Pairing instability near a lattice-influenced nematic quantum critical point

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We study how superconducting $T_c$ is affected as an electronic system in a tetragonal environment is tuned to a nematic quantum critical point (QCP). Including coupling of the electronic nematic variable to the relevant lattice strain restricts criticality only to certain high symmetry directions. This allows a weak-coupling treatment, even at the QCP. We develop a criterion distinguishing weak and strong $T_c$ enhancements upon approaching the QCP. We show that negligible $T_c$ enhancement occurs only if pairing is dominated by a non-nematic interaction away from the QCP, and simultaneously if the electron-strain coupling is sufficiently strong. We argue this is the case of the iron superconductors.

I. INTRODUCTION

The origin of high superconducting transition temperature $T_c$ of the copper and iron based systems remains to be well understood [1][5]. Among the various possibilities as likely causes of high $T_c$, one is that of the presence of a quantum critical point (QCP) in the vicinity of which the effective pairing interaction is strong, leading to enhanced $T_c$. In fact, $T_c$ boosted by an antiferromagnetic QCP remains among the more promising scenarios for these systems [6]. A related question, addressed here, is whether one expects similar enhancement of these systems [6].

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In this work we identify the missing element to be a symmetry-allowed coupling between the electronic nematic degree of freedom and a lattice shear strain mode. We show that, once this coupling is included in the theory of nematic criticality, the presence of a nematic QCP does not necessarily lead to significant enhancement of $T_c$. We identify the conditions under which the enhancement is negligible near the QCP. This occurs when the following two conditions are simultaneously satisfied. Namely, (i) the pairing is dominated by a non-nematic interaction away from the QCP, and (ii) if the electron-strain coupling is sufficiently large. Note, condition (i) does not trivialize the problem since, by itself, it does not preclude the nematic term to dominate near the QCP and provide significant $T_c$ enhancement. Our result provides a route to understand qualitatively why $T_c$ is unaffected by the nematic QCP in FeSe$_{1−x}$S$_x$.

The main physics ingredient of our work is enshrined in the standard theory of elasticity for an acoustic instability involving Ising-nematic symmetry, such as a second order tetragonal-orthorhombic transition. It is well known that, in this case the divergence of the correlation length, which manifests as vanishing acoustic phonon velocity, is restricted to two high-symmetry directions [20][21][22]. This is because along the generic directions the non-critical shear strains, that are invariably present in a solid, come into play and cutoff criticality. The physics of this cutoff can be also understood as follows.

Consider a translation symmetry preserving second order phase transition involving a local variable $x(r)=\lambda_0 + \sum_{\mathbf{q}\neq0} \lambda_q e^{i\mathbf{q}\cdot\mathbf{r}}$, where $\lambda_0$ is the order parameter. Within the Landau paradigm the free energy has mean field and fluctuation contributions. The former has the structure $F_{MF} = (a/2)\lambda_0^2 + (A/4)\lambda_0^4$, while the latter, to Gaussian order, is related to the action $S_{\text{fluc}} = \sum_{\mathbf{q}\neq0} (b + q^2) |\lambda_q|^2$. While in usual theories $b = a$, in those involving crystalline strains $b(\mathbf{q})$ is no longer a parameter but, rather, a function of the Brillouin zone angles $\mathbf{q}$ containing information about the crystalline anisotropy [21][22]. In other words, the concept of correlation length becomes angle-dependent. In this situation, the condition $b(\mathbf{q}) = a$ is satisfied only for certain high symmetry directions, and only along these directions the correlation length diverges at the transition defined by...
The above property is inherited by the electronic nematic subsystem once its coupling with the strain is included. This leads to two important conclusions of this paper. (i) Under certain standard assumptions, the weak coupling BCS analysis remains valid arbitrarily close to the nematic QCP. (ii) We identify the criterion for the weak coupling BCS analysis, which is close to a nematic/structural QCP that is driven by the coupling  with Π(ˆq, 0) becomes anisotropic in the presence of the nemato-elastic coupling. In the non-nematic phase the angular dependence of r(ˆq) has tetragonal symmetry. (a) Variation of r(ˆq) on the plane (red line) at the nematic QCP. It is zero only along the high-symmetry directions  (blue arrows). (b) For finite , r(ˆq) ∝ .

A crucial ingredient in the model is the symmetry-allowed nemato-elastic term linking with the local orthorhombic strain , defined as where and is the uniform macroscopic strain, and is the atomic displacement. is non-zero only in the symmetry-broken nematic/orthorhombic phase. This coupling can be written as , where has dimension of energy.

The effect of the nemato-elastic term on criticality has been discussed earlier. Here, for the sake of completeness, we recapitulate the main points. (i) It shifts the QCP to , where has dimension of density of states and is the bare orthorhombic elastic constant. Thus, is a dimensionless parameter that measures the strength of the nemato-elastic coupling. In the following we take , . (ii) The nemato-elastic coupling leads to hybridization of with the acoustic phonons (see Fig. 3(a)), which renormalizes the nematic susceptibility to where is the density, is the polarization index, and is the polarization vector for the bare acoustic phonons with angle-dependent velocity and dispersion . The above follows simply from integrating out the lattice variables. Evidently, is independent of the magnitude , and has four-fold symmetry of the tetragonal unit cell in the non-nematic phase. Thus, the nemato-elastic term makes the mass of the form , which is a collective mode of the nematic variable , which is a measure of the strength of the nemato-elastic coupling. In the presence of the nemato-elastic coupling, , r(ˆq) = 0 plane (red line) at the nematic QCP . It is zero only along the high-symmetry directions  (blue arrows). (b) For finite , r(ˆq) ∝ .

In what follows the frequency dependence of the susceptibility is consistent with the fact that only along  the frequency dependence is consistent with the fact that only along  the frequency dependence is consistent with the fact that only along }
FIG. 3: (color online) Diagrammatic representation of the relevant microscopic processes. (a) The bare electron-nematic susceptibility (single wavy-line) is dressed (double wavy-line) by the nemato-elastic coupling (red crosses). The dashed line is an acoustic phonon. (b) The pairing potential $W_{k,k'}$ consists of the dressed nematic interaction of strength $U$, and a non-nematic interaction $V_{k,k'}$ (gluon-line) of strength $V$. The former interaction vertex is accompanied by a form factor $f_{k,k'}$. The interesting regime is $V > U$, i.e., when pairing is dominated by the non-nematic interaction away from the nematic QCP.

as follows. In all likelihood, the pairing in the FeSC and the cuprates is mediated not just by the nematic fluctuations. In addition, there is, e.g., short wavelength spin/charge fluctuations or Mott correlations that mediate pairing. Consequently, it is physical to expect that, close to a nematic QCP, the pairing potential has a nematic component which is a strong function of $r$ (included in $\chi(q)$), and it has a non-nematic component which does not vary with $r$ (represented by $V^{(s,d)}$). Note, in what follows the precise microscopic origin and structure of $V^{(s,d)}$ is not relevant. Besides this physical relevance, as we show below, the inclusion of $V^{(s,d)}$ is crucial to distinguish the two limiting cases of “strong” and “weak” enhancement of $T_c$ upon tuning the system to the nematic QCP with $r \rightarrow r_0$.

Our goal is to study how $\lambda (r)$ changes as the system is tuned to the QCP, from which we can deduce the variation of $T_c \sim \Lambda e^{-1/\lambda}$, where $\Lambda \ll E_F$ is the high-energy cutoff of the pairing problem. Note, an important consequence of the coupling $g$ is that, it is now possible to consider the case where $T_c (r_0) < T_{FL}$, the Fermi liquid scale. For $T < T_{FL}$ the dynamics of the nematic pairing potential is irrelevant, and the problem can be treated within BCS formalism.

In the above model $\lambda (r)$ increases monotonically as the system approaches the QCP, since the nematic interaction itself is attractive and monotonic. However, the crucial question is whether this increment is significant. To address this issue quantitatively, we define $\delta \lambda \equiv \lambda (r) - \lambda (r=1)$, and we distinguish between “strong” and “weak” enhancements of $T_c$, depending on whether $\delta \lambda \gg \lambda (r=1)$ or not, respectively. Qualitatively, this criteria distinguishes between whether pairing is dominated by long wavelength nematic fluctuations or by a non nematic pairing interaction at the QCP.

III. RESULTS

The momentum anisotropy of the susceptibility $\chi(q)$ due to the coupling $g$ can be modeled as follows. (a) For $q_z \leq q_{2d}$, we get $\chi^{-1}(q) \approx r(q) + q^2_{2d}/(2k_F)^2$. The anisotropic mass $r(q)$ has tetragonal symmetry, and satisfies $r(q_{1,2}) = 0$ at the QCP. The simplest function consistent with these requirements is $r(q) = (r - r_0) + r_0 q_z / q_{2d}^2 + r_0 \cos^2 2\delta q_z$, where $\delta q_z$ is the azimuthal angle of $q$ (see Fig. [2]). This region of $q$-space also contains the critical modes. (b) For $q_z \geq q_{2d}$, the nemato-elastic coupling can be neglected and $\chi(q) \approx \chi^{-1}_0(q) = r + q^2_{2d}/(2k_F)^2$. However, this does not imply singular susceptibility at the QCP, since its location is shifted from $r = 0$ to $r = r_0$. In this region of $q$-space the modes are, thus, non-critical.

The main qualitative physics can be already illustrated by considering the simplest case of a single band with a cylindrical Fermi surface around the Brillouin zone center, and where the non-critical pairing term supports $s$-wave gap with $V_{k,k'}^{(s)} = V > 0$. The details of the calcu-
As importantly, the opposite limit of weak $T_c$ enhancement, which is relevant for understanding the phase diagram of FeSe$_{1-x}$S$_x$, occurs if $1 \gg r_0 \gg (U/V)^2$ (see Fig. 4). Physically, this implies a situation where the following two conditions are simultaneously satisfied. (i) The pairing is dominated by a non-nematic interaction away from the QCP (since $V \gg U$), and (ii) the electron-strain coupling is sufficiently large (since $r_0 \gg (U/V)^2$). Note, condition (i) does not trivialize the issue since, by itself, it does not preclude the nematic term to dominate near the QCP and provide significant $T_c$ enhancement. In fact, this is why condition (ii) comes into play. The origin of condition (i) lies in the physical expectation that the energy scale generated by the electron-lattice interaction is well below the Fermi energy, i.e., $r_0 \ll 1$.

Besides the case of the isotropic $s$-wave gap, we also study the following situations in the Appendix. (i) An extended $s$-wave gap, since the lattice-renormalized nematic interaction is intrinsically anisotropic, and it can give rise to angular variations of the gap. (ii) Motivated by the cuprates, we consider the case where the nematic interaction $V_{\mathbf{k},\mathbf{k}'} = V \cos 2\phi_{\mathbf{k}} \cos 2\phi_{\mathbf{k}'}$ favors a $d$-wave gap with $\Delta_{\mathbf{k}} = \Delta_0 \cos 2\phi_{\mathbf{k}}$. (iii) Motivated by the FeSC we study a system with Fermi pockets at $(0,0)$, $(\pm \pi,0)$, and $(0,\pm \pi)$, with a form of $V_{\mathbf{k},\mathbf{k}'}^{(s)}$ that leads to $s_{\pm}$-gap. In all these cases we find that qualitatively $\lambda(r)$ is described by Eq. (4), except with different numerical pre-factors. We conclude that the above criterion for $T_c$ enhancement in Eq. (5) is robust.

IV. CONCLUSION

The strength of the nemato-elastic coupling can be estimated as $r_0 \sim (T_s - T_0)/T_F$, where $T_0$ is the nominal nematic transition temperature of the electron subsystem in the absence of this coupling (see Fig. 1), accessible from, say, electronic Raman scattering [15]. In FeSe we get $T_0 \sim 10$ K, and $T_s \sim 90$ K [31]. We estimate the Fermi temperature from the bottom of the smallest electron pocket as measured by photoemission above $T_s$, which is around 25 meV in FeSe [17, 92]. Thus, for FeSe$_{1-x}$S$_x$ we estimate $r_0 \sim 0.3$ and $T_{FL} \sim 40$ K. Note, the condition $T_c < T_{FL}$ needed for a weak-coupling theory, is well-respected in this case. A similar estimate for Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ yields $r_0 \sim 0.05$ and $T_{FL} \sim 10$ K [28]. Since, in this system the maximum $T_c \sim 25$ K is comparable to $T_{FL}$, a more careful quantitative analysis is needed.

The estimation of $U$ and $V$ requires a full microscopic theory of pairing, that is currently unavailable. Consequently, a quantitative application of the theory to real systems is not possible at present. However, experimentally it is clear that FeSe$_{1-x}$S$_x$ has a nematic QCP around $x \approx 0.16$, but the superconducting $T_c(x)$ remains remarkably flat around this doping [17, 19]. This can be due to strong nemato-elastic effect violating the condition
in Eq. (5). In turn, this would imply that the pairing interaction in FeSe is mostly non-nematic in origin. A similar case can also be made for Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, where quantum critical nematic fluctuations have been detected only over a narrow doping range of $x = 0.65 - 0.75$ in the low-$T$ superconducting phase [14]. It is remarkable that over the same doping range $T_0$ the pairing interaction is non-nematic in origin in these materials. Thus, the dome-like structure of $T_c(x)$ hardly varies, implying that even here the lattice cutoff is operational. Thus, the dome-like structure of $T_c(x)$ over a wider doping range in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ is likely due to the antiferromagnetic QCP, while the absence of a magnetic QCP in FeSe$_{1-x}$S$_x$ results in a flat $T_c(x)$.

To summarize, we argued that nemato-elastic coupling can play a crucial role in determining if superconducting $T_c$ is strongly enhanced in the vicinity of a nematic quantum critical point. We showed that, in the presence of a significant non-nematic pairing interaction, strong nemato-elastic coupling implies that the nematic fluctuations do not boost $T_c$ significantly. Based on existing experiments on FeSe$_{1-x}$S$_x$ and on Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ we argued that this is likely the case of the iron-based superconductors. This would imply that the main pairing interaction is non-nematic in origin in these materials. More generally, from the perspective of material design for high temperature superconductivity, we conclude that (a) hard crystals are better suited for boosting $T_c$ near a nematic quantum critical point, and that (b) the lattice cutoff can be also avoided provided the non-nematic pairing potential is strong enough to guarantee $T_c(r = 1)$ $T_{FL}$, in which case the physics of Refs. [7-10] will be operational.

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Appendix A

In this appendix we provide the technical details for the calculation of the BCS eigenvalue $\lambda$ defined in Eq.(2) of the main text which is

$$\lambda \Delta_k = \nu_{FS} \int_{FS'} W_{k,k'} \Delta_{k'}. $$

The interaction potential is $W_{k,k'} = V_{k,k'}^{s,d} + U f_{k,k'}^2 \chi(k' - k)$. The form factor $f_{k,k'} = (h_k + h_{k'})/2$, where $h_k$ transforms as $k_x^2 - k_y^2$ in the $k_x - k_y$ plane. A simple choice is $h_k = \cos(2\phi_k)$, where $\phi_k$ is the azimuthal angle of $k$. Note that the nematic pairing potential is intrinsically anisotropic in the presence of the nemato-elastic coupling. This anisotropy can be taken into account by dividing the momentum space into two regions (a) $q_z > q_{2d}$, and (b) $q_z \leq q_{2d}$, and by working with asymptotic forms of $\chi$ in these two regions. Therefore, the pairing potential can be broken in three parts

$$W_{k,k'} = V_{k,k'}^{s,d} + U f_{k,k'}^2 \chi(k' - k)|_{q_z > q_{2d}} + U f_{k,k'}^2 \chi(k' - k)|_{q_z \leq q_{2d}}$$

The asymptotic forms of $\chi$ in the two regions are described in the main text. Note, the critical manifold is contained in the third term above, while the second term above involves non-critical modes. Furthermore, we will assume that $V > U$, where $V$ is the strength of the non-nematic pairing potential $V_{k,k'}^{s,d}$. Physically this implies that sufficiently far from the nematic QCP the pairing is dominated by the non-nematic term. As noted in the main text, the opposite limit of $U > V$ is trivial, since if the nematic potential already dominates pairing far away from the QCP, then, irrespective of the strength of the nemato-elastic coupling, it will invariably lead to large enhancement because the dominant pairing potential grows (even if it stays finite) as the QCP is approached.

(a) s-wave superconductivity with a uniform gap and a cylindrical Fermi surface (FS). We will assume that the non-nematic pairing potential is a constant with $V_{k,k'}^{s,d} = V$. Since Eq. (2) of the main text is restricted to the Fermi surface, $q_{2d} = 2k_F |\sin(\frac{2q_z k_F}{c})|$, and $\cos^2(2\phi_q) = \cos^2(\phi_q + \phi_q')$. The FS integral turns into angular integrals $\lambda = < W_{k,k'} >$ where

$$f > \int_0^{2\pi} \frac{du dv}{(2\pi)^2} f(u,v),$$

and $u = \phi_k + \phi_k'$ and $v = \phi_k - \phi_k'$. This mean value is to be estimated to lowest order in the parameter $r \leq 1$ which governs the nearness to the QCP (see Fig. 1, main text).

The contribution from the second term of Eq. (A1) is given by

$$U(\cos^2 u \cos^2 v \frac{1}{r + (1 - \cos v)/2}) \approx \frac{U}{2\sqrt{r}}.$$ 

Note, in the above estimation typical $q_z \sim \pi/c$, where $c$ is unit cell length along the $z$-direction, while typical $q_{2d} \approx r^{1/2}$. Therefore, to leading order in $r$ the constraint $q_z \geq q_{2d}$ is automatically satisfied in the above estimation, even though the angular integrals are performed freely.

The third term of Eq. (A1) involves momentum dependence along the $z$-direction, and therefore, the estimation of its contribution to $\lambda(r)$ involves averaging along the length of the cylindrical Fermi surface. Anticipating that the typical momentum transfer along $z$ is small compared to Fermi wavevector $k_F$ we can write $f_{FS} \rightarrow \int_0^{2\pi} \frac{dz}{\pi} f_{0,0} d(k_z/k_F)$. This implies that the contribution from the third term of Eq. (A1) is given by
where $c_1 = 8/3 - 2 \ln 2 \approx 1.28$. This leads to the equation

$$\lambda(r \geq r_0) / \nu_{FS} = V + \frac{U}{2 \sqrt{r}} = \frac{U}{\pi} \left( \ln \max[r - r_0, r_0] + c_1 \right),$$

which is equation (4) of the main text. Note, the leading $r$-dependence comes from the non-critical modes, rather than the critical ones which have a rather limited volume in momentum-space. The critical contribution gives only to a weak logarithmic dependence which can be ignored to leading order in $r$.

It is clear from the above that there will be considerable $T_c$ enhancement close to the nematic QCP defined by $r = r_0$ only if in this regime the nematic contribution dominates. This, in turn, is possible only if the nematolastic coupling is weak enough such that

$$r_0 < (U/V)^2.$$

This is the condition mentioned in equation (5) of the main text.

In the following we consider few other cases and we show explicitly that the structure of Eq. (4) remains the same, only numerical pre-factors change. This implies that the conclusion obtained in Eq. (5) is robust.

(b) s-wave superconductivity with higher order gap harmonics. Keeping s-wave symmetry we can introduce anisotropy in the gap function by considering higher order harmonics as $\Delta(k) = \Delta_0 + \sqrt{2} \Delta_4 \cos(4\phi_k)$. The second term of r.h.s is the normalized first higher order s-wave harmonic. We proceed to project the gap equation onto each orthogonal polynomial to get the secular equation

$$\lambda \Delta_0 = \lambda_{00} \Delta_0 + \lambda_{10} \Delta_1,$$

$$\lambda \Delta_4 = \lambda_{40} \Delta_0 + \lambda_{44} \Delta_4,$$

where we have defined $\lambda_{nn'} = \langle W_{kk'} g_n g_{n'} \rangle$, with $g_n$ the $n$-th orthogonal cosine polynomial. The secular system implies that the physical $T_c$ is to be given by the largest value of the matrix $(\lambda_{nn'})$. With the above ansatz for the gap we get

$$\lambda = \frac{\lambda_{00} + \lambda_{44}}{2} + \sqrt{(\frac{\lambda_{00} - \lambda_{44}}{2})^2 + \lambda_{30}^2}.$$

The calculation is then identical to case (a). Ignoring the log corrections from the critical manifold, we find to lowest order in $r$

$$\lambda(r \geq r_0) / \nu_{FS} = V + (1 + \frac{1}{2 \sqrt{r}}) \frac{U}{2 \sqrt{r}},$$

which is same as in case (a) except for a numerical pre-factor. It is also possible to do the calculation in the limit of an infinite number of s-wave harmonics, and we find that the superconducting eigenvalue goes as $\lambda(r) = V + U/\sqrt{r}$.

(c) d-wave superconductivity. Motivated by the cuprates, we take a non-nematic pairing interaction which promotes d-wave superconductivity $V_{kk'}^{d} = 2V \cos(2\phi_k) \cos(2\phi_{k'})$ on top of the nematic pairing potential. With a d-wave gap ansatz $\Delta(k) = \Delta_0 \cos(2\phi_k)$, we find

$$\lambda(r \geq r_0) / \nu_{FS} = V + \frac{3U}{4\sqrt{r}}.$$

Thus, once again the BCS eigenvalue is the same as in Eq. (4) except for a numerical pre-factor.

(d) The multiband case of Fe-based superconductors. Motivated by the physics of the Fe-based superconductors, we now consider a three band model with one hole band centered around the $(0,0)$ point of the Brillouin zone and two electron pockets located at $(\pi,0)$ and $(0,\pi)$ respectively, in the one-Fe/unit cell representation. The non-nematic pairing potential is now a matrix in the band space, and we take it to be

$$V_{kk'}^{n} = -V \begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 0 & -1/2 \\ 1/2 & -1/2 & 0 \end{pmatrix}.$$

Note, Eq. (2) is written with the convention that repulsive interactions have negative sign and attractive ones have positive sign. Thus, the above interaction implies that the non-nematic pairing potential is only inter-band, and that it is repulsive for the electron-hole pairing term, while it is attractive for the electron-electron pairing term. This invariably leads to a $s_\pm$ gap, which in the three-band language has the form $\Delta_0(1,-1,-1)$, which is the most discussed gap structure for these systems. Note, the nematic pairing potential is attractive, and is, by definition, intra-band. For circular Fermi surfaces, and assuming that the gaps on each of the pockets are constant, we get, following the case (a)

$$W_{kk'} = V \begin{pmatrix} x & -1/2 & -1/2 \\ -1/2 & 2x & 1/2 \\ -1/2 & 1/2 & 2x \end{pmatrix},$$

where $x = U/(2 \sqrt{rV})$. This leads to a BCS eigenvalue

$$\lambda(r \geq r_0) / \nu_{FS} = \frac{1}{4} \left( V + \frac{3U}{\sqrt{r}} + \sqrt{9V^2 + \frac{U^2}{r} + \frac{4UV}{\sqrt{r}}} \right).$$
Since the only energy scales here are $V$ and $U/\sqrt{T}$, it is simple to check that significant $T_c$ enhancement is only possible if the condition in Eq. (5) holds. Note also that, while the magnitudes of the gaps become different on the hole and the electron pockets with the inclusion of the nematic pairing, both for small and for large $x$ there is a change in the sign of the gap between the hole and the electron surfaces.

We conclude that in all the above cases the condition for significant $T_c$ enhancement is given by Eq. (5), while in the opposite limit there is hardly any impact of the QCP on the $T_c$. 

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