

Quantum Critical Elasticity

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We discuss elastic instabilities of the atomic crystal lattice at zero temperature. Because of long-range shear forces of the solid, at such transitions the phonon velocities vanish, if at all, only along certain crystallographic directions, and, consequently, the critical phonon fluctuations are suppressed to a lower dimensional manifold and governed by a Gaussian fixed point. In the case of symmetry-breaking elastic transitions, a characteristic critical phonon thermodynamics arises that is found, e.g., to violate Debye's T^3 law for the specific heat. We point out that quantum critical elasticity is triggered whenever a critical soft mode couples linearly to the strain tensor. In particular, this is relevant for the electronic Ising-nematic quantum phase transition in a tetragonal crystal as discussed in the context of certain cuprates, ruthenates, and iron-based superconductors.

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Quantum fluctuations close to an instability of the ground state result in fascinating, exotic behavior even at finite T that is often at odds with conventional properties of materials [1]. However, most of the recent interest has focused on instabilities associated with the electronic degrees of freedom in metals and insulators [2–4]. In contrast, zero temperature instabilities of the atomic crystal lattice have attracted much less attention. While distortive instabilities associated with the softening of an optical phonon have been studied in the context of quantum critical paraelectrics [5–7], quantum phase transitions involving the elastic degrees of freedom, namely, uniform strains and acoustic phonons, have remained largely unexplored even though such transitions are ubiquitous in various phases of matter such as insulators, metals, and superconductors. It is the aim of this work to fill this gap, and to study the critical thermodynamics associated with elastic *quantum* criticality (EQC).

Elastic *classical* criticality, i.e., elastic instabilities at a finite critical temperature T_c have been already studied and classified by Cowley [8] and Schwabl and collaborators [9–12]. These works identified the importance of shear rigidity, a property that distinguishes crystals from liquids and gases. This rigidity and the concomitant long-range forces restrict criticality to an m -dimensional subspace in a d -dimensional Brillouin zone, with $m \leq d$, making the transitions mean-field type for $d = 3$ [9,13]. This physics is also crucial for EQC, setting them apart from the paradigm of a conventional quantum phase transition, i.e., without any long range forces, involving electrons in metals and insulators [14]. Compared to finite T elastic transitions, in EQC one needs to take into account the dynamics of the acoustic phonons. As a result, we find, for example, that Debye's T^3 law for specific heat $C_p = T(\partial S/\partial T)_p$ is violated in a characteristic manner close to symmetry-breaking EQC.

The following are our main results. From a study of the statics and the dynamics of the critical acoustic phonons, we construct the scaling form of the free energy associated with all the different universality classes of EQC. This allows us to obtain, in addition to the specific heat, other thermodynamic quantities such as the thermal expansion $\alpha = (1/V)(\partial V/\partial T)_p$, and the ratio $\Gamma = \alpha/C_p$. The latter is a variant of the well-known Grüneisen parameter [15], and it can be identified with the relative change of temperature upon adiabatically changing the pressure, $\Gamma = 1/(V_m T)(\partial T/\partial p)_S$ with the molar volume V_m . The quantity Γ has proven useful in the investigation of quantum criticality in general as it necessarily diverges at a pressure-tuned quantum critical point with characteristic power laws [16–21]. Note that until now Γ has been theoretically studied only in situations where the crystal lattice acts as a nonintrusive probe and itself remains noncritical. We also derive a general expression for the exponent θ characterizing the dependence of the transition temperature $T_c(r) \sim |r|^\theta$ on the tuning parameter r of the quantum phase transition.

According to elasticity theory [22], the macroscopic stability of the crystal requires that all eigenvalues of the elastic constant matrix C_{ijkl} be positive. This guarantees that the acoustic phonon velocities, determined by the eigenvalues of the dynamical matrix $M_{ik}(\mathbf{q}) = C_{ijkl}q_j q_l$, are finite, where \mathbf{q} is the phonon momentum. At an elastic transition a specific eigenvalue of C_{ijkl} vanishes and, 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 [8–12]. Importantly, at the instability the phonon velocity goes to zero only for momenta along certain high symmetry directions for which the phonon triggers only the critical strain mode. However, for a generic direction the phonon

excites the noncritical strains with finite elastic constants as well, and consequently their velocity stays finite at the transition. Thus, elastic criticality can be classified as type 0, I, or II depending on the dimensionality $m = 0, 1, 2$, respectively, of the critical phonon subspace [8]. The fact that the phonons remain noncritical in a $(d - m)$ -dimensional subspace distinguishes elastic transitions from conventional ones, for which $m = d$. In the following we study two types of EQC, namely those that involve breaking of a point group symmetry of the unit cell (in which case $m = 1, 2$), and those that do not (in which case $m = 0$).

Symmetry-breaking elastic transitions.—If the EQC 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.

The Landau potential for the order parameter ε , being either a singlet or a doublet, reads

$$\mathcal{V}(\varepsilon) = \frac{r}{2}\varepsilon^2 + \frac{u}{4!}(\varepsilon^2)^2 + \sigma\varepsilon. \quad (1)$$

A second-order quantum phase transition obtains for a positive quartic coupling $u > 0$ if the tuning parameter r goes to zero, $r \rightarrow 0$, at $T = 0$ and $\sigma = 0$. This occurs when the corresponding elastic constant listed in the second column of Table I vanishes. The strain in general couples to an externally applied stress σ_{ij} . However, in most of the cases the appropriate σ is a shear stress. The tuning

TABLE I. Continuous symmetry-breaking elastic transitions [8,9,11]. 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 [8]. Modifications arise for tetragonal crystals with a finite c_{16} .

Elastic transition	Constant	Strain	Type
Orthorhombic \rightarrow monoclinic	c_{44}	ε_{23}	I
Orthorhombic \rightarrow monoclinic	c_{55}	ε_{13}	I
Orthorhombic \rightarrow monoclinic	c_{66}	ε_{12}	I
Tetragonal \rightarrow orthorhombic	$c_{11}-c_{12}$	$\varepsilon_{11}-\varepsilon_{22}$	I
Tetragonal \rightarrow orthorhombic	c_{66}	ε_{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

parameter, $r = r(p)$, will in general depend on hydrostatic pressure p , which arises from anharmonicities that mix the irreducible representations, in particular, from a third order term that couples the order parameter ε to the trace of the strain, $\mathcal{V}_{\text{int}} \sim \text{tr}\{\varepsilon_{ij}\}\varepsilon^2$.

Decomposing the phonon wave vector, $\mathbf{q} = (\mathbf{p}, \mathbf{k})$, into an m -dimensional soft component \mathbf{p} and a noncritical $(d - m)$ -dimensional component \mathbf{k} with $m = 1, 2$ for type I and II, respectively, the phonon dispersion close to criticality, $r \rightarrow 0^+$, assumes the anisotropic form [10]

$$\omega^2 \sim r\mathbf{p}^2 + a\mathbf{p}^4 + b\mathbf{k}^2 + \dots \quad (2)$$

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 $\mathbf{k}^2 \rightarrow \mathbf{k}^4$. It amounts to introducing an effective spatial dimensionality $d_{\text{eff}} = m + 2(d - m) = 2d - m$ with $d = 3$. The resulting scaling, $r \sim \mathbf{p}^2$ and $\omega^2 \sim \mathbf{p}^4, \mathbf{k}^4$, determines the correlation length exponent $\nu = 1/2$ and $z = 2$, respectively [23]. As a result of the enhanced effective dimensionality d_{eff} , the EQC is above its upper critical dimension $d_{\text{eff}} + z = 8 - m > d_c^+$ with $d_c^+ = 4$ for any $m = 1, 2$ and is governed by the Gaussian fixed point, thereby justifying the above scaling. Evaluating the Gaussian fluctuations of the critical phonon modes, we find that the resulting free energy can be cast in the scaling form

$$\mathcal{F}_{\text{cr}} = T^{(d_{\text{eff}}+z)/z} f\left(\frac{r}{T^{1/(\nu z)}}\right), \quad (3)$$

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

With the help of Eq. (3) the critical phonon thermodynamics is easily derived and summarized in Fig. 1. In the quantum critical regime (i) in Fig. 1, we find, in particular, a critical contribution to the phonon specific heat, $C_{\text{cr}} \sim T^{3-m/2}$, i.e., $C_{\text{cr}} \sim T^{5/2}$ and $C_{\text{cr}} \sim T^2$ for type I and type II transitions, respectively, signalling a breakdown of Debye's T^3 law. The volume thermal expansion, α , is determined by the pressure dependence of the tuning parameter r so that $\alpha_{\text{cr}} \sim T^{2-m/2}$ at $r = 0$. The critical Grüneisen ratio defined as $\Gamma_{\text{cr}} = \alpha_{\text{cr}}/C_{\text{cr}}$ obeys $\Gamma_{\text{cr}} \sim 1/T^{1/(\nu z)}$ with $\nu z = 1$ as expected from scaling considerations [16]. In the limit $T \ll r$ of regime (ii) in Fig. 1, on the other hand, Debye's T^3 law is recovered, however, with a critically enhanced prefactor, $C_{\text{cr}} \sim r^{-m/2} T^3$. The Grüneisen ratio diverges $\Gamma_{\text{cr}} = (m/6)[1/V_m(p - p_c)]$ 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 phonon signatures vanish with a relatively high power of T and, in fact, might be subleading, for example, compared to gapless particle-hole excitations in metals.

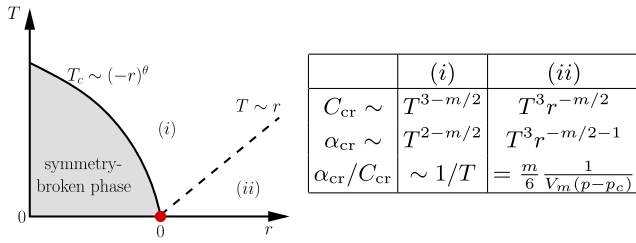


FIG. 1 (color online). Left panel: Phase diagram for a symmetry-breaking elastic quantum phase transition. The tuning parameter r vanishes when tuning the corresponding elastic constant to zero, see second column of Table I. The critical phonon thermodynamics exhibits a crossover at $T \sim r$ giving rise to two regimes (i) and (ii). The phase boundary, $T_c \sim (-r)^\theta$, is determined by the exponent θ , see text. Right panel: Critical phonon specific heat C_{cr} , phonon thermal expansion α_{cr} and Grüneisen 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.

We now turn to the discussion of the exponent governing the phase boundary $T_c \sim (-r)^\theta$ near the quantum critical point in Fig. 1. It is determined by the perturbative renormalization of the tuning parameter, $r \rightarrow R(T) = r + \delta r(T)$, which induces a T dependence, and $R(T_c) = 0$. For metals one generically expects a temperature dependence $\delta r \sim T^2$ so that $T_c \sim \sqrt{-r}$ and $\theta = 1/2$. The situation is more interesting for solids where the phonons provide the leading contribution to thermodynamics, e.g., insulators or fully gapped superconductors. In this case, the renormalization of r is determined by the self-interaction of critical phonon degrees of freedom. An explicit calculation, presented in the Supplemental Material [24], yields $\theta = 2/(6 - m)$. The $m = 1$ result agrees with a previous calculation in the context of quantum critical piezoelectric ferroelectrics [6].

Tetragonal-to-orthorhombic transition.—As an illustration of a particular example, we discuss in some further detail the tetragonal-to-orthorhombic transition which is described by the order parameter $\varepsilon_{11} - \varepsilon_{22}$, see Table I. In this case, the critical phonon becomes soft for momenta along diagonals in the $q_1 - q_2$ plane, i.e., $\mathbf{q} \propto (1, \pm 1, 0)$, and the critical manifold is thus one-dimensional corresponding to type I with $m = 1$. For finite but small deviations from the $q_1 = q_2$ manifold the critical phonon dispersion is given by (see Supplemental Material [24]),

$$\rho\omega^2(\mathbf{q}) \approx \frac{c_{11} - c_{12}}{2} q_+^2 + \frac{2c_{11} + 2c_{12} + c_{66}}{4} q_-^2 + \frac{c_{44}}{4} q_3^2 + a q_+^4. \quad (4)$$

Here $q_\pm = (q_1 \pm q_2)/\sqrt{2}$, and $|q_+| \gg (|q_3|, |q_-|)$, and ρ is the ionic mass density. As $c_{11} - c_{12} \rightarrow 0$ at the transition, the dependence on q_+ is determined by the last term $a q_+^4$

that derives from higher order terms of the strain potential. In the vicinity of the second critical manifold $q_1 = -q_2$ the dispersion is obtained by interchanging $q_+ \leftrightarrow q_-$ in the above. Importantly, the dispersion in other directions does not soften and remains noncritical as the remaining elastic constants stay finite.

An interesting aspect of this particular transition is that the tetragonal symmetry can also be explicitly broken by $\sigma = (p_2 - p_1)/2$, where p_i is the uniaxial pressure along the $i = 1, 2$ direction. This is reflected in the linear thermal expansion $\beta_i = -(1/V_m)(\partial S/\partial p_i)_T$. Whereas the sum $\beta_1 + \beta_2$ is expected to show similar behavior as the volume thermal expansion, α , the uniaxial thermal expansion, defined by the difference $\beta_\sigma \equiv \beta_2 - \beta_1 = -(1/V_m)(\partial S/\partial \sigma)_T$, is more singular. Minimization with respect to the order parameter yields $\varepsilon = -\sigma/r$ in the linear regime of small $|\sigma| \ll \sqrt{r^3/u}$, and $\varepsilon \sim \sigma^{1/3}$ in the nonlinear regime of large $|\sigma| \gg \sqrt{r^3/u}$. Taking the renormalization $r \rightarrow R(T)$ into account, one obtains in the former case $\beta_\sigma^{\text{cr}} \sim \sigma \partial_T(1/R(T))$. The resulting T dependence is singular in regime (i) with $\beta_\sigma^{\text{cr}} \sim \sigma T^{-(1+1/\theta)}$, where the exponent θ was introduced earlier, while in regime (ii) β_σ is analytic in T . In the nonlinear regime of σ and small temperatures, on the other hand, the effective modulus is determined by $r_{\text{eff}} = \partial_\varepsilon^2 \mathcal{V} \approx (u/2)\varepsilon^2 \sim \sigma^{2/3}$ and $\beta_\sigma^{\text{cr}} \sim T^3(\partial(r_{\text{eff}}^{-1/2})/\partial \sigma) \sim T^3 \sigma^{-4/3}$. The accompanying uniaxial Grüneisen ratio at $r = 0$ diverges $\beta_\sigma^{\text{cr}}/C_{\text{cr}} = 1/(9V_m \sigma)$ with the universal prefactor $1/9$ as σ is reduced.

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, ε , of the strain tensor which is itself invariant under all crystal symmetry operations, changes in a critical manner. An example is the isostructural volume collapse transition in a cubic crystal where the singlet, $\varepsilon = \text{tr}\{\varepsilon_{ij}\}$, represents fluctuations of the volume, $\int_V d\mathbf{r} \varepsilon(\mathbf{r}) = \delta V$.

The corresponding Landau potential generally contains all powers of ε . The cubic term, however, can be made to vanish by appropriately shifting $\varepsilon \rightarrow \varepsilon + \varepsilon_0$ by a constant ε_0 so that the potential assumes the same form as that of Eq. (1), $\mathcal{V}(\varepsilon) = (r/2)\varepsilon^2 + (u/4!)\varepsilon^4 - h\varepsilon$, 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 different expectation values of ε . This line terminates in a second-order quantum critical end point

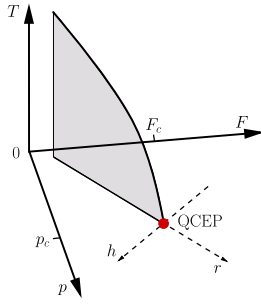


FIG. 2 (color online). Phase diagram with a solid-solid QCEP. A line of first-order solid-solid quantum phase transitions and a line of finite temperature, T , second-order transitions meet at the QCEP and enclose a surface of first-order transitions at finite T (shaded area).

(QCEP) at a critical field, F_c , and pressure, p_c , with $h(F_c, p_c) = r(F_c, p_c) = 0$, see Fig. 2.

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

A hallmark of solid-solid end points is the breakdown of Hooke's law. Minimizing the potential at $r = 0$ one obtains $\varepsilon \sim h^{1/3} \propto (p - p_c)^{1/3}$ at the critical field $h(F_c, p) \propto p - p_c$ resulting in a nonlinear strain-stress relation with mean-field exponent $1/\delta = 1/3$ and a divergent compressibility $\partial_p \varepsilon \sim |p - p_c|^{-2/3}$. The resulting energy depends nonanalytically on the tuning parameter h , $\mathcal{V}_{\min} \sim |h|^{4/3}$. 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 nonuniversal and depends on the T dependence of the tuning parameters, e.g., $h = h(p, F, T)$, induced by noncritical degrees of freedom. Setting $h(p, F, T) = h_0(p, F) + aT^x$, with e.g., $x = 2$ for a metal, one obtains at $r = 0$ a critical contribution to the specific heat and thermal expansion, $C_{\text{cr}}/T = -\partial_T^2 \mathcal{V}_{\min} \sim |h_0|^{1/3} T^{x-2}$ and $\alpha_{\text{cr}} = \partial_T \partial_p \mathcal{V}_{\min} \sim T^{x-1} |h_0|^{-2/3}$, respectively, for $T \rightarrow 0$. The critical Grüneisen ratio in this limit is given by $\Gamma_{\text{cr}} = \alpha_{\text{cr}}/C_{\text{cr}} = [1/3(x-1)][1/V_m(p-p_c)]$ for $h_0 \propto p - p_c$ and the prefactor now depends on x .

Influence of disorder.—We briefly comment on the influence of disorder on EQC. Usually, one distinguishes the effect of *random mass* and *random field* disorder describing disorder configurations that, respectively, preserve or explicitly break the symmetry associated with the order parameter, see Ref. [25] for a review in the context of structural transitions. In the case of symmetry-breaking EQC the importance of the former is decided by a modified

Harris criterion. Because of the enhanced spatial correlation volume $\xi^{d_{\text{eff}}}$ with $d_{\text{eff}} = 6 - m$, random mass disorder is irrelevant or marginal for $m = 1, 2$, respectively, as $2 \leq d_{\text{eff}}\nu = (6 - m)/2$. On the other hand, random field disorder, if present, is relevant and is expected to modify the criticality [26].

Linear coupling to soft, electronic modes.—Besides being of fundamental interest, the notion of EQC is actually relevant whenever a critical mode Φ , e.g., of electronic origin, couples linearly to strain, $\mathcal{L}_{\text{int}} = \gamma_1 \Phi \varepsilon$. In this case, the elastic moduli obtain a strong perturbative renormalization by the critical 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 of the same order as the elastic moduli themselves. For classical elastic criticality, this is well known [27,28] and has been experimentally confirmed for the classical metaelectric end point in KH_2PO_4 [29]. The Mott end point at finite T is also governed by critical elasticity [30]. Such a crossover to elastic criticality is also expected for the quantum case.

A crossover to a symmetry-breaking EQC should occur whenever an electronic order parameter Φ breaks a point-group symmetry of the crystal. This is in particular the case for Ising-nematic ordering associated with a Pomeranchuk instability of a Fermi surface [31] described by the order parameter $\Phi = \Psi^\dagger (\partial_1^2 - \partial_2^2) \Psi$, where Ψ^\dagger and Ψ are fermionic creation and annihilation operators, respectively. Such a transition that breaks discrete rotation symmetry of a Fermi surface has been discussed for ruthenates, cuprates, and, recently, for Fe-based superconductors [32]. In a tetragonal crystal the order parameter Φ generically couples linearly to the strain component $\varepsilon_{11} - \varepsilon_{22}$, thereby triggering a tetragonal-to-orthorhombic elastic transition. Such a structural transition, and the associated quantum phase transition are currently being studied in systems such as $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ and FeSe tuned by pressure. In these systems, even if the primary order parameter Φ is of electronic origin [33–37], the resulting quantum criticality is eventually governed by the long-range shear forces of the crystal with the concomitant critical phonon thermodynamics as presented in Fig. 1 [38], provided the transition itself stays continuous [39]. Similarly, a crossover to a solid-solid QCEP is expected whenever the order parameter couples linearly to a strain component that is invariant under point group operations. Examples of such cases include the metaelectric and metamagnetic QCEP [40,41], as well as the Kondo volume collapse transition at $T = 0$ [42,43].

Summary.—We studied all the different universality classes of elastic transitions of a crystalline lattice at zero temperature, namely, those that break point-group symmetries spontaneously and solid-solid quantum critical end points. Elastic quantum criticality is triggered whenever the

order parameter couples linearly with strain. Consequently, they are relevant for studying a wide range of correlated electron systems such as ruthenates, cuprates, and certain Fe-based superconductors.

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