of the alternating (AFM) spins running along one of the lattice axis, while in the other direction the spins are ordered ferromagnetically.[3] In the tetragonal notations, the structure vectors are commensurate: $\boldsymbol{Q_1}=(0,\pi)$ and $\boldsymbol{Q_2}=(\pi,0)$. With the local picture of interacting Fe spins and the two Heisenberg exchange interactions constants J_1 (nn) and J_2 (nnn), such a ground state realizes itself at the inequality $J_2>J_1/2$. Accompanying orthogonal lattice distortions can be understood, as in Ref. 5, in terms of a "spin-Peierls" effect, i.e., the variation in the exchange integrals at the lattice deformation.[7]

The present materials, however, are semimetals. Pnictides are better described in terms of an itinerant scheme. The consensus is that the energy spectrum obtained in the "first-principles" calculations[8] presents a good starting point. According to Ref. 8, the electron spectrum bears the multiband character. There are Fermi surfaces (FSs) for the two hole (h) pockets at the Γ point (0, 0) and two electronic (e) pockets located in the tetragonal (unfolded)[9] reciprocal lattice at $(0,\pi)$ and $(\pi,0)$. An approximate nesting between the e and h pockets is believed to be responsible for a spin-density wave (SDW) instability with the two vectors $\boldsymbol{Q_1}$ and $\boldsymbol{Q_2}$ mentioned above.[9] The main features of this spectrum have been reproduced in many numerical calculations for all classes of the new Fe-based materials. In Ref. 10 this spectrum has been directly observed for LaFePO in the de Haas–van Alphen (dHvA) experiments. Below we accept this model. With $T_c\sim 50$ K, $T_m\sim T_{\rm str}\sim 100-200$ K, and the Fermi energy $E_F\sim 0.1-0.2$ eV for the pockets' sizes, the model is expected to allow a mean-field treatment both for SC and magnetic phenomena.[11]

"First-principles" calculations provide a reasonable description of the ground-state properties, albeit some disagreements are not uncommon in the literature (see Ref. 12). However, subtleties, especially in a vicinity of phase transitions, remain beyond the reach of numerical analysis.

Among advantages of the "nesting" model[9,13,14] is that its formalism is practically identical to the well-studied BCS scheme for SC. It is a weak-coupling mean-field scheme if $T_{\rm SDW}\ll E_F$. (Fluctuations become important only in a narrow temperature interval $|\Delta T|/T_0=\mathrm{Gi}\ll 1$, as given by sort of a Levanyuk-Ginzburg criteria Gi.) The Landau functional near the transition can be derived exactly as it has been done for superconductivity near T_c.[15]

Nevertheless, we prefer not to write equations explicitly. Numerous unknown parameters that include parameters of the e and h pockets, interactions, and six elastic moduli for the tetragonal symmetry of pnictides should make it useless. For the sake of transparency we hold, where possible, the discussion on the qualitative level.

The mathematical analogy of the model[13,14,16] with the Cooper pairing in a BCS-type scheme stems from a logarithmic divergence for the scattering in the e-h channel in Fig. 1(a), which has the following form:

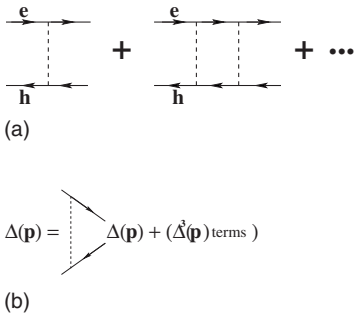

FIG. 1. (a) The logarithmic nesting model. (b) Mean-field equations near T_c.

$$V(\boldsymbol{p}-\boldsymbol{p}')T\sum_{\omega_n}\int \frac{\nu(E_F)d\epsilon' d\Omega_{\boldsymbol{p}'}}{(i\omega_n-\epsilon_e')(i\omega_n-\epsilon_h')} = V\nu(E_F)\ln(\bar{\omega}/T,\delta), \tag{1}$$

where

$$\epsilon_h = -\epsilon_e + \delta \tag{2}$$

are e and h energies, while δ accounts for deviations from the ideal nesting. With the notations $\boldsymbol{\Delta_1}$ and $\boldsymbol{\Delta_2}$ for the triplet (SDW) order parameters corresponding to the structure vectors $\boldsymbol{Q_1}=(0,\pi)$ and $\boldsymbol{Q_2}=(\pi,0)$, the equations for Δ's have the same structure as in SC theory,[15] as demonstrated in Fig. 1(b). Let T_0 be the "bare" transition temperature in the absence of coupling to the lattice. The Landau functional[17] near T_0 is of the form,

$$\Omega = \int \frac{A\nu}{2}\left[\tau\Delta^2 + b_0\frac{\Delta^4}{T_0^2} + c_0\xi_0^2(\boldsymbol{\nabla}\boldsymbol{\Delta})^2\right]d\boldsymbol{r}, \tag{3}$$

where $\nu \equiv \nu(E_F)$ is the characteristic density of states (DOS). A, c_0, and b_0 are constants and $\tau=(T-T_0)/T_0$; $\xi_0=v_F/2\pi T_0$. The functional (3) is the starting point in the general theory of the second-order phase transitions.[17,18] To account for interactions with the lattice, one adds to Eq. (3) a coupling to the lattice of the form

$$H_{\rm str} = -q\int \hat{u}(\boldsymbol{r})\hat{\Delta}(\boldsymbol{r})^2 d\boldsymbol{r}, \tag{4}$$

and the elastic energy itself that we also write schematically as

$$H_{\rm el} = \int K\hat{u}^2 d\boldsymbol{r}, \tag{5}$$

where K is an elastic modulus (such as the bulk modulus, for instance); the notation $\hat{u}$ stands for components of the strain tensor,

$$u_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right). \tag{6}$$

For magnetic phenomena, Eq. (4) describes magnetoelastic interactions and q is called the striction constant. The total Gibbs energy near the phase transition is

$$\Phi = \Omega(\tau) + H_{\rm el} + H_{\rm str}. \tag{7}$$

In the itinerant model of Eq. (1), the parameters Δ_1 and Δ_2 are built on the Bloch wave functions. These spatial features present in the SDW parameters immediately lead to the quadratic coupling between Δ's and acoustic degrees of freedom ($\boldsymbol{Q}=0$) given by Eq. (4). An estimate of the striction constants in Eq. (4) follows directly from the logarithmic contribution of Eq. (1). Indeed, elastic deformations change the parameter δ in Eq. (3) that controls the degree of the nesting,

$$\delta \equiv \delta(u) = \delta_0 + \lambda\hat{u}. \tag{8}$$

From Eq. (1) and Fig. 1(b) it is seen that

$$\tau \to \tau + \lambda\frac{\hat{u}}{T_0}. \tag{9}$$

Making use of Eq. (3), we estimate

$$q \sim \frac{\nu\lambda}{T_0} \sim \nu\left(\frac{E_F}{T_0}\right) \tag{10}$$

(taking λ on order of characteristic atomic energy E_F).

Return to Eqs. (4)–(7) and assume homogeneous $\hat{u}$. Minimizing Φ over $\hat{u}$, we obtain

$$K\hat{u} = q\left(\frac{\int \Delta^2 d\boldsymbol{r}}{V}\right) \tag{11}$$

(with V for the volume). The effective Landau functional $\tilde{\Omega}$ is

$$\tilde{\Omega}_{\rm min} = \Omega(\tau) - \left(\frac{1}{2K}\right)\left[q\frac{\int \Delta^2(\boldsymbol{r})d\boldsymbol{r}}{V}\right]^2. \tag{12}$$

In the mean field $\Delta^2(\boldsymbol{r})=$const, and Eq. (12) reproduces the result of Ref. 6: the functional Ω acquires a negative contribution to the biquadratic term in Eq. (3). Should the total be negative, the transition becomes first order. [Higher-order terms in the expansion (3) become necessary.]

In the presence of an external homogeneous deformation, $\hat{u}_{\rm ext}$ substitution into Eq. (9), $\tau \to \tau+\lambda(\hat{u}_{\rm ext}/T_0)$, leads to

$$\Omega_{\rm eff} = \Omega\left(\tau + \lambda\frac{\hat{u}_{\rm ext}}{T_0}\right). \tag{13}$$

Differentiating, we find

$$\frac{\partial^2\Omega_{\rm eff}}{\partial\hat{u}_{\rm ext}^2} = \frac{\lambda^2}{T^2}\frac{\partial^2\Omega}{\partial\tau^2} = -\frac{\lambda^2 C(\tau)}{T_0}, \tag{14}$$

where $C(\tau)$ is the specific heat. According to Eq. (14), already in the Landau mean-field approach the jump ΔC in the specific heat at the transition is accompanied by a negative steplike change in elastic moduli. The variation is of the atomic order. Therefore, the lattice would become unstable, and the second-order character of a transition changes to the first-order one.

In Refs. 6 and 19, the attention has been drawn to the fact that the specific heat $C(T)$ in Eq. (14) actually has a singularity at T_0,

$$C(T) \propto |\tau|^{-\alpha}. \tag{15}$$

[α is the so-called scaling index for the specific heat $C(T)$.] As to the order parameter, it appears below T_0 (see Ref. 17; §148, p. 484),

$$\Delta(T) \propto (-\tau)^{\beta} (\tau < 0). \tag{16}$$

Therefore, an elastic instability is ubiquitous for any magnetic transition. In the model chosen above, the instability occurs inside a narrow temperature interval controlled by the Levanyuk-Ginzburg parameter. Provided that layered pnictides can be treated, in the first approximation, as two-dimensional (2D), we write

$$\left| \frac{\Delta T}{T_0} \right| \equiv G_i^{2D} \sim \left(\frac{T_{SDW}}{E_F} \right) \ll 1. \tag{17}$$

By the order of magnitude, the same parameter also controls the width of the hysteresis.

Note that even for homogeneous lattice deformations, the magnetoelastic coupling [Eq. (4)] leads to Eq. (12), with the present biquadratic term that describes nonlocal interactions for the order parameter Δ. In Ref. 6 inhomogeneous fluctuations result in the cancellation of the nonlocal term (12) for the isotropic (liquid) media. However, the nonlocal coupling terms are always present for any anisotropic solid. As it was mentioned above, the problem could be rigorously solved in Ref. 6 only for the elastically isotropic solid (i.e., for a solid characterized by the bulk and shear moduli). In all other cases, the nonlocal term (12) that comes about due to exchange by acoustic phonons becomes strongly anisotropic. We now simplify the model[6] by restricting our consideration to homogeneous lattice fluctuations. Inhomogeneous fluctuations should not qualitatively change the physics of the problem.

With this in mind, one can rewrite Eq. (3) in the form

$$\Phi = \frac{K}{2}\hat{u}^2 + \Omega\left(\tau + \frac{\lambda}{T_0}\hat{u}\right) - \hat{\sigma}\hat{u}, \tag{18}$$

where $\Omega(\tau + \frac{\lambda}{T_0}\hat{u})$ is the exact functional (3), i.e., the functional that would describe the second-order phase transition driven by the order parameter Δ neglecting striction effects. In particular, it has the contribution Ω_{sing} responsible for the singular behavior of the specific heat $C(T)$ [Eq. (15)]. The term $-\hat{\sigma}\hat{u}$ stands for the applied external stress ($\hat{\sigma}$ is a proper component of the stress tensor; this term is needed at calculations of the temperature behavior of elastic moduli across the transition.)

In the presence of nonzero stress $\hat{\sigma} \neq 0$, fluctuations take place around the present equilibrium point $\hat{u}_{ext}$,

$$\hat{u}_{ext} = \frac{\hat{\sigma}}{K}. \tag{19}$$

Rewriting in Eq. (18) $\hat{u} \to \hat{u} + \hat{u}_{ext}$, we obtain

$$\Phi = -\frac{\hat{\sigma}^2}{2K} + \frac{K}{2}\hat{u}^2 + \Omega\left(\tau + \frac{\lambda}{T_0}\hat{u} + \frac{\lambda\hat{\sigma}}{T_0 K}\right). \tag{20}$$

The contribution $\lambda\hat{\sigma}/(T_0 K)$ in the argument of $\Omega(x)$ [Eq. (20)] shifts the transition temperature T_0 under the applied stress,

$$T_0(\hat{\sigma}) = T_0 - \frac{\lambda\sigma}{K}. \tag{21}$$

The Gibbs energy (20) must be minimized over fluctuations of (homogeneous) deformations $\hat{u}$,

$$\frac{\delta\Phi}{\delta\hat{u}} = K\hat{u} + \frac{\lambda}{T_0}\Omega'(x) = 0, \tag{22}$$

where

$$x = \tau + \frac{\lambda}{T_0}u + \frac{\lambda\sigma}{T_0 K}. \tag{23}$$

One may easily recognize in Eqs. (20) and (22) the analogy to equations in Ref. 6 describing the transitions in the elastically isotropic solid body.

To be now more specific, note that the elastic energy of homogeneous deformations for the tetragonal lattice can be rewritten in terms of the even irreducible representation of the D_{4h} group,

$$A_{1g}: u_{xx} + u_{yy}, u_{zz}; B_{1g}: u_{xx} - u_{yy}; B_{2g}: u_{xy}; E_g: u_{zx}, u_{zy}. \tag{24}$$

In principle, any distortion in Eq. (24) perturbs the electronic spectrum and, hence, affects the nesting features. Therefore, the number of the independent striction constants q's in Eq. (4) [or λ's in Eqs. (8) and (9)] may be large. In view that the layered character of pnictides makes them close to two-dimensional systems, the nesting parameter δ in Eq. (8) is controlled mainly by the strain components in Eq. (24) that do not have the z indices. Rewriting the 2D part of the elastic energy (5) in the form

$$H_{el} = \frac{K}{2}(u_{xx} + u_{yy})^2 + \frac{\mu_1}{2}(u_{xx} - u_{yy})^2 + 2\mu_2 u_{xy}^2, \tag{25}$$

with three independent moduli according to Eq. (24) and three magnetoelastic constants q_i [or λ_i in Eqs. (8) and (9)] and taking into account the uniaxial symmetry along $(0,\pi)$ or $(\pi,0)$ directions for the parameters Δ_1 and Δ_2, we simplify the problem further and rewrite Eq. (9) as

$$\tau \to \tau + \frac{\lambda_+}{T_0}u_+ + \frac{\lambda_-}{T_0}u_-, \tag{26}$$

where $u_+ = u_{xx} + u_{yy}$ and $u_- = u_{xx} - u_{yy}$. The second term is responsible for the orthorhombic deformation of the lattice.

For the actual calculations, one would need the expression for $\Omega(\tau)$. In our case the fluctuations are strong only in a narrow vicinity of the phase transition, and we expect that the first-order transition occurs inside the same interval. Therefore, only the *singular* part $\delta\Omega_{sing}(\tau)$ is of importance. We limit ourselves by the first fluctuation correction to the mean field Ω, which we calculate in exactly the same manner as in Ref. 17 (see §147, problem, p. 482). The minor differ-

ence is that for the strongly anisotropic pnictides, one needs to introduce in Eq. (3) the in-plane and out-of-plane coherence lengths $\xi_{0\|} \gg \xi_{0\perp}$. After an elementary calculation it follows:

$$\delta\Omega_{\rm sing}(\tau) = -\,{\rm const}(T_0\xi_{0\|}^{-2}\xi_{0\perp}^{-1})|\tau|^{3/2} \equiv -B|\tau|^{3/2}, \quad (27)$$

where const is a numeric factor that depends on the model details. [Strictly speaking, the values of B in Eq. (27) differ by a factor of $2^{3/2}$ on the two sides of T_0 (Ref. 17) (see §146, footnote on p. 475).] For the singularity in the specific heat, Eq. (27) gives

$$\delta C(\tau) = \frac{3}{4T_0}B|\tau|^{-1/2}. \quad (28)$$

Comparing Eq. (28) with the normal specific heat $C_n \sim \nu T_0$ leads to the criterion,

$$\frac{B}{\nu T_0^2}|\tau|^{-1/2} \equiv \alpha|\tau|^{-1/2} \ll 1. \quad (29)$$

[In the strictly 2D limit ($\xi_{\perp 0} \to \infty$) one would obtain the criteria (17)]. With Eqs. (14) and (23) one finds that corrections to the elastic moduli of Eq. (25) become strong in the same order of magnitude temperature interval Eq. (17) [or Eq. (29)] if both K and μ are of the atomic scale.

To demonstrate the emergence of the first-order transition from Eqs. (20) and (22), assume—for simplicity sake—$\alpha = 1/2$ in Eq. (15), i.e., extrapolate Eq. (27) over the whole fluctuation interval. From Eq. (22) (for each $u_{+,-}$) it follows:

$$Ku_+ = \frac{3}{2}B\frac{\lambda_+}{T_0}\frac{x}{|x|}|x|^{1/2}; \quad u_-\mu_1 = \frac{3}{2}B\frac{\lambda_-}{T_0}\frac{x}{|x|}|x|^{1/2}. \quad (30)$$

With the notations

$$\alpha_+ = \frac{3}{2}B\frac{\lambda_+^2}{KT_0^2}, \quad \alpha_- = \frac{3}{2}B\frac{\lambda_-^2}{\mu_1 T_0^2}, \quad (31)$$

$$\frac{\lambda_+ u_+}{T_0} = \rho, \quad \frac{\lambda_- u_-}{T_0} = \mu, \quad x \equiv \tau + \rho + \mu, \quad (32)$$

we rewrite Eq. (30) as

$$\frac{1}{\alpha_+}\rho = \frac{x}{|x|}|x|^{1/2}, \quad \frac{1}{\alpha_-}\mu = \frac{x}{|x|}|x|^{1/2} \quad (33)$$

or

$$\alpha_+^{-1}\rho = \alpha_-^{-1}\mu, \quad x = \tau + \rho\left(1 + \frac{\alpha_-}{\alpha_+}\right) = \tau + \upsilon. \quad (34)$$

Finally, with

$$\upsilon = (\alpha_+ + \alpha_-)\frac{x}{|x|}x^{1/2}, \quad (35)$$

we arrive to the single equation

$$x = \tau + (\alpha_+ + \alpha_-)\frac{x}{|x|}x^{1/2}. \quad (36)$$

Equation (36), such as Eq. (13) of Ref. 6, reveals the typical features of a first-order transition. At small enough τ, there are three solutions for x. If coefficients B in Eq. (27) are equal on both sides of T_0, the transition takes place at $\tau = 0$, where

$$x_+ = -x_- = (\alpha_+ + \alpha_-)^2 \quad (37)$$

determines the jumps of u_+, u_- at the transition (note that at negative $x_- \neq 0$, the driving parameter, according to Eq. (16), is finite). The area of hysteresis is determined by the equation

$$2 = (\alpha_+ + \alpha_-)|x|^{-1/2}. \quad (38)$$

These results qualitatively agree with the observed simultaneous onset both of orthorhombic distortions and the "stripe" SDW order in the iron system $A22$.[4] The distortion (32) just accompany the magnetic transition. In case of the "1111" class, the temperature $T_{\rm str}$ for the onset of the orthorhombic deformation precedes the onset of the magnetic order at T_m.[3] The two temperatures are rather close: $\Delta T = T_{\rm str} - T_m > 0$ is on order of 10–20 K, so that by order of magnitude $\Delta T/T_{\rm str} \sim 0.1$ falls into the range of Eq. (17) with $E_F \sim 0.1$–0.2 eV taken for the pockets' depths obtained in "first-principle" calculations.[8,20] Such closeness seen among most of REFeAsO [e.g., compare La (Ref. 3) and Nd (Ref. 21)] is strongly in favor that the structural transition is directly related to the magnetic instability. In the language of local Fe spins, the attempt was made in Ref. 22 to ascribe the temperature interval separating $T_{\rm str}$ and T_m to the appearance of a "nematic phase" that comes about due to strong spin fluctuations above T_m. We suggest that both transitions have the common origin and come about as the result of the lattice instabilities caused by the striction. Indeed, according to Eq. (14), the striction triggers softening of elastic moduli as temperature approaches the transition interval (17) or Eq. (29). Assume that it takes place more strongly for modulus μ_1 in Eq. (25). Recall that the orthorhombic distortion is the symmetry change by itself and for the tetragonal lattice is characterized by the symmetry parameter $u_- = u_{xx} - u_{yy}$. So far as the dependence $\delta\Omega_{\rm sing}(\tau + (\lambda_-/T_0)u_-)$ on u_- is the only form of the nonlinear elastic energy, the above analysis applies. However, when the renormalized modulus $\mu_{1\rm eff}$ becomes small, other nonlinear terms ever present in the lattice must be also taken into account. As the result, the Landau functional for the parameter $u_- = u_{xx} - u_{yy}$ also depends on those contributions. The higher-order terms in u_- becoming important when renormalized $\mu_{1\rm eff}$ is small nearby magnetic T_0. The mean-field treatment of the present symmetry parameter u_- could then be applied in the usual way for the second-order tetraorthotransition at $T_{\rm str}$.

Experimentally, the structural distortions at $T_{\rm str}$ appear in the weak first-order transition.[3] That last result immediately follows from the fact that by symmetry, the orthorhombic transition in the tetragonal lattice infers its *own quadratic striction*. Indeed, the following cubic terms are allowed in the tetragonal lattice by the symmetry reasons:

$$q_\| u_+ u_-^2 + q_\perp u_{zz} u_-^2, \quad (39)$$

in addition to the elastic terms

$$\frac{K}{2}u_+^2 + \frac{K_\perp}{2}u_{zz}^2. \tag{40}$$

In terms of our models (1), (3), and (7), the fact that $T_m < T_{str}$ should mean that the nonzero distortion u_- below T_{str} makes the nesting condition (1) worse.

Let us add a few final comments to the analyses above. The order of magnitude estimate of the in-plane lattice distortions at low enough temperatures follows from Eqs. (10) and (11):

$$u \sim \frac{q}{K} \sim \frac{\nu E_F}{KT_0}T_0^2 \sim \frac{T_0}{E_F} \sim 10^{-2} - 10^{-3} \tag{41}$$

that agrees well with the experimental data of Refs. 23–25. The hysteresis ΔT from Eq. (38) agrees by the order of magnitude with data.[4]

There are no experimental data for the volume change $\Delta V/V$. The lattice deformation along the c axis, in principle, could be obtained from Eqs. (39) and (40) together

$$u_{zz} \sim \frac{q_\perp}{K_\perp}u_-^2. \tag{42}$$

In Eq. (42) both $q_\perp$ and $K_\perp$ are expected to be small in a layered material. These parameters remain unknown in the oxypnictides.

Equation (14) together with Eq. (27) provides another observable feature. At temperatures above T_0 the fluctuation corrections to the elastic moduli should behave as

$$\sim (T - T_0)^{-1/2}, \tag{43}$$

while in the 2D limit of isolated planes

$$\sim (T - T_0)^{-1}. \tag{44}$$

The data[25] do not allow to distinguish between the exponents in Eqs. (43) and (44).

To summarize, in the frameworks of multiband electronic spectrum with nesting features, the theoretical scheme is elaborated to treat striction in iron pnictides. Magnetoelastic coupling changes the second-order character of magnetic transition. The transition becomes of the first order. Whether the transition bears strong or weak first-order character may depend on details. Provided that $T_0 \ll E_F$, the weak first-order transition is predicted. The model, when applied to the layered FeAs systems, leads to estimates of the correct order of magnitude. Discontinuities of all parameters at the transition are due to lattice instabilities. Magnetoelastic interactions may split the magnetic (SDW) transition at T_m and the orthorhombic deformations at $T_{str} > T_m$. The model predicts a noticeable precursory temperature dependence above the transition temperature in the elastic moduli.

The obtained results are in good qualitative agreement with peculiarities of the phase diagram of present parent or underdoped FeAs materials well above the temperature of superconducting transition.

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