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Over the last two decades, quantum phase transitions (QPTs) have emerged as one of main themes in condensed matter physics. These transitions occur at exactly zero temperature when the variation of a parameter such as pressure, chemical composition or magnetic field leads to a qualitative change of the ground state. Critical fluctuations associated with continuous quantum phase transitions are rooted in Heisenberg's uncertainty principle and follow quantum instead of classical statistical mechanics. Quantum critical points (QCPs) can control sizable regions of the phase diagram over substantial energy and temperature scales. Celebrated consequences include non-Fermi-liquid behavior in metals and exotic superconductivity. From a conceptual point of view, quantum phase transitions have emerged as a new ordering principle for low-energy phenomena that allows one to explore regions of the phase diagram where more conventional approaches are inadequate. Very recently, quantum phase transitions have also established exciting links between condensed matter, string theory, atomic physics, and quantum information theory.

Funding by the Deutsche Forschungsgemeinschaft (DFG, German Science Foundation) has allowed to join forces of German groups working in this fascinating area of condensed matter physics. The DFG Research Unit “Quantum phase transition” (FOR 960) has considerably strengthened their prominent role in this field. In this Research Unit we primarily focused on quantum phase transitions in metallic solids, i.e., systems where the electronic, magnetic, and lattice properties are governed by the occurrence of a QCP. In a collaborative effort of experiment and theory, we studied several classes of materials with strong electronic correlations at QCPs: intermetallic *f*-electron compounds, weak itinerant transition-metal magnets, and transition-metal oxides and sulfides. In many cases, the QCP was characterized by vanishing magnetic order induced by a loss of magnetic moments due to electronic interactions, notably the Kondo effect, or competing frustrated interactions. One of the central objectives was to widen the range of materials exhibiting a QPT in order to separate materials-related issues from fundamentally new physics.

QPTs are characterized by an interplay of thermal and quantum fluctuations [1–3]. At a continuous QPT, the energy of order-parameter fluctuations,  $\hbar/\tau$  exceeds the thermal energy  $k_B T$ . (Here,  $\hbar$  and  $k_B$  are the Planck and Boltzmann constants, and  $\tau$  is the typical lifetime of a fluctuation, with  $\tau \rightarrow \infty$  near criticality.) This implies that a fully quantum mechanical description of the order-parameter dynamics is required. As  $\hbar/k_B T$  reflects the extension of the system in the (imaginary) time direction, a QPT occurring at  $T = 0$  affects the system's finite-temperature behavior by virtue of finite-size scaling. Remarkably, such quantum critical behavior may persist up to rather high temperatures [4]. Microscopically, the unusual properties in the quantum critical regime, such as fractional power laws in thermodynamic quantities, can be ascribed to the thermal occupation of the unconventional elementary excitations of the quantum critical ground state – these excitations are often distinct from standard quasiparticles. While this is a fascinating issue in its own right, the

presence of electronic degrees of freedom at a QCP adds complexity: Near a metallic QCP, low-energy order-parameter fluctuations and low-energy electron-hole excitations coexist, which provides a major challenge for both experiment and theory.

On a phenomenological level, correlated metals may be treated using the Landau theory of Fermi liquids, where the effect of the interactions is cast into a few phenomenological parameters such as the electron's effective mass and the so-called Landau parameters [5,6]. In a number of instances, this model holds even when the effective mass  $m^*$  exceeds the free-electron mass by a factor of several hundred [7]. Because of its great success, the Landau Fermi-liquid theory is considered as the standard model of metals.

Metals with strong correlations are often close to a magnetic instability – this applies in particular to rare-earth intermetallic systems with their delicate balance between magnetic order (due to the RKKY interaction) and paramagnetic ground state (due to the Kondo effect). By now, several dozens of heavy-fermion compounds have been found to display magnetic QPTs. Two of them,  $\text{CeCu}_{6-x}\text{Au}_x$  and  $\text{YbRh}_2\text{Si}_2$ , both discovered and investigated by groups of our Research Unit, have become model systems in the field.  $\text{CeCu}_{6-x}\text{Au}_x$  [8,9] exhibits a QCP at a critical concentration  $x_c \approx 0.1$  where long-range incommensurate antiferromagnetic order sets in towards larger Au concentration. Subsequently, the stoichiometric compound  $\text{YbRh}_2\text{Si}_2$  which is close to a QCP [10,11] has attracted a great deal of attention. It exhibits a possible disintegration of heavy quasiparticles at the QPT [12–14] and ferromagnetic fluctuations [15] close to antiferromagnetic order [16]. Heavy-fermion behavior has also been detected in several  $3d$  and  $4d$  transition-metal oxides.  $\text{LiV}_2\text{O}_4$  is a prototypical example [17,18] which is believed to be close to a QCP.

On the theory side, magnetic QPTs in metals have been traditionally described in the framework of the Hertz-Millis-Moriya (HMM) picture [19–21], which is based on a formulation in terms of the magnetic order parameter only. It assumes the presence of quasiparticles, which undergo singular scattering due to the abundance of low-lying magnetic fluctuations at the QCP. It is known that the HMM approach breaks down for ferromagnets as well as for two-dimensional antiferromagnets – in both cases the low-energy electrons render the gradient expansion in the order-parameter field theory singular. This is related to the presence of multiple dynamic exponents, which formally requires a consistent theoretical treatment of both order-parameter and electron-hole dynamics – this is a formidable task where initial steps have been undertaken recently [22,23].

Still, the HMM approach is expected to work for three-dimensional antiferromagnets, such as the heavy-fermion compounds mentioned above. However, the theory appears to be inconsistent with certain experimental results. This has triggered more radical theoretical approaches, postulating a break-down of conventional quasiparticles. A particular set of ideas is based on a critical point involving Mott localization of the  $4f$  electrons [24–27]. This would imply that the Fermi surface collapses, and critical physics emerges on the whole Fermi surface. A recently proposed alternative scenario instead puts forward a strong-coupling version of magnetic quantum criticality, which may also cause power-law spectral functions on the whole Fermi surface [28,29]. Experimentally, some materials do seem to follow a HMM scenario while others, notably  $\text{CeCu}_{6-x}\text{Au}_x$  and  $\text{YbRh}_2\text{Si}_2$ , do not – the distinction between both classes of materials still remaining unclear. Thus, it is fair to say that many of the phenomena at metallic QCPs are not fully understood at present; we refer to a review article [3] and, of course, to the various articles in this volume for more details.

Many novel features of a quantum critical point arise from the fact that the relevant energy scale, e.g., given by the magnetic ordering temperature, goes to zero. Therefore small perturbations, otherwise masked by the “high-energy” scale of magnetic interactions, may acquire importance. Hence it is feasible that new phases

arise in the vicinity of a QCP. For instance, unconventional heavy-fermion superconductors [30] and the high-temperature cuprate superconductors are strong candidates for QPTs because of their proximity to magnetic order. In fact, a host of different systems has been discovered in recent years, where unconventional superconductivity often emerges in the vicinity of a QPT [31–34]. For the archetypal heavy-fermion superconductor  $\text{CeCu}_2\text{Si}_2$ , long-range antiferromagnetic order of the itinerant (spin-density wave) type [35] and superconductivity coexist at slightly expanded unit-cell volume [36], while two different variants of superconductivity may be separated by volume compression [37]. Hence, these superconducting phases are candidates for a variety of novel pairing mechanisms, such as magnetic, quadrupolar and valence fluctuations, while systems lacking inversion symmetry [32] promise novel behavior that requires a description in terms of mixtures of pairing symmetries. Yet, the emergence of novel phases is not restricted to superconductivity but includes also more exotic behavior, like reduced dimensionality [12, 38], phases with partial or “hidden” order [39–41], and deconfinement of excitations [42, 43].

In this volume of *European Physical Journal: Special Topics* we discuss recent results emanating from our research within the Research Unit. The content of this volume is organized as follows. Chapters 1 and 2 present results on rare-earth intermetallic compounds with focus on Ce- and Yb-based systems. Research on quantum criticality in these systems in the past focused on antiferromagnetic QCPs. Recently, however, several ferromagnets were shown to be close to a QPT which can be tuned by changing the ligand composition, e.g.,  $\text{CeFeAs}_{1-x}\text{P}_x\text{O}$ ,  $\text{YbNi}_4(\text{P}_{1-x}\text{As}_x)_2$ ,  $\text{CeTi}_{1-x}\text{V}_x\text{Ge}_3$ . Another new aspect is the investigation of geometrically frustrated rare-earth systems, which has begun only recently. Here the hexagonal compounds  $\text{YbAgGe}$  and  $\text{CePdAl}$  where the Yb or Ce atoms occupy a distorted kagomé lattice in the  $ab$  plane that structurally is repeated in the  $c$  direction, are geometrically frustrated. The main difference is that  $\text{CePdAl}$  exhibits a uniaxial anisotropy with the  $c$  direction as easy direction while  $\text{YbAgGe}$  has a planar anisotropy of the easy  $ab$  plane.  $\text{CePdAl}$  can be driven to a QCP by replacement of  $\sim 15$  at% Pd by Ni. The role of frustration of one-third of the Ce atoms in  $\text{CePdAl}$  is an important issue: does this compound sustain a spin-liquid state at low temperature, as does  $\text{Pr}_2\text{Ir}_2\text{O}_7$  that has likewise been investigated in our Research Unit. The latter system is shown to exhibit quantum critical scaling. For  $\text{CeCu}_{6-x}\text{Au}_x$  where a QCP can be accessed by tuning Au concentration and, for  $x > 0.1$ , hydrostatic pressure  $p$  or magnetic field, the unusual quantum criticality and near-equivalence of  $x$  and  $p$  tuning was shown by elastic and inelastic neutron scattering while field tuning apparently leads to the more conventional universality class of quantum criticality.

Chapter 3 deals with the theory of elastic quantum phase transitions, i.e., transitions where electronic degrees of freedom couple to those of the crystal lattice. While at first sight, this topic seems off the main issue of this volume, it bears considerable relevance to the recently discovered iron-based superconductors where in the so-called 122 classes, e.g.,  $\text{BaFe}_2\text{As}_2$ , antiferromagnetism gives way to superconductivity upon partial substitution of Fe by Co, As by P, or Ba by K. Here, too, a QCP has been suggested to exist beneath the superconducting “dome”. Associated with the destruction of antiferromagnetism with increasing temperature for a given substitutional system, is an orthorhombic–tetragonal transition usually at somewhat higher temperature. Also,  $\text{CeCu}_{6-x}\text{Au}_x$  undergoes a monoclinic–orthorhombic transition at  $T_{mo} \approx 200$  K for  $x = 0$ , where  $T_{mo}$  vanishes for  $x = 0.14$ , i.e., close to the antiferromagnetic QCP. Hence, structural effects are likely to gain more importance for electronically driven QPTs.

Chapter 4 introduces a number of advanced experimental techniques that decisively supported our work, such as UHV-compatible crystal growth, vibrating coil magnetometry at mK temperatures, and neutron Lamor diffraction. Neutron

depolarisation imaging was used to detect inhomogeneities in ferromagnetic single crystals, viz., distributions of Curie temperatures and magnetic-moment magnitudes. In particular, the cluster glass  $\text{CePd}_{1-x}\text{Rh}_x$  has been investigated in detail and yields insights into the nature of spin freezing in the presence of Kondo correlations.

As to transition-metal oxides, Chapter 5 presents a comprehensive experimental investigation of  $\text{La}_y\text{Cu}_3\text{Ru}_x\text{Ti}_{4-x}\text{O}_{12}$  which with varying Ru concentration  $x$  passes from an antiferromagnetic Mott insulator with colossal dielectric constant ( $x = 0$ ) to a  $d$ -electron derived heavy-fermion metal ( $x = 4$ ). The experimental studies comprise measurements of the magnetic susceptibility, specific heat, electrical resistivity, ESR, and  $^{63}\text{Cu}$  NMR. These experiments were supported by DFT calculations to unravel the roles of Ru  $4d$  and Cu  $3d$  magnetic moments. The bulk of the data suggest for  $x = 4$  the presence of a heavy-fermion state with a Kondo temperature of 200 K. On decreasing  $x$ , the electronic properties of the Ru moments evolve from those of a coherent Kondo lattice to a single-ion Kondo behavior. Concomitantly, the Cu moments become successively localized, with the possibility of a QCP at the metal-to-insulator transition for  $x \approx 2.25$  indicated by the simultaneous formation of a spin-glass phase.

In Chapter 6, the development of a functional renormalization group (fRG) approach to quantum magnets is presented in a systematic manner taking into account all two-particle correlations. This approach enables an unbiased analysis of quantum spin models and allows one to compute the RG flow of the wave-vector dependent spin susceptibility. The latter can be employed to deduce instabilities towards ordered states, and the absence thereof indicates regimes of spin-liquid behavior. The fRG approach is applied to two-dimensional Heisenberg models with geometric frustration and used to construct zero-temperature phase diagrams.

Chapter 7 presents an in-depth study of the phase transition in the itinerant ferromagnet  $\text{Sr}_{1-x}\text{Ca}_x\text{RuO}_3$  (SCRO). While the Curie temperature  $T_C$  decreases monotonically with  $x$ , with  $T_C \rightarrow 0$  for  $x \approx 0.7$ , the critical exponents derived from scaling plots of the magnetization isotherms close to  $T_C$  reveal an unusual behavior. While the pure compound  $\text{SrRuO}_3$  exhibits mean-field values of exponents  $\beta$ ,  $\gamma$  and  $\delta$ , these exponents change continuously with  $x$ . For  $x = 0.7$ , quantum critical scaling is observed, again with unusual exponents strongly differing from the Hertz-Millis-Moriya theory. Moreover, an anomalously low dynamical exponent  $z = 1.76$  for an itinerant ferromagnet was directly inferred from the temperature dependence of the specific heat (the HMM theory predicts  $z = 3$  or 4 for a clean or disordered ferromagnet). Epitaxial tensile and compressive strain was imposed on SCRO thin films prepared by pulsed laser deposition. In both cases, a reduction of  $T_c(x = 0)$  and  $|dT_c/dx|$  was found.

Chapter 8 reviews theoretical concepts on critical quasiparticles, i.e., cases where single-particle spectra develop power-law singularities as a result of quantum criticality. Two examples are treated in detail: the first is a pseudogap single-impurity Kondo model where the host of a Kondo impurity exhibits a pseudogap, as experimentally realized in graphene and other semimetals as well as in some unconventional superconductors. The second example concerns a strong-coupling description of magnetic quantum criticality in metals that was developed to understand Kondo and heavy-fermion systems near the onset of antiferromagnetism [28,29], also with the aim to explain the unusual behavior of  $\text{CeCu}_{6-x}\text{Au}_x$  and  $\text{YbRh}_2\text{Si}_2$ . This theory utilizes the concept of Landau quasiparticles, but allows for an energy-dependent quasiparticle residue corresponding to an energy-dependent effective mass. Energy relaxation couples quasiparticles across the critical Fermi surface, not just at “hot spots”. Many of the unusual features of the above compounds can be understood within this model.

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