Quantum critical elasticity

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An elastic instability of a crystal at zero temperature, \( T = 0 \), gives rise to characteristic quantum critical signatures at finite \( T \). Close to such instabilities, critical fluctuations are suppressed due to long-range shear forces of the solid so that the phonon velocities either remain finite or vanish only along certain crystallographic directions. We consider spontaneous symmetry-breaking elastic quantum phase transitions as well as solid-solid quantum critical endpoints and discuss their quantum critical thermodynamics. We point out that quantum critical elasticity prevails whenever a critical, soft mode couples linearly to the strain tensor. In particular, this is relevant for certain iron-based superconductors exhibiting an electronic Ising-nematic quantum phase transition in a tetragonal crystal host.

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A characteristic of crystals is their shear rigidity that distinguishes them, in particular, from liquids and gases [1]. This rigidity and the concomitant long-range shear forces can fundamentally influence critical phenomena in a crystal host. Whenever the associated order parameter possesses the same symmetry as a representation of the strain field, they strongly hybridize so that the critical properties close to a zero temperature instability are eventually governed by quantum critical elasticity.

Such a strong entanglement of critical and elastic degrees of freedom occurs in the recently discovered iron-based superconductors. Certain materials such as Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) and FeSe exhibit a nematic instability driven by electronic degrees of freedom whose order parameter strongly couples to strain and triggers a tetragonal-to-orthorhombic elastic transition [2]. Interestingly, this transition is second order and the critical temperature can be tuned to zero by doping, see Fig. 1. The resulting quantum critical point is located well-inside the superconducting dome close to optimal doping where, in all likelihood, the electronic system is fully gapped [3]. This opens the unique possibility of observing thermodynamic signatures of the critical elastic medium without being masked by a Fermi-liquid background, and motivates us to develop the theory of such quantum criticality.

In the context of classical phase transitions, the coupling between elastic and critical degrees of freedom (of magnetic, ferroelectric or electronic origin) were intensively investigated in the 1970ies, see e.g. [4–9]. Depending on the symmetries of the critical system two scenarios are distinguished. In the first case, the order parameter \( \Phi \) can only couple quadratically to the strain field \( \varepsilon \), and the elastic interaction \( L_{\text{int}} = \gamma_2 \Phi^2 \varepsilon \), with the coupling constant \( \gamma_2 \), remains perturbative as long as the specific heat exponent is negative, \( \alpha = 2 - \nu d < 0 \), with the correlation exponent \( \nu \) and the dimensionality \( d \). This corresponds to the requirement that the renormalization of the elastic constants arising in lowest order perturbation theory due to the correlator \( \langle \Phi^2 \Phi^2 \rangle \) stays non-singular. Whereas for classical critical systems this criterion can be violated, it is fulfilled in most of the cases for quantum critical theories, though see [10], for which this criterion (in the absence of long-range interaction) becomes \( \nu(d + \varepsilon) > 2 \) with the dynamical exponent \( \varepsilon \). In such a perturbative situation, the crystal only acts as a diagnostic tool to probe quantum critical properties [11–16]. The critical fluctuations exert via the elastic coupling an internal pressure to which the crystal responds resulting in a characteristic change of the lattice constants as a function of the tuning parameter of the transition, which can be measured with the help of thermal expansion \( \alpha = (1/V)(\partial V/\partial T)_p \). An important quantity is the relative change of temperature upon adiabatically changing the pressure, \( \Gamma = (1/V_m)(\partial T/\partial p)_S \), with the molar volume \( V_m \), which is a variant of the well-known Grüneisen parameter [17, 18], and it can be identified with the ratio, \( \Gamma = \alpha/C_p \), where \( C_p = T(\partial S/\partial T)_p \)

![Figure 1](https://example.com/figure1.png)

Figure 1: Sketch of the phase diagram of iron-based superconductors with a tetragonal-orthorhombic quantum phase transition located within a superconducting dome transition temperature \( T_c(x) \). The phase boundary \( T_S \) is expected to asymptotically follow \( T_S(x) \sim (x_c - x)^{2/5} \), see text.
is the specific heat. The quantity $\Gamma$ necessarily diverges at a pressure-tuned quantum critical point with characteristic power-laws thus allowing to identify and classify quantum phase transitions [11].

More interesting is the second case, where the symmetries allow for a linear coupling between order parameter and strain, $\mathcal{L}_{\text{int}} = \gamma_1 \Phi \varepsilon$. In this case, the elastic moduli obtain a strong renormalization by the order parameter susceptibility $\delta C \sim \gamma_1^2 \langle \Phi \Phi \rangle$ that is singular by definition and drives the crystal unstable. Upon approaching the phase transition, a crossover to elastic criticality occurs when this renormalization becomes on the same order as the elastic moduli themselves. The nature of the transition then completely alters, and it is governed by the universality class of elastic phase transitions with the strain tensor becoming a primary order parameter. This case is in fact relevant for the iron-based systems with $\Phi$ being a nematic order parameter composed of either charge, spin or orbital degrees of freedom of the electrons [19–23]. Even if the fluctuations of $\Phi$ trigger the orthorhombic transition, the resulting quantum criticality differs drastically from critical electron nematicity that obtains without coupling to the crystal lattice [24].

Classical elastic transitions have been studied and classified by Cowley [25] and Schwabl and collaborators [26–29], and the same classification is relevant for transitions at $T = 0$. At an elastic transition an eigenvalue of the elastic constant matrix $C_{ijkl}$ vanishes. Depending on the degeneracy of this particular eigenvalue the strain order parameter is either a singlet, doublet or triplet of the irreducible representations of the crystal class. A peculiar aspect of elastic transitions is the intrinsic anisotropy of the phonon system. The phonon velocities are determined by the eigenvalues of the dynamical matrix $M_{nk}(\hat{q}) = C_{ijkl} \hat{q}_i \hat{q}_j$ with $\hat{q} = q/|q|$. These eigenvalues generically remain finite even if one of the elastic matrix $C_{ijkl}$ vanishes. Only for certain high symmetry directions of the wavevectors $\hat{q}$, the polarizations of the phonons might generate the pure critical strain mode so that the phonon velocity vanishes for this specific $\hat{q}$. For a generic direction, however, the phonon excites the non-critical strains as well, and its velocity remains finite. As a consequence, one can differentiate three types of elastic transitions where the phonon velocities remain finite either for all $\hat{q}$, vanish along certain directions of $\hat{q}$, or vanish if the phonons propagate in a particular plane [33]. The phonons thus remain non-critical in a $(3 - m)$-dimensional subspace with $m = 0, 1, 2$ corresponding to type 0, I or II, respectively, in the classification of Cowley [25]. Importantly, as a result of the restricted critical subspace even the classical critical theory is at $(m = 2)$ or above $(m = 1)$ its upper critical dimension [26–31]. The emergence of a restricted critical subspace is one major distinction between elastic and conventional criticality (i.e., in the absence of long-range forces).

Here, we consider elastic instabilities of the crystal lattice at $T = 0$ and investigate the arising quantum critical properties. The elastic instability might be intrinsic, i.e., induced by the anharmonicity of the strain potential or triggered by a coupling to another soft mode, as discussed above. We distinguish two cases, namely transitions that do and those that do not break a crystal symmetry. The tetragonal-to-orthorhombic transition in the iron-based systems falls in the first category. Note, however, that we do not consider here distortive quantum phase transitions characterized by the softening of an optical phonon. Such transitions have been studied in detail in the context of quantum critical paraelectrics [32–34].

**Symmetry-breaking elastic transitions** – If the quantum critical elasticity can be associated with the breaking of a crystal symmetry, the strain order parameter assumes a zero expectation value in the symmetric, undistorted phase. Depending on the presence or absence of a cubic invariant in the Landau potential for the order parameter, the transition is expected to be of first or second order. Of particular interest are second-order transitions that are accompanied by critical fluctuations which induce unusual behavior at finite $T$. In Table I, we list the elastic transitions associated with spontaneous crystal-symmetry breaking. Most of these transitions are of type I with a strain order parameter that is a singlet. The exceptions are listed in the last two rows that possess a doublet order parameter and are characterized by phonon velocities that vanish within one- as well as two-dimensional subspaces, i.e., type I and II, respectively.

| elastic transition    | constant | strain | type |
|-----------------------|----------|--------|------|
| orthorhombic $\rightarrow$ monoclinic | $c_{44}$ | $\varepsilon_{23}$ | I    |
| orthorhombic $\rightarrow$ monoclinic | $c_{55}$ | $\varepsilon_{13}$ | I    |
| orthorhombic $\rightarrow$ monoclinic | $c_{66}$ | $\varepsilon_{12}$ | I    |
| tetragonal $\rightarrow$ orthorhombic | $c_{11} - c_{12}$ | $\varepsilon_{11} - \varepsilon_{22}$ | I    |
| tetragonal $\rightarrow$ orthorhombic | $c_{66}$ | $\varepsilon_{12}$ | I    |
| tetragonal $\rightarrow$ mono- or triclinic | $c_{44}$ | $(\varepsilon_{23}, \varepsilon_{13})$ | I+II |
| hexagonal $\rightarrow$ mono- or triclinic | $c_{44}$ | $(\varepsilon_{23}, \varepsilon_{13})$ | I+II |

Table I: Second-order elastic transitions [25–27]. Second column: component of the elastic constant matrix in Voigt notation that goes to zero at the transition; third column: the strain order parameter; fourth column: type of the transition in the classification of Cowley [25]. Modifications arise for tetragonal crystals with a finite $\varepsilon_{16}$.
couples to an externally applied stress $\sigma_{ij}$. However, in most of the cases the appropriate singlet $\sigma$ is a shear stress. The tuning parameter $r = r(T, p)$ will depend on temperature $T$ and hydrostatic pressure $p$. The temperature dependence might be induced either by phonon excitations or by an elastic coupling to other degrees of freedom. The pressure dependence effectively arises from anharmonicities that mix the irreducible representations, in particular, from a third order term that couples the singlet to the trace of the strain, $\gamma_{int} \sim \text{tr}\{\varepsilon_{ij}\} \varepsilon^2$.

The elastic quantum phase transition is above its upper critical dimension for any $m = 1, 2$. It is governed by mean-field theory specified for the singlet case in Eq. [4], and the critical phonon excitations can be treated perturbatively. Their wave vector can be decomposed, $q = (p, k)$, into an $m$-dimensional soft component $p$ and a $(3 - m)$-dimensional stiff component $k$ with $m = 1, 2$ for type I and II, respectively. Close to criticality, $r \to 0^+$, the phonon dispersion assumes the anisotropic form [28]

$$\omega^2 \sim rp^2 + ap^4 + bk^2 + \ldots$$  \hspace{1cm} \text{(2)}

with finite constants $a$ and $b$, and the dots represent other terms not relevant for the following discussion. In order to deal with this anisotropic spectrum, a possibility is to perform the substitution $k^2 \rightarrow k'^2$. It amounts to introducing an effective spatial dimensionality $d_{eff} = m + 2(d - m) = 2d - m$ with $d = 3$. The resulting scaling $r \sim p^2$ and $\omega^2 \sim p^4$, $k'^4$ determines the correlation length exponent $\nu = 1/2$ and $z = 2$, respectively [33]. The contribution of the critical phonon modes to the free energy can then be cast in a scaling form [11]

$$\mathcal{F}_{\text{ct}} = T \frac{d_{eff}}{T_{1/(\nu z)}} f\left(\frac{r}{T_{1/(\nu z)}}\right),$$  \hspace{1cm} \text{(3)}

where the function $f$ possesses the asymptotics $f(x) = \text{const.}$ for $x \to 0$ and $f(x) \sim x^{\nu z} e^{-x^{2})} = x^{-m/2}$ for $x \to \infty$.

With the help of Eq. (3) the critical phonon thermodynamics is easily derived and summarized in Fig. 2. Close to criticality $r \approx 0$ (regime (i) in Fig. 2) one obtains a critical contribution to the phonon specific heat, $C_{\text{ct}} \sim T^{3-m/2}$, i.e., $C_{\text{ct}} \sim T^{5/2}$ and $C_{\text{ct}} \sim T^2$ for type I and type II transitions, respectively. The volume thermal expansion, $\alpha$, is determined by the pressure dependence of the tuning parameter $r$ so that $\alpha_{\text{ct}} \sim T^{2-m/2}$ at $r = 0$.

The critical Grüneisen ratio defined as $\Gamma_{\text{ct}} = \alpha_{\text{ct}}/C_{\text{ct}}$ obeys $\Gamma_{\text{ct}} \sim 1/T^{1/(\nu z)}$ with $\nu z = 1$ as expected from scaling considerations [11]. In the limit $T \ll r$ (regime (ii) in Fig. 2), on the other hand, we obtain $C_{\text{ct}} \sim r^{-m/2} T^3$, and a universal divergence $\Gamma_{\text{ct}} = \frac{m}{2} \frac{\nu z}{V_m(p-p_c)}$ with a universal prefactor $m/6$ i.e., 1/6 and 1/3 for type I and II, respectively, where we used $r(T = 0, p) \propto p - p_c$ with the critical pressure $p_c$. Note that the critical signatures vanish with a relatively high power of $T$ and, in fact, might be subleading compared to gapless particle-hole excitations in metals so that the critical phonon contributions would be difficult to identify. The analysis of quantum critical elasticity should be feasible however when the electrons are fully gapped as in the iron-based superconductors.

Relevance to Fe-superconductors – The tetragonal-to-orthorhombic transition in the iron-based superconductors is described by the order parameter $\varepsilon_{11} - \varepsilon_{22}$ within the 1-2 plane, see Table I, and belongs to type I in the classification of Cowley ($m = 1$). Near the quantum critical point this gives a specific heat $C_{\text{ct}} \sim T^{5/2}$ in regime (i), while in regime (ii), $C_{\text{ct}} \sim T^3/\sqrt{T}$, the standard $T^2$-dependence of phonons is critically enhanced by a factor $1/\sqrt{T}$ where $r \propto x - x_c$ with the pressure-dependent critical doping $x_c(p)$. As a function of doping, the Grüneisen parameter is expected to diverge in this regime as $\Gamma_{\text{ct}} = -1/(6V_m(x - x_c))(dx_c/dp)$. To the best of our knowledge, the critical elastic contribution has not been taken into account in analyzing low-$T$ heat capacity data of the materials near the critical doping. The phase boundary $T_S(x)$ at lowest $T$ directly follows from the $T$-dependence of $r$. As the electrons are gapped, the leading contribution are expected to derive from phonon-phonon interactions and an explicit calculation yields $\delta r \sim T^{5/2}$ as in quantum critical piezoelectric ferroelectrics [33], implying $T_S(x) \sim (x_c - x)^{2/5}$, see Fig. 1.

Interestingly, the associated symmetry of this specific elastic transition can also be explicitly broken by applying a uniaxial pressure $\sigma = (p_2 - p_1)/2$ within the 1-2 plane. This is reflected in the uniaxial thermal expansion $\beta_i = -(1/V_m)(\partial S/\partial p_i)T$ with $i = 1, 2$. Whereas the sum $\beta_1 + \beta_2$ is expected to show similar behavior as the volume thermal expansion, $\alpha$, the difference $\beta_0 - \beta_1 = -(1/V_m)(\partial S/\partial \sigma)T$ is more singular. Minimization with respect to the order parameter yields $\varepsilon = -\sigma/r$ for small $|\sigma| \ll \sqrt{T^3/\alpha}$ and $\varepsilon \sim \sigma^{1/3}$

![Figure 2: Left panel: Phase diagram for a symmetry-breaking elastic quantum phase transition. The tuning parameter $r(T = 0)$ vanishes for tuning the corresponding elastic constant to zero, see second column of Table I. The finite-temperature phase boundary is determined by the temperature dependence of $r(T)$ induced either by phonons or by elastic coupling to some other degrees of freedom. The critical phonon thermodynamics exhibits a crossover at $T \sim r$ giving rise to two regimes (i) and (ii). Right panel: Critical phonon specific heat $C_{\text{ct}}$, phonon thermal expansion $\alpha_{\text{ct}}$ and Grünneisen ratio in the regimes (i) and (ii) for pressure tuning $r(T = 0) \propto p - p_c$; $m = 1, 2$ for type I and II, respectively.](image-url)
for large $|\sigma| \gg \sqrt{r/r_*}$. For small uniaxial pressures $\sigma$ the critical part $\beta_{\sigma}^c \sim \sigma^2/|r|$ is linear in $\sigma$ and its $T$-dependence is determined by the one generated for the tuning parameter $r = r(T)$. For larger pressures and small temperatures, on the other hand, the effective modulus is determined by $r_{\text{eff}} = r_{\text{eff}}^0 \approx \approx \frac{u}{2} e^2 \sim \sigma^{2/3}$ and $\beta_{\sigma}^c \sim T^3(\partial r_{\text{eff}}^{-1/3}/\partial \sigma) \sim T^3 \sigma^{-4/3}$. The associated critical Grüneisen ratio divergence at $r = 0$ then reads $\beta_{\sigma}^c/\sigma_{\text{cr}} = 1/(9 V_{\text{min}} \sigma)$ with the universal prefactor $1/9$.

**Isostructural elastic transitions** - The remaining elastic transitions not listed in Table I are generically not of second order. Exceptions are specific points in the phase diagram where the symmetry is enhanced by additional fine-tuning, and particular interesting examples of this class are isostructural transitions. Here, the expectation value of a certain singlet representation of the strain tensor, $\varepsilon$, which is itself invariant under all crystal symmetry operations, changes in a critical manner.

The corresponding Landau potential generally contains all powers of $\varepsilon$. The cubic term, however, can be made to vanish by appropriately shifting $\varepsilon \to \varepsilon + \varepsilon_0$ by a constant $\varepsilon_0$ so that the potential assumes the same form as that of Eq. (1),

$$V(\varepsilon) = \frac{r}{2} \varepsilon^2 + \frac{u}{4!} \varepsilon^4 - h \varepsilon,$$  

where $h$ is to be identified, though, with an additional tuning parameter. In order to reach the second-order quantum critical point both parameters, $h$ and $r$, must then be tuned to zero at $T = 0$, for example, as a function of an external field $F$ and pressure $p$. The criterion $h(F,p) = 0$ and $r(F,p) < 0$ defines a line of first-order quantum phase transitions in the $(F,p)$ phase diagram between isostructural solids characterized by a different $\varepsilon$. This line terminates in a second-order quantum critical endpoint (QCEP) at a critical field, $F_{\text{c}}$, and pressure, $p_{\text{c}}$, with $h(F_{\text{c}},p_{\text{c}}) = r(F_{\text{c}},p_{\text{c}}) = 0$, see Fig. 3.

At this **solid-solid quantum critical point** a true mean-field transition occurs without critical microscopic fluctuations. Due to the high symmetry of the order parameter $\varepsilon$, the isostructural transitions are all of type 0 in the Cowley classification with a non-critical phonon sector. This peculiar aspect is rooted in the presence of shear moduli that, in particular, distinguishes the solid-solid QCEP from the liquid-gas analogue.

Such a solid-solid QCEP is expected to be induced by any zero temperature instability associated with an emergent $\mathbb{Z}_2$ symmetry so that a linear coupling of the Ising order parameter to strain is allowed. An example is the metamagnetic QCEP [30, 57], where $F$ corresponds to a magnetic field, that will be preempted by a solid-solid QCEP due to magnetoelastic coupling. Similar reasoning would apply to a metaelectric QCEP where the polarization changes in a critical manner at some finite electric field. The mean-field character of the metaelectric endpoint that exists at finite temperature in KH$_2$PO$_4$ was explicitly demonstrated already in Ref. [35]. Moreover, the Kondo volume collapse transition at $T = 0$ also corresponds to a solid-solid QCEP [39, 40]. A famous analogue at finite temperature is the $\gamma - \alpha$ transition of Ce [41, 42], and also the Mott endpoint at finite $T$ is predicted to fall in the same category [41].

A hallmark of solid-solid endpoints is the breakdown of Hooke’s law. Minimizing Eq. (4) at $r = 0$ one obtains $\varepsilon \sim h^{1/3} \propto (p - p_c)^{1/3}$ at the critical field $h(F_{\text{c}},p) \propto p - p_c$ resulting in a non-linear strain-stress relation with mean-field exponent $1/3 = 1/3$ and a divergent compressibility $\partial p \varepsilon \sim |p - p_c|^{-2/3}$. The resulting energy depends non-analytically on the tuning parameter $h$, $V_{\text{min}} \sim |h|^{4/3}$. However, due to the absence of critical microscopic fluctuations there is no diverging correlation length, and, as a consequence, the usual scaling hypothesis for critical phenomena is not applicable. As a result, the thermodynamics at finite $T$ for a solid-solid QCEP is non-universal and depends on the $T$-dependence of the tuning parameters, e.g., $h = h(p,F,T)$, induced by non-critical degrees of freedom. Setting $h(p,F,T) = h_0(p,F) + a T^x$, with e.g. $x = 2$ for a metal, one obtains at $r = 0$ a critical contribution to the specific heat and thermal expansion, $C_{\text{cr}}/T = -\partial^2 V_{\text{min}} \sim |h_0|^{1/3}T^{x-2}$ and $\alpha_{\text{cr}} = \partial T \partial \varepsilon V_{\text{min}} \sim T^{x-1}|h_0|^{-2/3}$, respectively, for $T \to 0$. The critical Grüneisen ratio in this limit is given by $\Gamma_{\text{cr}} = \alpha_{\text{cr}}/C_{\text{cr}} = \frac{1}{12 (x-1)} \left( \frac{1}{V_{\text{min}}(p - p_c)} \right)$ for $h_0 \propto p - p_c$ and the prefactor now depends on $x$.

In summary, any quantum critical system that allows a linear coupling of its order parameter to the strain tensor will eventually be governed by quantum critical elasticity. The resulting continuous symmetry-breaking elastic transitions are accompanied with a phonon softening giving rise to quantum critical phonon thermodynamics, that is summarized in Fig. 2. These predictions are relevant for the Fe-based superconductors close to their elastic quantum critical point.

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