Elastic coupling and spin-driven nematicity in iron-based superconductors

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Spin-driven nematic order that has been proposed for iron-based superconductors is generated by pronounced fluctuations of a striped density wave state. On the other hand it is a well known fact that the nematic order parameter couples bilinearly to the strain, which suppresses the fluctuations of the nematic order parameter itself and lowers the upper critical dimension, yielding mean-field behavior of the nematic degrees of freedom for $d > 2$. This is consistent with the measured Curie-Weiss behavior of the nematic susceptibility. Here we reconcile this apparent contradiction between pronounced magnetic fluctuations and mean-field behavior of the nematic degrees of freedom. We show, by developing a φ^4 theory for the nematic degrees of freedom, that the coupling to elastic strain does not suppress the fluctuations that cause the nematic order in the first place (magnetic fluctuations), yet it does transform the Ising-nematic transition into a mean-field transition. In addition, we demonstrate that the mean-field behavior occurs in the entire temperature regime where a softening of the shear modulus is observed.

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I. INTRODUCTION

In many iron-based superconductors, a structural phase transition that sets at in at the temperature T_s, from the high-temperature tetragonal phase into an orthorhombic phase, has been shown to closely track the magnetic transition at T_m [1–4], i.e., $T_s \geqslant T_m$. In 1111 materials the structural and magnetic phase transitions are split and of second order. On the other hand, in the 122 family the transitions are either joint and of first order or split and second order. In $Ba(Fe_{1-x}Co_x)_2As_2$, where the transitions are split, the lower, magnetic transition is weakly first order for $x < 0.02$ [1,2].

From elastoresistance measurements [5] there is very strong evidence that the nematic state is driven by electronic excitations. This is fully consistent with the comparatively large resistivity-anisotropy measurements [6,7] with the softening of the elastic modulus over a wide temperature range [8–12], with strong signatures in the electronic Raman response in the normal [10,13–19] and superconducting [20] states, and with the observation of anisotropies in various additional observables, such as thermopower [21], optical conductivity [22,23], torque magnetometry [3], and in STM measurements [24] and NMR measurements [25].

To explain the origin of the nematic phase in pnictides, an orbital fluctuation based scenario [26–31] and a theory for spin-driven nematicity [4,32,33] have been proposed. In the latter, spin-fluctuations, associated with striped magnetic order, can generate the emergent electronic nematic order at temperatures above the Neel temperature [4,32–35]. Nematic degrees of freedom couple to the lattice [9,36,37] and induce the structural phase transition to the orthorhombic phase. Scaling of the shear modulus and the NMR spin-lattice relaxation rate for 122 systems, discussed in Ref. [8], strongly support the spin-driven nematicity scenario. Here the presence of the magnetic fluctuations associated with the stripe density wave phase proves crucial for stabilizing the nematic phase. On the other hand, nematic order was also observed in FeSe, a material where spin-magnetic order is only generated via application of external pressure, while a structural transition along with a softening of the lattice occurs at ambient pressure in a fashion very similar to the 122 iron pictides [38–40]. This led to the suggestion that this system might be driven by orbital fluctuations. Alternatively, given the observed small Fermi surfaces of FeSe [41,42] almost degenerate imaginary charge density and spin density waves are expected [43–46]. Therefore, a mechanism based on fluctuating and possibly ordered striped imaginary charge density waves was proposed that is conceptually very similar to the striped spin-driven mechanism [43].

In Ref. [32] the phase diagram of striped density wave induced nematicity was investigated. At a finite temperature phase transition, it was found that preemptive nematic order emerges via split phase transitions for some regime of the parameter space of the model, while in other cases a joint first-order transition occurs, all in good agreement with experiment. Clearly, fluctuations were crucial to derive this rich phase diagram.

On the other hand: the behavior near the nematic transition seems to display generic mean-field behavior, including the Curie-Weiss behavior of nematic susceptibility [12,47,48]. In addition, it was noted already in the 1970s [49–52] that fluctuations of an order parameter that couples linearly to an elastic deformation are suppressed. This is the case for the nematic order parameter, which couples linearly to orthorombic distortion via the nemato-elastic coupling. This can lead to mean-field behavior, instead of $d = 2$ or $d = 3$ Ising-like behavior that is expected in the absence of the coupling to strain [49–51]. In the context of the iron-based systems, this effect was already stressed by Cano *et al.* [37] and in Ref. [53], where quantum critical elasticity was investigated. Given these observations and the fact that fluctuations were essential for the derivation of the aforementioned phase diagram, it seems worthwhile exploring whether the strain-coupling-induced mean-field behavior of the nematic degrees of freedom can change the conclusions of Ref. [32].

To address this problem, we start from a model of a spin-driven nematic phase, similar to that of Ref. [32], and include

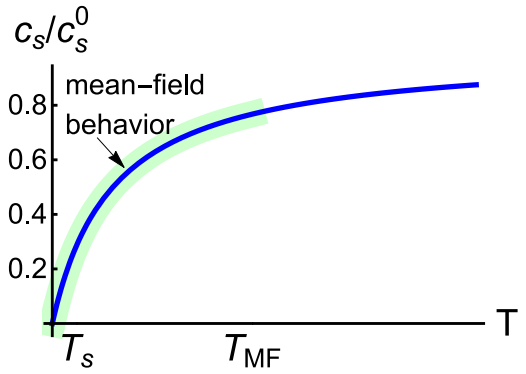

FIG. 1. The regime in which the mean-field behavior of the nematic degrees of freedom can be expected (shaded light green region). The figure shows the softening of the elastic modulus c_s, Eq. (49), denoted by a solid blue line, as one approaches the structural transition from the high-temperature tetragonal phase. $T_{\rm MF}$ indicates the characteristic temperature where mean-field behavior of nematic degrees of freedom sets in upon approaching the transition at T_s. The mean-field regime coincides with the regime of strong elastic modulus renormalization (see the main text for the explanation).

the coupling to elastic strain. We then determine an effective order parameter theory of the nematic order parameter in the presence of strain. Integrating out strain results in the appearance of the nonanalytic terms in the propagator for nematic fluctuations, that are direction dependent, similar to what was found in Refs. [54–56], where spin models in the presence of dipolar interactions were examined. These nonanalytic terms lead to mean-field behavior of the nematic transition and are shown to give rise to a Curie-Weiss susceptibility over a sizable temperature range. Yet the strain coupling does not affect the very existence of nematic order and of the split structural and magnetic transition temperatures. Thus, elastic strain changes the universality class of the nematic phase transition (not of the magnetic transition) but does not destroy the nematic phase itself. In addition, we find that the mean-field behavior occurs in the entire temperature regime where a softening of the shear modulus is observed; see Fig 1. This is one of our principal results.

Another alternative explanation for Curie-Weiss behavior due to nematic quantum criticality was recently proposed in Ref. [57].

The outline of the paper is as follows. In Sec. II we briefly introduce the model for spin-driven nematicity. In Sec. III we develop a φ^4 theory for the nematic fluctuations and estimate the Ginzburg regime, showing that nematic fluctuations are expected to be large in the absence of the coupling to the lattice. In Sec. III B we include the nemato-elastic coupling and analyze the nature of the nematic transition using a renormalization group approach. We show that the coupling to the lattice introduces nonanalytic direction-dependent terms in the propagator for nematic-fluctuations. This results in softening only along certain directions in the momentum space. As a consequence, the upper critical dimension becomes lower compared to the case without coupling to the strain. We find $d_{uc} = 2$ and the nematic transition becomes mean-field for $d > 2$. Finally, In Sec. IV we summarize our results.

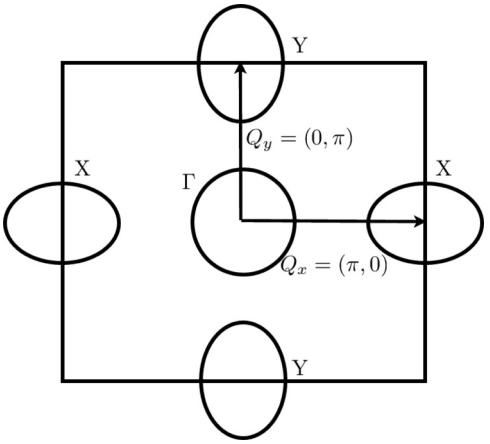

FIG. 2. Band structure: The model consists of the central hole-like Γ band and the electron-like X and Y bands, shifted by $\mathbf{Q}_X = (\pi/a, 0)$ and $\mathbf{Q}_Y = (0, \pi/a)$, respectively.

II. THE MODEL

In what follows, we will work with a 1-Fe unit cell with lattice constant a. We begin by considering a continuum model valid near the second-order phase transition, with diverging correlation length that includes coupled magnetic and elastic degrees of freedom characterized by the action

$$S = S_\Delta + S_{\rm ph} + S_c, \tag{1}$$

with partition function

$$Z = \int \mathcal{D}\mathbf{u}\, \mathcal{D}(\Delta_x \Delta_y) e^{-S}. \tag{2}$$

Here, S_Δ represents the the action of the magnetic degrees of freedom, $S_{\rm ph}$ the phononic actions, and S_c the coupling between magnetic degrees of freedom and phonons.

In order to develop a long-wavelength theory for the magnetic degrees of freedom, it is sufficient to analyze the symmetry of the ordered state. The iron-based systems are characterized by magnetic order with ordering wave vectors $\mathbf{Q}_x = \pi \mathbf{e}_x/a$ and $\mathbf{Q}_y = \pi \mathbf{e}_y/a$; see Fig. 2. Let us denote spin fluctuations associated with $\mathbf{Q}_x$ and $\mathbf{Q}_y$ ordering wave vectors $\Delta_{\mathbf{x}}$ and $\Delta_{\mathbf{y}}$, respectively. Both order parameters individually describe collinear order, i.e., they are formed out of the manifold $O(3)/O(2)$. Naively, one would expect for the total system a manifold $O(3)/O(2) \times O(3)/O(2)$ for the order parameters. However, either quantum or thermal fluctuations (in the case of localized spins) or simple mean-field interactions (in the case of itinerant spins) bring these down to $O(3)/O(2) \times Z_2$. Then the most general expansion of the magnetic action is (see also Refs. [18,32])

$$S_\Delta = \int_x \left[r_0 \left(\Delta_x^2 + \Delta_y^2\right) + (\nabla \Delta_x)^2 + (\nabla \Delta_y)^2 \right] + \int_x \left[\frac{u}{2N} \left(\Delta_x^2 + \Delta_y^2\right)^2 - \frac{g}{2N} \left(\Delta_x^2 - \Delta_y^2\right)^2 \right]. \tag{3}$$

Here, $\int_x \cdots = \int d^d x \cdots$. Similarly, we will use below $\int_q \cdots = \int \frac{d^d q}{(2\pi)^d} \cdots$ for integrations over momenta. The parameter r_0 tunes the distance from the magnetic phase transition, and u and g denote the magnetic and nematic

coupling constants respectively. In a model based on itinerant electrons these constants can be expressed as an integral over certain combinations of Green's functions across different bands [18,32]. Here we do not distinguish between localized or itinerant magnetism and merely use the above phenomenological form for the magnetic energy that is basically dictated by symmetry as long as $g > 0$. The results that we will subsequently obtain are valid regardless of the detailed microscopic nature of magnetism and must be the subset of a more complicated analysis of, e.g., a multi-orbital Hubbard model. One of the efficient approaches to spin-driven nematicity is the large-N expansion, where N denotes the number of components of the vectors $\Delta_{x,y}$. The validity of the large-N approach for the present model follows from the comparison of numerical investigations of the $J_1 - J_2$ Heisenberg model [58] and from an analysis of the $\epsilon = 4 - d$ expansion, formally valid for all N in Ref. [32]. In our analysis we are using a continuum model. For an anisotropic system of moderately or weakly coupled layers, it is more appropriate to avoid the continuum limit in the third dimension. In Ref. [32] such a model was analyzed where $q^2 \to q_x^2 + q_y^2 + A_z(1 - \cos q_z)$, where $q_{x,y}$ are still in the continuum limit while q_z goes from $-\pi$ to π. It was then shown that such an anisotropic three-dimensional system behaves very similarly to a model in the continuum limit, yet with dimension d intermediate between 2 and 3, i.e., $2 < d < 3$. In what follows we will pursue this continuum approach with variable dimensionality.

The static phonon part of the action for the acoustic modes in the B_{1g} channel is given as

$$S_{\rm ph} = N \int_q c_s(\mathbf{q})(q_x u_x - q_y u_y)^2. \tag{4}$$

Here $\mathbf{u} = (u_x, u_y)$ is the phonon displacement field, $c_s(\mathbf{q})$ is the sound velocity, and $\mathbf{q}$ momentum along soft direction. $c_s(\mathbf{q})$ is determined by the elastic constants of the material. It holds for a tetragonal symmetry,

$$c_s(\mathbf{q}) = c_s^0 + \mu_1 \cos^2\theta + \mu_2 \sin^4\theta \sin^2(2\phi), \tag{5}$$

where $c_s^0 = c_{11} - c_{12}$ is the bare value of the sound velocity, and μ_1 and μ_2 are expressed in terms of the combinations of elastic constants of the system (for details see the Appendix A). The coefficient N in $S_{\rm ph}$ was introduced to generate a consistent expansion in large N.

Finally, the key magneto-elastic coupling is

$$S_c = \lambda_{\rm el} \int_x \left(\Delta_x^2 - \Delta_y^2\right)(\partial_x u_x - \partial_y u_y), \tag{6}$$

where $\lambda_{\rm el}$ is the magneto-elastic coupling constant and $\partial_x u_x - \partial_y u_y$ the orthorhombic distortion.

III. COLLECTIVE NEMATIC FLUCTUATIONS AND φ^4 THEORY OF NEMATIC DEGREES OF FREEDOM

In order to develop a theory for collective nematic degrees of freedom, we first perform a Hubbard-Stratonovich transformation of the two quartic terms in the magnetic part S_Δ of the action Eq. (3) to obtain

$$S_\Delta[\varphi,\lambda] = \frac{1}{2}\int_x \left(\frac{N}{u}\lambda^2 + \frac{N}{g}\varphi^2\right) + \int_x \begin{pmatrix}\Delta_x\\ \Delta_y\end{pmatrix}^T \mathcal{G}^{-1}[\lambda,\varphi]\begin{pmatrix}\Delta_x\\ \Delta_y\end{pmatrix}, \tag{7}$$

where

$$\mathcal{G}^{-1}[\lambda,\varphi] = \begin{pmatrix} r_0 + i\lambda + \varphi - \nabla^2 & 0\\ 0 & r_0 + i\lambda - \varphi - \nabla^2\end{pmatrix}. \tag{8}$$

We shift $\varphi \to \varphi + \lambda_{\rm el}(\partial_x u_x - \partial_y u_y)$ and integrate out the magnetic modes. It follows

$$S = \frac{N}{2}\int_x \left(\frac{1}{u}\lambda^2 + \frac{1}{g}\varphi^2\right) + N\int_q c_s(\mathbf{q})(q_x u_x - q_y u_y)^2 - \frac{\lambda_{\rm el} N}{g}\int_x \varphi(\partial_x u_x - \partial_y u_y) + \frac{N}{2}\,\mathrm{tr}\ln\mathcal{G}^{-1}[\lambda,\varphi], \tag{9}$$

where $c_s(\mathbf{q})$ is given by Eq. (5) with $c_s \to c_s + \lambda_{\rm el}^2/g$. Finally, we integrate over the phonon degrees of freedom, which leads to

$$S = \frac{N}{2}\int_q \left[\frac{1}{u}\lambda_q\lambda_{-q} + \left(\frac{1}{g} + \frac{\lambda_{\rm el}^2}{c_s(q)}\right)\varphi_q\varphi_{-q}\right] + \frac{N}{2}\,\mathrm{tr}\ln\mathcal{G}^{-1}[\lambda,\varphi]. \tag{10}$$

This action is an exact reformulation of our initial model. It is the starting point of our subsequent analysis.

We concentrate on finite-temperature transitions and, for the moment, focus on the tetragonal phase, where the nematic order parameter is zero. We write

$$\lambda(x) = -i\psi_0 + \eta(x), \tag{11}$$

where ψ_0 is determined by the saddle-point equation that becomes exact at leading order in $1/N$. Nonzero ψ_0 amounts to a fluctuation renormalization of the magnetic correlation length. $\eta(x)$ denotes the fluctuating part of $\lambda(x)$. Similarly, for the Green's function matrix we can write

$$\mathcal{G}^{-1}[\lambda,\varphi] = \mathcal{G}_0^{-1} - \mathcal{V}[\eta,\varphi], \tag{12}$$

where

$$\mathcal{G}_0^{-1} = (r - \nabla^2)I, \tag{13}$$

with $r = r_0 + \psi_0$, and

$$\mathcal{V}[\eta,\varphi] = -\begin{pmatrix} i\eta + \varphi & 0\\ 0 & i\eta - \varphi\end{pmatrix}. \tag{14}$$

We expand:

$$\mathrm{tr}\ln\mathcal{G}^{-1}[\lambda,\varphi] = \mathrm{tr}\ln\mathcal{G}_0^{-1} + \mathrm{tr}\ln(1 - \mathcal{G}_0\mathcal{V}) \approx \mathrm{tr}\ln\mathcal{G}_0^{-1} - \tfrac{1}{2}\,\mathrm{tr}(\mathcal{G}_0\mathcal{V})^2 - \tfrac{1}{3}\,\mathrm{tr}(\mathcal{G}_0\mathcal{V})^3 - \tfrac{1}{4}\,\mathrm{tr}(\mathcal{G}_0\mathcal{V})^4. \tag{15}$$

Now one can write the action as $S = S_0 + S_2 + S_3 + S_4$, with

$$S_0 = -\frac{N}{2}\int_x \frac{\psi_0^2}{u} + \frac{N}{2}\,\mathrm{tr}\ln \mathcal{G}_0^{-1}, \tag{16}$$

and the quadratic part

$$S_2 = \frac{N}{2}\int_q \begin{pmatrix}\eta(q)\\ \varphi(q)\end{pmatrix}^T D^{-1}(q)\begin{pmatrix}\eta(-q)\\ \varphi(-q)\end{pmatrix}, \tag{17}$$

where

$$D^{-1}(q) = \begin{pmatrix} D_\eta^{-1}(q) & 0 \\ 0 & D_\varphi^{-1}(q)\end{pmatrix}, \tag{18}$$

with $D_\eta^{-1}(q) = \frac{1}{u} + \Pi(q,r)$ and $D_\varphi^{-1}(q) = \frac{1}{g} + \frac{\lambda^2}{c_s(q)} - \Pi(q,r)$. The self-energy part is given by

$$\Pi(q,r) = \int_k \frac{1}{r+k^2}\frac{1}{r+(\mathbf{k}+\mathbf{q})^2} \approx L_2 r^{\frac{d}{2}-2} - b_\varphi q^2, \tag{19}$$

with

$$b_\varphi = -r^{\frac{d}{2}-3}\left(\frac{4}{d}L_4 + \frac{d-4}{d}L_3\right), \tag{20}$$

and we defined

$$L_n = \int_p \frac{1}{(1+p^2)^n} = \frac{\Gamma\left(n-\frac{d}{2}\right)}{(2\sqrt{\pi})^d\Gamma(n)}. \tag{21}$$

The cubic action is given by

$$S_3 = -N\int_{p,q} T(p,q)\varphi(-p)\varphi(p-q)\eta(q), \tag{22}$$

where

$$T(p,q) = i\int_k G_0(k)G_0(k-q)G_0(p+k-q) \tag{23}$$

is the triangular loop that appears in Fig. 3.

The quartic terms give the following contribution to the action:

$$S_4 = -\frac{N}{4}L_4 r^{d/2-4}\int_{q_1,q_2,q_3} \varphi_{q_1}\varphi_{q_2}\varphi_{q_3}\varphi_{-q_1-q_2-q_3}. \tag{24}$$

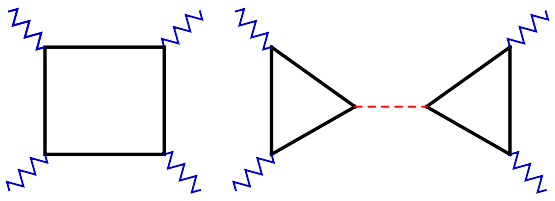

FIG. 3. Diagrammatic contributions to u_φ. Full lines denote the spin-fluctuation propagators G_0, wavy lines the propagators D_φ and dotted lines the propagator D_η (see the main text). The diagram on the left is proportional to L_4 and gives a negative contribution to u_φ. The diagram on the right contains two triangles T given by Eq. (23), connected by a propagator D_η. This diagram becomes larger as the dimensionality d is lowered and it provides a positive contribution to u_φ.

Since the action S is quadratic in η, we can integrate the η-fields from the action, and use that

$$\int \mathcal{D}\eta \exp\left\{\int_q\left[-\frac{N}{2}\eta(q)D_\eta^{-1}(q)\eta(-q) + Nj(q)\eta(q)\right]\right\} = \exp\left\{-\frac{N}{2}j(q)D_\eta(q)j(-q)\right\}, \tag{25}$$

with $j(q) = \int_p T(p,q)\varphi(-p)\varphi(p-q)$.

The resulting field theory for the nematic fluctuations is therefore of the form

$$S_\varphi/N = \frac{1}{2}\int_q\left(r_\varphi + \frac{\lambda_{\mathrm{el}}^2}{c_s(\mathbf{q})} + b_\varphi q^2\right)\varphi_q\varphi_{-q} + \frac{u_\varphi}{4}\int_x \varphi^4, \tag{26}$$

where

$$\begin{aligned} u_\varphi &= -L_4 r^{\frac{d}{2}-4} + \frac{2uL_3^2 r^{d-6}}{1+uL_2 r^{\frac{d}{2}-2}},\\ r_\varphi &= \frac{1}{g} - L_2 r^{\frac{d}{2}-2},\\ b_\varphi &= r^{\frac{d}{2}-3}\left(\frac{4}{d}L_4 + \frac{d-4}{d}L_3\right). \end{aligned} \tag{27}$$

We note that there are two contributions to the quartic term u_φ: the mean-field-like term $\propto L_4$, which is negative, and the second term $\propto L_3^2$, which is depicted in Fig. 3 on the right. As we have shown above, the second term arises from the contraction of η propagators coming from two triangular loops T. This term yields a positive contribution, and it is responsible for the change in sign of the quartic coupling constant and thus for the possibility to have second-order split magnetic and nematic transitions. Analyzing both contributions shows that the term proportional to L_3^2 becomes increasingly more important for lower space dimensionality d. Thus, low-dimensional fluctuations are responsible for preemptive nematic order. If $d < 4$, $r^{\frac{d}{2}-2} \gg 1$ as $r \to 0$, and we get for sufficiently large magnetic correlation length that

$$u_\varphi = \left(\frac{2L_3^3}{L_2} - L_4\right)r^{\frac{d}{2}-4}. \tag{28}$$

To avoid confusion, we stress that $r \propto \xi^{-2}$ determines the magnetic correlation length ξ, while $r_\varphi \propto \xi_\varphi^{-2}$ yields the nematic correlation length. The former vanishes at the critical point T_N of striped magnetic order, while the latter is zero at a nematic second-order transition. We find that the quartic coupling constant u_φ, given by Eq. (28), can therefore only be positive for $d < 3$. Thus, only for very large correlation length and $d < 3$ is it possible that we obtain a second-order transition. We remind the reader that an anisotropic three-dimensional system is described in terms of an intermediate dimensionality $2 < d < 3$; see Ref. [32].

Finally, we comment on the splitting between the nematic and the magnetic transitions. The condition for the second-order nematic transition (for which $u_\varphi > 0$ is required) to occur is that $\tilde{r}_\varphi = r_\varphi + \frac{\lambda_{\mathrm{el}}^2}{c_s^0} = 0$, with r_φ given by Eq. (28). This gives

$$\frac{1}{g} - L_2 r^{\frac{d}{2}-2} + \frac{\lambda_{\mathrm{el}}^2}{c_s^0} = 0, \tag{29}$$

which occurs at the finite (but large) value of the magnetic correlation length $\xi \propto r^{-\frac{1}{2}}$. In other words, the nematic transition preempts the magnetic transition and occurs at a slightly higher temperature $T_s > T_N$. The temperature difference is dictated by the value of the nematic coupling constant g and the size of the nemato-elastic coupling constant.

A. The case without coupling to strain

Let us first analyze the case $\lambda_{\rm el} = 0$ without coupling to the lattice. We still need to determine whether, for a given set of coupling constants u, g, the correlation length ever becomes large enough to yield a positive sign for u_φ. In order to determine the location of the tricritical point of the nematic degrees of freedom (i.e., where u_φ changes its sign), we use the fact that at the nematic transition and for $\lambda_{\rm el} = 0$ it holds that $r_\varphi = 0$, i.e., $L_2 r^{\frac{d}{2}-2} = \frac{1}{g}$, which we solve to determine $r(g)$:

$$r(g) = \left(\frac{2^d \pi^{d/2}}{\Gamma\left(2-\frac{d}{2}\right) g}\right)^{\frac{2}{d-4}}. \tag{30}$$

We use this result to express r in Eq. (28) in terms of g and obtain with $\alpha = u/g$:

$$u_\varphi = \frac{4-d}{24 g^{\frac{8-d}{4-d}}} \frac{2\alpha(3-d)-(6-d)}{1+\alpha} \left(\frac{2^d \pi^{d/2}}{\Gamma\left(2-\frac{d}{2}\right)}\right)^{\frac{4}{4-d}}. \tag{31}$$

Thus, if $d < 3$ one only obtains a second-order transition for

$$\alpha > \alpha_c = \frac{6-d}{2(3-d)}. \tag{32}$$

This result was obtained in Ref. [32] from an analysis of the equation of state of the nematic order parameter.

Let us next estimate the size of the Ginzburg regime, i.e., the regime of strong critical fluctuations of the nematic order parameter without coupling to strain. One expects such critical nematic fluctuations for $d \leqslant 4$, if $u_\varphi > 0$. The Ginzburg regime is most easily estimated if we determine the natural dimensionless coupling constant $\hat{u}_\varphi$. To this end we substitute $\varphi = \mu\phi$ and $q = \gamma k$, where $\gamma^2 = r_\varphi / b_\varphi$ and $\mu = b_\varphi^{\frac{d}{4}} r_\varphi^{-\frac{d+2}{4}}$ such that

$$S = \frac{1}{2}\int_k (1+k^2)\phi_k\phi_{-k} + \frac{\hat{u}}{4}\int_{k_{1,2,3}} \phi_{k_1}\phi_{k_2}\phi_{k_3}\phi_{-k_1-k_2-k_3}, \tag{33}$$

with dimensionless coupling constant

$$\begin{aligned}\hat{u} &= u_\varphi \gamma^{3d} \mu^4 \\ &= \frac{u_\varphi r_\varphi^{\frac{d-4}{2}}}{b_\varphi^{d/2}}.\end{aligned} \tag{34}$$

We obtain

$$\hat{u}_\varphi = \Upsilon_d \, (g r_\varphi)^{\frac{d-4}{2}}, \tag{35}$$

with coefficient

$$\Upsilon_d = \frac{(48\pi)^{d/2}(4-d)^{1-\frac{d}{2}}}{24\Gamma\left(2-\frac{d}{2}\right)} \frac{2\alpha(3-d)-(6-d)}{(1+\alpha)}. \tag{36}$$

Let us define $f = g r_\varphi$. If $f \to 0$, the coupling $\hat{u}_\varphi$ diverges. This is expected as we are below the upper critical dimension.

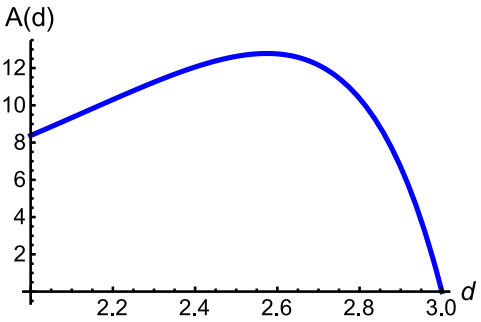

FIG. 4. Slope $A(d)$ of the coefficient Υ_d, near α_c, for $2 < d < 3$. The dimensionality $2 < d < 3$ effectively describes a three-dimensional but anisotropic system; see Ref. [32]. The slope is always bigger than 1, except in the region around $d = 3$. This signifies a strong fluctuation regime (except near $d = 3$).

The Ginzburg regime f_{Ginz} is determined by $\hat{u}_\varphi(f) \approx 1$. Thus, we analyze the coefficient $\Upsilon_d(\alpha)$. Close to the tricritical point ($\alpha \approx \alpha_c$), $\Upsilon_d(\alpha)$ vanishes like $\Upsilon_d(\alpha) = A(d)\frac{\alpha-\alpha_c}{\alpha_c}$, where $A(d)$ is the slope.

Except for d near $d = 3$, we find that the slope is always bigger than unity; see Fig. 4. We recall that a dimensionality below $d = 3$ effectively describes a three-dimensional yet anisotropic system [32]. A slope bigger than unity already suggests a broad fluctuation regime, except for a region near the tricritical point.

B. Critical behavior with coupling to strain

Next, we include the coupling to strain; i.e., we analyze the action S_φ of Eq. (26) for finite $\lambda_{\rm el}$. This problem is similar to the one of a magnetic system with additional dipolar interactions. In Refs. [54,55] the critical behavior of uniaxial magnets with dipolar interactions in d dimensions was investigated using a renormalization group approach. It was found that in the presence of the dipolar interaction the upper critical dimension is lowered from $d = 4$ (for the model including only exchange interaction) to $d = 3$ (for the model containing both the exchange interaction and the dipolar interaction). This is because the dipolar interactions generate nonanalytic direction-dependent terms in the spin propagator, similar to the nonanalyticities that occur in the propagator in the case of second-order elastic phase transitions, where the order parameter is a component of the strain tensor and where an acoustic phonon emerges as a soft mode [51]. Due to the direction dependence of the propagator in an elastic phase transition [51], the softening occurs only along certain directions, which leads to the mean-field behavior already in $d = 3$ for systems where the softening occurs in $(m = 1)$-dimensional subspace, and for $d = 3$ and $m = 2$ logarithmic corrections were found to occur.

As seen from Eqs. (5) and (26), the coupling of the nematic fluctuations to orthorhombic distortion generates similar direction-dependent nonanalytic terms in the propagator for nematic fluctuations, and only certain directions in momentum space remain soft. In fact, for a tetragonal system, one finds that (see the Appendix A for the detailed derivation) the softening

occurs in an $(m = 1)$-dimensional submanifold, in particular along the directions $q_x = \pm q_y$ and $q_z = 0$.

If we rescale the field to eliminate the coefficient b_φ, the action Eq. (26) can be written in the form

$$S_\varphi = \frac{1}{2}\int_q \left(r_\varphi + \frac{\lambda_{\rm el}^2}{c_s(q)} + q^2\right)\varphi_q\varphi_{-q} + \frac{u_\varphi}{4}\int_{q_1,q_2,q_3}\varphi_{q_1}\varphi_{q_2}\varphi_{q_3}\varphi_{-q_1-q_2-q_3}, \tag{37}$$

with $c_s(q)$ given by Eq. (5) and μ_1,μ_2 are given in the AppendixA. We analyze this action using a one-loop renormalization group approach. We define $\tilde{r}_\varphi = r_\varphi + \frac{\lambda_{\rm el}^2}{c_s^0}$. The flow equations for this φ^4 theory are straightforward, and we obtain the usual result (see for example Ref. [59]):

$$\frac{d\tilde{r}_\varphi}{dl} = 2\tilde{r}_\varphi + 3u_\varphi\frac{d}{dl}\int_q^> D_\varphi(q),$$
$$\frac{du_\varphi}{dl} = (4-d)u_\varphi - 9u_\varphi^2\frac{d}{dl}\int_q^> D_\varphi^2(q). \tag{38}$$

The momentum integration is performed over momenta between $\Lambda/b < q < \Lambda$, where Λ is the cutoff and $b = e^{-l}$. The propagator for nematic fluctuations in the presence of the coupling to the lattice is given by

$$D_\varphi^{-1}(q) \approx \tilde{r}_\varphi + q^2 + h_2\Lambda^2\sin^4\theta\sin^2 2\phi + h_1\Lambda^2\cos^2\theta, \tag{39}$$

where we introduced $h_i\Lambda^2 = -\frac{\lambda^2}{(c_s^0)^2}\mu_i$. Simple power counting arguments show that the coupling constants h_i are relevant and they grow according to

$$\frac{dh_i}{dl} = 2h_i. \tag{40}$$

This flow equation will not be modified by interaction corrections, as the elimination of high energy modes cannot generate nonanalytic corrections of the type $q_z^2/q^2 \sim \cos^2\theta$ or $q_x^2q_y^2/q^4 \sim \sin^4\theta\sin^2 2\phi$. Thus, we have

$$h_i(l) = h_i e^{2l}. \tag{41}$$

In addition we have

$$\frac{d\tilde{r}_\varphi}{dl} = 2\tilde{r}_\varphi + 3u_\varphi\Lambda^{d-2}A(h_1,h_2) - 3u_\varphi r\Lambda^{d-4}B(h_1,h_2),$$
$$\frac{du_\varphi}{dl} = (4-d)u_\varphi - 9u_\varphi^2\Lambda^{d-4}B(h_1,h_2), \tag{42}$$

with

$$A(h_1,h_2) = K_{d-1}\int\frac{\sin^{d-2}\theta d\theta d\phi}{(2\pi)^2}f(\theta,\phi),$$
$$B(h_1,h_2) = K_{d-1}\int\frac{\sin^{d-2}\theta d\theta d\phi}{(2\pi)^2}f^2(\theta,\phi). \tag{43}$$

We used $\int\cdots = \int_0^\pi d\theta\int_0^{2\pi}d\phi\cdots$ as well as

$$f(\theta,\phi) = \frac{1}{1+h_1\cos^2\theta + h_2\sin^4\theta\sin^2(2\phi)}. \tag{44}$$

Furthermore, $K_d = \frac{2\pi^{d/2}}{(2\pi)^d}/\Gamma(\frac{d}{2})$. For large h_i the main contribution to the integrals in Eq. (43) comes from the vicinity $\theta \approx \pi/2$ and $\phi \approx 0$ and one finds that

$$A(h_1,h_2) \sim \frac{1}{2}\frac{K_{d-1}}{(2\pi)^2}(h_1h_2)^{-1/2},$$
$$B(h_1,h_2) \sim \frac{1}{4}\frac{K_{d-1}}{(2\pi)^2}(h_1h_2)^{-1/2}.$$

Therefore we introduce the effective coupling constant

$$G = \frac{u_\varphi}{\sqrt{h_1h_2}}, \tag{45}$$

such that

$$\frac{dG}{dl} = (2-d)G - 9G^2\Lambda^{d-4}\frac{K_{d-1}}{4(2\pi)^2}. \tag{46}$$

which flows to zero for $d > 2$, leading to mean-field behavior above $d = 2$ [49–51].

Next, we would like to estimate the temperature range in which the mean-field behavior can be expected, and in which the Curie-Weiss behavior of nematic degrees of freedom can be observed. The scaling $A,B \simeq (h_1h_2)^{-1/2}$ breaks down when one of the h_i becomes of order 1; see Eq. (43). Let us assume that this happens at length $l = l^*$, such that $h_1(l^*) \approx 1$. One finds that $h_2(l^*) = \frac{h_2(0)}{h_1(0)}$, and that for $d = 2$, $u_\varphi(l^*) = \frac{u_\varphi(0)}{h_1(0)}$. The nematic correlation length is given by $\xi_\varphi(l^*) = \sqrt{h_1(0)}\xi_\varphi(0)$. The analysis will break down when the correlation length becomes smaller than the lattice spacing a, i.e., for $\xi_\varphi(l^*) < a$. Therefore, we expect the mean-field behavior to be valid only for

$$\xi_\varphi(0) > \frac{a\Lambda c_s^0}{\sqrt{\lambda_{\rm el}^2\mu_1}} \approx \sqrt{\frac{c_s^0}{\lambda_{\rm el}^2}}, \tag{47}$$

where $\lambda_{\rm el}$ is the nemato-elastic coupling constant, and c_s^0 and μ_1 represent the combinations of various elastic constants of the material (see the Appendix). In Eq. (47) we have used that $\mu_i \sim c_s^0$ (see Ref. [60] for experimental data) and that $a\Lambda \sim 1$. The susceptibility of the nematic order parameter is given by $\chi_\varphi = r_\varphi^{-1} = \xi_\varphi^2$. Therefore, the condition for the mean-field behavior reduces to the following condition for the nematic susceptibility:

$$\chi_\varphi > \frac{c_s^0}{\lambda_{\rm el}^2}. \tag{48}$$

In Ref. [9], it was shown that the elastic modulus c_s softens as one approaches the structural transition and that it effectively measures the nematic susceptibility through

$$c_s^{-1} = \left(c_s^0\right)^{-1}\left(1 + \frac{\lambda_{\rm el}^2}{c_s^0}\chi_\varphi\right). \tag{49}$$

We see that when the nematic susceptibility becomes of the order $\chi_\varphi \sim \frac{c_s^0}{\lambda_{\rm el}^2}$ strong renormalization of the elastic modulus will take place. Therefore, we have explicitly shown that the mean-field behavior, Eq. (48), occurs in the entire regime where the suppression of the elastic modulus takes place; see Fig. 1 for details. This is exactly what has been observed experimentally [12,47,48]. We add that this conclusion is valid

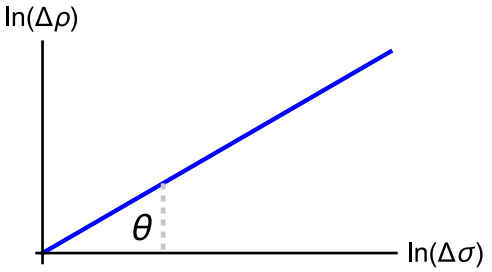

FIG. 5. Prediction for the resistivity anisotropy. For a mean-field nematic transition, one expects the resistivity anisotropy $\Delta\rho$ to vary like $\Delta\rho \sim (\Delta\sigma)^{1/\delta}$, where $\Delta\sigma$ is the externally applied stress, and $\delta = 3$ in the mean-field theory. The angle θ in the picture is thus $\theta = \arctan(\frac{1}{3})$.

regardless of the detailed microscopic origin of nematicity. Curie-Weiss behavior due to the coupling to the lattice is expected in the entire temperature regime where a softening of the elastic constant is observed. For several iron based systems, this regime can be as high as 300–350 K [9,12,47,48].

Note that another implication of our result is that the mean-field behavior implies further resistivity anisotropy $\Delta\rho$ near the structural transition $\Delta\rho \sim (\Delta\sigma)^{1/\delta}$, with $\delta = 3$, where $\Delta\sigma$ is the externally applied stress; for details see Fig. 5.

IV. CONCLUSION

In the spin-driven nematic scenario magnetic fluctuations associated with the striped magnetic order cause the formation of the nematic state: the state with no magnetic order, but broken Z_2 symmetry. Therefore, fluctuations are crucial for the existence of the nematic state. However, experimentally it has been measured that the nematic degrees of freedom behave mean-field-like in a very broad temperature range; in particular, the Curie-Weiss dependence of the nematic susceptibility was observed. At first sight, these two observations might seem to be in contradiction.

The present paper reconciles these two statements and determines the temperature regime where a Curie-Weiss behavior of the nematic susceptibility is expected. In particular, we show that the coupling to the lattice suppresses the fluctuations of the nematic order parameter itself, which renders the nematic transition mean-field, but it does not affect the magnetic transition or the very existence of the nematic phase. Starting from a microscopic model of a spin-driven nematic phase, which also explains the emergence of the nematic phase at a slightly higher temperature than the Neel temperature (separated magnetic and nematic transitions), we constructed the φ^4 theory of the nematic degrees of freedom. First we ignored the coupling to the lattice, and, by analyzing the quartic coefficient, we showed that nematic fluctuations are characterized by a rather large Gizburg regime. Next, we added the coupling between nematic degrees of freedom to elastic strain to the φ^4 theory and analyzed this using the renormalization group procedure. We have found that, due to the nemato-elastic coupling which introduces direction-dependent terms in the propagator for nematic fluctuations, rendering only certain directions soft, the nematic transition becomes mean-field for $d > 2$. Most importantly, the nemato-elastic coupling does not suppress fluctuations that cause the nematic order in the first place (i.e., magnetic fluctuations); it only suppresses the fluctuations of the nematic order parameter itself. We have found that the nematic transition happens at large but finite magnetic correlation length, such that one obtains split magnetic and nematic transitions, with the nematic transition being mean-field-like (rather than in the Ising universality class), while the magnetic transition is expected to behave in a non-mean-field-like fashion.

Finally, we found that the mean-field behavior of the nematic degrees of freedom should occur in the entire regime where there is a significant softening of the elastic modulus. This is in excellent agreement with the experiments, where Curie-Weiss behavior of the nematic susceptibility was measured across a rather large temperature range [9,12,47,48] (up to 300–350 K for some iron-based superconductors), which coincides with the temperature range in which a significant reduction of the elastic modulus was observed.

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APPENDIX A: MOMENTUM DEPENDENCE OF THE ELASTIC CONSTANT $c_s(q)$

The elastic part of the free energy of a tetragonal system is given by

$$F_{\rm el} = \frac{c_{11}}{2}\left(\epsilon_{xx}^2 + \epsilon_{yy}^2\right) + \frac{c_{33}}{2}\epsilon_{zz}^2 + \frac{c_{44}}{2}\left(\epsilon_{xz}^2 + \epsilon_{yz}^2\right) + \frac{c_{66}}{2}\epsilon_{xy}^2 + c_{12}\epsilon_{xx}\epsilon_{yy} + c_{13}(\epsilon_{xx} + \epsilon_{yy})\epsilon_{zz}, \quad \text{(A1)}$$

where $\epsilon_{ij} = \frac{\partial_i u_j + \partial_j u_i}{2}$, and u_i is the ith component of the phonon displacement field.

The dynamic matrix M is defined from $F_{\rm el} = \frac{1}{2}u_i(q)M_{ij}(q)u_j(q)$. It can be expressed as

$$M_{ij} = \sum_{m,l} q_m q_l \frac{\partial^2 F_{\rm el}}{\partial\epsilon_{im}\partial\epsilon_{lj}}. \quad \text{(A2)}$$

For a tetragonal system the dynamic matrix is given by

$$M(\mathbf{q}) = \begin{pmatrix} c_{11}q_x^2 + c_{66}q_y^2 + c_{44}q_z^2 & (c_{12}+c_{66})q_xq_y & (c_{13}+c_{44})q_xq_z \\ (c_{12}+c_{66})q_xq_y & c_{66}q_x^2 + c_{11}q_y^2 + c_{44}q_z^2 & (c_{13}+c_{44})q_yq_z \\ (c_{13}+c_{44})q_xq_z & (c_{13}+c_{44})q_yq_z & c_{44}(q_x^2+q_y^2) + c_{33}q_z^2 \end{pmatrix}. \quad \text{(A3)}$$

The phonon frequencies ω in a tetragonal system can be determined from the dynamic matrix M, via $\det(\omega^2\rho - M(\mathbf{q})) = 0$, where ρ denotes the density. A vanishing elastic constant corresponds to a vanishing sound velocity. Here, we are interested in the case $c_{11} - c_{12} \to 0$.

The soft directions, along which the sound velocity vanishes correspond to the two lines in the xy plane (i.e., $q_z = 0$): $q_x = q_y$ and $q_x = -q_y$. Along these directions we have that $\omega^2\rho = (c_{11} - c_{12})q_x^2 \to 0$. Now, if one calculates the dispersion in the vicinity of such a line, for example $q_x = q_y$, one finds that

$$\omega^2\rho \approx (c_{11} - c_{12})\frac{(q_x + q_y)^2}{2} + \frac{(q_x - q_y)^2}{2}\left[c_{11} + c_{66} - \frac{(c_{11} - c_{66})^2}{c_{12} + c_{66}}\right] + c_{44}q_z^2, \tag{A4}$$

where $q_z \ll q_x$ and $q_x - q_y \ll q_x$. Choosing the angle parametrization such that $q_x = q\sin\theta\cos(\phi + \frac{\pi}{4})$ and $q_y = q\sin\theta\sin(\phi + \frac{\pi}{4})$, we get $\omega^2\rho \approx c_s(\mathbf{q})q_+^2$, with $q_+ = (q_x + q_y)$ being the soft momentum and

$$c_s(\mathbf{q}) = \frac{(c_{11} - c_{12})}{2} + \mu_1\sin^4\theta\sin^2 2\phi + \mu_2\cos^2\theta, \tag{A5}$$

with

$$\mu_1 = \frac{1}{8}\left[c_{11} + c_{66} - \frac{(c_{11} - c_{66})^2}{c_{12} + c_{66}}\right], \quad \mu_2 = c_{44}. \tag{A6}$$

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