Lattice Effects on Nematic Quantum Criticality in Metals

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Theoretically, it is commonly held that in metals near a nematic quantum critical point the electronic excitations become incoherent on the entire "hot" Fermi surface, triggering non-Fermi-liquid behavior. However, such conclusions are based on electron-only theories, ignoring a symmetry-allowed coupling between the electronic nematic variable and a suitable crystalline lattice strain. Here, we show that including this coupling leads to entirely different conclusions because the critical fluctuations are mostly cut off by the noncritical lattice shear modes. At sufficiently low temperatures the thermodynamics remain Fermi-liquid type, while, depending on the Fermi surface geometry, either the entire Fermi surface stays cold, or at most there are hot spots. In particular, our predictions are relevant for the iron-based superconductors.

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Introduction.—At an Ising nematic quantum critical point (QCP) in solids, discussed often in the context of the iron-based superconductors, cuprates, ruthanates, and quantum Hall systems, the ground state transforms from one having discrete rotational symmetry to another in which this symmetry is broken (see Fig. 1) [1–8]. An ideal example is the tetragonal to orthorhombic structural transition at a temperature T_S in the iron superconductors (FeSC), which is driven by electronic correlations, and where $T_S \to 0$ with doping [6–9]. Besides the FeSC, a nematic QCP is often invoked in the context of several other correlated metals, notably the cuprates [1–3]. Consequently, a topic of immediate relevance is how the quantum fluctuations associated with this QCP affect the low temperature properties of a metal.

At present it is widely believed that the effective electron-electron interaction becomes long ranged near the nematic QCP [10–13]. As a result the electrons become unusually massive and short-lived, leading to non-Fermi-liquid (NFL) behavior both in thermodynamics and in single electron properties almost everywhere on the Fermi surface. Thus, the specific heat coefficient $\gamma \equiv -\partial^2 F/\partial T^2$, where $F(T)$ is the free energy, diverges as $\gamma(T) \propto 1/T^{1/3}$ in space dimension $d = 2$, and as $\gamma \propto \log T$ in $d = 3$. Simultaneously, almost the entire Fermi surface gets "hot," and is characterized by a frequency dependent self-energy $\Sigma(i\omega_n) \propto |\omega_n|^{2/3}$ in $d = 2$, and by $\Sigma(i\omega_n) \propto \omega_n \log|\omega_n|$ in $d = 3$.

These results are based on the simplest treatment of the typical model describing itinerant electrons interacting with the critical nematic collective mode of the electrons themselves [10]. The latter is characterized by a susceptibility

$$\chi_0^{-1}(\mathbf{q}, i\Omega_n) = \nu_0^{-1}[r + q^2 + D(\mathbf{q}, i\Omega_n)], \qquad (1)$$

where ν_0 is a constant with the dimension of density of states, and $\mathbf{q}$ and Ω_n are the dimensionless momentum and Matsubara frequency, respectively. The dynamics of the collective mode is damped due to the excitation of particle-hole pairs close to the Fermi surface,

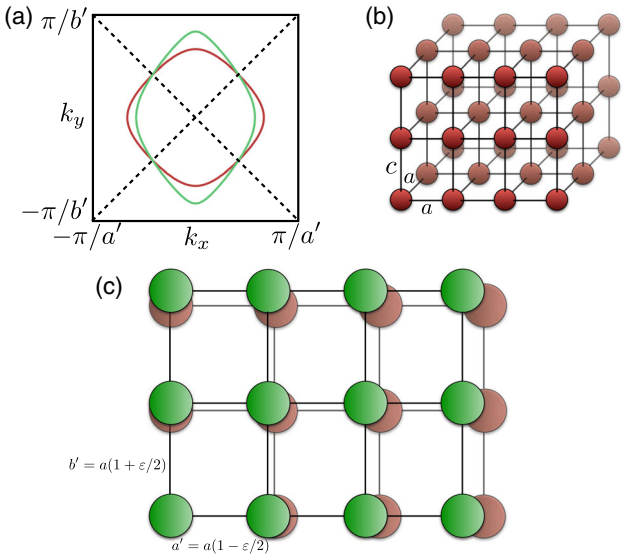

FIG. 1. Ising nematic phase transition involving $(x^2 - y^2)$ symmetry breaking. (a) The C_4 symmetric Fermi surface (red) distorts and becomes C_2 symmetric (green) in the nematic phase. (b) A tetragonal lattice with equivalent $\hat{x}$ and $\hat{y}$ directions. (c) View of its x-y plane, which distorts in the nematic phase, red and green circles being the original and the distorted atomic positions, respectively. In the nematic phase the unit cell lengths a' and b' along the two directions become inequivalent. ϵ is the orthorhombic strain. Even if the electron dispersion is two dimensional, in the presence of the lattice the third dimension is important (see text).

$D(\mathbf{q}, i\Omega_n) \propto |\Omega_n|/q$. At the QCP the tuning parameter vanishes, $r = 0$.

More recently, a lot of work has been done to improve the theory in $d = 2$ [14–19]. However, these works do not question the belief that the electronic properties are NFL type. In fact, it is widely accepted that quantum criticality involving a nonmodulating order parameter invariably leads to NFL physics.

Experimentally, the existence of NFL physics is well established in the pseudogap and strange metal phases of the cuprates [20]. NFL behavior has also been reported for certain, if not all, FeSC [21]. However, at present there is no definite evidence that the NFL physics is due to a nematic QCP, since there are other possible sources of NFL behavior, such as spin fluctuations and Mott physics.

Nematoelastic coupling.—The link between nematic QCP and NFL behavior is based on an electron-only theory. In practice, in a solid the electronic environment is sensitive to the lattice strains, and this gives rise to a symmetry-allowed nematoelastic coupling between the electron-nematic variable ϕ and a suitable component of the strain tensor of the type

$$\mathcal{H}_{\text{nem-latt}} = \lambda \int d\mathbf{r}\phi(\mathbf{r})\varepsilon(\mathbf{r}), \tag{2}$$

where λ is the coupling constant with the dimension of energy. For the sake of concreteness we assume ϕ to transform as $(x^2 - y^2)$ under the point group operations. Then, $\varepsilon(\mathbf{r}) = \varepsilon + i\sum_{\mathbf{q}\neq 0}[q_x u_x(\mathbf{q}) - q_y u_y(\mathbf{q})]e^{i\mathbf{q}\cdot\mathbf{r}}$ is the local orthorhombic strain, $\vec{u}(\mathbf{r})$ is the atomic displacement associated with strain fluctuation, and the uniform macroscopic strain $\varepsilon \neq 0$ in the symmetry-broken nematic or orthorhombic phase, see Fig. 1(c). The problem is well posed if we assume that the undistorted lattice is tetragonal, whose elastic energy is given by $F_E = \int d^d r C_{ijkl}\varepsilon_{ij}(r)\varepsilon_{kl}(r)/2$, $i = (x, y, z)$, where C_{ijkl} are the bare elastic constants (for an explicit expression in the more convenient Voigt notation used henceforth, see Ref. [22] and the Supplemental Material [23]).

Importantly, the above coupling shifts the nematic QCP, and it occurs already at a finite value of r given by

$$r = r_0 \equiv \lambda^2\nu_0/C_0, \tag{3}$$

where C_0 is the bare orthorhombic elastic constant. At this point the renormalized orthorhombic elastic constant $\bar{C}_0 \equiv C_0 - \lambda^2\nu_0/r$ vanishes, triggering a simultaneous orthorhombic instability. We take r_0 to be a small parameter; i.e., the effective energy scale generated by the coupling λ is small compared to the Fermi energy. Technically, this allows us to track how the properties of the familiar electron-only theory are recovered at a sufficiently high temperature.

Direction selective criticality.—This is an inherent property of acoustic instabilities of a solid whereby criticality, or the vanishing of the acoustic phonon velocity, is restricted to certain high-symmetry directions in the Brillouin zone such as $\hat{q}_{1,2} \equiv (\hat{q}_x \pm \hat{q}_y)/\sqrt{2}$ for a tetragonal-orthorhombic transition [26]. Along the remaining directions the noncritical strains come into play. This physics is well known from studies of structural transitions [27–29], and its relevance for the finite-T structural or nematic transition in FeSC has also been pointed out [30,31]. Our goal here is to study how this physics affects the metal's quantum critical properties.

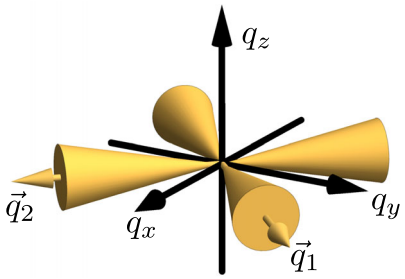

FIG. 2. Direction selective criticality. At the tetragonal-orthorhombic transition the critical directions in momentum space are restricted to $\hat{q} \approx \pm\hat{q}_{1,2} = \pm(\hat{q}_x \pm \hat{q}_y)/\sqrt{2}$ as indicated by the yellow cones. As a consequence, momentum scaling is anisotropic, see text.

In the presence of the nematoelastic coupling λ the strain and the electron-nematic degree of freedom hybridize, and the resulting mode inherits the above anisotropy. The hybridization can be incorporated by integrating out the strain fluctuations giving rise to a renormalization of the nematic susceptibility of Eq. (1), $\chi^{-1} = \chi_0^{-1} - \Pi$ with

$$\Pi(\mathbf{q}, i\Omega_n) = \frac{\lambda^2}{\rho}\sum_{\mu}(\mathbf{a}_{\mathbf{q}} \cdot \hat{u}_{\mathbf{q},\mu})^2/(\omega_{\mathbf{q},\mu}^2 + \Omega_n^2). \tag{4}$$

Here, ρ is the density, μ is the polarization index, $\mathbf{a}_{\mathbf{q}} \equiv (q_x, -q_y, 0)$, and $\hat{u}_{\mathbf{q},\mu}$ is the polarization vector for the bare acoustic phonons with angle-dependent velocity $\mathbf{v}^{(0)}_{\hat{q},\mu}$ and dispersion $\omega_{\mathbf{q},\mu} = \mathbf{v}^{(0)}_{\hat{q},\mu} \cdot \mathbf{q}$. To lowest order in r_0, the frequency dependence of Π can be dropped. Then, both the numerator and the denominator of Π are $O(q^2)$. This implies that the effect of the nematoelastic coupling is to soften the mass of the nematic fluctuations, albeit with an angular dependence; i.e., $r \to r(\hat{q}) \equiv r - \nu_0\Pi(\mathbf{q} \to 0, \Omega_n = 0)$. Note that $r(\hat{q})$ possesses the fourfold symmetry of the crystal lattice in the non-nematic phase. As shown in the Supplemental Material [23], an immediate consequence of this angular dependent mass is that criticality is restricted to the two high-symmetry directions $\hat{q} = \pm\hat{q}_{1,2}$ only, for which $r(\hat{q}) = 0$ at the QCP, see Fig. 2. The remaining directions stay noncritical since $r(\hat{q} \neq \hat{q}_{1,2}) > 0$ even at the QCP.

In the following we assume that all the bare elastic constants are of order C_0, such that the entire lattice effect can be modeled by the single parameter r_0. With this simplification, which does not change the results

qualitatively, the critical static nematic susceptibility is given by $\chi^{-1}(\mathbf{q} \approx \mathbf{q}_1) \propto r_0(q_2^2 + q_z^2)/q_1^2 + q_1^2$. Note that the criticality around $\mathbf{q}_2$ can be deduced by $q_1 \leftrightarrow q_2$. This leads to two important conclusions. First, even if the electronic subsystem has two-dimensional dispersion, as in the cuprates and the FeSC, the q_z dependence of $\chi(\mathbf{q})$ is generated by the lattice. Second, the direction selective criticality leads to anisotropic scaling with $(q_2, q_z) \sim q_1^2$ around $\mathbf{q}_1$, see Fig. 2. Since each noncritical direction scales as twice the critical one, this is equivalent to a theory with isotropic scaling in an enhanced effective space dimension $d_{\text{eff}} = 5$ [26,32,33]. Thus, the effect of fluctuations is weaker compared to the electron-only theory.

Fermi surface dependent dynamics.—The effect of the lattice is indirect. Since Π is essentially static at small r_0, the critical dynamics is generated by the excitation of particle-hole pairs in the Fermi sea, and is given by $D(\mathbf{q}, i\Omega_n)$ of Eq. (1). In electron-only theories this invariably leads to Landau damping along generic directions $\hat{q}$, and a dynamical exponent $z = 3$. However, with finite λ the lattice imposes that z is determined by $D(\mathbf{q} \approx \mathbf{q}_{1,2}, i\Omega_n)$, and the question is whether there is Landau damping along these directions. As we argue below, this depends on the Fermi surface, leading to two different universality classes.

The important point is that the interaction between the nematic collective mode and the electrons, given by $\mathcal{H}_{\text{nem-el}} \propto \sum_{\mathbf{q},\mathbf{k}} h_{\mathbf{k}} c^{\dagger}_{\mathbf{k}+\mathbf{q}/2} c_{\mathbf{k}-\mathbf{q}/2} \phi_{\mathbf{q}}$ in usual notations, is invariably accompanied by a form factor $h_{\mathbf{k}}$ that transforms as $(k_x^2 - k_y^2)$. Note that Landau damping requires electrons to scatter along the Fermi surface. This implies that the damping of a collective mode with momentum along $\hat{q}$ depends on the form factor at those particular points on the Fermi surface where $\hat{q}$ is tangential to the surface.

Ballistic nematicity: Consider the Fermi surface of the cuprates, shown in Fig. 3(a). The possibility of Landau damping with bosonic momentum $\mathbf{q}_1$ involve points on the Fermi surface that intersect the $k_x = -k_y$ dashed line, and along this line the form factor $h_{\mathbf{k}} = 0$. Thus, there is no Landau damping, and we get $D(\mathbf{q}_1, i\Omega_n) \propto \Omega_n^2/(v_F q_1)^2$, leading to ballistic critical dynamics at the lowest temperatures and frequencies, with the dynamical exponent $z = 2$ [34].

Damped nematicity: Now consider the typical Fermi surface of the FeSC with hole and electron pockets around the zone center, and around $(\pi, 0)$ and $(0, \pi)$, respectively, as shown in Fig. 3(b). For the same reason as above, the hole pocket does not give rise to Landau damping of the critical mode. But, since the centers of the electron pockets are shifted, $h_{\mathbf{k}}$ is finite everywhere on the electron Fermi surface, and the critical mode gets damped. This leads to the standard $D(\mathbf{q}_1, i\Omega_n) \propto |\Omega_n|/(v_F q_1)$ and exponent $z = 3$. The damping only involves certain hot spots of the electron pockets, on which we comment further below.

Critical thermodynamics.—For the sake of concreteness henceforth we assume that the electronic dispersion is two dimensional. The free energy of the nematic fluctuations is

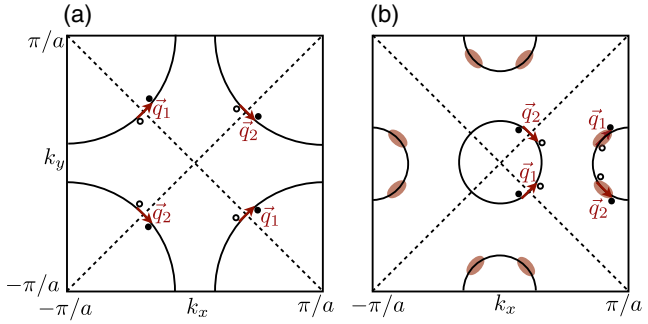

FIG. 3. Fermi surface dependent critical dynamics and the appearance of hot spots. Schematic Fermi surfaces of (a) the cuprates and (b) the iron-based superconductors. The form factor accompanying the interaction between the electrons and the nematic boson $h_{\mathbf{k}} \sim \cos k_x - \cos k_y = 0$ along the dashed lines. The critical bosons are restricted to the directions $\hat{q}_{1,2}$, see Fig. 2. Landau damping is only possible via the creation of particle-hole pairs at special points on the Fermi surfaces where $\hat{q}_{1,2}$ is tangential, provided the form factor remains finite. This is the case only for the electron pockets centered around $(\pi, 0)$ and $(0, \pi)$ in (b). Consequently, the critical dynamics is ballistic in (a) and damped in (b) at the lowest energy. For the same reason hot spots with reduced fermion lifetimes (red patches) appear only on the electron pockets of (b). The remaining Fermi surfaces stay "cold."

$F = (T/2)\sum_{\mathbf{q},\Omega_n} \log \chi^{-1}(\mathbf{q}, i\Omega_n)$, and the critical phase diagram is summarized in Fig. 4. There are two important regions in $\mathbf{q}$ space: (i) $\hat{q} \approx \hat{q}_{1,2}$ (shaded area in Fig. 2), and (ii) $q_z \gg (q_1, q_2)$. For region (ii), the entire nematoelastic coupling can be neglected, and we get the susceptibility of the electron-only theory with $\chi^{-1} \propto r_0 + q_{2d}^2 + |\Omega_n|/q_{2d}$, where $\mathbf{q}_{2d} = (q_1, q_2)$. Since it covers a larger volume in $\mathbf{q}$ space, the contribution from region (ii) gives the leading term. Thus, above the temperature scale $T_{\text{FL}} \sim r_0^{3/2} E_F$, where E_F is the Fermi energy in temperature units, we recover the usual electron-only theory with isotropic two-dimensional criticality and $\gamma(T) \propto 1/T^{1/3}$. However, for $T \ll T_{\text{FL}}$ this mode becomes massive giving a Fermi-liquid (FL) type contribution $\gamma(T) \propto 1/r_0^{1/2}$. In this low T-regime the nematoelastic coupling sets in, and direction selective criticality is restricted to region (i). The associated thermodynamics is as follows.

Ballistic nematicity (cuprates): In this case $D(\mathbf{q} \approx \mathbf{q}_1, i\Omega_n) \propto \Omega_n^2/q_1^2 + (q_2/q_1)^2|\Omega_n|/q_1$, where the last term indicates that Landau damping requires a finite q_2 component. The competition between these two terms yields an additional crossover scale $T^* \sim r_0^2 E_F$. For $T \ll T^*$ the dynamics is ballistic, giving the scaling $|\Omega_n| \sim q_1^2$. But above T^* the dynamics is damped, with the scaling $|\Omega_n| \sim r_0 q_1$. In both of these two regimes momentum scaling $(q_2, q_z) \sim q_1^2/r_0^{1/2}$ is anisotropic, and the anisotropy extends up to the temperature T_{FL}. The critical free energy can be estimated from the above scaling (for a detailed

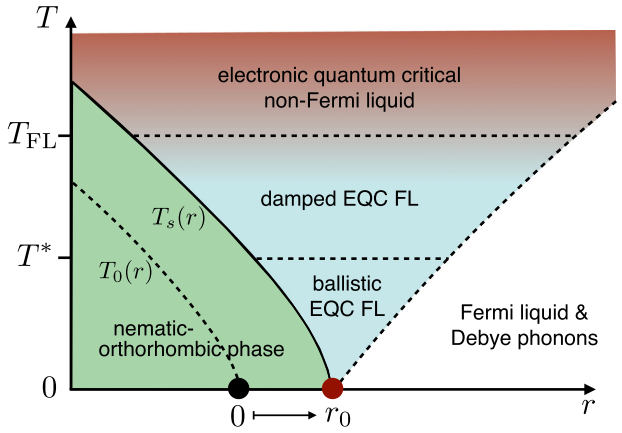

FIG. 4. Phase diagram with the Ising-nematic QCP. r is the control parameter. Nematoelastic coupling shifts the QCP from $r = 0$ (black circle) to $r = r_0$ (red circle), and the transition temperature from $T_0(r)$ to $T_s(r)$. $r_0 \ll 1$ is the ratio between the lattice-generated energy scale and Fermi energy E_F. Above the temperature scale $T_{\rm FL} \sim r_0^{3/2} E_F$ the nematoelastic coupling can be neglected, and the familiar electron-only theory of nematicity giving NFL physics is appropriate. $T_{\rm FL}$ is a crossover to Fermi-liquid physics. Below $T_{\rm FL}$ nematoelastic coupling is important, and criticality is direction selective (see Fig. 2), as in elastic quantum criticality (EQC). For the ballistic universality class, exemplified by the cuprates, there is an additional crossover at $T^* \sim r_0^2 E_F$. For the damped universality class, exemplified by the iron superconductors, $T^* = 0$. Their respective thermodynamics are given by Eqs. (5) and (6).

calculation see the Supplemental Material [23]). For $T \ll T_{\rm FL}$, including the noncritical contribution from region (ii), we get

$$\gamma(T) = \begin{cases} \frac{c_1}{r_0^{1/2} E_F} + \frac{c_2 T^{3/2}}{r_0 E_F^{5/2}}, & T \ll T^*, \\ \frac{c_1}{r_0^{1/2} E_F} + \frac{c_3 T^4}{r_0^6 E_F^5}, & T^* \ll T \ll T_{\rm FL}. \end{cases} \tag{5}$$

Note that the $T^{3/2}$ contribution appears also in the context of elastic quantum criticality (EQC), even in the absence of itinerant electrons [33].

Damped nematicity (FeSC): In this case there is finite Landau damping even for $\hat{q} = \hat{q}_1$ so that $D(\mathbf{q} \approx \mathbf{q}_1, i\Omega_n) \propto |\Omega_n|/(v_F q)$. There is no physics related to the crossover T^*. For $T \ll T_{\rm FL}$ this leads to

$$\gamma(T) = \frac{c_1}{r_0^{1/2} E_F} + \frac{c_4 T^{2/3}}{r_0 E_F^{5/3}}, \qquad T \ll T_{\rm FL}. \tag{6}$$

In the above $c_{1,\ldots,4}$ are numerical prefactors. For both cases, once the nematoelastic coupling sets in below $T_{\rm FL}$, the leading thermodynamics is Fermi-liquid type, while the critical contribution is subleading, in stark contrast to what the electron-only theory predicts. Note that in our theory we do not expect increased entropy in the nematic phase [35,36].

Electron self-energy.—We calculate at zero temperature the frequency dependence of the electron self-energy on the Fermi surface, i.e., $\Sigma_{\mathbf{k}_F}(i\omega_n) \propto h^2_{\mathbf{k}_F} S_{\hat{k}_F}(i\omega_n)$, where $S_{\hat{k}_F}(i\omega_n) = \int_{\mathbf{q},\nu_n} \chi(\mathbf{q}, i\nu_n) G_{\mathbf{k}_F+\mathbf{q}}(i\omega_n + i\nu_n)$, and G is the electron Green's function. As in the free energy calculation, regions (i) and (ii) of the $\mathbf{q}$ space are important. At sufficiently high frequency $|\omega_n| \gg T_{\rm FL}$ the contribution from region (ii) gives $S(i\omega_n) \propto |\omega_n|^{2/3}$, and the entire Fermi surface is hot (barring the points where $h_{\mathbf{k}_F} = 0$). Thus, at high frequency we recover the properties of the electron-only critical theory. For low frequency this contribution turns into a noncritical Fermi-liquid correction with $S(i\omega_n) \sim -i\omega_n / r_0^{1/2}$, which guarantees that the real part of the self-energy stays Fermi-liquid type everywhere on the Fermi surface.

The contribution from region (i) can lead to singular self-energy provided it involves electrons scattering parallel to the Fermi surface. This implies that at most we expect "hot spots" where electronic lifetimes are short, see Fig. 3. However, for the Fermi surface of the cuprates, as well as for the hole Fermi pockets of the FeSC, the vanishing form factor $h_{\mathbf{k}}$ at these points implies that the nematic fluctuation induced hot spots do not survive (the familiar hot-spot or Fermi-arc physics of the cuprates is presumably related to either spin fluctuations or Mott physics, which are not treated here). On the other hand, the nematic fluctuation induced hot spots do survive on the electron pockets of the FeSC for which $h_{\mathbf{k}} \approx 1$. As shown in the Supplemental Material [23], region (i) gives a subleading critical contribution to the self-energy $\Sigma(i\omega_n)_{\rm cr} \propto |\omega_n|^{4/3}/r_0^{1/2}$, which leads to a reduced lifetime for electrons at these hot spots. The arc lengths of the spots scale as $(|\omega_n|^{1/3}/r_0^{1/2}) k_F$, and thus their contribution to $\gamma(T) \propto T^{2/3}$, which is consistent with Eq. (6).

Discussion.—The nematoelastic coupling in Eq. (2) shifts not only the QCP, but also the finite-T transition from T_0 to T_S, see Fig. 4. Here, T_0 is the nominal nematic transition temperature of the electron subsystem in the absence of the coupling λ. Thus, the dimensionless parameter r_0 can be estimated as $r_0 \sim (T_s - T_0)/E_F$. Experimentally, T_0 is accessible from, say, electronic Raman scattering [8]. At present there is no clear experimental evidence of a nematic QCP in the cuprate phase diagram. Consequently, iron-based superconductors are better suited to study effects of nematoelastic coupling. In $BaFe_2As_2$ we get $T_0 \sim 90$ K [37], and $T_s \sim 138$ K. We estimate the Fermi temperature from the bottom of the electron bands as measured by photoemission, which are around 50 meV in $BaFe_2As_2$ [38]. Thus, overestimating the Fermi temperature $T_F \sim 1000$ K gives a conservative estimate of $r_0 \sim 0.05$, and $T_{\rm FL} \sim 10$ K, or more, near the nematic QCP of $Ba(Fe_{1-x}Co_x)_2As_2$.

For the iron-based superconductors we predict Fermi-liquid behavior below $T_{\rm FL}$ in thermodynamics and in

single-particle properties, except at hot spots on the electron pockets where noncanonical Fermi-liquid behavior is expected. Our predictions can be tested by photoemission, and by quasiparticle interference effects in tunneling spectroscopy upon suppression of the superconducting phase in these systems.

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