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Interplay of magnetic and structural transitions in iron-based pnictide superconductors

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The interplay between the structural and magnetic phase transitions occurring in the Fe-based pnictide superconductors is studied within a Ginzburg-Landau approach. We show that the magnetoelastic coupling between the corresponding order parameters is behind the salient features observed in the phase diagram of these systems. This naturally explains the coincidence of transition temperatures observed in some cases as well as the character (first or second order) of the transitions. We also show that magnetoelastic coupling is the key ingredient determining the collinearity of the magnetic ordering and we propose an experimental criterion to distinguish between a pure elastic from a spin-nematic-driven structural transition.

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The discovery of an unconventional high-temperature superconductivity in the F-doped arsenic-oxide LaFeAsO (Ref. 1) has given rise to a great interest on iron pnictide compounds. To date several families of Fe-based superconductors have been discovered and the superconducting transition temperature has been raised to above 50 K.[2] All of these systems display an intriguing competition between structural, magnetic, and superconducting transitions.[2,3] The parent compounds of the so-called 1111 and 111 families undergo a structural transition (ST) followed by a magnetic transition (MT) at a lower temperature[4] whereas in the 122 and 11 cases these two transitions take place simultaneously.[5–8] In any case these orderings are quickly suppressed by doping or by applying pressure, which eventually gives rise to superconductivity. The role, if any, of magnetic and elastic degrees of freedom in inducing this superconductivity is currently an open question. There is already a growing body of theoretical works advocating for spin fluctuation mediated superconductivity[9] but the isotope effect observed in both magnetism and superconductivity suggests that the elastic medium also plays a role.[10] It is therefore compelling to understand the connection between the ST and the MT in these systems.

The ST, for example, has been studied in Refs. 11–13, where it has been identified with a spin-nematic ordering but ignoring the possible softening of the lattice itself. This idea has been further elaborated in Ref. 14, where the observed softening of the lattice is interpreted as due to the fluctuations of the emerging nematic degrees of freedom. On the other hand, the study of the MT in Ref. 15 focuses on the role of the magnetoelastic (ME) couplings in producing a weak first-order MT by means of the Larkin-Pikin mechanism.[16] This latter is relevant only in the fluctuation dominated Ginzburg regime and is subjected to the condition of a MT with diverging specific heat in the absence of ME coupling. Furthermore, the collinearity of the magnetic moments is examined in Ref. 17 by using a purely electronic model.

In this paper we study the ST and the MT using a Ginzburg-Landau approach, in which the interplay between elastic and magnetic degrees of freedom is considered explicitly. This provides a general unified framework that goes beyond previous phenomenological approaches and rationalizes different experimental findings. We address, in particular, the simultaneity of the ST and MT, their character (first versus second order), the collinearity of the magnetic structure, and the spin-nematic scenario for the ST. Our study identifies a particular ME coupling [see Eq. (2) below] as the common key factor behind the salient features of the ST and MT in the Fe-based superconductors.

Our main results are the following. (i) We derive the general phase diagram of the ST and MT, which exhibits four qualitatively different regimes, as shown in Fig. 1. This explains why the simultaneous ST and MT in the 122 compounds are sometimes observed as second-order transitions[6] (Ia in Fig. 1) and sometimes as first order[5] (Ib in Fig. 1). Moreover, when the two transitions are separate but close enough, we predict the MT to be first order (IIa in Fig. 1). This richness of the phase diagram is due to the ME coupling. (ii) The collinearity of the magnetic moments is linked to the existence of the ME term allowed by symmetry. (iii) In regime II where the two transitions are separate, the ST can be a consequence of either a purely elastic instability of the lattice or due to a spin-nematic transition. Here we develop an experimental criterion to distinguish between these two possibilities. (iv) The fluctuations associated with the ST are shown to become critical only along certain lines of high symmetry in the Brillouin zone both for a pure elastic ST as well as for a spin-nematic-driven ST. Consequently, in both the scenarios the ST has a mean-field behavior.[13]

For concreteness we assume for the present discussion that the ST is a pure elastic one for which the order parameter is the shear strain u_{xy},[18] where subscripts refer to the principal axes of the tetragonal lattice [with two and four Fe atoms per unit cell for the 1111 and the 122 systems respectively, see Fig. 2(a)]. Thus $u_{xy} \neq 0$ implies the monoclinic distortion of the tetragonal unit cell observed experimentally, as illustrated in Fig. 2(b). The qualitative aspects of the current discussion remain unchanged for the case where the ST is spin-nematic driven, which we treat later. The description of the MT requires two Néel vectors,[19] $\mathbf{L}_1$ and $\mathbf{L}_2$, which can be associated with the spontaneous magnetizations $\mathbf{M}_1$ and $\mathbf{M}_2$ of the two interpenetrating Fe sublattices [Fig. 2(b)]. The

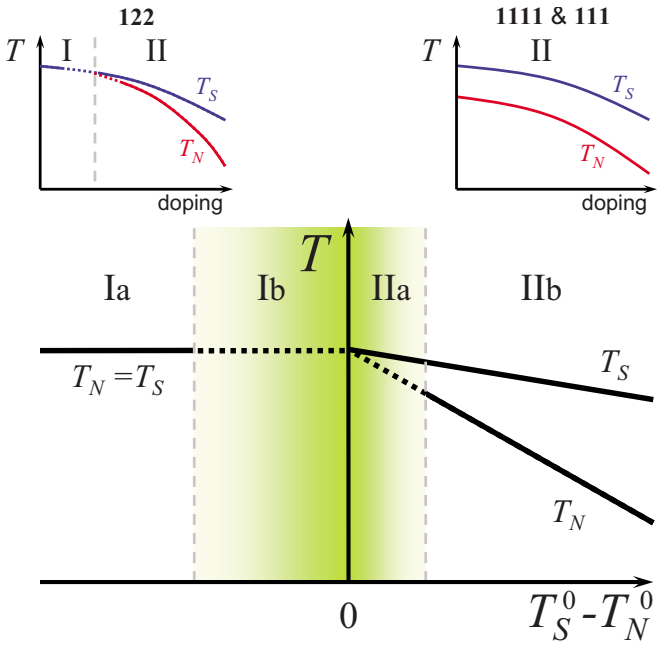

FIG. 1. (Color online) Schematic T vs doping diagrams for the structural and magnetic phase transitions (top panels) and general phase diagram T vs $T_S^0 - T_N^0$ determined by our Ginzburg-Landau theory Eq. (1) (bottom panel). Empirically $T_S^0 - T_N^0$ increases with doping. In the regions I the transitions are simultaneous while in regions II they occur at different temperatures T_S and T_N. Continuous (dotted) lines indicate second- (first-) order transitions. The background-color intensity indicates the strength of the discontinuity.

Ginzburg-Landau free energy then can be conveniently written as

$$F_{GL} = F_M + F_E + F_{\mathrm{ME}}. \tag{1}$$

Here the magnetic part is $F_M = \frac{1}{2}A(L_1^2 + L_2^2) + \frac{1}{4}B(L_1^4 + L_2^4)$. In principle, fourth order terms of the form $L_1^2 L_2^2$ and $(\mathbf{L}_1 \cdot \mathbf{L}_2)^2$ are also allowed by symmetry but we omit them because the former does not affect the results qualitatively while the latter is generated by the ME coupling (see below). In a continuum description the free energy for the elastic part is quite standard, and the case with a tetragonal symmetry is described by six elastic moduli and the various components of the strain tensor.[20] However, to simplify the discussion, in the following we consider explicitly only the critical strain u_{xy} and we write $F_E = \frac{1}{2}c_{66}u_{xy}^2 + \frac{1}{4}\beta u_{xy}^4$. The coefficients A and c_{66} are assumed to vary with the temperature as $A = A'(T - T_N^0)$ and $c_{66} = c'_{66}(T - T_S^0)$. T_N^0 and T_S^0 are the nominal MT and ST temperatures, respectively (not to be confused with the actual transition temperatures T_N and T_S), taken as the control parameters of our theory. According to Mermin-Wagner theorem, a finite T_N^0 implies that the magnetism is three dimensional. The remaining coefficients B, C, and β are taken as positive constants. As regards the ME term, the key contribution is[13–15]

$$F_{\mathrm{ME}} = g_1 u_{xy}(\mathbf{L}_1 \cdot \mathbf{L}_2), \tag{2}$$

where $g_1 > 0$ in order to be consistent with the experimental observation that the ferromagnetic Fe-Fe bonds are shorter than the antiferromagnetic ones in the collinear-Néel state. To our purposes, the standard magnetostriction $u_{ll}(L_1^2 + L_2^2)$ can be neglected because it does not change qualitatively the results. It is worth mentioning that, in the context of the cuprate superconductors, a similar free energy F_{GL} was used to study the structural transition of doped La_2SrCuO_4.[21]

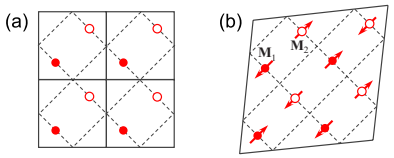

FIG. 2. (Color online) (a) Tetragonal Fe lattice (drawn as two interpenetrating sublattices) at temperatures $T > T_S, T_N$. (b) A monoclinic distortion of the tetragonal unit cell and a collinear Néel order in the two Fe sublattices take place at $T < T_S, T_N$.

The free energy in Eq. (1) is phenomenological in nature and its structure, which is based on symmetry considerations, is independent of the underlying microscopic theory. For example, the ST can be due to orbital ordering[22] or due to magnetic fluctuations.[14] Similarly, the magnetic part of the free energy can be understood from a band magnetism picture,[17] as well as from a localized magnetism viewpoint.[11,12] The appropriate microscopic description of the phase transitions is a current open problem.

A microscopic description of the phase transitions is important to establish how the various coefficients of the Ginzburg-Landau theory vary with physical parameters such as doping and pressure. Such a study is beyond the scope of the current paper. However, it is our empirical observation that the results are consistent with the current experiments if we assume that $T_S^0 - T_N^0$ increases with doping. It is likely that low doping influences the magnetic sector more (say, via the loss of nesting between electron and hole bands) than the elastic medium which is affected indirectly. Furthermore, sample quality can also alter these parameters[23] and, if the magnetism is anisotropic, T_N^0 can also depend strongly on the coupling between the magnetic planes.[11]

We anticipate that, experimentally, undoped and lightly doped 122 systems fall in regimes Ia and Ib in Fig. 1 with simultaneous transitions of second[6] and first[5] orders, respectively, and then enter regime IIa at higher doping where the ST is second order while the separate MT is first order.[7] On the other hand, the 1111 and 111 compounds appear to fall in the regime IIb, where the transitions are separate ($T_S > T_N$) and second order. Regime IIa has not yet been reported experimentally for these systems.

Within our framework, the fact that these transitions sometimes are observed separate and sometimes simultaneous is explained as follows. Note that, once the magnetic order sets in and the collinear-Néel state is formed, there is an effective shear stress that produces a monoclinic distortion via the ME term [Eq. (2)]. Thus, the MT in these systems implies a ST while the converse is evidently not true. This gives rise to the regimes I and II in the phase diagram shown in Fig. 1, which are defined by the conditions $T_S^0 < T_N^0$ and $T_S^0 > T_N^0$, respectively. Thus, as the temperature is lowered in regime II there is first the ST at $T = T_S^0$, where $c_{66} = 0$, followed by a separate MT at $T_N = T_N^0$

$+[g_1u_0(T_N)]/A'$, where $u_0(T)=\pm[(T_S^0-T)c_{66}'/\beta]^{1/2}$ is the value of the strain order parameter u_{xy} in the monoclinic phase at $T<T_S$. In the regime I, however, the system encounters the MT first at $T=T_N^0$, where $A=0$, but simultaneously the ST occurs due to the effective stress in the ME term. In this regime, unlike in II, there is no instability of the lattice because the elastic modulus c_{66} stays finite (and jumps across the transition).

The two regimes above are divided in their turn into subregimes Ia, Ib, IIa, and IIb according to the character, first or second order, of the MT. This is again due to the ME coupling and is not related to symmetry reasons such as the existence of cubic invariants. The point is that sufficiently close to $T_S^0=T_N^0$, the effective coefficient of the fourth-order term in the magnetic sector becomes negative turning the MT first order (in which case, one has to include higher order terms to bound the free energy from below). This is readily seen in the regime I ($T_S^0<T_N^0$), where the elastic sector is stable and one can ignore the u_{xy}^4 term in F_E. Indeed minimizing F_{GL} one gets $u_{xy}=-g_1(\mathbf{L}_1\cdot\mathbf{L}_2)/c_{66}$, which implies that the elastic sector generates an effective magnetic term of the form $-g_1^2(\mathbf{L}_1\cdot\mathbf{L}_2)^2/(2c_{66})$. The coefficient of this term is arbitrarily large near $T_S^0=T_N^0$. The MT into the collinear-Néel state turns first order when this term is sufficiently strong with the tricritical point given by $c_{66}=g_1^2/B$ and $A=0$. The logic is quite similar in the regime II ($T_S^0>T_N^0$), where one first has to expand $u_{xy}=u_0+\delta u_0$ in the monoclinic phase to then obtain (after further minimization) $\delta u_0=-g_1(\mathbf{L}_1\cdot\mathbf{L}_2)/(2|c_{66}|)$. This implies an effective magnetic term $-g_1^2(\mathbf{L}_1\cdot\mathbf{L}_2)^2/(4|c_{66}|)$ which drives the MT first order, with the tricritical point given by $A=g_1u_0(T_N)$ and $c_{66}=-g_1^2/(2B)$. In both the regimes the discontinuity is increased as the system approaches the point $T_S^0=T_N^0$ (indicated by the color intensity in Fig. 1). These results have to be contrasted to Ref. 15, where strong fluctuations are required and weaker first-order transitions with narrower hysteresis, are expected.

At this stage, the role of the ME coupling in favoring the collinear-Néel state observed experimentally[24] is quite straightforward. In regime II the collinearity is due to the term $g_1u_0(\mathbf{L}_1\cdot\mathbf{L}_2)$, which lifts the degeneracy of the transition temperatures for $\mathbf{L}_\pm=\frac{1}{\sqrt{2}}(\mathbf{L}_1\pm\mathbf{L}_2)$. This implies that only one between $\mathbf{L}_\pm$ is nonzero in the ordered state (which one in particular depends on the sign of u_0, i.e., on the ferroelastic domain). In regime I, however, the reason is different. In this case the set up of the collinear order is associated with the negative coefficient $-g_1^2/(2c_{66})$ in front of the term $(\mathbf{L}_1\cdot\mathbf{L}_2)^2$, generated by the ME coupling. Presumably, the vicinity to the structural instability, where c_{66} is small, makes the ME term strong enough to overcome any other contribution (due to, e.g., magnetic interactions) and thus forces collinearity.

In region II of the phase diagram there are two different physical scenarios to conceptualize the ST, namely, a pure ferroelastic transition and a transition induced by a spin-nematic ordering. (a) In the first scenario we have a proper ferroelastic instability in F_E caused by the vanishing of the elastic modulus c_{66} (the case described until now). An immediate consequence is that the temperature range over which the monoclinic distortion has square-root behavior $u_0(T)\propto(T_S-T)^{1/2}$ is the same as the temperature range over which the elastic modulus is expected to have a linear dependence $c_{66}\propto|T-T_S|$. (b) The second scenario arises from the possibility that above T_N the system enters a spin-nematic state in which the two Néel vectors are zero in average but fluctuate in phase.[25] The description of this state requires the introduction of an additional Ising order parameter σ which is independent of but has the same symmetry properties as $\mathbf{L}_1\cdot\mathbf{L}_2$. Now the system is expected to undergo a pseudoproper ferroelastic transition driven by the nematic ordering. This case can be treated if we replace F_E in Eq. (1) by

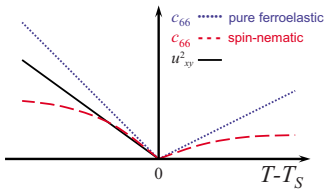

FIG. 3. (Color online) Expected temperature dependence of the squared spontaneous strain u_{xy}^2 and the elastic modulus c_{66} in scenarios (a) proper ferroelastic instability and (b) driven by spin-nematic ordering. Large deviations from a linear behavior in c_{66} as compared to u_{xy}^2 indicate spin-nematic ordering.

$$\tilde{F}_E=\frac{a}{2}\sigma^2+\frac{b}{4}\sigma^4+\frac{c_{66}}{2}u_{xy}^2+\frac{\beta}{4}u_{xy}^4+g_2u_{xy}\sigma, \tag{3}$$

where $a=a'(T-T_n^0)$ with T_n^0 being the nominal-nematic transition temperature while all other coefficients are T-independent (including c_{66} for this discussion). In the absence of the ME coupling of Eq. (2) the structural-nematic transition, below which $u_{xy}\propto\sigma\neq0$, occurs at $T_{SN}^0=T_n^0+g_2^2/(c_{66}a')$, where the effective elastic modulus $\tilde{c}_{66}=c_{66}-g_2^2/a$ vanishes. The arguments given earlier for the phase diagram and the collinearity of the magnetic order hold equally well for this case, except now T_S^0 in Fig. 1 has to be replaced by T_{SN}^0. However, in this case the range of temperatures over which $\tilde{c}_{66}\propto|T-T_S|$ is restricted to the condition $|T-T_S|<g_2^2/(c_{66}a')$. This range is in principle different from the one over which the monoclinic distortion has square-root dependence, and gives a different behavior compared to case (a). This difference, schematically represented in Fig. 3, can be used as a quantitative criterion to distinguish experimentally between the pure ferroelastic and the spin-nematic-induced scenarios. These considerations are based on a mean field analysis of the ST, which we justify in the following.

Previous studies on ferroelastics[26] have shown that a second-order ST, like in the proper ferroelastic scenario (a), displays a mean-field behavior. This follows from the fact that at the transition point, where the elastic modulus $c_{66}=0$, the phonon velocity remains finite everywhere in the Brillouin zone ($\mathbf{q}$ space), except along the two lines of high symmetry $q_x=0$ and $q_y=0$ on the $q_z=0$ plane. Consequently, except for these "soft" lines, the long-wavelength critical excitations associated with the strain field u_{xy} are gapped and the transition in three dimensions is mean-fieldlike.[26] The contribution of these excitations to F_E can be written as $\delta F_E=\frac{1}{2}\Sigma_{\mathbf{q}\neq0}c_{66}(\mathbf{q})|u_{xy}(\mathbf{q})|^2+\cdots$, where the ellipsis denotes noncritical modes and interaction terms. Near the soft lines

$$c_{66}(\mathbf{q}) \approx c_{66} + c_1 \cos^2\theta + c_2 \sin^2 2\varphi \sin^4\theta + \kappa q^2 \quad (4)$$

where θ and φ represent the polar and the azimuthal angles, respectively, in $\mathbf{q}$ space.[26] Here the κq^2 contribution is due to harmonic terms in the free energy with higher order spatial derivatives (the usual stiffness associated with collective excitations) and c_1 and c_2 are constants that depend on the elastic moduli of the system.[27] In the scenario (b) the situation is slightly more subtle. Indeed, if we ignore the coupling $g_2 u_{xy}\sigma$, it appears that the nematic transition, which belongs to the Ising class, is in three dimensions below its upper critical dimension and therefore it is not mean-field type. However, the ME coupling gives rise to anisotropic corrections to the mass of the σ field. In fact the resulting mass term can be written as $F_\sigma = \frac{1}{2}\Sigma_{\mathbf{q}\neq 0} a(\mathbf{q})|\sigma(\mathbf{q})|^2$, where $a(\mathbf{q}) = a - g_2^2/c_{66}(\mathbf{q})$. As a consequence, in this scenario too, the long-wavelength critical excitations are gapped except along the two soft lines.[28] So the ST is mean field type in both the scenarios.

We finally discuss some limitations of our study. We have restricted ourselves to magnetic states describable in terms of the Néel vectors $\mathbf{L}_1$ and $\mathbf{L}_2$. This includes the collinear $(\pi,0)$ [or $(0,\pi)$] "stripe" order observed experimentally. In the case of a different magnetic ground state the corresponding Ginzburg-Landau theory may have a different form with structural and magnetic orderings not necessarily coupled. This seems to be the case in $BaMn_2As_2$, where a *G*-type antiferromagnetic order is found and no structural distortion is observed.[29] The same applies to 11 Fe chalcogenides, for which, in addition, the question of whether the magnetic order is intrinsic or arises from nonstoichiometry, i.e., due to interstitial Fe ions inducing weak charge localization, is still open.[30] Critical fluctuations are also not considered in our theory. While we expect that they will not change the nature of the ST, they certainly will enhance the effects of the Larkin-Pikin mechanism[16] on the MT. We do expect therefore an enlargement of the first order MT region (Ib and IIa in Fig. 1). All these considerations, as well as making contact with microscopic theories, deserve deeper investigation in future studies.

In summary, we have shown that the magnetoelastic coupling Eq. (2) plays a key role in producing the specific features of the structural and magnetic transitions in the Fe-based superconductors. This coupling is responsible for the simultaneity of the transitions observed in the 122 systems and explains the different characters (first order and second order) of the transitions reported so far. It also naturally explains the collinearity of the magnetic order. We have also addressed the question of the possibility of a spin-nematic-driven structural transition, indicating an experimental way to distinguish this type of scenario from a proper ferroelastic transition.

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[19] The two sublattice magnetizations associated with the $(\pi,0)$ [or $(0,\pi)$] orderings observed experimentally can be defined as $\mathbf{M}_1 = \mathbf{L}_1 \cos(\mathbf{Q}\cdot\mathbf{R}_1)\cos(\pi z)$ and $\mathbf{M}_2 = \mathbf{L}_2 \cos(\mathbf{Q}\cdot\mathbf{R}_2)\cos(\pi z)$, where $\mathbf{Q} = (\pi,\pi)$ and $\mathbf{R}_{1(2)}$ are points on the Fe sublattice 1(2). The observed moments are $\sim 0.3-0.7\mu_B$ in the 1111 and 111 and $\sim 1.5\mu_B$ in the 122 compounds.
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