Variation of shear moduli across superconducting phase transitions

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(Received 10 October 2019; revised manuscript received 21 January 2020; accepted 24 March 2020; published 10 April 2020)

We study how shear moduli of a correlated metal change across superconducting phase transitions. Using a microscopic theory we explain why for most classes of superconductors this change is small. The Fe-based and the A15 systems are notable exceptions where the change is boosted by five orders of magnitude. We show that this boost is a consequence of enhanced nematic correlation. The theory explains the unusual temperature dependence of the orthorhombic shear and the back-bending of the nematic transition line in the superconducting phase of the Fe-based systems.

DOI: 10.1103/PhysRevB.101.144502

I. INTRODUCTION

An important topic in high-temperature superconductivity is to understand the interplay between superconducting and nematic orders. The issue arises naturally for the Fe-based systems for which the two orders are ubiquitously present [1–12]. The relevance of nematicity to understand the pseudogap state of the cuprates is currently under active investigation as well [13–21].

One reason for this interplay can be fluctuations of the two orders, and the effect of nematic fluctuations on superconductivity has been studied theoretically [22–28]. Experimentally, two different trends have been reported. In $NaFe_{1-x}Co_xAs$ an increase in $T = 0$ penetration depth near a nematic quantum critical point (QCP) has been inferred [29]. But for $FeSe_{1-x}S_x$ the superconducting transition T_c is unaffected by the nematic QCP [30–32]. A second cause of the above interplay can be a third degree of freedom such as antiferromagnetic fluctuations which can enhance nematic correlation, but which are themselves suppressed in a singlet superconductor [33]. What is less examined is the effect of the superconducting order itself on the nematic properties of electrons in solids. The goal of the current paper is to study the last from a microscopic point of view.

For such a study a shear strain of a suitable symmetry is an appropriate nematic order parameter, even if the nematic transition is driven by electronic spin and orbital fluctuations [34,35]. This is because, due to electron-strain coupling, the nematic transition at temperature T_s itself manifests as a structural instability. Consequently, tracking the change in the shear elastic constant $c_s(T)$ across T_c is a practical method to study the interplay. For simplicity we restrict our study to the case where $T_c > T_s$.

More concretely, for $T \sim T_c$, the free energy per unit volume involving the shear strain u_s and the superconducting order parameter Δ can be written as

$$F = (c_s/2)u_s^2 + (a/2)|\Delta|^2 + (b/4)|\Delta|^4 + (\lambda/2)u_s^2|\Delta|^2. \quad (1)$$

Here Δ has dimension of energy, while (a, λ) have that of density of states (DOS), $a = a_0(T - T_c)$, and $b > 0$. The fourth term, which captures the interplay, describes how the shear elastic constant is modified across T_c. In the above we assumed that Δ belongs to a one-dimensional irreducible representation of the unit cell point group, and that there is no second nearly critical symmetry channel for superconductivity [4,5,36].

From Eq. (1) it follows that $c_s(T)$ itself is continuous at T_c, but its temperature derivative jumps at T_c with the jump given by $(dc_s/dT)_{T_c^+} - (dc_s/dT)_{T_c^-} = \lambda a_0/b$. In other words, $c_s(T)$ has a kink at T_c which encodes information about the interplay parameter λ. The magnitude of this kink can be quantified by $\delta c_s/|c_s^m|$, where $\delta c_s \equiv \lambda\Delta_0^2 \sim c_s^s - c_s^m$. Here c_s^s is the zero-temperature elastic constant in the superconducting phase, c_s^m is inferred from the $T = 0$ extrapolation of $c_s(T)$ in the metal phase, and $\Delta_0 \equiv \Delta(T = 0)$.

A literature search reveals that in most known classes of superconductors the ratio $\delta c_s/|c_s^m|$ is "small" and is of order 10^{-6}. Examples include conventional Bardeen-Cooper-Schrieffer (BCS) systems [37,38], cuprates such as $La_{2-x}Sr_xCuO_4$ at various dopings (see Figs. 7 and 8 in Ref. [39]), and heavy fermion systems UPt_3 and URu_2Si_2 [40,41]. From an Ehrenfest-type thermodynamic argument it is known that $\delta c_s/|c_s^m|$ is related to the ratio between the superconducting condensation energy and the Fermi energy, which is typically small [42,43]. This provides a simple way to understand this small ratio without a microscopic analysis.

However, there are two classes of superconductors, namely, the Fe-based [33,44–47] and the A15 systems [48–50], for which this ratio is "large" with $\delta c_s/|c_s^m| \sim 10^{-1}$. Clearly, this increase of $\delta c_s/|c_s^m|$ by *five* orders of magnitude compared to the standard behavior cannot be understood purely from thermodynamics, and a microscopic approach is needed. With this motivation, here we develop such a microscopic theory of the coupling λ that encodes the interplay between the two orders.

Our main results are the following. First, we show that in systems with negligible nematic correlation $\lambda/\mathcal{N}_F$ is small, where $\mathcal{N}_F$ is DOS at Fermi level. This is due to a cancellation of the low-energy electronic contribution that is not imposed by symmetry. We show that this cancellation is related to the general property that the quadrupolar charge susceptibility of an electronic system remains approximately unchanged between its metallic and superconducting phases. This explains the small ratio of $\delta c_s/|c_s^m|$ for most superconductors. Second, we show that for systems with large nematic correlation length $\xi \gg l$, where l is the interatomic distance, the parameter λ is boosted by $(\xi/l)^4$. This accounts for the five orders of magnitude increase in $\delta c_s/|c_s^m|$ seen in the A15 and the Fe-based systems. Together, these two results provide a broad and unifying principle to understand $\delta c_s/|c_s^m|$ across various families of superconductors. Third, we show that the sign of λ, that controls cooperation or competition between the two orders, is nonuniversal and that it depends on the band structure.

II. MICROSCOPIC THEORY

Our main message can be illustrated by considering a one-band metal in a tetragonal lattice. The relevant elastic constant can be written as

$$c_s(T) \equiv c_0 - \alpha^2 \chi_n(T). \tag{2}$$

Here c_0 is the modulus of the bare elastic medium, which we assume to be temperature independent, and α is the electron-strain interaction energy, such that in the presence of a finite strain the electron dispersion changes as $\epsilon_{\mathbf{k}} \to \tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \alpha u_s h_{\mathbf{k}}$. To be concrete we take u_s to be the orthorhombic strain that transform as $(x^2 - y^2)$, in which case $h_{\mathbf{k}} \sim \cos k_x - \cos k_y$. The precise nature of the shear mode and the associated form factor is unimportant. Likewise, the spatial symmetry of Δ (i.e., s, p, or d wave) plays no role, and we take it as s wave for simplicity. The quantity $\chi_n \equiv \lim_{\mathbf{q}\to 0} \chi_n(\mathbf{q}, \omega = 0)$, where $\chi_n(\mathbf{q}, 0)$ is the static nematic susceptibility of the electrons. Thus, the role of the lattice variables is simply to probe the electronic properties, in particular how χ_n changes across T_c.

At this point it is convenient to distinguish the two situations discussed in the following subsections.

A. Away from nematic instability

When the system is far away from nematic/orthorhombic instability the nematic correlation length is negligible, and therefore $\chi_n^{s/m}(\mathbf{q}, 0) \approx \Pi_n^{s/m}(\mathbf{q}, 0)$, where $\Pi_n^{s/m}(\mathbf{q}, 0)$ is the bare nematic susceptibility. We added superscripts (s, m) to denote superconducting and metallic phases, respectively. In the superconducting phase the bare nematic susceptibility is

$$\Pi_n^s(\mathbf{q}, 0) = -\frac{2}{\beta V} \sum_{\omega_n, \mathbf{k}} f_{\mathbf{k},\mathbf{q}}^2 [G_{\mathbf{k}+\mathbf{q}}(i\omega_n) G_{\mathbf{k}}(i\omega_n) - F_{\mathbf{k}+\mathbf{q}}(i\omega_n) F_{\mathbf{k}}(i\omega_n)],$$

where β is inverse temperature, V is volume, $f_{\mathbf{k},\mathbf{q}} \equiv (h_{\mathbf{k}} + h_{\mathbf{k}+\mathbf{q}})/2$ is the nematic form factor, $G_{\mathbf{k}}(i\omega_n) = -(i\omega_n + \epsilon_{\mathbf{k}})/(\omega_n^2 + E_{\mathbf{k}}^2)$, $F_{\mathbf{k}}(i\omega_n) = \Delta/(\omega_n^2 + E_{\mathbf{k}}^2)$, and $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}$. An overall factor two is due to spins. The equivalent expression for $\Pi_n^m(\mathbf{q}, 0)$ is obtained by setting $\Delta = 0$.

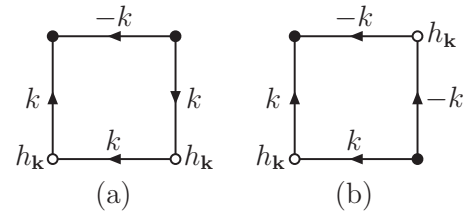

FIG. 1. Diagrammatic representation of the coupling λ that controls the interplay between superconducting and nematic orders; see Eq. (1). λ is a four-point function with two particle-hole (open circles) vertices with nematic form factor $h_{\mathbf{k}}$ and two particle-particle (closed circles) vertices; see Eq. (3). Solid lines are electron Green's functions. $k = (\mathbf{k}, \omega)$ denote momentum and frequency.

Equations. (1) and (2) give $\lambda = -(\alpha^2/2)[\partial^2 \chi_n^s/(\partial|\Delta|^2)]_{|\Delta|=0}$. Thus, λ is a four-point function that can be obtained from $\Pi_n^m(0, 0)$ by inserting two particle-particle vertices (see Fig. 1). This leads to the microscopic expression

$$\lambda = \lambda_0 \equiv -\frac{2\alpha^2}{\beta V} \sum_{\omega_n, \mathbf{k}} h_{\mathbf{k}}^2 \big[2G_{\mathbf{k}}^0(i\omega_n)^3 G_{\mathbf{k}}^0(-i\omega_n) + G_{\mathbf{k}}^0(i\omega_n)^2 G_{\mathbf{k}}^0(-i\omega_n)^2\big], \tag{3}$$

with $G_{\mathbf{k}}^0(i\omega_n)^{-1} \equiv i\omega_n - \epsilon_{\mathbf{k}}$. The above frequency sum is simple to perform. We define the B_{1g} density of states as $\mathcal{N}_{B_{1g}}(\epsilon) \equiv (1/V) \sum_{\mathbf{k}} h_{\mathbf{k}}^2 \, \delta(\epsilon - \epsilon_{\mathbf{k}})$, and we get

$$\lambda_0 = -\frac{\alpha^2}{2} \int_{-\infty}^{\infty} d\epsilon \mathcal{N}_{B_{1g}}(\epsilon) \frac{d^2}{d\epsilon^2} [\tanh(\beta\epsilon/2)/\epsilon].$$

We expand $\mathcal{N}_{B_{1g}}$ around the Fermi energy as $\mathcal{N}_{B_{1g}}(\epsilon) \approx \mathcal{N}_{B_{1g}}(0) + \epsilon \mathcal{N}'_{B_{1g}}(0) + (\epsilon^2/2)\mathcal{N}''_{B_{1g}}(0) + \cdots$, where primes imply derivatives with respect to energy. Remarkably, the term proportional to $\mathcal{N}_{B_{1g}}(0)$, which is the contribution from the low-energy excitations, *vanishes*. Since the term proportional to $\mathcal{N}'_{B_{1g}}(0)$ is trivially zero, the first nonzero contribution is proportional to $\mathcal{N}''_{B_{1g}}(0)$. We get

$$\lambda_0 = -\alpha^2 \mathcal{N}''_{B_{1g}}(0) \{\log[\Lambda/(2T)] + \mathcal{C}_1\}, \tag{4}$$

where $\mathcal{C}_1 \equiv \gamma - 3/2 - \log(\pi/4)$, γ is the Euler constant, and Λ is a high-temperature cutoff. The logarithmic temperature dependence above has the same origin as the familiar $\log(T)$ dependence of the particle-particle susceptibility in BCS theory.

The cancellation of the low-energy electronic contribution is important, and consequently it is useful to understand better its physical origin. Clearly, the cancellation is not dictated by any symmetry. Instead, it is a consequence of the property that the *bare* quadrupolar charge susceptibility of electrons remains nearly unchanged across a metal to superconductor transition. This can be demonstrated by the following calculation.

The frequency sum in the expression for $\Pi_n^s(0, 0)$ gives

$$\Pi_n^s(0, 0) = \frac{1}{V} \sum_{\mathbf{k}} h_{\mathbf{k}}^2 \frac{\partial}{\partial \epsilon_{\mathbf{k}}} \left[\frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh \frac{E_{\mathbf{k}}}{2T}\right].$$

If we neglect the energy dependence of the B_{1g} density of states $\mathcal{N}_{B_{1g}}(\epsilon)$, which is appropriate for the low-energy electronic contribution, after the energy integral we get

$$\Pi_n^s(0,0)_{\rm low} = \Pi_n^m(0,0)_{\rm low} = 2\mathcal{N}_{B_{1g}}(0). \tag{5}$$

In the above the subscript "low" implies the low-energy contribution. In other words, from the perspective of the low-energy electrons $\Pi_n^s(0,0)$ is independent of Δ. This property is reminiscent of that of the uniform charge susceptibility $\partial n/\partial\mu$, where n is the electron density and μ the chemical potential. It is known that the Thomas-Fermi screening length, which is controlled by the uniform charge susceptibility, remains practically unchanged when a metal turns into a superconductor [51]. The above discussion implies that if $\Pi_n^s(0,0)$ is expanded around $\Pi_n^m(0,0)$ in powers of $|\Delta|^2$, order by order the prefactors would be zero if we neglect the energy dependence of $\mathcal{N}_{B_{1g}}(\epsilon)$. The coupling λ_0 in Eq. (3) is related to the prefactor at order $|\Delta|^2$ in this expansion.

The above low-energy cancellation has the following consequences. First and most importantly, we conclude that for superconductors with negligible nematic correlation $\delta c_s/|c_s^m| \sim (T_c/E_F)^2$, where E_F is the Fermi energy. This follows from the estimate $\mathcal{N}''_{B_{1g}}(0) \sim \mathcal{N}_F/E_F^2$, and by estimating the electron-phonon interaction energy α as the geometric mean of the typical electronic and elastic energy scales, i.e., $(\alpha^2\mathcal{N}_F/c_s) \sim 1$ [52]. For renormalized Fermi liquids such as the heavy fermions, in Eq. (3) the bare $G^0_{\mathbf{k}}(i\omega_n)$ has to be replaced by the quasiparticle propagator $\tilde{G}_{\mathbf{k}}(i\omega_n)^{-1} \equiv (i\omega_n/Z - \epsilon_{\mathbf{k}})$, where $Z < 1$ is the quasiparticle weight. This gives $\lambda_0 \sim Z^4\alpha^2\tilde{\mathcal{N}}_F/\tilde{E}_F^2$, where the tilde implies renormalized quantities. Since $\tilde{E}_F \sim ZE_F$, and $\tilde{\mathcal{N}}_F \sim \mathcal{N}_F/Z$, we get $\delta c_s/|c_s^m| \sim Z(T_c/E_F)^2$. In other words, compared to conventional superconductors, $\delta c_s/|c_s^m|$ for heavy fermions is further reduced by a factor of Z. Thus, the above estimation, backed by a microscopic calculation, explains the order of magnitude of $\delta c_s/|c_s^m|$ reported for most known superconductors, the Fe-based and the A15 systems being exceptions. Second, the sign of λ_0, which governs whether the two orders cooperate or compete, is nonuniversal, and it depends on the sign of $\mathcal{N}''_{B_{1g}}(0)$. Third, due to the absence of the low-energy contribution the coupling $\lambda \sim \lambda_0$ is nearly temperature independent. This is consistent with the weak T dependence of χ_n of several Fe-based systems at doping away from the nematic instability [53–55].

B. Near a nematic instability

The above considerations need modification if the system is in the vicinity of a nematic instability and the nematic correlation length $\xi \gg l$, where l is the interatomic distance. For the sake of simplicity we assume that the nematic instability is a Pomeranchuk transition, i.e., spontaneous deformation of the Fermi surface. Accordingly, we postulate the presence of an interaction $\mathcal{H}_I = -(g/2)\sum_{\mathbf{q}} O_n(-\mathbf{q})O_n(\mathbf{q})$, with $g > 0$ having a dimension of inverse DOS, and where $O_n(\mathbf{q}) \equiv \frac{1}{\sqrt{V}}\sum_{\mathbf{k},\sigma} f_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k},\sigma}$, is the quadrupolar charge operator. Such a phenomenological interaction has been widely used to study nematic instability in metals [8,22,25,27,35,56]. In this case the increase of the nematic correlation length $\xi(T)$ with lowering temperature can be described using random phase approximation, and the nematic susceptibility can be written as $\chi_n^i(\mathbf{q},0) = \Pi_n^i(\mathbf{q},0)/[1 - g\Pi_n^i(\mathbf{q},0)]$, where $i = (s,m)$. As in the case away from the nematic instability, we have $\lambda \propto [\partial^2\chi_n^s/(\partial|\Delta|^2)]_{|\Delta|=0}$, and taking into account that $\partial\Pi_n^s(0,0)/\partial|\Delta| = 0$ due to gauge invariance, we conclude

$$\lambda = \lambda_{\rm renorm} \equiv \lambda_0(\xi/l)^4, \tag{6}$$

where $(\xi/l)^2 = 1/[1 - g\Pi_n^m(0,0)]$. From the above equation we deduce the following. (1) Close to a nematic instability $g\Pi_n^m \sim 1$, or equivalently $\xi \gg l$. Elastoresistivity measurements in Fe-based systems have shown an increase of χ_n by a factor 100 [2]. Since, $\chi_n \sim (\xi/l)^2$, we get $\xi/l \sim 10$. Therefore λ and eventually $\delta c_s/|c_s^m|$ can be boosted by at least four orders of magnitude, even though the bare coupling λ_0 is small. Note that the identification that electronic nematic correlation is significant in the A15 systems is an important conclusion of our study. The behavior of $c_s(T)$ below T_c in the A15 systems was understood in Ref. [57] using a model [58] with a particular dispersion that disagrees with later band structure results [59]. No such special dispersion is assumed in our theory. (2) In the metal phase the nematic susceptibility $\chi_n^m(T) \propto (\xi(T)/l)^2 \sim \mathcal{N}_F\Lambda/(T - T_0)$. Here T_0 is the nematic transition temperature of the electron-only subsystem, with $T_0 = T_s - \alpha^2\Lambda\mathcal{N}_F/c_0 \lesssim T_s$. This implies that the renormalized λ has power-law temperature dependence with $\lambda_{\rm renorm} \propto (\xi(T)/l)^4 \propto 1/(T - T_0)^2$. This is to be contrasted with case (a) where the bare coupling λ_0 has weak logarithmic T dependence.

The enhancement of λ implied by Eq. (6) has the following two consequences.

1. $c_s(T)$ across superconducting T_c

Since $\chi_n^m(T) \propto 1/(T - T_0)$ while $\lambda_{\rm renorm} \propto 1/(T - T_0)^2$ has a stronger T dependence, it is clear that, for λ_0 above a positive threshold, the softening of $c_s(T)$ in the metal phase will turn into a hardening in the superconducting phase. This can be illustrated from the following phenomenological modeling. We write $c_s(T)/c_0 = 1 - a_0P(T)/[1 - b_0P(T)]$, where $a_0 \equiv \alpha^2\mathcal{N}_F/c_0$ and $b_0 \equiv g\mathcal{N}_F$ are constants, and $P(T)$ is the dimensionless bare nematic polarization. In the metallic phase we postulate $P(T \geqslant T_c) = \Lambda/(T + T_1)$, with $T_1 \gg T_c$ such that $P(T)$ is weakly T-dependent around T_c. As noted above, in the superconducting phase the bare polarization has an additional term proportional to $\lambda_0\Delta(T)^2$. We assume the mean-field scaling $\Delta(T)^2 = \Delta_0^2(1 - T/T_c)$, and we write the bare interplay coupling λ_0 in terms of a dimensionless parameter $t_2 \equiv \lambda_0\Delta_0^2/(\alpha^2\mathcal{N}_F)$. This implies $P(T \leqslant T_c) = \Lambda/(T + T_1) - t_2(1 - T/T_c)$. It follows that, for sufficiently large and positive $t_2 > \Lambda T_c/(T_c + T_1)^2$, the elastic constant $c_s(T)$ starts hardening immediately below T_c, as seen in electron and holed doped $BaFe_2As_2$ [33,44,46,47]. On the other hand, for $t_2 < 0$ (or equivalently $\lambda_0 < 0$) the elastic softening enhances in the superconducting phase. It is likely that this latter trend is relevant for $FeSe_{1-x}S_x$ at large doping where $T_c > T_s$ [60]. These two trends are illustrated in Fig. 2, for which we use $a_0 = 0.22$, $b_0 = 49.8$, $T_1/\Lambda = 50$, $T_c/\Lambda = 0.2$, while $t_2 = 1.3 \times 10^{-4}$ and $t_2 = -0.2 \times 10^{-4}$ for the red (dark) and green (light) lines, respectively. For intermediate values of t_2 the T

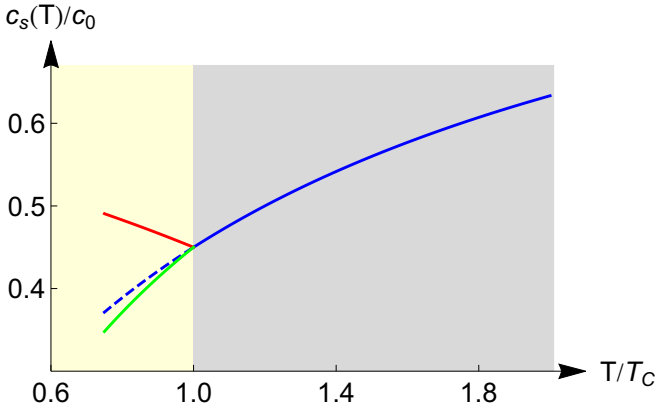

FIG. 2. Kink in the T dependence of the shear elastic constant $c_s(T)$ at a superconducting transition T_c. The system is close to a nematic instability, and the nematic correlation length increases with lowering T. For sufficiently large $\lambda_0 > 0$ the elastic constant hardens immediately upon entering the superconducting phase (red/dark line), as seen in the Fe-based systems. For $\lambda_0 < 0$ the elastic constant softens more rapidly in the superconducting phase (green/light line). The dashed line is the extrapolation of the metallic behavior.

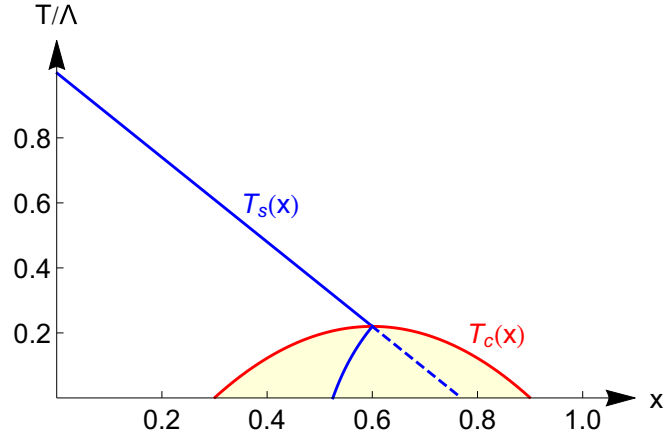

FIG. 3. Back-bending of the nematic transition line (solid blue line) $T_s(x)$ in the superconducting phase (shaded light yellow) due to strong interplay between the two orders. The blue dashed line is the hypothetical nematic transition if the interplay is ignored.

dependence of $c_s(T)$ interpolates between these two limiting behaviors.

2. *Back-bending of $T_s(x)$ in the superconducting phase*

As noted above, for λ_0 greater than a positive threshold the shear modulus $c_s(T)$ hardens for $T \leqslant T_c$ (red/dark line in Fig. 2). An immediate consequence of this behavior is the back-bending of the nematic/orthorhombic transition line $T_s(x)$ in the superconducting phase, as shown in Fig. 3. Here x is a hypothetical tuning parameter that, in practice, can be related to doping or pressure. To illustrate the back-bending we consider the same model of $P(T)$ as above, and we introduce an x dependence to the temperature scales $T_1(x)/\Lambda = 49.02 + 1.3x$ and $T_c(x)/\Lambda = 0.22 - 2.44(x - 0.6)^2$, and to the parameter $t_2(x) = 3 \times 10^{-3}[T_c(x)/\Lambda]^2$. Thus, in this model $T_c(x)$ has a domelike structure, and the $T_s(x)$ is linearly decreasing with x. The two transition lines meet at $x = 0.6$, and if the interplay is ignored $T_s(x)$ continues the trend (dashed lines Fig. 3) in the superconducting phase. However, once the interplay is taken into account, the hardening of $c_s(T)$ for $T < T_c$ implies that there cannot be a nematic transition for $x > 0.6$ in the superconducting phase. Moreover, since the hardening increases with lowering T, it necessarily implies that $T_s(x)$ back-bends in the superconducting phase, as reported in electron-doped $BaFe_2As_2$ [61].

III. SUMMARY

To summarize, we examined the thermodynamic signatures of the interplay between superconducting and nematic instabilities. In particular, we studied microscopically the properties of the coupling λ between the two orders; see Eq. (1). This is related to how the shear elastic constant $c_s(T)$ changes across a superconducting transition. We explained why in most systems λ (in suitable unit) is small and nearly temperature independent, which leads to $\delta c_s/|c_s^m| \sim 10^{-6}$ as seen in most classes of superconductors. The situation is different if, due to an imminent nematic instability, the nematic correlation length $\xi \gg l$, where l is the interatomic distance. In this case $\lambda \propto [\xi(T)/l]^4$ has strong T dependence, and it can be boosted by several orders of magnitude. This leads to large $\delta c_s/|c_s^m| \sim 10^{-1}$, as seen experimentally in the Fe-based and A15 superconductors. If the bare coupling λ_0 is above a positive threshold, it leads to hardening of $c_s(T)$ for $T \leqslant T_c$ and to the back-bending of the nematic transition line in the superconducting phase, as seen in doped $BaFe_2As_2$. Finally, we predict that the nematic susceptibility $\chi_n(T)$ of the A15 systems will show a Curie-Weiss-type increase with lowering T. This can be verified using electronic Raman response and elastoresistivity techniques.

ACKNOWLEDGMENTS

We are thankful to L. Bascones, G. Blumberg, A. Chubukov, Y. Gallais, F. Hardy, P. Hirschfeld, D. Maslov, P. Massat, C. Meingast, A. J. Millis, J. Schmalian, and K. Sengupta for insightful discussions. I.P. acknowledges financial support from ANR Grant No. ANR-15-CE30-0025. P.K. and B.M.A. acknowledge support from the Independent Research Fund Denmark, Grants No. DFF-6108-00096 and No. DFF-8021-00047B.

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