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Colloquium: Heavy-electron quantum criticality and single-particle spectroscopy
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Angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM) have become indispensable tools in the study of correlated quantum materials. Both probe complementary aspects of the single-particle excitation spectrum. Taken together, ARPES and STM have the potential to explore properties of the electronic Green function, a central object of many-body theory. In this article, we explicate this potential with a focus on heavy-electron quantum criticality, especially the role of Kondo destruction. We discuss how to probe the Kondo destruction effect across the quantum critical point using ARPES and STM measurements. We place particular emphasis on the question of how to distinguish between the signatures of the initial onset of hybridization-gap formation, which is the “high-energy” physics to be expected in all heavy-electron systems, and those of Kondo destruction, which characterizes the low-energy physics and, hence, the nature of quantum criticality. We survey
I. INTRODUCTION

A major objective of quantum materials research is to link observable properties to the nature of quantum mechanical many-body ground states properties and to the characteristics of the excitation spectrum above the ground state. In particular, it aims at understanding and predicting the emergence of novel phases in terms of a minimal set of variables, most notably symmetries and broken symmetries of the ground state and the ensuing classification of the excitation spectrum. The typical energy window commonly involved in the materials of interest can cover a wide range, from a few percent of a meV to several eV. A well-known example is the high-temperature superconductors, which have stimulated research since their discovery more than 30 years ago.

The quest for a unified understanding of different classes of quantum materials has led to the notion of quantum critical points (QCPs) as an economic and powerful way of organizing their phase diagrams (Coleman and Schofield, 2005; Kirchner et al., 2013; Sachdev, 1999; Si and Steglich, 2010). Such continuous zero-temperature phase transitions not only separate different ground states but also give rise to a characteristic behavior; this is the quantum-critical fan, which can extend to comparatively large energies and temperatures, cf. Fig. 1. Within this fan, universal scaling behavior is expected up to some material-specific high-energy cutoff. Among the materials classes that are currently attracting particular interest are the cuprates, iron pnictides, pyrochlore iridates, transition metal dichalcogenides, and heavy-electron compounds. An underlying theme of most if not all these materials classes is the tendency of their charge carriers to localize in response to the large effective Coulomb repulsion experienced by the itinerant degrees of freedom. The tendency towards localization gives rise to the bad-metal behavior of these materials.

In heavy-electron compounds, which most commonly are based on Ce, Yb, and U, the primary degree of freedom is the \( f \) electron. In the lanthanide-based materials, the \( 4f \) electron is localized close to the ionic core as a result of atomic physics and thus has a characteristic energy of order eV. For the same reason, the wavefunction overlap between the \( 4f \) orbitals and the band (or \( c \)) electrons, \( \text{i.e.} \), the hybridization, is typically small. As a result, the \( 4f \) electron appears localized at high temperatures or energies in the entire range of phase space as long as the valency of the lanthanide ion remains near its localized limit. In this regime each \( 4f \) electron contributes a finite amount \( \sim \ln N_f \) to the entropy, where \( N_f \) is the angular momentum degeneracy. \( N_f \) is affected by spin-orbit coupling and the crystal electric fields but as long as \( N_f > 1 \), the spin entropy remains macroscopically large.

Similar arguments in principle apply to actinide-based heavy-electron compounds (Fisk et al., 1985). In contrast to their \( 4f \) counterparts, \( 5f \) orbitals are substantially less localized. As a result, the associated heavy-electron bands are more dispersive, \( f - c \) hybridization is stronger and crystal electric fields are less-well defined. Collectively, these properties frequently lead to more complex behaviors compared to Ce- or Yb-based intermetallics (Lawrence et al., 2011), and so we will use the lanthanide-based heavy-electron materials as exemplary of the essential physics. As temperature is lowered and the ground state is approached, the spin entropy associated with the localized \( 4f \) (\( 5f \)) electron needs to
be quenched. Evidently, the system possesses several options for releasing this entropy, which lead to different ground states. At zero temperature, the system can transition from one ground state to another upon changing coupling constants in the Hamiltonian. At values of these coupling constants where the ground state energy is non-analytic, the system undergoes a quantum phase transition. Experiments, however, are performed at non-zero temperatures. The challenge, then, is how to distinguish the approach to different ground states with only a limited, intermediate temperature window accessible to experiment. This task is made even more difficult given that high-energy properties are largely insensitive to the changes in the coupling constants that take a system through different ground states.

The primary tools for exposing the underlying physics that accompanies the entropy release as the temperature or energy is lowered include spectroscopic methods that can trace excitations over some energy range of interest. For example, spin excitations can be probed with the help of inelastic neutron scattering. Among the various spectroscopic techniques, angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy/spectroscopy (STM) stand out as these allow to most directly trace properties of the one-particle Green function, the basic building block in almost every many-body theory.

We survey and compare recent ARPES and STM experiments performed on quantum critical heavy-electron compounds that are located close to ground state instabilities at the border of magnetism. In particular, we focus on how critical Kondo destruction (Coleman et al., 2001; Si et al., 2001), i.e., the breakdown of Kondo entanglement at zero temperature right at the onset of magnetism, is reflected in ARPES and STM data at elevated temperatures.

The Colloquium is organized as follows. After a brief introduction of quantum criticality in heavy-electron systems, we recapitulate the relation between ARPES and STM measurements and their link with the single-particle Green function. We then discuss recent STM measurements on YbRh$_2$Si$_2$, a heavy-electron antiferromagnet that features a Kondo-destruction QCP as a function of applied magnetic field, before turning to high-resolution ARPES measurements on the Cerium-115 family that consists of CeMIn$_5$ ($M=$Co,Rh,Ir). We close with an outlook on current challenges and future directions. To facilitate the reading, each of Sections II-V ends with a brief summary of the salient points discussed in the section.

II. QUANTUM CRITICALITY

Quantum phase transitions occur at zero temperature and like their finite temperature counterparts, they can be either first order or continuous (Gegenwart et al., 2008; v. Löhneysen et al., 2007; Sachdev, 1999; Si and Steglich, 2010). In contrast to the finite temperature case where thermal fluctuations drive the transition, quantum fluctuations, encoded already at the Hamiltonian level, are responsible for the occurrence of a quantum phase transition. A classical transition can be accessed by vary-
ing the temperature through a critical value $T_c$, while the zero-temperature transition is approached by tuning a non-thermal control parameter, denoted $\delta$ in Fig. 1, to its critical value ($\delta_c$). If the transition is continuous, characteristic, critical scaling ensues in its vicinity which reflects the singular behavior of the ground state wave-function at $\delta_c$. At non-zero temperatures, this singular behavior leads to the quantum critical fan in which characteristic behavior is observed in various quantities below a system-specific cutoff energy, see Fig. 1.

In stoichiometric heavy-electron compounds containing, e.g., Ce or Yb elements, 4f electrons in a partially-filled 4f shell are strongly correlated, provided the Ce or Yb ions possess a valence close to +III. The spin-orbit interaction and the crystal electric field generated by the ligands surrounding the Ce or Yb ion in the crystalline environment reduce the degeneracy of the 4f shell. Most commonly, the lowest-lying atomic 4f-levels correspond to a Kramers doublet. As a result, the 4f electrons behave as a lattice of effective spin-1/2 local moments. This leads to an effective description in terms of the Kondo lattice Hamiltonian:

$$ H_{KL} = H_0 + \sum_{ij} I_{ij} S_i \cdot S_j + \sum_i J_K S_i \cdot s_i^f, \quad (1) $$

where $H_0 = \sum_{k,\sigma} \varepsilon_k c_{k,\sigma}^\dagger c_{k,\sigma}$ describes the conduction electrons. The RKKY interaction $I_{ij}$ and the Kondo coupling $J_K$ typically are antiferromagnetic, i.e., $I_{ij} > 0$, $J_K > 0$. The competition between these two types of interactions lies at the heart of the microscopic physics for heavy-electron systems (Doniach, 1977).

In the heavy-electron compounds described by the Kondo lattice Hamiltonian, Eq. (1), a QCP may arise from tuning the ratio of RKKY to Kondo interactions, which is parameterized by the non-thermal control parameter $\delta = T_{K}^0 / I$. Here, the Kondo scale (for the $N_f = 2$ case) is $T_{K}^0 \approx \rho_0^{-1} \exp\left(-1/\rho_0 J_K\right)$, with $\rho_0$ being the density of states of the conduction electrons at the Fermi energy, whereas $I$ parameterizes the RKKY interaction. This RKKY exchange interaction between the localized moments is mediated by the conduction electron spin density. It is perturbatively generated from the Kondo coupling term $\sim J_K$, resulting in $I_{ij}(J_K)$. In Eq. (1), we have added $I_{ij}$ as an independent exchange interaction to facilitate the discussion of the phase diagram, because tuning the ratio between the explicit $I_{ij}$ and $J_K$ is more convenient. It accesses the quantum phase transition that otherwise would have been induced in the tuning of $\delta$ through the variation of the ratio of $J_K$ to the conduction electron bandwidth $2D \sim 1/\rho_0$. Formally, one may think of Eq.(1) as arising from a more complete starting Hamiltonian through the process of integrating out additional conduction electron degrees of freedom; this procedure results in the explicit $I_{ij}$ term in the effective Hamiltonian of Eq.(1). One needs to be sure that there is no double counting of the explicit and generated contributions to $I_{ij}$, and this can be consistently done in practice. For a technical discussion of this point we refer the reader to Ref. (Si et al., 2005).

On the paramagnetic side, the ground state is characterized by the amplitude of the static Kondo singlets that...
are formed between the local moments and conduction electron spins (Hewson, 1993). For a Kondo-destruction QCP, this static Kondo-singlet amplitude is continuously suppressed when the system approaches the QCP from the paramagnetic side (Si et al., 2014, 2001; Zhu et al., 2003).

As illustrated in Fig. 2(a), the Kondo-destruction energy scale $E_{loc}^{\ast}$ goes to zero as the control parameter $\delta$ approaches the QCP at $\delta_c$ from the paramagnetic side, and the antiferromagnetic order sets in when $\delta$ goes across $\delta_c$. The Kondo destruction goes beyond the Landau framework of quantum criticality. The latter is based on order-parameter fluctuations, which in the present context of antiferromagnetic heavy-electron systems is referred to as a spin-density-wave (SDW) QCP (Hertz, 1976; Millis, 1993; Moriya, 1985). It arises when $E_{loc}^{\ast}$ stays non-zero when decreasing $\delta$ to $\delta_c$, and approaches zero only inside the ordered regime at $\delta < \delta_c$. In this case, the asymptotic quantum critical behavior at energies below $E_{loc}^{\ast}(\delta_c)$ is the same as in the type of phase diagram shown in Fig. 1(b), where $E_{loc}^{\ast}$ is not part of the critical physics.

The Kondo destruction gives rise to a dynamical spin susceptibility which displays unusual scaling at the QCP (Si et al., 2014, 2001). This includes a fractional exponent (Glossop and Ingersent, 2007; Grempel and Si, 2003; Zhu et al., 2003, 2007) in the singular dependence on frequency ($\omega$) and temperature ($T$), and $\omega/T$ scaling. These features have in fact been observed by inelastic neutron scattering measurements on the $5f$ electron system $\text{UCu}_{6-x}\text{Pd}_x$ (Aronson et al., 1995) and the $4f$ electron-based metal $\text{CeCu}_{6-x}\text{Au}_x$ (Schröder et al., 2000). For $\text{CeCu}_{6-x}\text{Au}_x$ at its critical doping $x_c \approx 0.1$, the exponent in the $\omega/T$ scaling analysis (Schröder et al., 2000) was found to be $\alpha = 0.75(5)$, which compares well with the value $\alpha = 0.72-0.78$ calculated at the Kondo-destruction QCP (Glossop and Ingersent, 2007; Grempel and Si, 2003; Zhu et al., 2003, 2007). In the case of a standard SDW QCP, no such $\omega/T$ scaling is expected as this QCP is described by a Ginzburg-Landau functional above its upper critical dimension (Hertz, 1976; Millis, 1993; Moriya, 1985).

In the single-particle excitations, the collapse of $E_{loc}^{\ast}$ implies a sudden reconstruction of the Fermi surface across the QCP. To contrast this picture with the more traditional scenario of an SDW transition (Hertz, 1976; Millis, 1993; Moriya, 1985), where critical fluctuations are tied to nesting properties of the Fermi surface, we will refer to quantum criticality exhibiting critical Kondo destruction as local quantum criticality (Coleman et al., 2001; Pépin, 2007; Senthil et al., 2004; Si et al., 2001). At zero temperature,

- for $\delta > \delta_c$, the Fermi surface is large and is given by the combination of the $4f$ and conduction electrons. A non-zero amplitude of the static Kondo singlet will be referred to as defining a Kondo-screened ground state. It produces a Kondo resonance, which reflects electronic excitations produced by entanglement of the $4f$-moments with the conduction electrons. The Kondo effect is responsible for the large mass enhancement and a small quasiparticle weight $z_L$ [Fig. 2(b)]. There is a small gap for the single-particle excitations at the small Fermi surface.

- for $\delta < \delta_c$, the Fermi surface is small as determined by the conduction electrons alone. This is because, when the amplitude of the static Kondo singlet vanishes, there is no longer a well-defined Kondo resonance. We refer to this state as a Kondo-destruction ground state.

A. High-energy excitations, temperature evolution and mass enhancement

Figure 2(a) also contains a high-energy scale $T_0$ which describes the initial onset of dynamical Kondo correlations. This scale is generally affected by the presence of higher crystal electric field doublets (or quartets) that together form the 4$f$ multiplet (Chen et al., 2017; Cornut and Coqblin, 1972; Kroha et al., 2003; Pal et al., 2019). It is important to note that this scale smoothly evolves across the QCP at $\delta_c$. The development of the hybridization gap is associated with the initial onset of dynamical Kondo correlations, as illustrated in Fig. 3, and will appear on both sides of $\delta_c$.

For $\delta > \delta_c$, the temperature evolution of the physical properties reflects the flow of the system towards the Kondo-screened ground state. For instance, the initial onset of dynamical Kondo correlations results in the Kondo-screened ground state; the single-particle excitations develop into fully coherent heavy-quasiparticles at the large Fermi surface as the temperature is lowered below $T_{FL}$, the crossover temperature into the paramagnetic Fermi-liquid state.

For $\delta < \delta_c$, the initial onset of dynamical Kondo correlations still takes place, even though it does, in the end, not lead to a well-defined Kondo resonance and the Kondo-singlet amplitude vanishes in the ground state. Still, as the temperature is further lowered, vestiges of the Kondo effect will be observed at any non-zero temperature. In particular, the effective mass is a dynamical quantity, measuring the dispersion of the Landau quasiparticles, and is enhanced through the dynamical Kondo effect; further discussions of this point can be found in Refs. (Cai et al., 2019; Si et al., 2014).
The unusual $\omega/T$ scaling of the dynamical spin susceptibility sets apart the QCP featuring critical Kondo destruction from the more traditional QCP based on the Landau framework of order-parameter fluctuations. It means that the dynamical susceptibility $\chi(\omega, T)$, in the regime where scaling operates, can be scaled to depend on $\omega$ or $T$ only through the combination $\omega/T$. Such scaling has been observed in CeCu$_{6-x}$Au$_x$ at its antiferromagnetic QCP (Schröder et al., 1998) and indicated for YbRh$_2$Si$_2$ (Friedemann et al., 2010). Recent measurements of the optical conductivity in thin films of YbRh$_2$Si$_2$ have demonstrated a singular response in the charge sector with an $\omega/T$ scaling (Prochaska et al., 2020). A scaling form of this kind for both the optical conductivity and dynamical spin susceptibility is strongly suggestive of the presence of $\omega/T$ scaling in the single-

**D. Summary of Section II**

For heavy-electron metals, the Landau form of quantum criticality corresponds to an SDW QCP. A new type of quantum criticality has been advanced, in the form of a Kondo-destruction (local) QCP. It goes beyond the Landau framework in that, the critical destruction of Kondo entanglement characterizes the physics beyond the slow fluctuations of the magnetic order parameter. The Kondo destruction is characterized by a new energy scale, $E_{loc}^\ast$, vanishing at the QCP, as illustrated in Fig. 2(a); a sudden reconstruction from large to small Fermi surface as the system is tuned from the paramagnetic side through the QCP, along with a vanishing quasiparticle weight on approach of the QCP from both sides, as illustrated in Fig. 2(b).

**III. ARPES, STM, AND THE SINGLE-PARTICLE GREEN FUNCTION**

The unusual $\omega/T$ scaling of the dynamical spin susceptibility sets apart the QCP featuring critical Kondo destruction from the more traditional QCP based on the Landau framework of order-parameter fluctuations. It means that the dynamical susceptibility $\chi(\omega, T)$, in the regime where scaling operates, can be scaled to depend on $\omega$ or $T$ only through the combination $\omega/T$. Such scaling has been observed in CeCu$_{6-x}$Au$_x$ at its antiferromagnetic QCP (Schröder et al., 1998) and indicated for YbRh$_2$Si$_2$ (Friedemann et al., 2010). Recent measurements of the optical conductivity in thin films of YbRh$_2$Si$_2$ have demonstrated a singular response in the charge sector with an $\omega/T$ scaling (Prochaska et al., 2020). A scaling form of this kind for both the optical conductivity and dynamical spin susceptibility is strongly suggestive of the presence of $\omega/T$ scaling in the single-
sufficiently low $\omega$ the Kondo screening discussed above is related to a pole in velocity. The lifetime of a quasiparticle is given by the form $\Sigma(\omega, k, T)$. This Green function can quite generally be cast into the form

$$G(\omega, k, T) = \frac{1}{\omega - \varepsilon_k - \Sigma(\omega, k, T)},$$

where $\varepsilon_k$ is the bare electron dispersion and the proper selfenergy $\Sigma(\omega, k, T)$ encodes the effects of electron-electron interaction. In a Fermi liquid, this function can be decomposed into two parts,

$$G(\omega, k, T) = G_{\text{coh}}(\omega, k, T) + G_{\text{incoh}}(\omega, k, T),$$

where the incoherent part is non-singular close to the Fermi surface while the coherent part $G_{\text{coh}}$ near $E_F$ describes the quasiparticle contribution and assumes the form

$$G_{\text{coh}}(\omega, k, T) = \frac{z}{\omega - v_F(k - k_F) + i\Gamma(\omega, T)}.$$

The amplitude of the static Kondo screening discussed above is related to a pole in the selfenergy, which in the Fermi liquid regime can at sufficiently low $\omega$ and $T$ be written

$$\Sigma(\omega, k, T) = \frac{a}{\omega - b} + \delta\Sigma(\omega, k, T),$$

where $a$ and $b$ are parameters that capture the strength of Kondo screening and energy of the Kondo resonance, respectively. The pole in $\Sigma$ shift the Fermi momentum from its initial, 'small' value to a new, 'large' value as long as $a \neq 0$. In contrast to the SDW QCP case, where $a \neq 0$ on either side of the critical point, Kondo screening is critically destroyed at the local QCP and $a = 0$ in the antiferromagnetic side with a Fermi surface that is separated by the QCP, in which the Hall coefficient is determined by the conduction electrons alone.

The Hall effect turns out to be a particularly useful quantity in this context as it is a measure of the carrier density on either side of the QCP. This is a consequence of the Fermi liquid nature of the two phases separated by the QCP, in which the Hall coefficient is completely determined by the renormalized dispersion of the single-electron excitations, to the leading order of elastic scattering (quenched disorder) when it is nearly isotropic, and is independent of the quasiparticle weight $z$ or any Landau parameters, regardless of the strength of electron-electron (and electron-phonon) interactions. This can been seen through the kinetic equations of a Fermi liquid, or using the Kubo formalism (Bethe-Matieb and Nozières, 1966; Kohno and Yamada, 1988) and related Feynman-diagrammatic means (Khodas and Finkel’stein, 2003).

The dynamical spin susceptibility $\chi(\omega, k, T)$ and also the optical conductivity $\sigma(\omega, T)$ can be written as convolutions of the Green function with itself and specific vertex functions. On the other hand, ARPES and STM measurements depend directly on $G(\omega, k, T)$. Single-electron spectroscopies are thus, at least in principle, particularly useful in distinguishing between the two types of quantum criticality.

**B. ARPES and STM**

ARPES and STM measurements probe the single-particle spectrum and thus give access to the spectral function $2\pi A(E, k) = -\text{Im} G(\omega = E + i\delta, k, T)$. Although the single-particle Green function appears in the theoretical description of both ARPES and STM, both spectroscopic techniques are complementary. While ARPES directly probes the single-particle excitations as a function of energy and momentum, STM measures a conductance that is local in real space. Both methods are surface sensitive, albeit to different degrees. Furthermore, through variation of the photon energy, the bulk sensitivity of ARPES can be enhanced. By construction, ARPES only probes the occupied part of the single-particle excitation spectrum, which, especially at low temperatures, leads to a sharp cutoff at the Fermi energy (Hüfner, 2003). ARPES therefore measures only part of the full spectral function, i.e. the imaginary part of the retarded Green function below the Fermi energy. A sketch of the spectral function of a Fermi liquid is shown in Fig. 4 (a). It consists of contributions from the quasiparticle pole and an incoherent background. The quasiparticle pole contributes a factor $z$ to the total area beneath the spectral function, while the incoherent background contributes $(1 - z)$ times the total area. $z$ is commonly called the wave-function renormalization factor and it is inversely proportional to the quasiparticle mass in a Fermi liquid. The evolution of $z$ with tuning parameter is plotted schematically in Fig. 2(b) where we see that $z$ vanishes at a local QCP. The position of the quasiparticle pole as a function of momentum defines the dispersion. Per se, ARPES is not able to distinguish between the quasiparticle peak and the incoherent part of the spectral function. Provided the energy and momentum resolution is not a limiting factor, however, the characteristic broadening $\delta k$ of the quasiparticle peak in energy ($\sim |k - E_F|^2$) and with temperature ($\sim T^2$) should be discernible in the momentum distribution curves provided by ARPES. The weight of the quasiparticle peak, in principle, could also be extracted based on the total incoherent part. However, since ARPES only probes occupied states, the complete spectral function is inaccessible. Although, inverse photoemission is in principle able to probe states above
the Fermi energy, it is haunted by rather poor energy resolution.

\[ \delta \epsilon \]

\[ A(E, k) \]

\[ E_F \]

\[ E(k) \]

\[ E_F \]

\[ k_F^L, k_F^S \]

\[ \delta > \delta_c \]

\[ \delta < \delta_c \]

\[ E_F \]

\[ |k_F - E_F|^2 \]

\[ \text{FIG. 4 Electronic characteristics of the Fermi liquid state of a Kondo lattice: (Color online) (a) Spectral density of a Fermi liquid: The quasiparticle pole at \( k_F \) has a characteristic width \( \delta \epsilon \) that increases with the distance from the Fermi energy \( E_F \) as \( \delta \epsilon \sim |E_F - k_F|^2 \). A similar broadening occurs due to finite-temperature effects. The incoherent part of \( A(E, K) \) vanishes at \( E_F \). (b) Quasiparticle dispersion in the Fermi liquid to either side of the QCP: \( k_F^L \) and \( k_F^S \) refer to large and small Fermi surfaces, respectively. Across a Kondo-destruction QCP, the one-electron spectrum is gapless at \( k_F^L \) and develops a small gap at \( k_F^S \) for \( \delta > \delta_c \), and the converse is valid for \( \delta < \delta_c \). The flattening of the dispersion near \( k_F^S \) for \( \delta < \delta_c \) (dashed blue curve) reflects the effective mass enhancement due to the dynamical Kondo effect.} 

In general, when interpreting ARPES spectra, one needs to keep in mind that in order to relate the photoemission intensity to the spectral function, the one-electron dipole matrix element enters, which generally is unknown. In addition, \( k_z \) broadening can be important, where \( k_z \) is the component of the electron momentum perpendicular to the surface, and depends on the photon energy (Strocov, 2003; Wadati et al., 2006).

STM, on the other hand, measures a local-in-real-space conductance. In the linear-response regime, the current-voltage characteristics is related to the local density of states (DOS) of the material under investigation (Bardeen, 1961; Terroff and Hamann, 1985). Therefore, at low bias voltage and temperature, the spatially resolved spectral density can be obtained. As the applied bias voltage shifts the chemical potential at which the local density of states is probed, STM is, unlike ARPES, not confined to only occupied states. It is, however, important to realize that the assumption that the spectral function is independent of the bias voltage has to break down at some sample-dependent value of the bias voltage beyond which the tunneling current can no longer be related to the local density of states. Moreover, the properties of the STM tip, e.g. its DOS, may affect the results.

C. Probing quantum criticality in the Kondo lattice

One of the strongest diagnostic tools to distinguish the local QCP from the SDW QCP are Hall conductivity measurements, as the local QCP manifests itself by a jump of the Hall coefficient across the QCP. This is a consequence of the Hall coefficient being inversely proportional to the carrier density (in the isotropic case or, in general, the curvatures of the quasiparticle dispersion on the Fermi surface) while being independent of the quasiparticle weight \( z \) in a Fermi liquid. The continuous nature of the local QCP is ensured by the vanishing of the quasiparticle weight from either side of the transition. For an SDW QCP, on the other hand, \( z \) will remain non-zero (except at isolated points on the Fermi surface) as \( \delta \) is tuned through \( \delta_c \).

In a Kondo lattice at sufficiently high temperatures, where in first approximation the effect of the RKKY interaction can be ignored, the single-impurity Anderson model is expected to capture the overall physical behavior. This model is given by

\[ H_{\text{AND}} = \sum_{\sigma} \varepsilon f_{\sigma}^\dagger f_{\sigma} + \sum_{k,\sigma} \delta \epsilon c_{k,\sigma}^\dagger c_{k,\sigma} \]

\[ + \frac{U}{2} \sum_{\sigma \neq \sigma'} f_{\sigma}^\dagger f_{\sigma'}^\dagger f_{\sigma} f_{\sigma'} + \sum_{k,\sigma} \left( V_k f_{\sigma}^\dagger c_{k,\sigma} + h.c. \right) \]

where \( f_{\sigma}^\dagger \) (\( f_{\sigma} \)) is the set of local 4f electron creation (destruction) operators of spin projection \( \sigma \). The conduction electron operators are \( c_{\sigma}^\dagger \) and \( c_{\sigma} \). The band structure of the conduction electrons is encoded in \( \varepsilon_{k,\sigma} \), and the matrix element \( V_k \) that mixes 4f and c electrons is referred to as the hybridization. (For the case of the periodic Anderson model in the local moment limit, with the 4f electron occupancy being close to unity, it reduces to the Kondo-lattice model given in Eq. (1) when the charge degrees of freedom of the 4f electrons are projected out (Schrieffer and Wolff, 1966; Zamani et al., 2016a.).)

STM spectra of single-site Kondo problems possess the structure of Fano resonances (Fano, 1961) and depend on the ratio of tunneling into the Kondo impurity vs tunneling into the embedding host. This ratio is encoded in the so-called Fano parameter. Rigorous derivations of the tunneling current and the form of the Fano parameter are given in (Plilhal and Gradzuk, 2001; Schiller and Hershfield, 2000; Ujjasgy et al., 2000). If tunneling occurs predominantly into the conduction band the measured local DOS features the suppression of conduction electron states near the Fermi energy as the Kondo
effect develops. The first scanning tunneling studies of dense Kondo systems appeared about a decade ago (Ay- 
najian et al., 2010; Ernst et al., 2010; Schmidt et al., 2010). The pronounced variation of STM spectra with
the type of surface for Kondo lattice compounds is largely
due to variations in the Fano parameter, see e.g. Fig. 10
for tunneling into differently terminated surfaces. This
has been explicitly demonstrated based on mean field
and dynamical mean field theory approximations for the
Kondo lattice (Benlagra et al., 2011; Figgins and Morr,
2010; Maltseva et al., 2009; Wölfe et al., 2010). At suf-
ciently high temperatures, however, STM spectra in the
vicinity of each Ce moment are expected to be similar to
those for the single-ion Kondo case. Kondo screening is a
predominantly local phenomenon and thus its onset and
evolution are easily probed in real space, i.e., via STM.
For a study of the single-particle Green function in the
paramagnetic Fermi liquid regime of the Kondo lattice
far away from any QCP, in the context of photoemission,
see Refs. (Costi and Manini, 2002; Reinert et al., 2001).
ARPES measurements at similar temperatures, around
and above the energy scale $T_D$, provide the band struc-
ture $\epsilon_k$ of the occupied conduction electron states. A flat
band near the $4f$ electron atomic level $\epsilon$ (see Eq. (6)),
which is far from the Fermi energy, and the formation of a
flat band near the Fermi energy induced by the Kondo
effect at each Ce moment, reflect the $4f$ electron spectral
weight. This can be enhanced using resonant ARPES, see
Chen et al., 2017).

At (sufficiently) low temperatures, in the Fermi liq-
uid regime to either side of the QCP at $\delta_c$ [Fig. 2(a)], the
band structure is shown in Fig. 4(b). For $\delta < \delta_c$, the small
Fermi surface prevails and the band structure is that of
the blue dashed line crossing the Fermi energy $E_F$ at $k_F^S$.
Still, incoherent spectral weight, a vestige of incomplete
Kondo screening, develops but is ultimately gapped near
$k_F$. For $\delta > \delta_c$, the Fermi surface incorporates the $4f$
moments and the Fermi wavevector changes from $k_F^P$
at high temperatures (without the $4f$ moments) to $k_F^P$
at low temperatures. On this side of the QCP, any spectral
weight near $k_F^S$ is due to incoherent single-particle excita-
tions and is ultimately gapped. In other words, for $\delta > \delta_c$
in the Fermi liquid regime the spectral weight near the
blue dashed line of Fig. 4(b) has developed a small gap
at $k_F^S$. This should in principle be directly detectable via
ARPES, provided the energy and momentum resolution
is sufficiently high, and low enough temperatures can be
reached.

On the other hand, the change $k_F^S$ to $k_F^P$ has only
indirect vestiges in real space as the Fermi liquid is a
momentum-space concept. The ensuing difficulties when
tracing single-electron excitations in real space can al-
ready be read off from Fig. 4(b): The Fermi liquid is de-
scribed by a low-energy effective theory and is valid only
in the vicinity of $k_F$. (The spectral function is a more
general concept but it only assumes a form similar to that
shown in Fig. 4(a) in the Fermi liquid regime.) Fourier
transforming the momentum-resolved spectral function
to real space necessarily will sum up spectral weight out-
side of the Fermi liquid regime, where the characteristic
broadening that identifies the quasiparticle peak is no
longer valid.

One possible way forward is to perform quasiparti-
tle interference (QPI) experiments to map out the band
structure near the Fermi energy (Derry et al., 2015; Yaz-
dani et al., 2016). We will return to this possibility in
Section VI. Another is to perform isothermal STM mea-
surements at low temperatures through the phase dia-
gram connecting $\delta < \delta_c$ with $\delta > \delta_c$. While this by itself
does not provide any direct information on the size of the
Fermi surface, it has been recently demonstrated that
such a measurement is able to pick up the critical slowing
down at the Kondo-destruction energy scale (Seiro et al.,
2018), as discussed in the next Section.

D. Summary of Section III

The nature of quantum criticality in heavy-electron
metals is manifested in the evolution of the single-particle
excitations across the QCP. It is natural to probe this
behavior using the ARPES and STM spectroscopies,
given that they are established means of studying single-
particle excitations in metals. However, there is challenge
to this task, mostly because heavy-electron systems have
the distinction that the required energy scale is very low.

For ARPES, this requirement poses a challenge to
access the quantum critical behavior, as is the limi-
tation that even the state-of-the-art setups cannot yet
reach temperatures below about 1 K. Still, ARPES
should be informative in elucidating i) the onset of hy-
bridization gap, which represents the high-energy physics
for the quantum criticality of heavy-electron metals
[see Fig. 2(a)]; and ii) the evolution of the dynamical
Kondo effect as temperature is lowered towards either
the antiferromagnetic/paramagnetic ground state or the
quantum-critical regime.

STM spectroscopy has superb energy resolution and
can reach low temperatures, but more demanding setups
(such as those suited for QPI) are needed to access the
information in the momentum space. Still, STM probes
the single-particle physics in a way that is complementary
to ARPES. In addition, it provides a promising means to
probe the isothermal evolution of single-particle excita-
tions at low temperatures, across the Kondo-destruction
energy scale.

IV. QUANTUM CRITICALITY IN YbRh$_2$Si$_2$

YbRh$_2$Si$_2$ is a prototype system for local quantum cri-
ticality, as illustrated by its temperature $(T)$-magnetic
The temperature vs. field phase diagram of YbRh$_2$Si$_2$ from (Custers et al., 2003). The blue regions mark Fermi liquid behavior, i.e., $\rho(T) - \rho(0) \sim T^2$, while orange indicates the quantum critical area of the phase diagram where $\rho(T) - \rho(0) \sim T^c$, with $c \approx 1$. The continuous line in the quantum critical region is the $E'$-line as derived from thermodynamic and transport properties. (b) Normalized Hall coefficient across the critical field for different temperatures. The inverse of $R_H$ is a measure of the carrier density. The lower $T$, the sharper is the crossover. At $T = 0$ and $B = B_c$, a jump of $R_H$ corresponds to the sudden localization of 4$f$ electrons as $B$ is taken through $B_c$ from above. From (Paschen et al., 2004). (c) Comparison between the isothermal magnetotransport crossover width and the crossover field as specified by the ratio of the FWHM/2 to the crossover inflection field, $B_{int}$. FWHM denotes the full width at half maximum. From (Paschen et al., 2016). (d) The “sharpness” of the crossover: The FWHM vanishes in a linear-in-$T$ fashion indicating a jump of $R_H$ at $B_c$ in the zero-temperature limit.

FIG. 6 Divergence of the A coefficient at the QCP in YbRh$_2$Si$_2$ (Color online): The effective mass diverges on approach to the critical field $B_c = \mu_0 H_c$ from either side of the QCP. Data for $H \parallel c$ have been scaled by a factor of 11. Adapted from Ref. (Gegenwart et al., 2002).

For $B < B_c$, the mass enhancement is also large. This is compatible with the large $C/T$ measured in the antiferromagnetic state, although to reliably extract $\gamma$ is a challenge because of the interference of the large specific-heat feature at the magnetic transition temperature $T_N$. The mass enhancement can be more reliably extracted from the $A$-coefficient, because the effect of the magnetic transition at $T_N$ on the resistivity is relatively minor. The evolution of the $A$-coefficient with $B$ is consistent with the destruction of the Kondo effect as the QCP is approached from the non-magnetic side as well as the dynamical Kondo effect inside the antiferromagnetic phase.

The effect of increasing temperature on the Hall crossover can be quantified in terms of the ratio of the crossover width to the crossover magnetic field. For $T \gtrsim 0.5$ K, the ratio quickly increases towards unity, as shown in Fig. 5(c). This implies that, for such temperatures, YbRh$_2$Si$_2$ falls in the quantum critical fluctuation regime already for zero magnetic field. Thus, the single-electron spectral weight will be significant at both the small and large Fermi surfaces. In this temperature range, significant spectral weight is thus to be expected at the large Fermi surface. The ARPES measurements in YbRh$_2$Si$_2$, which have been reported for $T > 1$K (Kummer et al., 2015), are consistent with this prediction (Paschen et al., 2016).

The temperature evolution of the single-particle excitations in YbRh$_2$Si$_2$ has been studied by STM measurements, which were first carried out down to 4.6 K in Ref. (Ernst et al., 2011) and were recently extended down to 0.3K (Seiro et al., 2018). The lattice Kondo
effect has been identified with the feature at a particular bias, -6meV. The initial onset of this feature takes place near 25K, which corresponds to $T^{\ast}_{0}$, an estimate of $T_{0}$ based on the (spin) entropy $S$ and defined through $S(T^{\ast}_{0}/2) = 0.4R\ln 2$, where $R$ is the ideal gas constant, see Table I. At $B = 0$, the measurements down to $T = 0.3K$ show an increase in the spectral weight [Fig. 7(a)]. This is compatible with the dynamical Kondo effect at non-zero temperatures.

The STM experiments have also determined the isothermal $B$-dependence of the peak width, at the lowest measured temperature $T = 0.3K$. It shows a minimum near $B^{\ast}(T = 0.3K)$, as shown in Fig. 7(b). This observation is consistent with a critical slowing down associated with the Kondo-destruction energy scale that was implicated by magnetotransport and thermodynamic measurements (Friedemann et al., 2010; Gegenwart et al., 2007; Paschen et al., 2004). As such, it represents the most direct evidence so far for the Kondo-destruction quantum criticality based on a single-particle measurement in YbRh$_2$Si$_2$.

Summary of Section IV

We now summarize the salient results on YbRh$_2$Si$_2$ discussed in this section.

High-energy features: STM experiments for YbRh$_2$Si$_2$ at $B = 0$ clearly observe the initial onset of dynamical Kondo correlations around $T_{0}$, a comparatively high temperature, as expected for any Kondo-lattice system regardless of the nature (Kondo-screened or Kondo destruction) of its ground state. This is consistent with the observation of a hybridization gap in the optical spectrum (Kimura et al., 2006). As temperature is further lowered below $T_{0}$, 4f electron spectral weight is expected to develop, and this has also been clearly observed.

Low-energy isotherms: STM experiments for YbRh$_2$Si$_2$ have been carried out as a function of magnetic field at $T = 0.3K$. The Kondo-lattice spectral peak shows a critical slowing-down feature at $B^{\ast}$, the Kondo-destruction scale previously determined from magnetotransport and thermodynamic measurements. As such, the STM results are consistent with local quantum criticality.

V. THE CERIUM-BASED 115 FAMILY: PHOTOEMISSION VS. TUNNELING SPECTROSCOPY

The Cerium-based 115 family is comprised of compounds CeMIn$_5$ where $M = Co, Rh, or Ir$. These compounds are stoichiometric and can be grown in a very clean form. All three compounds crystallize in the HoCoGa$_5$ structure type and thus possess tetragonal unit cells. Due to their proximity to quantum criticality, they have contributed considerably to a global understanding of quantum critical heavy-electron materials (Park and Thompson, 2009; Si, 2006). While CeCoIn$_5$ and CeIrIn$_5$ under ambient conditions are low-temperature superconductors, CeRhIn$_5$ is an antiferromagnet (Movshovich et al., 2001; Petrovic et al., 2001b). In addition, substituted variants, e.g. by Cd substitution on the In site or by substitution of Ce, have also been investigated. For a review, see (Thompson and Fisk, 2012).

A. CeIrIn$_5$

CeIrIn$_5$ at ambient pressure is a heavy-electron superconductor with a transition temperature $T_{c} = 0.40K$ (Petrovic et al., 2001a). After almost two decades of study, the origin of superconductivity remains controversial, though there is growing support for a magnetically-driven mechanism (Chen et al., 2015). In spite of this controversy, superconductivity in CeIrIn$_5$ has attracted recent attention because of its unusual strain tunability (Bachmann et al., 2019).

In contrast to CeCoIn$_5$ or even CeRhIn$_5$, CeIrIn$_5$ has been comparatively less studied by STM and ARPES.
Early ARPES studies led to different conclusions concerning the formation of 4f-derived flat bands (Fujimori et al., 2006, 2003). More recently, a high-resolution ARPES study by Chen et al. mapped out the full band-structure of CeIrIn₅ (Chen et al., 2018a). Interestingly, this study was able to resolve the complete fine structure of both the 4f⁵/₂ and 4f⁷/₂ peaks in the measured energy-distribution curves (EDCs) and momentum-distribution curves (MDCs), which may be a reflection of the comparatively stronger 4f − c hybridization than in CeCoIn₅ (Chen et al., 2018a).

To the best of our knowledge, no scanning tunneling spectroscopy of CeIrIn₅ is available, apart from an STM investigation that focuses on the structural properties of CeIrIn₅ surfaces (Ernst et al., 2010; Wirth et al., 2014). Our main focus in this section will therefore be on CeCoIn₅ and CeRhIn₅.

B. CeCoIn₅

CeCoIn₅ has attracted interest not only for its comparatively high superconducting transition temperature T_c ~ 2.3K but also for an overall phenomenology that resembles that of the underdoped cuprates.

The strong interest in CeCoIn₅ includes early photoemission studies which, however, have led to contradictory results concerning the localized vs. itinerant nature of the 4f electrons (Koitzsch et al., 2008, 2013, 2009). Optical conductivity measurements of CeCoIn₅ show the existence of a hybridization gap at high energies which starts forming at comparatively high temperatures (Burch et al., 2007; Singley et al., 2002) and recent STM studies of CeCoIn₅ are in line with these findings (Allan et al., 2013; Aynajian et al., 2012; Zhou et al., 2013). De Haas-van Alphen (dHvA) studies performed at low temperatures indicate that the Fermi surface of CeCoIn₅ includes the 4f electrons and that therefore the Fermi surface of CeCoIn₅ is large (Settai et al., 2001; Shishido et al., 2002). This conclusion is further corroborated by band-structure calculations that treat the 4f electrons as fully itinerant (Hauke et al., 2010).

CeCoIn₅ under ambient conditions is believed to be located close to an antiferromagnetic QCP of the SDW type and can be tuned to a quantum phase transition by applying a magnetic field (Ronning et al., 2005; Singh et al., 2007; Zaum et al., 2011). The STM study by Aynajian et al. also reported an interesting energy-over-temperature (ω/T) scaling of the local conductance of CeCoIn₅ which sets in around 60K (Aynajian et al., 2012). It is worth recalling that STM probes the single-electron response while the dynamic spin susceptibility measures the magnetic fluctuation spectrum. As ω/T scaling is not expected in the dynamical spin susceptibility at a QCP of the SDW type, the observation of dynamical scaling in the local conductance suggests that the SDW nature applies, at least at ambient conditions, only at asymptotically low energies. In any case, the observation of ω/T scaling does appear to be in line with the linear-in-temperature behavior of the resistivity below 20K (Kummer et al., 2011b) as shown in Fig. 8. Further support in favor of such an ω/T scaling in CeCoIn₅ for the single-particle excitations near the Γ point has come from a recent high-resolution ARPES study (Chen et al., 2017).

The ARPES study by Chen et al. reported the first 3D Fermi-surface mapping of CeCoIn₅ and provided a measurement of the full band structure of this heavy-electron system (Chen et al., 2017). Due to the large temperature range of the study from 14K to 310K, Chen et al. were able to demonstrate that the formation of the 4f-derived flat band sets in at temperatures far above the coherence temperature. This finding is significant, although not entirely unexpected. It demonstrates not only the slow evolution of the Kondo screening process but also the likely role of a Kondo effect on the excited crystal field levels (Chen et al., 2017; Pal et al., 2019). These results contrast with a temperature-independent Fermi surface in YbRh₂Si₂ that was inferred from the state of the art ARPES measurements in a temperature window from 1K to 100K (Kummer et al., 2015). An earlier laser-based ARPES study of YbRh₂Si₂ reported a T-dependent bandstructure below 100K (Mo et al., 2012). In this regard, we note that Chen et al. suggested that ARPES at temperatures larger than 100K may be required in YbRh₂Si₂ due to the large effect of the crystal field levels (Chen et al., 2017). This is consistent with T_{coh} ≈ 160K in this compound, see Table I.

High-resolution ARPES results on CeCoIn₅ that are largely compatible with those of Chen et al. (Chen et al., 2017) have also been reported by Jang et al. (Jang et al., 2017). Though ARPES measurements on heavy-electron compounds have been a major experimental achievement,
It is instructive to analyze the high-resolution ARPES data of Chen et al. for the temperature-dependent band structure of CeCoIn$_5$ in light of the expectation that the Fermi surface of this compound should contain the $4f$ electrons at sufficiently low temperatures. In other words, in terms of Fig.2, CeCoIn$_5$ is located on the $\delta > \delta_c$ side of the $E^\loc_F$ line. Note, however, that Fig.2 presents one type of specific cut through the global heavy-electron phase diagram (Si, 2006) and does not contain CeCoIn$_5$ which is believed to be in close proximity to an SDW QCP.

The red continuous line in the right-hand panel of Fig.9(a) is a fit of the data to the mean field expression for the single level, single band Anderson lattice model. The circles in Fig.9(a) are obtained from the maximum in the EDCs and interpreted as the dispersion of the quasiparticle band. This leads to the value of $k'_F$, where $k'_F$ is the projected zero-temperature Fermi momentum. Such a fit should not be taken too literally. As mentioned above, mean field approaches may in principle be suitable to address the conduction bands at comparatively high energies and temperatures or the low-energy behavior on either the small or the large Fermi volume side in a limited energy range. They do, however, generically fail to describe the crossover from the high to the low energy/temperature behavior. In addition, there is the general difficulty of constructing the correct mean field theory. The effective model for a system like CeCoIn$_5$ should not be the single level, single band Anderson lattice model. Nonetheless, the mean field construction provides an estimate for the change in Fermi wavevector from its high-temperature value $k_F$ to $k'_F$. If $k'_F = k_F$, the $4f$ electrons remain localized and do not contribute to the Fermi volume. As discussed above and also briefly mentioned in Ref. (Chen et al., 2018b), if the Fermi surface of CeCoIn$_5$ expands from $k_F$ to $k'_F$ as the zero-temperature fixed point is approached, the bandstructure in the vicinity of $E_F$ should resemble that sketched in Fig.4(a) and the spectral weight close to $k_F$ needs to vanish as $T \to 0$ so that the incoherent spectral weight at the Fermi energy is gapped out. The detection of such a, possibly very small, gap is challenging in view of the limited energy resolution and $k_z$ broadening effects of ARPES experiments as discussed in Section III. Note that, although it is expected that $k'_F \neq k_F$ in CeCoIn$_5$, results shown in Fig.9(a) are indicative of a spectral weight increase near and at $k_F$ as the temperature is lowered from $T = 60K$ to $T = 17K$. This is most likely not an artifact due to the limited energy resolution of the measurement, indicating that the single-particle excitations are not of the form depicted in Fig.4(a). This is also corroborated by the strange metal behavior, encoded in an approximately linear-in-temperature dependence of the resistivity over a wide temperature window above the superconducting transition.
tion temperature \(T_c \approx 2.3\)K (Petrovic et al., 2001b). In Fig. 8, the temperature dependence of the resistivity \(\rho\) of CeCoIn\(_5\) is shown together with the magnetic resistivity, \(\rho_{\text{m}}\), the difference between the resistivities of CeCoIn\(_5\) and its non-magnetic reference compound LaCoIn\(_5\).

The ARPES study of Chen et al. also indicated the presence of \(\omega/T\) scaling in the EDCs near the \(\Gamma\) point in an intermediate temperature range (Chen et al., 2017). This is reproduced in Fig. 9(c). Already at around 90K, the EDCs multiplied by \(T_{\text{EDC}}\) (with \(x_{\text{EDC}} \approx 0.36\)) collapses on a function depending only on \(\omega/T\). This, however, should not be interpreted as reflecting an \(\omega/T\) scaling of all single-particle excitations, which would imply a strict linear-in-\(T\) behavior of the resistivity. Indeed, this scaling seems to be confined to the vicinity of the \(\Gamma\) point and is absent in the angle-integrated EDCs. Moreover, this peculiar scaling exists only in an intermediate \(T\) range and fails below 20K, as shown in Fig. 9(c). This conclusion appears to be compatible with the findings reported in (Aynajian et al., 2012), taking into account that tunneling into states with small lattice momenta is favored over tunneling into large-momentum states (Huang et al., 2015; da Silva Neto et al., 2013; Tersoff and Hamann, 1985). This demonstrates that ARPES and STM indeed provide information on the single-particle Green function that can be directly compared to each other. It is, however, noteworthy that the temperature exponents accompanying this \(\omega/T\) scaling in the intermediate temperature range from 20K to around 70K differ somewhat depending on the measurement technique. While the STM-derived exponent is \(x_{\text{STM}} \approx 0.53\), the best fit of the ARPES data was obtained for \(x_{\text{EDC}} \approx 0.36\). The difference between the ARPES and STM results is most likely due to the dependence of the STM current on the degree of tunneling into \(f\) and \(c\) electron states. This dependence is encoded in the Fano parameter.

STM studies on CeCoIn\(_5\) (and to a much lesser extent, on CeRhIn\(_5\) and CeIrIn\(_5\)) have been performed by several groups (Allan et al., 2013; Aynajian et al., 2012, 2014; Ernst et al., 2010; Haze et al., 2018; Zhou et al., 2013). In Fig. 10(a) and (b), results are shown for the local tunneling conductance of CeCoIn\(_5\) very lightly doped with mercury (Hg) as well as CeRhIn\(_5\) at different temperatures and on two different surfaces (Aynajian et al., 2012). The Hg-doping induced disorder in CeCoIn\(_5\) generates impurity scattering at the dopant sites which in turn can be systematically used to obtain lattice momentum-resolved information of the local DOS through QPI (Derry et al., 2015). This use of QPI to extract the band structure near \(E_F\) in the low-temperature limit, however, also has potential shortcomings that were already alluded to in Section III.

### C. CeRhIn\(_5\)

CeRhIn\(_5\) is an antiferromagnet with a Néel temperature of \(T_N = 3.8K\) at ambient pressure and has predominantly localized moments (Hegger et al., 2000). Under pressure, \(T_N\) can be suppressed to zero, thus tuning the system to a QCP at a critical pressure \(p_c\). De Haas-van Alphen studies of CeRhIn\(_5\) across the QCP display a clear jump of the dHvA frequencies at \(p_c\), see Fig. 11(a), which implies that the Fermi surface changes discontinuously at the QCP (Shishido et al., 2005). This compound therefore likely hosts a Kondo-destruction QCP at \(\delta_c = p_c\) (\(\delta\) was defined in Section II). This conclusion is further corroborated by an effective mass that tends to diverge on approach to \(p_c\), Fig. 11(b). The latter reflects the vanishing of the wavefunction renormalization factor \(\delta\), depicted in Fig. 2(b), as the QCP is reached from either above or below \(p_c\). In addition, transport measurements

![Fig. 10 Tunneling spectroscopy of CeCoIn\(_5\) and CeRhIn\(_5\) (Color online): local conductance vs applied bias voltage for different temperatures on (a) Ce-terminated surfaces and (b) Co (respectively Rh)-terminated surfaces. The peak-dip-peak structure in conductance of CeCoIn\(_5\) (panel (a)) is typical of a hybridization gap that is not obvious in CeRhIn\(_5\), even at the lowest temperature. (Data taken from (Aynajian et al., 2012)).](image)

![Fig. 11 De Haas-van Alphen measurements on CeRhIn\(_5\) (Color online): (a) Jump of the dHvA frequencies at \(p_c\) indicating a reconstruction of the Fermi surface as the QCP is crossed. (b) Diverging effective mass upon approaching \(p_c\) from above and below (Data taken from (Shishido et al., 2005)).](image)
provide evidence for the Kondo-destruction QCP (Park et al., 2006, 2008). These low-energy quantum critical features are accompanied by experiments measuring high energy properties. The optical conductivity of CeRhIn$_5$ has been reported in (Mena et al., 2005) and shows the formation of a weak hybridization gap at high frequencies as temperature is lowered below the crossover scale $T_0$.

Despite evidence for the existence of a QCP featuring critical reconstruction of the Fermi surface in CeRhIn$_5$ under pressure, APRES and STM investigations of this compound are comparatively rare. This is largely due to difficulties in preparing a suitable surface and to the present impossibility of making these measurements under applied pressure. Early non-resonant ARPES investigations of CeRhIn$_5$ reported that the 4$f$ electrons in this compound are predominantly itinerant (Moore et al., 2002), whereas a second non-resonant ARPES study argued that the 4$f$ electrons are nearly localized (Fujimori et al., 2003).

Scanning tunneling spectroscopy data on Ce- and on Rh-terminated surfaces of CeRhIn$_5$ show no clearly discernible Fano resonances, at least at around 20K (Aynajian et al., 2012), see Fig.10(a) and (b). Interestingly, these results seem incompatible with high-resolution resonant ARPES data, Fig. 12, which point to the development of the 4$f$-electron spectral weight near the Fermi energy, although the weight transfer is much weaker than in CeCoIn$_5$, Fig.12 (Chen et al., 2018b). The spectral weight transfer depicted in Fig.12 for the three bands crossing the Fermi surface also show that, in the temperature range studied, spectral weight transfer occurs mainly near the $\gamma$ band crossing. The difference between the ARPES measurements of (Chen et al., 2018b) and the STM investigation of (Aynajian et al., 2012) is likely due to the increased surface sensitivity of STM. One possibility is that the Kondo temperature at the surface is reduced due to the reduced hybridization; a second is that the cleaving process to obtain suitable surfaces appears to be more problematic for CeRhIn$_5$ and CeIrIn$_5$ than for CeCoIn$_5$. In fact, very recent STM results (Haze et al., 2019) on epitaxially grown CeRhIn$_5$ with well-defined surfaces are very much in line with the ARPES measurements of (Chen et al., 2018b). As in the case of the STM images of YbRh$_2$Si$_2$ [see Fig. 7(a)], these data are consistent with the dynamical Kondo effect taking place near the small Fermi surface.

**D. Further considerations**

We now turn to several additional points that cut across specific Ce-115 families. First, the connection between the different Ce-115 families deserves further studies. As already discussed, isothermal dHvA measurements in CeRhIn$_5$ provide evidence for a sudden Fermi surface reconstruction at $p_c$. Intriguingly, frequencies of dominant $\alpha$ orbits at $p > p_c$ for CeRhIn$_5$ are very similar to those found for the large Fermi surface of CeCoIn$_5$ at atmospheric pressure (Shishido et al., 2005). No Fermi-surface reconstruction has been found in CeCoIn$_5$. It is possible that a sudden Fermi-surface reconstruction can still be found in CeCoIn$_5$ under a new tuning parameter, such as negative pressure. But it may also be that such an effect simply does not exist in CeCoIn$_5$, reflecting its inherent difference from CeRhIn$_5$. For example, the $4f-c$ hybridization is much larger in CeCoIn$_5$ than in CeRhIn$_5$, as evident in their STM spectra (Fig. 10). As argued recently, this difference in overall hybridization can be traced to an anisotropic spatial extent of their 4$f$ orbitals that is set by details of the crystal electric field wavefunction (Sundermann et al., 2019; Willers et al., 2015).

Second, an alternative explanation for the jump of the dHvA measurements across $p_c$ in CeRhIn$_5$ has been proposed in Ref. (Watanabe and Miyake, 2010). It was suggested that the 4$f$-valence fluctuations lead to a rapid valence change near $p_c$ and a strongly first order antiferromagnetic transition. The latter implies a large jump of the order parameter and, thus a large reconstruction of the Fermi surface. So far, however, all experimental evidence points to a continuous transition at $p_c$. In addition, canonical valence-fluctuating systems such as CeSn$_3$ (CePd$_3$) have specific-heat coefficients of 53 (37) mJ/(mol K$^2$), an effective Kondo temperatures of 770 (1120) K (Lawrence et al., 1981). In those cases, the 4$f$-occupancy $n_f$ will be far from 1 or 0 and, consequently, the entropy in the valence-fluctuation sector, which one can estimate by $R [n_f \ln n_f^{-1} + (1 - n_f) \ln(1 - n_f)^{-1}]$, will be a sizable fraction of $R \ln 2$. By contrast, in the quantum critical regime of CeRhIn$_5$, the specific heat coefficient is very large [$\gamma \approx 1.25$ J/(mol K$^2$)] (Park and Thompson, 2009), implying that $n_f$ is exceedingly close.

![FIG. 12 EDCs of CeRhIn$_5$ vs temperature (Color online): The energy distribution curves show the evolution of spectral weight with temperature near the Fermi energy $E_F$ for the three bands that cross $E_F$, labelled $\alpha$, $\beta$ and $\gamma$-band. Data were taken at along the $\Gamma$M direction at $k_{\parallel} = -0.57 \AA^{-1}$ ($\alpha$-band), $k_{\parallel} = -0.3 \AA^{-1}$ ($\beta$-band), and $k_{\parallel} = -0.124 \AA^{-1}$ ($\gamma$-band) and with an uncertainty of $\delta k_{\parallel} \sim 0.03 \AA^{-1}$ for each of the three $k_{\parallel}$-values. (From (Chen et al., 2018b)).](image)
to 1. Thus, the valence-fluctuation sector will have a tiny entropy compared to the nearly $R \ln 2$ entropy in the spin sector, and can hardly be the main driver of the critical fluctuations. In other words, the quantum criticality should primarily be driven by physics of the Kondo limit (Park et al., 2006, 2008). Similar arguments apply to CeCoIn$_5$, CeIrIn$_5$, YbRh$_2$Si$_2$, and CeCu$_{5.9}$Au$_{0.1}$.

E. Summary of Section V

We close this section by summarizing the status of ARPES and STM investigations in Cerium-based 115 systems, as discussed in this section.

By andlarge, theexisting STLand ARPES results on the Cerium-based 115 family are consistent with each other, given the requirements of surface quality and the associated difficulties. The recent high-resolution ARPES investigation of these 115 materials also shows that none of the three compounds follows the low-temperature band-structure expectations of the heavy-electron phenomenology, encoded in Fig. 4(a). This is in line with other measurements, in particular transport measurements, which suggest that none is in a Fermi liquid regime in the range where the ARPES measurements were made. Further, the limited energy resolution of state-of-the-art ARPES is still posing a major challenge in the heavy-electron materials class in which the associated energy scales are typically very small.

High-energy features: Existing ARPES and STM investigations of the 115 members show the initial onset of dynamical Kondo correlations around the $T_0$ temperature scale [Fig. 2(a)] and the concomitant onset of hybridization-gap formation. This is in line with optical conductivity measurements on these compounds (Chen and Wang, 2016). Comparing ARPES and STM data for the same compound gives complementary results that are compatible with each other, and provide evidence for the existence of the hybridization-gap onset scale $T_0$.

Low-energy features: Neither in CeCoIn$_5$ nor CeRhIn$_5$ has ARPES been able to confirm unambiguously the existence of either $k_F^L$ or $k_F^S$. While this may not be surprising due to the limited energy and momentum resolution currently available to ARPES, this finding is also compatible with the absence of Fermi liquid signatures in the investigated temperature range in these compounds; in this range, Fermi liquid signatures are absent as well in transport and thermodynamic properties. Isothermal measurements of dHvA have shown a sudden reconstruction of the Fermi surface across the pressure-induced QCP in CeRhIn$_5$, which provides strong evidence for a Kondo-destruction QCP.

VI. PROGRESS, CHALLENGES AND PROSPECTS

A. High energy Kondo features

We have stressed that the initial onset of dynamical Kondo correlations or hybridization is expected, at the $T_0$ scale of Fig. 2, for all heavy-electron systems regardless of the nature of their ground states.

This scale is evident in YbRh$_2$Si$_2$ by STM and optical conductivity. Similarly, the formation of a hybridization gap was manifested in CeRhIn$_5$ by optical conductivity measurements (Mena et al., 2005) and, recently, by STM measurements (Haze et al., 2019). Also for CeCu$_6$, which is near a QCP that is accessed by introducing Au-substitution for Cu, a hybridization gap has been observed by optical conductivity (Marabelli and Wachter, 1990). This captures the high-energy $T_0$ scale for the onset of hybridization-gap formation [Fig. 2(a)], and indeed evolves smoothly across the critical substitution $x_c = 0.1$ based on photoemission measurements (Klein et al., 2008). The $T_0$ scale is also evidenced by recent time-resolved measurements in the critical substitution range (Pal et al., 2019; Wetli et al., 2018). Here, a terahertz irradiation pumps the system and disturbs the correlations between the local moments and conduction electrons. We can expect the underlying Kondo coupling to produce an initial echo at a time corresponding to $h/(k_B T_0)$. Such a finite time scale is indeed observed both away from and at the QCP. Note that the Fermi liquid scale of CeCu$_6$ is 0.2K (see Table I), which is not accessible by current experiments done at temperature above 1.5K. Nonetheless, it is conceivable that future experiments may probe not only the echo effect at $h/(k_B T_0)$, but also the scaling time regime much beyond $h/(k_B T_0)$.

Table I compiles high-temperature and Fermi liquid energy scales of the heavy-electron compounds discussed in this Colloquium. This table lists both $T_0^{hyb}$, the initial onset of the hybridization gap, and $T_0^{en}$, based on the (spin) entropy $S$. These two high-energy scales can differ by as much as an order of magnitude, which is not too surprising given that the crossover of Kondo lattice systems from the high-temperature incoherent regime towards the low-temperature coherent/quantum critical/ordered regime is rather broad. This regime can be made even broader when the excited crystal field levels are involved. In practice, we propose to use

$$T_0 = \sqrt{T_0^{hyb} T_0^{en}}$$

(7)

as a measure of the crossover Kondo scale. Defined in this way, we can infer from Table I that $T_0$ is $\sim 62K$ in YbRh$_2$Si$_2$, $\sim 50K$ in CeCoIn$_5$, $\gtrsim 25K$ in CeRhIn$_5$, and $\gtrsim 13K$ in CeCu$_6$. 
TABLE I Characteristic high- and low-temperature scales for several heavy-electron compounds located in the vicinity of quantum criticality. Here, $T_{FL}$ is a temperature scale below which the Landau Fermi liquid $T^2$ resistivity is observed. $T_{hyb}^B$ is a ‘high temperature’ estimate for the onset of the hybridization gap, and is estimated from the optical conductivity $\sigma(\omega, T)$ (Figs. 3, 13) with the exception of CeRhIn$_5$, where existing $\sigma(\omega, T)$ data only indicate that $8K < T_{hyb}^B < 300K$ (Mena et al., 2005). $T_{en}^B$ is a ‘low-temperature’ estimate of $T_B$ based on the (spin) entropy $S$, using a procedure for the single-impurity Kondo model with constant conduction electron density of states (for which $T_B = T_{en}^B = T_K^B$). $S(T_{en}^B/2) = 0.4R\ln2 \approx 0.277R$, where $R = 8314.5\ mJ/(mol\ K)$ is the ideal gas constant. (LMT) designates the lowest measured temperature for the electrical resistivity $\rho$.

For YbRh$_2$Si$_2$ at the critical field, $T_{FL}$ has been estimated from $\rho(T)$ and using the result that $\rho(T) \sim T$ down to the LMT of 8mK (Taupin et al., 2015), making the listed value to be an upper bound. The hybridization gap onset in $\sigma(\omega < T)$ is assumed to be the same for $0 \leq B \leq 2T$. Similarly, changes of $T_{en}^B$ are assumed to be small for fields $0 \leq B \leq 2T$, where the specific heat at 20K is only weakly field-dependent for $B \leq 2T$, see (Gegenwart et al., 2006).

For CeRhIn$_5$, the QCP is located at $p_c = 2.35GPa$ and $H_c$ with $\mu_0H_c \lesssim 10T$, see (Park et al., 2008).

(1) This value for $T_{hyb}^B$ has been estimated from the ARPES data of (Chen et al., 2018b) for ambient conditions, see also Fig. 12.

For CeCu$_{6-x}$Au$_x$ ($x_c = 0.1$), $\rho(T)$ is linear in $T$ down to the LMT 20mK; hence, the listed value is also an upper bound. The estimate of $T_{hyb}^B$ in CeCu$_{6-x}$Au$_{0.1}$ is supported by the specific heat data of (Löhneysen et al., 1994).

The references in this table are arranged such that in each row the first reference provides $T_{FL}$, the second contains estimates for $T_{hyb}^B$ and the third provides results on the low-temperature (spin) entropy.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$T_{FL}/K$</th>
<th>$T_{hyb}^B/K$</th>
<th>$T_{en}^B/K$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>YbRh$_2$Si$_2$</td>
<td>0.07</td>
<td>$\sim 160$</td>
<td>$\approx 24$</td>
<td>(Gegenwart et al., 2006; Kimura et al., 2006; Trovarelli et al., 2000)</td>
</tr>
<tr>
<td>YbRh$_2$Si$_2$</td>
<td>$&lt; 0.008$</td>
<td>$\sim 160$</td>
<td>$\approx 24$</td>
<td>(Gegenwart et al., 2006; Kimura et al., 2006; Taupin et al., 2015)</td>
</tr>
<tr>
<td>(B=B$_c$, B</td>
<td></td>
<td>c)</td>
<td>0.135</td>
<td>$\sim 160$</td>
</tr>
<tr>
<td>CeCoIn$_5$</td>
<td>0.14</td>
<td>$\gtrsim 100$</td>
<td>$\approx 25$</td>
<td>(Mena et al., 2005; Paglione et al., 2007; Petrovic et al., 2001b)</td>
</tr>
<tr>
<td>(B=6T)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CeRhIn$_5$</td>
<td>$&lt; 0.15$</td>
<td>$\gtrsim 60^{(1)}$</td>
<td>$\approx 10$</td>
<td>(Chen et al., 2018b; Park et al., 2008; Park and Thompson, 2009)</td>
</tr>
<tr>
<td>CeCu$_6$</td>
<td>0.2</td>
<td>$\gtrsim 40$</td>
<td>$\approx 4$</td>
<td>(Amato et al., 1987; Fischer et al., 1987; Marabelli and Wachter, 1990)</td>
</tr>
<tr>
<td>CeCu$_{6-x}$Au$_x$ ($x_c = 0.1$)</td>
<td>$&lt; 0.02$ (LMT)</td>
<td>$\gtrsim 40$</td>
<td>$\approx 4$</td>
<td>(Fischer et al., 1987; Löhneysen et al., 1994; Marabelli and Wachter, 1990)</td>
</tr>
</tbody>
</table>

B. Isothermal evolution at low temperatures

We have discussed in Section II that, to assess the nature of quantum criticality (Kondo destruction vs. SDW), the isothermal evolution of quasiparticle spectral weight at low temperatures is particularly informative. In YbRh$_2$Si$_2$, this has been done through STM measurements as a function of magnetic field at $T = 0.3\ K$, and the results (Seiro et al., 2018) support the Kondo-destruction scale that had been inferred from magnetotransport and thermodynamic measurements (Friedemann et al., 2010; Gegenwart et al., 2007; Paschen et al., 2004). Further STM measurements at lower temperatures will clearly be instructive. Whether related STM studies can be carried out in 115 systems is at the present time unclear, because the QCP is realized at a relatively large pressure (CeRhIn$_5$) or possibly at negative pressure (CeCoIn$_5$ and CndRhIn$_5$) (Pham et al., 2006; Sidorov et al., 2002). In these latter two cases, applying uniaxial tension might open the possibility of both ARPES and STM studies in a regime that would access their respective QCP. Similar isothermal studies by ARPES appears to be difficult, due to the low temperature that is needed, and also because ARPES cannot be performed in the presence of a magnetic field.

C. Outlook

As discussed above (see Section III), STM is a real space probe and thus generally lacks momentum resolution. It is, however, possible to extract information on the band structure near the Fermi energy using Friedel oscillations that occur near defects (Petersen et al., 2000, 1998). Since STM is a surface probe, QPI only provides a projected bandstructure. Furthermore, the standard approach which is based on Born scattering is known to be insufficient in many cases (Toldin et al., 2013). This limitation notwithstanding, it will be instructive to obtain bandstructure information through Fourier transform-STM on either side of the QCP to interpret QPI spectra in the quantum critical fan of the QCP.

Critical Kondo destruction is accompanied by a partic-
FIG. 13 Optical conductivity $\sigma(\omega, T)$ and evolution of the hybridization gap (Color online): (a) Although the hybridization gap in CeRhIn$_5$ (top) is overall less pronounced than that in the optical conductivity of CeCoIn$_5$ (bottom), the overall features for both compounds are in accordance with general expectations (see Fig. 3): at the highest measured $T$ a broad Drude peak exists out of which a hybridization gap develops below $\sqrt{\omega D}$ as $T$ is lowered (Data taken from (Mena et al., 2005)). (b) The hybridization gap in YbRh$_2$Si$_2$ evolves over a large $T$ region, starting well above 100K. As the data are taken at zero external field, the system is located on the $\delta < \delta_c$ side (see section II) and a Drude peak is therefore expected in $\sigma(\omega, T)$ at small $\omega$ and sufficiently low $T$. (Data taken from (Kimura et al., 2006)). (c) In CeCu$_6$, the optical conductivity develops a hybridization gap at around $\hbar \omega \approx 1$meV below 50K which is flanked towards higher energies by a pronounced peak. (Data taken from (Marabelli and Wachter, 1990)).
warrant et al., 2008; Kirchner et al., 2013; Si and Paschen, 2013; Stewart, 2001). A case in point is CeNiAsO, a heavy-electron relative of the high-Tc Fe-based oxypnictides. Here, the recent neutron scattering experiments provide evidence for a local-moment antiferromagnetic order, whose ordering wavevector is determined by the RKKY interaction mediated by the conduction-electron states near the small Fermi surface (i.e., the Fermi surface of the conduction electrons alone, with the 4f-electrons localized) (Wu et al., 2019), and transport measurements have suggested the possibility of a Kondo-destruction QCP induced by either pressure or P-for-As doping (Luo et al., 2014).

More broadly, there is the question of where to look for new examples of Kondo-destruction criticality. If the f–c hybridization is too strong, magnetic order would more likely be of the SDW type that, when tuned to $T = 0$, would result in a conventional QCP. Thus, weaker hybridization is expected to be a more favorable setting to access a possible Kondo-destruction QCP. Alternatively, a low carrier density gives a small Fermi surface in a Kondo lattice and delays the full development of a Kondo singlet state with decreasing temperature. CeNi$_2$As$_2$−$\delta$ appears to be an example of such a case with evidence of Kondo-destruction quantum criticality (Luo et al., 2015). Finally, in the absence of tuning hybridization or carrier density, increasing frustration, whether through crystal structure or reduced dimensionality, offers an exciting opportunity for discovering new examples (Fritsch et al., 2014; Si, 2006; Tokiwa et al., 2015; Zhao et al., 2019).

VII. CONCLUSION

We have reviewed and compared recent ARPES and STM investigations on heavy-electron materials close to magnetic instabilities with a focus on Kondo-destruction quantum criticality. Real-space and momentum-space spectroscopies combine the power of both methods (Crepaldi et al., 2013; Nicoara et al., 2006) which has proven to be useful in the study of complex materials such as the cuprate high-temperature superconductors (Markiewicz, 2004; Shen and Davis, 2008) and the Kondo insulator SmB$_6$ (Matt et al., 2018). In the context of Cerium- and Ytterbium-based rare earth intermetallics as well as actinide-based compounds, such a combination seems particularly promising given that much of the excitement and interest generated by these materials derives from the interplay of local and itinerant degrees of freedom; while Kondo screening is primarily a local phenomenon, a possible Fermi-volume increase is best addressed in momentum space. Method-specific constraints, limited energy resolution and the need for very low temperatures in order to resolve a Fermi momentum change across a Kondo-destruction quantum critical point pose unique challenges to both ARPES and STM investigations.

On the other hand, combining ARPES and STM results with other measurements, like resistivity and magnetotransport measurements, neutron scattering and optical conductivity investigations, can provide a consistent picture of Kondo-destruction quantum criticality that emerges as a function of some non-thermal tuning parameter and enables one to locate a specific compound in the general phase diagram of heavy-electron materials. This appears particularly relevant in the present context in order to aide a separation of bulk and surface contributions as both ARPES and STM are primarily surface sensitive. The change in symmetry and $c$–$f$ hybridization that typically occurs at surfaces can in Kondo systems substantially modify low-energy scales as compared to their bulk value.

We have emphasized the distinction between the spectroscopic properties that reflect the high-energy Kondo physics, such as the formation of the hybridization gap, and those that are capable of probing the nature of quantum criticality, such as low-temperature isothermal measurements across the quantum critical point. The latter has become possible in the STM measurements of YbRh$_2$Si$_2$, which corroborates the Kondo-destruction energy scale that had been extracted by isothermal magnetotransport and thermodynamic measurements. In CeRhIn$_5$, strong evidence for Kondo destruction in the one-electron excitation spectrum has been provided by quantum oscillation measurements across the critical pressure. It will certainly be instructive to explore further signatures of beyond-Landau quantum criticality in these and other heavy-electron systems.

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