

Emergent Properties of the Periodic Anderson Model: A High-Resolution, Real-Frequency Study of Heavy-Fermion Quantum Criticality

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(Received 5 January 2024; revised 8 August 2024; accepted 17 September 2024; published 7 November 2024)

We study paramagnetic quantum criticality in the periodic Anderson model (PAM) using cellular dynamical mean-field theory (CDMFT), with the numerical renormalization group (NRG) as a cluster impurity solver. The PAM describes itinerant c electrons hybridizing with a lattice of localized f electrons. At zero temperature, it exhibits a much-studied quantum phase transition from a Kondo phase to a Ruderman-Kittel-Kasuya-Yosida (RKKY) phase when the hybridization is decreased through a so-called Kondo breakdown quantum critical point (KB QCP). There, Kondo screening of f spins by c electrons breaks down, so that f excitations change their character from somewhat itinerant to mainly localized, while c excitations remain itinerant. Building on *Phys. Rev. Lett.* **101**, 256404 (2008), which interpreted the KB transition as an orbital-selective Mott transition, we here elucidate its nature in great detail by performing a high-resolution, real-frequency study of various dynamical quantities (susceptibilities, self-energies, and spectral functions). NRG allows us to study the quantum critical regime governed by the QCP and located between two temperature scales, $T_{\text{FL}} < T_{\text{NFL}}$. In this regime, we find fingerprints of non-Fermi-liquid (NFL) behavior in several dynamical susceptibilities. Surprisingly, CDMFT self-consistency is essential to stabilize the QCP and the NFL regime. The Fermi-liquid (FL) scale T_{FL} decreases toward and vanishes at the KB QCP; at temperatures below T_{FL} , FL behavior emerges. At $T = 0$, we find the following properties. The KB transition is continuous. The f quasiparticle weight decreases continuously as the transition is approached from either side, vanishing only at the KB QCP. Therefore, the quasiparticle weight of the f band is nonzero not only in the Kondo phase, but also in the RKKY phase; hence, the FL quasiparticles comprise c and f electrons in both phases. The Fermi surface (FS) volumes in the two phases differ, implying a FS reconstruction at the KB QCP. Whereas the large-FS Kondo phase has a two-band structure as expected, the small-FS RKKY phase unexpectedly has a three-band structure. We provide a detailed analysis of quasiparticle properties of both the Kondo and, for the first time, also the RKKY phase and uncover their differences. The FS reconstruction is accompanied by the appearance of a Luttinger surface on which the f self-energy diverges. The volumes of the Luttinger and Fermi surfaces are related to the charge density by a generalized Luttinger sum rule. We interpret the small FS volume and the emergent Luttinger surface as evidence for f -electron fractionalization in the RKKY phase. Finally, we compute the temperature dependence of the Hall coefficient and the specific heat, finding good qualitative agreement with experiments.

DOI: [10.1103/PhysRevX.14.041036](https://doi.org/10.1103/PhysRevX.14.041036)

Subject Areas: Condensed Matter Physics,
Strongly Correlated Materials

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I. INTRODUCTION

For more than 20 years, quantum criticality in heavy-fermion (HF) systems has remained a subject of ongoing experimental and theoretical research [1–3]. In this paper, we study several open theoretical questions within a canonical model for HF systems, the periodic Anderson model (PAM) in three dimensions. Our new insights are derived from real-frequency results with unprecedented energy resolution at arbitrarily low temperatures. To set the scene, we begin with a survey of the state of the field, focusing, in particular, on aspects relevant for the subsequent discussion of our own results. Readers well familiar with HF physics may prefer to skip directly to Sec. IE, which offers an outline of our own work and results.

A. Heavy-fermion compounds and phenomena

HF compounds are a class of strongly correlated systems. They contain partially filled, localized f orbitals featuring strong local Coulomb repulsion. These localized orbitals hybridize with weakly interacting itinerant conduction bands (c bands) [4]. Particularly interesting is the appearance of a so-called Kondo breakdown (KB) quantum critical point (QCP) [5–7], which is the subject of this work. The most prominent HF compounds featuring a KB QCP derive their f orbitals from Yb or Ce. Examples are YbRh_2Si_2 , $\text{CeCu}_{6-x}\text{Au}_x$, or the so-called Ce-115 family, including CeCoIn_5 or CeRhIn_5 . In the following, we first introduce HF materials, in general, and then focus on experimental and theoretical aspects of the KB QCP.

In HF systems, the hybridization between c and f electrons in combination with the strong local repulsion of f electrons generates Kondo correlations [4]. The strong repulsion effectively leads to the formation of local moments in the f orbitals. These experience an effective antiferromagnetic interaction with the c electrons due to hybridization. This promotes singlet formation between c and f electrons, similar to the Kondo singlet formation in the single-impurity Kondo or Anderson models [8]. At temperatures below some scale T_{FL} , these Kondo correlations ultimately lead to the formation of a Fermi liquid (FL) with quasiparticles (QPs) composed of both c and f electrons. Because of the local nature of the f electrons, these QPs usually have a large effective mass, hence the name heavy fermions.

If Kondo correlations are strong, the f electrons effectively become mobile and contribute to the density of mobile charge carriers. This especially affects the Fermi surface (FS) volume [9–14] and the Hall number n_{H} [15], which are both proportional to the charge density in a FL.

Kondo correlations compete with Ruderman-Kittel-Kasuya-Yosida (RKKY) [16–19] correlations. The RKKY interaction is an effective exchange interaction between f electrons mediated by the c electrons. If the c band is close to half filling, this interaction is antiferromagnetic and

promotes f - f singlet formation. This competes with the aforementioned c - f singlet formation [20].

It is believed that quantum criticality in HF systems is largely driven by this competition between RKKY and Kondo correlations [4,19,20]. Many HF materials can be tuned through a QCP by varying, e.g., magnetic fields, pressure, or doping [1,2]. At these QCPs, a transition from the Kondo-correlated heavy FL to some other, often magnetically ordered, phase occurs. In some HF materials, this quantum phase transition may be understood in terms of a spin density wave (SDW) instability of the heavy FL, i.e., a magnetic transition in an itinerant electron system, described by Hertz-Millis-Moriya theory [21–24]. The antiferromagnetic ordering occurring at this SDW QCP leads to a doubling of the unit cell, but QPs remain intact across the transition. In particular, the charge density involved in charge transport does not change abruptly across the SDW QCP. It is, therefore, expected that the Hall coefficient, which is sensitive to the carrier density, likewise does not abruptly change at such a QCP [6,7]. Furthermore, in $d = 3$ spatial dimensions, such a QCP is essentially described by a ϕ^4 theory above its upper critical dimension. The long-wavelength order parameter fluctuations are, therefore, Gaussian. Because of that, ω/T scaling of dynamical susceptibilities, a clear sign of an interacting fixed point [24], is not expected at a SDW QCP.

Interestingly, however, there is a large class of HF materials which show QCPs not compatible with the spin density wave scenario [1]. Examples include YbRh_2Si_2 [25–28], $\text{CeCu}_{6-x}\text{Au}_x$ [29], CeRhIn_5 [30,31], and CeCoIn_5 [32]. In these materials, experimental observations point toward a sudden localization of the f electrons as the QCP is crossed from the Kondo correlation-dominated heavy FL phase. In contrast to the SDW scenario, QPs seem to be destroyed at this QCP [6,7,28]. It, thus, seems that the Kondo correlations between f and c electrons suddenly break down at the QCP, hence the name KB QCP.

B. Experimental phenomena at the KB QCP

In the following, we briefly summarize some experimental results indicative of the sudden breakdown of Kondo correlations and a corresponding sudden localization of the f electrons. We first focus on results close to $T = 0$ that indicate that the f electrons localize. After that, we discuss some remarkable dynamical and finite-temperature properties of the KB QCP. We focus on universal phenomena and omit material-specific aspects.

Fermi-liquid behavior at low T .—In most HF systems, FL behavior is observed at temperatures below some FL scale T_{FL} , on either side of the KB QCP (on the RKKY side, the FL is often antiferromagnetically ordered). Below T_{FL} , $\sim T^2$ behavior of the resistivity and $\sim T$ behavior of the specific heat is usually observed [27,28,33,34].

FS reconstruction at $T = 0$.—A smoking gun signal of a KB QCP is a sudden reconstruction of the FS at $T = 0$. In a FL, the volume of the FS is connected to the density of charge carriers by Luttinger’s theorem [9,10,35,36]. Thus, a sudden change in the FS volume is also a sign for partial localization of charge carriers. A sudden change in the carrier density has been observed in terms of a sudden jump of the Hall number $n_H \sim 1/R_H$ (where R_H is the Hall coefficient) in many HF materials, including YbRh_2Si_2 [26,37], $\text{CeCu}_{6-x}\text{Au}_x$ [29], and CeCoIn_5 [32]. Further evidence for a FS reconstruction is due to de Haas–van Alphen (dHvA) frequency measurements, with sudden jumps of dHvA frequencies observed in CeRhIn_5 [30,31] and CeCoIn_5 [32,38,39]. More direct access to the FS is provided by angle-resolved photoemission (ARPES) measurements [3], which have by now been performed on several HF compounds like CeCoIn_5 [40–43], CeRhIn_5 [44], YbRh_2Si_2 [45–47], or YbCo_2Si_2 [48]. Close to criticality, ARPES data on HF compounds are to date not quite conclusive yet, since low-temperature scans across the KB QCP (often tuned by magnetic field or pressure) are challenging.

Possible absence of magnetic ordering.—The KB QCP is not necessarily accompanied by magnetic ordering [32,49,50]. In CeCoIn_5 , antiferromagnetic order occurs only well away from the KB QCP inside the RKKY-dominated phase where the f electrons are localized [32]. Furthermore, while for pure YbRh_2Si_2 antiferromagnetic ordering sets in at the KB QCP, this may be changed by chemical pressure [49]. In this way, the jump of n_H can be tuned to occur either deep in the antiferromagnetic phase or deep in the paramagnetic phase. This fact suggests that the KB QCP is not tied to magnetic ordering [49,51–53].

Continuous suppression of the FL scale to zero.—The above-mentioned sudden FS reconstruction suggests that the KB QCP marks a transition between two FL phases with different densities of mobile carriers. Observations on various different materials suggests that this transition is continuous: The FL scale T_{FL} decreases continuously to zero at the KB QCP [28,34], and the QP mass at the QCP diverges in many compounds [29,30,33] from both sides of the transition.

Onset scale for c - f hybridization.—Besides the FL scale T_{FL} , another important scale in HF compounds is the scale below which c - f hybridization begins to build up. We denote this scale by T_{NFL} , for reasons explained later. (It is often also denoted T_0 .) This scale is visible, for instance, in scanning tunneling spectroscopy (STS) experiments [3] or in optical conductivity measurements in terms of a distinct gap in the STS or optical spectra, called the hybridization gap. T_{NFL} is then the temperature below which hybridization gap formation sets in. This scale has been determined in many different HF compounds via STS, for instance, in CeCoIn_5 [54],

CeRhIn_5 [55], and YbRh_2Si_2 [56,57], or via optical conductivity measurements, e.g., in YbRh_2Si_2 [58,59], CeRhIn_5 [60], CeCoIn_5 [60,61], and $\text{CeCu}_{6-x}\text{Au}_x$ [62]. These experiments unambiguously show that T_{NFL} is virtually unaffected by the distance to the KB QCP or whether the f electrons are (de)localized at $T = 0$.

Strange-metal behavior.—Close to the KB QCP, there is a vast scale separation between T_{NFL} and the FL scale, giving rise to an intermediate quantum critical region with NFL behavior. In this NFL region, a linear-in-temperature resistivity is measured universally for all of the above-mentioned materials [25,32,63–66]. Furthermore, YbRh_2Si_2 [25,28], $\text{CeCu}_{6-x}\text{Au}_x$ [29,64], and CeCoIn_5 [67] feature a $\sim T \ln(T)$ dependence of the specific heat. Both observations are in stark contrast to the $\sim T^2$ dependence of the resistivity and $\sim T$ dependence of the specific heat expected from a FL [15]. Recent shot-noise measurements on YbRh_2Si_2 nanowires further indicate the absence of QP in the strange-metal region [68].

Furthermore, dynamical susceptibilities exhibit ω/T scaling [69] at the KB QCP. This was initially observed for the dynamical magnetic susceptibilities in $\text{UCu}_{5-x}\text{Pd}_x$ [70], $\text{CeCu}_{6-x}\text{Au}_x$ [71], and $\text{CeCu}_{6-x}\text{Ag}_x$ [72] and very recently also for the optical conductivities of both YbRh_2Si_2 [63] and $\text{CeCu}_{6-x}\text{Au}_x$ [73]. Note that ω/T scaling is a clear sign for a non-Gaussian QCP [24]; i.e., the critical fixed point is an interacting one. Particularly interesting, too, are the recent observations of ω/T scaling for the optical conductivity, as it shows that the critical behavior is not limited to the magnetic degrees of freedom only but also includes the charge degrees of freedom.

In summary, the following phenomena seem to be almost universal for the KB QCP: (i) a sudden jump of n_H as the KB QCP is crossed at $T = 0$; (ii) a sudden reconstruction of the FS as the KB QCP is crossed at $T = 0$; (iii) a diverging QP mass as the KB QCP is approached from either side at $T = 0$; (iv) a $\ln(T)$ dependence of $\gamma = C/T$ at finite temperatures above the KB QCP; (v) a linear-in- T dependence of the resistivity at finite temperatures above the KB QCP; (vi) ω/T scaling of dynamical susceptibilities at finite temperatures above the QCP. All of these phenomena are not compatible with a magnetic transition in an itinerant electron system. To the best of our knowledge, a full understanding of the KB QCP has not yet been achieved.

C. Theory of the KB QCP: Basics and challenges

Below, we introduce the basic models which have been proposed to describe the essentials of HF physics, including the KB QCP. We further review some basic intuitive, qualitative notions associated with the physics of these models. Then, we give a qualitative overview of the challenges faced when attempting to describe the KB QCP. Concrete approaches for tackling those challenges are reviewed in the next subsection.

The universal physics of HF systems is believed to be described by the PAM:

$$H_{\text{PAM}} = \sum_{i\sigma} \epsilon_f f_{i\sigma}^\dagger f_{i\sigma} + \sum_i U f_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger f_{i\downarrow} + \sum_{i\sigma} V (c_{i\sigma}^\dagger f_{i\sigma} + \text{H.c.}) + \sum_{\mathbf{k}\sigma} \epsilon_{c\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}, \quad (1)$$

which we consider here on a three-dimensional cubic lattice. Here, $f_{i\sigma}$ and $c_{i\sigma}$ annihilate an f or c electron with spin $\sigma \in \{\uparrow, \downarrow\}$ at site i , respectively, $c_{\mathbf{k}\sigma}$ is the discrete Fourier transform of $c_{i\sigma}$, while $\epsilon_f = \epsilon_f^0 - \mu$ and $\epsilon_{c\mathbf{k}} = \epsilon_{c\mathbf{k}}^0 - \mu$, with $\epsilon_{c\mathbf{k}}^0 = -2t \sum_{a=x,y,z} \cos(k_a)$, denote the local f energy and c -band dispersion relative to the chemical potential μ , respectively. The f electrons experience a strong local repulsion U and hybridize with the c electrons with hybridization strength V .

At $U = 0$, the PAM features a two-band structure, with a band gap determined by the hybridization strength V (therefore also often called the hybridization gap). The hybridization thereby shifts the FS such that both f and c electrons are accounted for, and QPs in the vicinity of the FS are hybrid c - f objects. The low-energy physics of the Kondo-correlated FL phase can be thought of as a renormalized version of the $U = 0$ case. The interaction does not destroy the low-energy hybridization between c and f electrons but merely renormalizes it. When approaching the KB QCP from the Kondo-correlated phase, the interaction renormalizes the hybridization to ever smaller values. The point where the hybridization renormalizes to zero and c and f electrons decouple at low energies marks the KB QCP [74]. In the RKKY-correlated phase, c and f electrons have been argued to remain decoupled, so that the FS is that of the free c electrons, with QPs of purely c electron character [3,74]. Surprisingly, we find a somewhat different scenario. Indeed, we show in the present work that even in the RKKY-correlated phase QPs close to the FS are c - f hybridized; see Sec. VIC.

Description of the strange metal.—Arguably the most challenging aspect of the KB QCP is the strange-metal behavior at finite temperatures above the QCP. There are by now various routes to microscopically realize NFL behavior; see Ref. [75] for an extensive recent review. Rigorous results on NFL physics can, for instance, be obtained from Sachdev-Ye-Kitaev models [75] or from impurity models featuring quantum phase transitions [76], e.g., multichannel Kondo impurities [77–80] or multi-impurity models [81–91]. Despite considerable recent progress [92–94], it is to date not fully clarified to what extent known routes to NFL physics connect to the strange-metal behavior observed experimentally in HF materials.

Description of the Fermi surface reconstruction.—Another challenging issue is to explain how the FS can change its size in the first place. The volume of the FS is fixed to be proportional to the particle number by the

Luttinger sum rule [9,10], which involves the combined particle number of the c and f electrons [10]. While the FS volume matches the Luttinger sum rule prediction in the Kondo-correlated phase, this is not the case in the RKKY-correlated phase, where the f electrons seem to be missing from the FS volume. A theoretical description of the KB QCP also needs to correctly describe both the Kondo- and RKKY-correlated phases, which is far from straightforward especially in the latter case. Nevertheless, this aspect of the KB QCP is better understood and intuitively more accessible than the strange-metal physics.

D. Theory of the KB QCP: Approaches

The KB QCP has been subject to many theoretical studies in the past, using both analytical and numerical approaches. Below, we briefly list what has been achieved so far and point out the main issues of the corresponding approaches.

Numerically exact methods.—Significant progress on physical phenomena can be made based on exact solutions obtained with controlled numerical methods. The main advantage is that such an approach is highly unbiased: The bare PAM or the closely related Kondo lattice model (KLM) is solved exactly, potentially in some simplified geometry and usually in some constrained parameter regime. Results have so far been obtained with quantum Monte Carlo (QMC) methods [95–106] and the density matrix renormalization group [107], some of which have reported evidence of a Kondo breakdown [103,104,107]. Even though reports of dynamical or transport properties are scarce, numerically exact studies can provide valuable benchmarks for less-controlled approaches.

Slave-particle theories.—Considerable conceptual progress on KB physics has been achieved using slave-particle approaches [108–113]. These approaches decompose the degrees of freedom of the PAM or the KLM in terms of additional fermionic or bosonic degrees of freedom (often called partons) which are subject to gauge constraints, to ensure the mapping is exact [108–111,113–115]. While the parton decomposition does not render the models solvable, it allows for more flexibility when constructing approximate solutions. For instance, a certain effective low-energy form of the Hamiltonian and some effective dynamics of the gauge fields (which are static after the initial exact mapping) are usually assumed. The effective theory can then be solved by means of approximate methods, for instance, by taking certain large N limits and/or resorting to static mean-field theory.

One of the early successes of slave-particle approaches is the prediction of a RKKY phase in which f electrons are localized and do not contribute to the FS in terms of an orbital-selective Mott phase [110,111,113]. The missing FS volume in the RKKY phase was linked to emergent topological excitations of fractionalized spins [110,111,116], thus coining the term fractionalized FL

(FL*). It was further established that a continuous transition between Kondo- and RKKY-correlated phases can exist [111], including a FS reconstruction accompanied by a sudden jump in the Hall coefficient [117]. Recently, by considering spatially disordered interactions [94,115], it has been possible to account for a strange-metal-like $\sim T \ln T$ resistivity using a slave-particle approach (though to our knowledge, a $\ln T$ correction to the $\sim T$ resistivity has not been reported in YbRh_2Si_2 [118], which shows the most extensive strange-metal regimes of all known HF compounds).

Dynamical mean-field theory.—Dynamical mean-field theory (DMFT) [119,120] and its extensions [121–123] have been successfully used in many studies on HF systems [5,124–132] and have lead to valuable new insights. DMFT methods treat lattice models by mapping them on self-consistent impurity models.

The most prominent approach, which has lead to many insights, is the extended DMFT (EDMFT) approach to KLM [5,124,133–143]. EDMFT maps the KLM on a self-consistent Bose-Fermi-Kondo impurity model and is able to capture a KB QCP due to the local competition between Kondo screening and magnetic fluctuations. One of the main successes of EDMFT is the explanation of ω/T scaling of the dynamical spin structure factor in $\text{CeCu}_{6-x}\text{Au}_x$ [71] at the KB QCP. However, to the best of our knowledge, predictions of other thermodynamic and transport properties, like the linear-in- T resistivity or the $T \ln T$ dependence of the specific heat, are lacking to date. It is, therefore, still unclear whether the EDMFT approach correctly describes the experimentally observed strange-metal behavior. We expect, though, that these gaps in the literature will be filled in future studies.

A downside of the EDMFT approach is that full self-consistency leads to a first-order phase transition [124,144] at $T > 0$. A continuous transition can be recovered by insisting on a featureless fermionic density of states [145], at the cost of giving up self-consistency of the fermionic degrees of freedom, as is routinely done in KB QCP studies using EDMFT [136,137,139]. This downside of EDMFT has lead to the proposal of using two-site cellular DMFT (CDMFT) [121] to study Kondo breakdown physics [126]. Using exact diagonalization (ED) as an impurity solver, it was shown that a two-site CDMFT treatment of the PAM [Eq. (1)] can describe the KB QCP as an orbital-selective Mott transition (OSMT) at $T = 0$ [131,132], where the f electrons localize while the c electrons remain itinerant. Similar studies with QMC impurity solvers [130,146,147] were, however, not able to find signs of a KB QCP in the temperature range studied. Since ED suffers from limited frequency resolution while QMC has trouble reaching low temperatures, it is to date not clear to what extent CDMFT can describe KB physics. The ED study was further not able to establish conclusively whether the transition is first or second order.

E. Overview of our main results

In this work, we revisit the CDMFT approach of Refs. [131,132], now using the numerical renormalization group (NRG) [148,149] as an impurity solver. The NRG is numerically exact, produces spectral data directly on the real-frequency axis, and is able to access arbitrarily low temperatures and frequencies. NRG, therefore, eliminates the limitations of both ED and QMC for studying quantum critical phenomena. In particular, using NRG, we are able to settle the question of whether a two-site CDMFT approximation of the PAM on a simple cubic lattice is capable of describing a KB QCP. Furthermore, leveraging the high resolution of NRG, we find several new features of the RKKY phase which were not accessible to lower-resolution methods. Most important, NRG can explore the quantum critical regime governed by the QCP. We stick to the parameters used in Refs. [131,132] and vary the c - f hybridization strength V and temperature T [cf. Eq. (1) and Sec. II]. Similar in spirit as Ref. [131], we focus on purely paramagnetic solutions by artificially preventing the breaking of spin rotation symmetry. This is motivated by experimental observations which suggest that the KB QCP and magnetic ordering are distinct phenomena [32,49,150]. Here, we decide to focus on the paramagnetic KB QCP and refrain from the additional complications introduced by possible magnetic ordering. The interplay between KB physics and symmetry breaking will be considered in detail in future work.

The main goals of our work are to (i) establish that two-site CDMFT is able to describes a continuous KB QCP; (ii) establish that the QCP is governed by a NFL critical fixed point and characterize its properties; (iii) make progress on our understanding of the fate of c - f hybridization in the vicinity of the QCP; and (iv) explore to what extent CDMFT is able to qualitatively capture the experimental phenomena described in Sec. IB. In the process, we reveal several new aspects of the CDMFT solution. The remainder of this subsection is intended as a summary of our main results and a guide to where to find them in our paper.

1. The KB QCP is a continuous OSMT

Using NRG, we clearly establish that two-site CDMFT describes a continuous KB QCP. First and foremost, this is shown in Sec. III and Fig. 2, where we present the phase diagram obtained with CDMFT-NRG. Here, we establish the presence of two energy scales: the FL scale T_{FL} , below which we find FL behavior, and a NFL scale $T_{\text{NFL}} (\geq T_{\text{FL}})$, which marks the onset of c - f hybridization (cf. Figs. 11 and 12) and below which we find strange-metal-like NFL behavior in the vicinity of the QCP. We find that as V approaches a critical hybridization strength V_c from either side, T_{FL} continuously decreases to zero while T_{NFL} remains nonzero throughout. We identify V_c as the location of a KB QCP. While the FS volume in the Kondo-correlated phase at $V > V_c$ counts both the c and the f electrons, it counts only the c electrons in the

RKKY-correlated phase at $V < V_c$ (cf. Sec. VIII). The KB QCP thereby marks a continuous transition between two FL phases, which differ in their FS volumes (cf. Figs. 13 and 17 and their corresponding sections). The FS reconstruction, which occurs at the KB QCP, is accompanied by the appearance of a *dispersive* pole in the f -electron self-energy. This also implies the appearance of a Luttinger surface [11], the locus of points in the Brillouin zone at which the f self-energy pole lies at $\omega = 0$ (cf. Secs. VI and VII). Reference [151] recently suggested that Luttinger surfaces may define spinon Fermi surfaces. The appearance of a Luttinger surface, therefore, suggests that the f electron is fractionalized (i.e., spinon degrees of freedom emerge at low energies as stable spin-1/2 excitations) in the RKKY phase. In the parlance of Refs. [110,111], this suggests that the RKKY phase is a fractionalized FL (FL*). We will explore this more concretely in future work. Following Refs. [131,132], *we therefore identify the KB QCP as a continuous OSMT, in which the f electrons partially localize while the c electrons do not.*

2. NFL physics at intermediate T close to the QCP

In the vicinity of the QCP, there is a scale separation between T_{FL} and T_{NFL} , giving rise to an intermediate NFL region extending down to $T = 0$ at V_c (cf. Fig. 2). Our evidence that this intermediate region is a NFL region is based on NRG finite-size spectra (Fig. 3), dynamical correlation functions (Fig. 4), and a $\sim T \ln T$ of the specific heat (Fig. 19). In a companion paper [152], we will present a detailed analysis of the optical conductivity, showing ω/T scaling, and the temperature dependence of the resistivity, showing linear-in- T behavior in the NFL regime. Moreover, our KB QCP for the PAM shows several similarities with QCPs found for the two-impurity and two-channel Kondo models (cf. Sec. X). Very surprisingly, we find a stable NFL fixed point even though the effective two-impurity model lacks the symmetries necessary to stabilize a NFL fixed point *without* self-consistency [82–85,87–89,153–156]. We find that the CDMFT self-consistency conditions are essential for the stability of the NFL fixed point (cf. Sec. IV and Appendix A4).

3. Fate of c - f hybridization across the KB QCP

One of our most surprising findings is that low-energy c - f hybridization is not destroyed as the KB QCP is crossed from the Kondo ($V > V_c$) to the RKKY phase ($V < V_c$). We elaborate this in detail in Secs. V–VIII. Indeed, we find that the QP weights for both the c and f electrons are nonzero in *both* $T = 0$ phases adjacent to the KB QCP, vanishing only *at* the KB QCP (Fig. 9). This is one of our most surprising results and in stark contrast to previous work. It implies that, contrary to widespread belief [3], the difference between the Kondo and RKKY phases is not due to nonzero versus zero f -electron QP weight. Instead, it is caused by a sign change of the effective

f -level position close to the center of the Brillouin zone (Fig. 9 and its discussion; Sec. VIII). We connect this sign change to the aforementioned emergence of a dispersive self-energy pole (Fig. 10 and its discussion). It, thus, reflects the orbital-selective Mott nature of the RKKY phase.

The nonzero f -electron QP weight and the dispersive self-energy pole leads to the emergence of a *third* band in the RKKY phase (cf. Figs. 13 and 14 and their discussion). The emergence of a third band in a model constructed from only two bands is our most striking and unexpected result. Its emergence is previewed in Fig. 1, showing the total (c and f) spectral function $A_{\mathbf{k}}(\omega)$: At high frequency ($|\omega| \lesssim 10^{-1}$, measured in terms of the bare c -electron half-band width), its structure remains qualitatively unaltered as the KB QCP is crossed—it seems as if, in both cases, there is a two-band structure characteristic for HF systems. However, as one enlarges further to lower frequencies, it becomes clear that the low-frequency physics is entirely different: A third band emerges in the RKKY phase, and the FS is shifted relative to that in the Kondo phase. The emergence of the third band is intimately tied to the emergence of a Luttinger surface (cf. Secs. VII and VIII). It was concluded in Ref. [151] that Luttinger surfaces may define spinon Fermi surfaces. From that perspective, the third band can be viewed as a direct manifestation of the fractionalization of the f electrons in the RKKY phase: Their spinon degrees of freedom become independent, long-lived excitation, giving rise to the third band. A more concrete investigation will be the subject of future work.

4. Relation to experiment

We repeatedly make contact to experimental observations in our manuscript. In Table I, we provide a list of experimental observations which are qualitatively reproduced by our CDMFT-NRG approach. We include references to the relevant experimental publications and reviews (without claim of completeness) and pointers to where our corresponding CDMFT results appear in this paper.

To conclude our overview, we summarize the structure of the paper: After reviewing CDMFT and NRG in Sec. II, we present and discuss the phase diagram in Sec. III. By detailed discussion of real-frequency dynamical susceptibilities and NRG finite-size spectra, we demonstrate in Sec. IV that T_{FL} vanishes at the QCP and gives rise to NFL behavior at intermediate temperatures below T_{NFL} . After reviewing expectations on single-particle properties in HF systems in Sec. V, a detailed discussion of single-particle properties of the self-consistent two-impurity Anderson model follows in Sec. VI. Using NRG, we show unambiguously that the f electron QP weight is finite in *both* the Kondo- and RKKY-correlated phases. In Sec. VII, we discuss how the single-particle properties of the self-consistent impurity model translate to lattice properties. There, we show that the FS indeed reconstructs across the KB QCP. In Sec. VIII, we discuss the details of this FS reconstruction in the context of

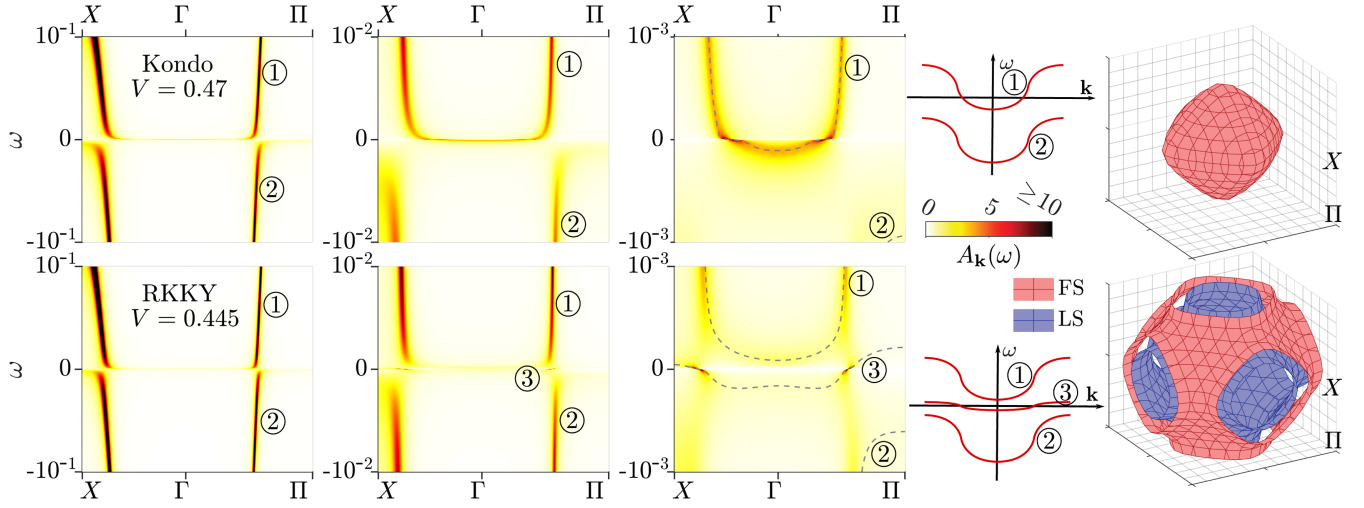


FIG. 1. Three left columns: $\mathbf{k}$ -dependent spectral function $A_{\mathbf{k}}(\omega)$ of the PAM at $T = 0$, enlarging frequencies $|\omega| \leq 10^{-1}$, 10^{-2} , and 10^{-3} . V is chosen close to the KB QCP, in either the Kondo phase (upper row) or the RKKY phase (lower row). At relatively high frequencies (first column), the spectral functions of both phases seem to have a similar structure, involving two bands, labeled ① and ②. However, enlarging to lower frequencies (second and third columns), we find a striking difference: In the RKKY phase, a narrow third band emerges at low frequencies, labeled ③, as indicated by the dashed lines in the third column and in the schematic sketch of the band structure in the fourth column. This difference also leads to different Fermi surfaces, shown on the far right as red surfaces; the blue surface shows the Luttinger surface in the RKKY phase. For more details, see Sec. VII.

Luttinger's theorem and present our results for the Hall coefficient. Section IX shows results on the specific heat. Finally, in Sec. X, we discuss the similarities and differences between the KB QCP in the PAM studied with two-site CDMFT and the impurity QCPs in the two-channel and two-impurity Kondo models. Section XI presents our conclusions and an outlook. We discuss technical details regarding CDMFT and NRG in Appendixes A and B; Appendixes C and D discuss how relevant energy scales are determined; see also Fig. 2 and its discussion.

II. MODEL AND METHODS

Although the CDMFT treatment of the PAM is well established [130–132], we describe it in some detail, to

introduce notation and terminology that is used extensively in subsequent sections.

Before starting, a general remark on notation. Matsubara propagators analytically continued into the complex plane are denoted $G(z)$, with $z \in \mathbb{C}$. The corresponding retarded propagators are $G(\omega^+)$, with $z = \omega + i0^+$, $\omega \in \mathbb{R}$. Ditto for self-energies.

A. Periodic Anderson model

We consider the PAM on a three-dimensional cubic lattice, where each lattice site hosts a noninteracting conduction c orbital and an interacting localized f orbital. The Hamiltonian H_{PAM} is given by Eq. (1). In this work, we set $t = 1/6$ so that the c -electron half-bandwidth is 1 and use the latter as unit of energy. Following the choices of

TABLE I. Left: experimental phenomena associated with heavy-fermion behavior that can be recovered qualitatively from the periodic Anderson model, treated using two-site CDMFT + NRG. Middle: references and reviews (without claiming completeness) which have inferred these phenomena from experimental data. Right: figures in this work or a follow-up paper [152] exhibiting these phenomena.

Phenomenon	Experiment	PAM, CDMFT
Phase diagram	[3,28,34]	Fig. 2
Sudden FS reconstruction	[30–32,38,39]	Figs. 13 and 17
Jump of Hall coefficient	[26,32,37]	Fig. 18, Appendix D
Control parameter dependence of T_{Hall}	[26]	Fig. 2
Divergent QP mass	[28–30,33]	Figs. 9 and 19
$T_{\text{FL}} \rightarrow 0$ at KB QCP	[3,28,34]	Fig. 2
Hybridization gap forms at T_{NFL} ; $T_{\text{NFL}} \neq 0$ at KB QCP	[3,54–62]	Figs. 2, 11, and 12
NFL: $\sim T \ln T$ specific heat	[25,28,29,67]	Fig. 19
NFL: linear-in- T resistivity	[25,32,63–66]	[152]
NFL: ω/T scaling	[63,70–73]	[152]

De Leo, Civelli, and Kotliar [131,132], we set the chemical potential to $\mu = 0.2$, the f -level energy to $\epsilon_f^0 = -5.5$, and the f -level Coulomb repulsion to $U = 10$, so that the system is electron doped. When exploring the phase diagram in Sec. III, we vary the c - f hybridization V and temperature T .

In the momentum representation, the lattice propagators can be expressed as

$$G_{\mathbf{k}}(z) = \begin{pmatrix} z - \epsilon_f - \Sigma_{f\mathbf{k}}(z) & -V \\ -V & z - \epsilon_{c\mathbf{k}} \end{pmatrix}^{-1} = \begin{pmatrix} G_{f\mathbf{k}}(z) & G_{fc\mathbf{k}}(z) \\ G_{fc\mathbf{k}}(z) & G_{c\mathbf{k}}(z) \end{pmatrix}. \quad (2)$$

The matrix elements in the second line in Eq. (2), defined by computing the matrix inverse stated in the first, are given by

$$G_{f\mathbf{k}}(z) = [z - \epsilon_f - \Delta_{f\mathbf{k}}(z) - \Sigma_{f\mathbf{k}}(z)]^{-1}, \quad (3a)$$

$$G_{c\mathbf{k}}(z) = [z - \epsilon_{c\mathbf{k}} - \Sigma_{c\mathbf{k}}(z)]^{-1}, \quad (3b)$$

$$G_{fc\mathbf{k}}(z) = \Sigma_{c\mathbf{k}}(z)G_{c\mathbf{k}}(z)/V = \Delta_{f\mathbf{k}}(z)G_{f\mathbf{k}}(z)/V, \quad (3c)$$

$$\Delta_{f\mathbf{k}}(z) = V^2[z - \epsilon_{c\mathbf{k}}]^{-1}, \quad (3d)$$

$$\Sigma_{c\mathbf{k}}(z) = V^2[z - \epsilon_f - \Sigma_{f\mathbf{k}}(z)]^{-1}. \quad (3e)$$

For brevity, we often omit momentum and/or frequency arguments. The f -hybridization function Δ_f and the one-particle irreducible f self-energy Σ_f describe, respectively, the effects of hybridization and interactions on f electrons. Their effects on c electrons are described by Σ_c , which is not one-particle irreducible and a function of Σ_f . In particular, hybridization leads to so-called hybridization poles in $\Sigma_c(z)$, which, in turn, cause so-called hybridization gaps in the spectral functions $A_c(\omega) = -(1/\pi)\text{Im}G_c(\omega^+)$ (discussed in detail in later sections).

B. Two-site cellular DMFT

We study the PAM using a two-site CDMFT approximation, considering a unit cell of two neighboring lattice sites as a cluster impurity and the rest of the lattice as a self-consistent bath. We choose to focus solely on solutions with SU(2) spin rotation symmetry, U(1) total charge symmetry, and inversion symmetry, i.e., solutions which treat sites 1 and 2 as equivalent. Enforcing these symmetries may induce artificial frustration in some regions of the phase diagram; in particular, they exclude the possibility of symmetry-breaking order such as antiferromagnetism. We have two reasons for nevertheless focusing only on non-symmetry-broken solutions. First, in some materials the antiferromagnetic QCP (AFM QCP) and the KB QCP do not coincide: in YbRh₂Si₂ they can be shifted apart by applying chemical pressure [49], and in CeCoIn₅ they naturally lie apart [32]. This strongly suggests that the onset

of antiferromagnetic order is not an intrinsic property of the KB QCP itself [150]. (The question why the AFM QCP often coincides with the KB QCP is interesting but not addressed in this paper.) Second, in experimental studies, symmetry-breaking order is usually absent in the quantum critical region. It is, therefore, of interest to understand the properties of the KB QCP and the NFL regime above it in the absence of symmetry breaking. Having chosen to exclude symmetry breaking, we refrain from studying the limit $V \rightarrow 0$, where its occurrence is increasingly likely for energetic reasons. Studies of symmetry-broken phases are left for future work.

The CDMFT approximation for the PAM, excluding symmetry breaking, leads to a self-consistent two-impurity Anderson model (2IAM) defined by [130–132]

$$H_{2\text{IAM}} = \sum_{i\sigma} \epsilon_f f_{i\sigma}^\dagger f_{i\sigma} + \sum_i U f_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger f_{i\downarrow} + \sum_{i\sigma} V (c_{i\sigma}^\dagger f_{i\sigma} + \text{H.c.}) - \sum_{ij\sigma} c_{i\sigma}^\dagger (t\tau^x + \mu\mathbb{1})_{ij} c_{j\sigma} - \sum_{ij\lambda\sigma} V_{ij\lambda} (c_{i\sigma}^\dagger a_{\lambda j\sigma} + \text{H.c.}) + \sum_{\lambda i\sigma} E_{\lambda i} a_{\lambda i\sigma}^\dagger a_{\lambda i\sigma}. \quad (4)$$

Here, $i \in \{1, 2\}$ labels the two cluster sites in the “position basis,” $\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, and $\tau^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. There are two spinful baths, with annihilation operators $a_{\lambda i\sigma}$. Both baths hybridize with both cluster sites, whose assumed equivalence implies $V_{ij\lambda} = V_{ji\lambda}$. These couplings, chosen to be real, and the bath energies $E_{\lambda i}$ together define the c -hybridization function

$$(\Delta_c)_{ij}(z) = \sum_{\lambda l} \frac{V_{il\lambda} V_{jl\lambda}}{z - E_{\lambda l}}. \quad (5)$$

The cluster correlators of the 2IAM are 2×2 matrix functions. In the cluster position basis, they are given by

$$G_f(z) = [z - \epsilon_f - \Delta_f(z) - \Sigma_f(z)]^{-1}, \quad (6a)$$

$$G_c(z) = [z + \mu + t \cdot \tau^x - \Delta_c(z) - \Sigma_c(z)]^{-1}, \quad (6b)$$

$$G_{fc}(z) = \Sigma_c(z)G_c(z)/V = \Delta_f(z)G_f(z)/V, \quad (6c)$$

$$\Delta_f(z) = V^2[z + \mu + t \cdot \tau^x - \Delta_c(z)]^{-1}, \quad (6d)$$

$$\Sigma_c(z) = V^2[z - \epsilon_f - \Sigma_f(z)]^{-1}. \quad (6e)$$

These have to be solved self-consistently, by iteratively computing Σ_f via an impurity solver and readjusting the dynamical mean field Δ_c (see Appendix A and Refs. [121,122]).

By SU(2) spin symmetry, the hybridization function Δ_c is spin diagonal and spin independent. The same is true for Δ_f , which is fully determined by Δ_c . Moreover, $1 \leftrightarrow 2$

inversion symmetry ensures that they are linear combinations of $\mathbb{1}$ and τ^x . They can, therefore, be diagonalized independently of ω using the Hadamard transformation $U_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, which maps τ^x to $\tau^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. It is, thus, convenient to correspondingly transform $H_{2\text{IAM}}$, expressing it through the bonding and antibonding operators

$$f_{\pm,\sigma} = \frac{1}{\sqrt{2}}(f_{1\sigma} \pm f_{2\sigma}), \quad c_{\pm,\sigma} = \frac{1}{\sqrt{2}}(c_{1\sigma} \pm c_{2\sigma}). \quad (7)$$

After reperiodization (discussed in Appendix A 3), these modes represent Brillouin zone regions centered at $\Gamma = (0, 0, 0)$ and $\Pi = (\pi, \pi, \pi)$, respectively [157,158]. The labels $\alpha \in \{+, -\}$ on $f_{\alpha\sigma}$ and $c_{\alpha\sigma}$ are, thus, called “momentum” labels. The $\pm$ modes are coupled only via the Coulomb interaction term, which can change the total charge in each channel only by 0 or ± 2 . This implies two $\mathbb{Z}_2$ symmetries: The number parity operators $\hat{P}_{\pm} = \hat{N}_{\pm} \bmod 2$ for the $+$ and $-$ channels are both conserved, with eigenvalues $P_{\pm} \in \{0, 1\}$. Because of the $P_{\pm}$ symmetry, the Green’s functions and self-energies are diagonal in the $\pm$ basis.

C. Numerical renormalization group

We solve the 2IAM using the full-density-matrix NRG [159–161]. Following Wilson [148,149], the bath’s continuous spectrum is discretized logarithmically, and the model is mapped onto a semi-infinite Wilson chain. We represent the impurity f and c orbitals by sites $n = -1$ and 0 , respectively, and the bath by sites $n \geq 1$. The hopping amplitudes for $n \geq 1$ decay exponentially, $\sim \Lambda^{-n/2}$, where $\Lambda > 1$ is a discretization parameter. This energy-scale separation is exploited to iteratively diagonalize the model, adding one site at a time while discarding high-energy states. For a “length- N ” chain (i.e., one with largest site index N), the lowest-lying eigenenergies have spacing $\sim \Lambda^{-N/2}$. By increasing N , one can, thus, resolve ever-lower energy scales.

We set up the Wilson chain in the momentum basis, in which the $\pm$ modes are coupled only via the interaction term on site -1 . To reduce computational costs, we use an interleaved chain [162,163] of alternating $+$ and $-$ orbitals. (Interleaving slightly lifts degeneracies, if present, of the sites being interleaved—but this is not an issue here, since the $\pm$ modes are nondegenerate due to τ^z contributions to hopping terms. Indeed, we have double-checked, especially close to the QCP, that our interleaved results are reproduced when using a computationally more costly standard Wilson chain geometry.) We exploit the SU(2) spin, U(1) charge, and both $\mathbb{Z}_2$ parity symmetries in our NRG calculations using the QSpace tensor library [164,165], further reducing computational costs. Together with interleaving, this allows us to achieve converged data using a fairly small NRG discretization parameter of $\Lambda = 3$ while keeping

$N_{\text{keep}} \leq 25000$ SU(2) multiplets. Because spectra close to the QCP can be quite sensitive to z shift (see Ref. [161] for the definition of z), we refrain from z averaging, i.e., use only the logarithmic grid of $z = 1$.

For further methodological details on achieving DMFT self-consistency and reperiodization, see Appendix A; for further information on NRG, see Appendix B.

III. PHASE DIAGRAM

Based on a detailed study of the dynamical properties of various local operators, described in Sec. IV B, we have established a phase diagram for the PAM, shown in Fig. 2(a). While its generic structure has been known for a long time [4,20,51–53,110,150], we reach orders of magnitude lower temperatures and better energy resolution than previously possible and characterize the various regimes through a detailed analysis of real-frequency correlators. We first focus on zero temperature, involving two distinct phases separated by a QCP, then discuss finite-temperature behavior, involving smooth crossovers between several different regimes.

Zero temperature.—At $T = 0$, we find two phases when tuning V , separated by a QCP at $V_c = 0.4575(25)$. For $V > V_c$, we find a Kondo phase, where the f and c bands are hybridized to form a two-band structure and the correlation between f -orbital local moments in the effective 2IAM is weak, as shown by the blue line in Fig. 2(b) and discussed below. This phase is a FL, with a Fermi surface (FS) whose volume satisfies the Luttinger sum rule [9,10] when counting both the f and c electrons (see Fig. 17, to be discussed later). We henceforth call a FS *large* or *small* if its volume accounts for both c and f electrons or only c electrons, respectively. The Kondo phase is adiabatically connected to the case of $U = 0$ and $V > 0$ and is, thus, a normal FL.

For $V < V_c$, we find a RKKY phase, where the local moments at nearest neighbors have strong antiferromagnetic correlations [see the blue line in Fig. 2(b) and its discussion below], while SU(2) spin symmetry is conserved by construction. This phase, too, is a FL, with a small FS accounting only for c electrons. While this phase, thus, appears to violate Luttinger sum rule, it still obeys a more general version of that rule [11,36,110]: We find a surface of poles of $\Sigma_{f\mathbf{k}}(z = 0)$ (Luttinger surface), which, together with the FS, accounts for the total particle number. We discuss this in detail in Secs. VII and VIII. In the RKKY phase, the FS coincides with the FS of the free c band, but the effective band structure differs from that of a free c band: There are *three* bands (see Figs. 1 and 13 below, to be discussed later), including a narrow QP band crossing the Fermi level. This narrow QP band is responsible for the FL behavior we observe in the RKKY phase. Based on Ref. [151] revealing that Luttinger surfaces may define spinon Fermi surfaces, we conjecture that the RKKY

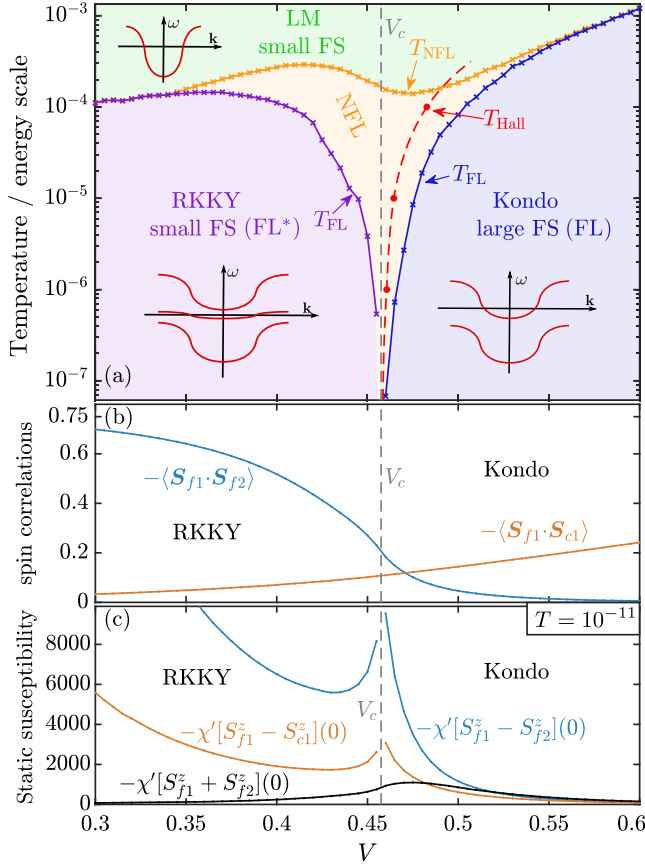


FIG. 2. (a) Paramagnetic phase diagram of the PAM as a function of the c - f hybridization V and temperature T (on a log scale). At $T = 0$, there are two distinct phases, the RKKY phase and the Kondo phase, separated by a QCP at $V_c = 0.4575(25)$. At $T > 0$, we find four different regimes, labeled LM (local moment), RKKY, Kondo, and NFL, connected via smooth crossovers. For the first three, associated band structures are depicted schematically in insets. (See Figs. 1 and 13–15 for the CDMFT band structure results.) The crossovers are characterized by the temperature scales T_{NFL} (orange solid line) and T_{FL} (purple and blue solid lines) below which NFL and FL behaviors emerge, respectively. The scales $T_{\text{NFL}}(V)$ and $T_{\text{FL}}(V)$ are determined by analyzing dynamical susceptibilities of the self-consistent 2IAM at $T = 0$, as explained in Sec. IV B and Appendix C. The red dots marked T_{Hall} (and the guide-to-the-eye red dashed line) indicate how the crossover from a large FS in the Kondo phase to the small FS in the RKKY phase evolves with temperature. T_{Hall} is determined by analyzing the Hall coefficient similar to Ref. [26] (see Fig. 18 and Appendix D). (b) Equal-time intersite f - f spin correlation $\langle \mathbf{S}_{f1} \cdot \mathbf{S}_{f2} \rangle$ and local c - f spin correlation $\langle \mathbf{S}_{f1} \cdot \mathbf{S}_{c1} \rangle$. (c) Static susceptibilities for the total f spin $S_{f1}^z + S_{f2}^z$, the intersite staggered f - f spin $S_{f1}^z - S_{f2}^z$, and the local staggered f - c spin $S_{f1}^z - S_{c1}^z$ of the effective 2IAM, all plotted at $T = 10^{-11}$ as a function of V .

phase is a fractionalized FL (FL*) [110,111]. We will explore this conjecture in more detail in future work.

Figure 2(b) shows the equal-time f - f intersite spin correlators $\langle \mathbf{S}_{f1} \cdot \mathbf{S}_{f2} \rangle$ and the local c - f $\langle \mathbf{S}_{f1} \cdot \mathbf{S}_{c1} \rangle$ of the

effective 2IAM at $T = 10^{-11}$, plotted as functions of V . $\langle \mathbf{S}_{f1} \cdot \mathbf{S}_{f2} \rangle$ smoothly evolves from $\simeq 0$ at $V = 0.6$ deep in the Kondo phase to $\simeq -0.75$ deep in the RKKY phase. On the other hand, the absolute value of $\langle \mathbf{S}_{f1} \cdot \mathbf{S}_{c1} \rangle$ smoothly decreases when going from the Kondo phase to the RKKY phase. This shows that the Kondo phase is dominated by local c - f correlations, indicative of spin screening, and has only weak nonlocal f - f spin correlations. By contrast, the RKKY phase is dominated by nonlocal antiferromagnetic f - f spin correlations and has only weak local c - f correlations. Note that equal-time spin correlations of the self-consistent 2IAM are continuous across the QCP and do not show nonanalytic behavior at V_c . Rather, we see below that the QCP is characterized by a zero crossing of the effective bonding f level (see discussion of Fig. 9 below). This is accompanied by a sharp jump of the FS and the appearance of a dispersive pole in the f self-energy (see the discussion of Figs. 13, 14, and 17 below).

Figure 2(c) shows static susceptibilities for the total f -spin $S_{f1}^z + S_{f2}^z$, the staggered intersite f - f -spin $S_{f1}^z - S_{f2}^z$, and the staggered local f - c -spin $S_{f1}^z - S_{c1}^z$, plotted versus V at $T = 10^{-11}$. [Susceptibilities are defined in Eq. (8) below.] While the total f -spin susceptibility evolves smoothly across the QCP, both staggered susceptibilities, which are related to intersite f - f singlet formation and Kondo singlet formation, respectively, show singular behavior near the QCP. This suggests that the latter arises from a competition between intersite f - f singlet formation and Kondo singlet formation. Furthermore, both staggered susceptibilities become very large deep in the RKKY phase, reflecting the tendency of this phase toward antiferromagnetic order.

Finite temperature.—When the temperature is increased from zero, both FL phases cross over, at a V -dependent scale $T_{\text{FL}}(V)$, to an intermediate NFL critical regime, characterized by the absence of coherent QP (see Fig. 15 and Sec. IV A). Importantly, the scale $T_{\text{FL}}(V)$ vanishes when V approaches V_c from either side; thus, the NFL regime extends all the way down to $T = 0$ at the QCP. With increasing temperature, the NFL regime crosses over, at a scale $T_{\text{NFL}}(V)$ [larger than $T_{\text{FL}}(V)$], to a local moment (LM) regime, which is adiabatically connected to $V = 0$. There, free c electrons are decoupled from f orbital local moments, resulting in a one-band structure. The crossover scales T_{NFL} and T_{FL} can be extracted from an analysis of dynamical susceptibilities at $T = 0$ (see Sec. IV B and Appendix C). To make qualitative contact with experimental results on YbRh_2Si_2 [26], we also show a scale T_{Hall} , which marks the crossover between large and small FS based on analyzing the Hall coefficient in a way which closely resembles the analysis done in Ref. [26] (see Fig. 18 and Appendix D). In qualitative agreement with the experimental data in Fig. 3 in Ref. [26], T_{Hall} depends on the tuning parameter (V in our case, B field in Ref. [26]) and bends toward the Kondo side of the phase diagram.

IV. TWO-STAGE SCREENING

The presence of two crossover scales, T_{NFL} and T_{FL} , implies that the evolution, with decreasing energy, from unscreened local f moments to a fully screened FL regime evolves through two stages. In this section, we study this evolution from two perspectives, focusing first on NRG finite-size spectra (Sec. IV A) and then on the dynamical properties of various local susceptibilities at $T = 0$ (Sec. IV B).

A. Finite-size spectra

We begin our discussion of the physical properties of the different regimes shown in Fig. 2(a) by studying NRG energy-level flow diagrams of the self-consistent effective 2IAM. Such diagrams show the (lowest) rescaled eigenenergies $\Lambda^{N/2} E_i(N)$ of a length- N Wilson chain as a function of the energy scale $\Lambda^{-N/2}$. Conceptually, the $E_i(N)$ form the finite-size spectrum of the impurity plus bath in a spherical box of radius $R_N \propto \Lambda^{N/2}$, centered on the impurity [148,166]: With increasing N , the finite-size level spacing, $\sim 1/R_N$, decreases exponentially. The resulting flow of the finite-size spectrum is stationary (N independent), while $\Lambda^{-N/2}$ lies within an energy regime governed by one of the fixed points, but changes when $\Lambda^{-N/2}$ traverses a crossover between two fixed points. We label eigenenergies by the conserved quantum numbers $(Q, 2S, P_+, P_-)$, where Q is the total charge relative to the ground state, S the total spin, and $P_{\pm} \in \{0, 1\}$ the number parity eigenvalues in the $\pm$ sectors.

Kondo phase.—Figure 3(a) shows the NRG flow diagram for the self-consistent 2IAM at $T = 0$ and $V = 0.46$, which is in the Kondo phase close to the QCP. The ground state has quantum numbers $(0, 0, 0, 0)$. As already indicated in the discussion of Fig. 2(a), we find a FL at low-energy scales and a NFL at intermediate-energy scales. In the FL region below $T_{\text{FL}} > V_c$, the low-energy many-body spectrum can be constructed from the lowest particle and hole excitations. These come with quantum numbers $(\pm 1, 1, 1, 0)$ and $(\pm 1, 1, 0, 1)$ for the bonding and antibonding channel, respectively, with the $P_{\pm}$ quantum numbers identifying the channel containing the excitation. The low-energy many-body spectrum can then be generated by stacking these single-particle excitations, leading to towers of equally spaced energy levels, characteristic for FL fixed points [149]. This directly shows that the Kondo phase is a FL featuring a QP spectrum at low energies.

At intermediate-energy scales between T_{FL} and T_{NFL} , the effective 2IAM flows through the vicinity of a NFL fixed point. Our calculations strongly suggest that this NFL fixed point also governs the low-energy behavior of the QCP at $T = 0$ and $V = V_c$. We, thus, identify this NFL fixed point with the critical fixed point of the QCP in the two-site CDMFT approximation. As pointed out in subsequent sections and summarized in Sec. X, this fixed point shares

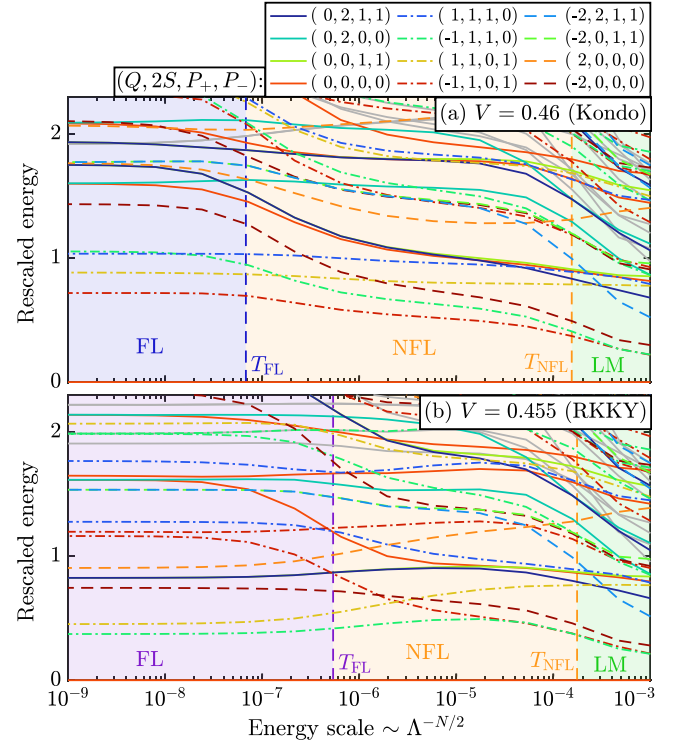


FIG. 3. NRG flow diagrams for the self-consistent effective 2IAM at $T = 0$, in (a) the Kondo phase at $V = 0.46$ and (b) the RKKY phase at $V = 0.455$, both close to the QCP. The rescaled eigenenergies are plotted as functions of the energy scale $\Lambda^{-N/2}$, for odd values of N . The vertical dashed lines indicate the scales T_{FL} and T_{NFL} . Quantum numbers for selected energy levels are indicated in the legend. Energy levels with total charge $|Q| = 0, 1$, or 2 are shown using solid, dash-dotted, or dashed lines, respectively.

several similarities with the NFL fixed points of the two-channel Kondo model (2CKM) [77,78,167–171], the two-impurity Kondo model (2IKM) [87–89,153–156], and the 2IAM *without* self-consistency [82–85], which is closely related to the 2IKM. One may, therefore, argue that it is not surprising to find such a NFL fixed point also in a self-consistent solution of the 2IAM. On the other hand, the NFL fixed points of the 2IKM and the 2IAM are known to be *unstable* to breaking $\pm$ mode degeneracy or particle-hole symmetry [82,83,86,89]. Furthermore, for the 2IKM and the 2IAM, the RKKY interaction has to be inserted by hand as a direct interaction, because if $\pm$ mode symmetry and particle-hole symmetries are present (as needed to make the NFL fixed point accessible), then these symmetries prevent dynamical generation of an antiferromagnetic RKKY interaction [172]. It has, therefore, been argued that this NFL fixed point is artificial and not observable in real systems [172–174]. From this perspective, the behavior found here for our effective *self-consistent* 2IAM is indeed unexpected and remarkable: Although it lacks particle-hole symmetry or $\pm$ mode

degeneracy and we do not insert the RKKY interaction by hand, it evidently *can* be tuned close to a QCP controlled by a NFL fixed point with 2IKM-like properties.

We note in passing that self-consistency is crucial to reach the NFL fixed point—we checked that naively tuning V without self-consistency leads to a continuous crossover without a QCP (see also Appendix A 4 for more details). It is not entirely clear to us why the self-consistency stabilizes the NFL fixed point, though we suspect the Luttinger sum rule [9,10] to play a crucial role. We discuss the Luttinger sum rule in more detail in Sec. VIII. We also remark that, for the non-self-consistent 2IKM mentioned above, frequency-independent or only weakly frequency-dependent hybridization functions were used in the analyses of prior studies which concluded that its NFL fixed requires some special symmetries to be stable. By contrast, for the self-consistent 2IAM studied here, the self-consistent hybridization functions acquire a rather strong frequency dependence in the vicinity of the KB QCP and appear to become singular at the QCP itself (see Appendix A 4). Regarding the energy level structure of the self-consistent 2IAM, we did *not* find obvious similarities to the NFL fixed point of the 2IKM; i.e., the level structure seems quite different.

RKKY phase.—Figure 3(b) shows the NRG flow diagram for the self-consistent 2IAM at $V = 0.455 < V_c$, which is in the RKKY phase close to the QCP. Again, a NFL is found at intermediate energies and a FL fixed point at low energies. This directly establishes that the RKKY phase, too, is a FL described by a QP spectrum at low energies. However, note that, close to the QCP, the level structure of the FL fixed point in the RKKY phase ($V = 0.455$) is quite different from that in the Kondo phase ($V = 0.46$). This suggests that these Fermi liquids are not smoothly connected. Indeed, we see in Sec. VIII that their FS volumes differ. This implies different scattering phase shifts and, hence, different NRG eigenlevel structures, consistent with the fact that the level structures in Figs. 3(a) and 3(b) differ strikingly in the FL regimes on the left.

B. Dynamical susceptibilities

The characteristic level structure of RG fixed points governs the behavior of dynamical properties at $T = 0$, causing striking crossovers at the scales T_{FL} and T_{NFL} . In this section, we extract these from the dynamical susceptibilities of local operators.

Let O be a local operator acting nontrivially only on the cluster impurity in the self-consistent 2IAM. We define its dynamical susceptibility as

$$\chi[O](\omega^+) = -i \int_0^\infty dt e^{i\omega^+ t} \langle [O(t), O^\dagger(0)] \rangle, \quad (8)$$

where $\langle \cdot \rangle = \text{Tr}(\rho \cdot)$ denotes a thermal expectation value. When ω lies within an energy range governed by a specific

fixed point, the imaginary part of such a susceptibility typically displays power-law behavior, $\chi''[O](\omega) = -(1/\pi) \text{Im} \chi[O](\omega^+) \sim \omega^\alpha$. When ω traverses the crossover region between fixed points, the exponent α changes, indicating a change in the degree of screening of the local fluctuations described by O . A log-log plot of χ'' versus ω , thus, consists of straight lines with slope α in regions governed by fixed points, connected by peaks or kinks (see Fig. 4). We, thus, define the crossover scales T_{NFL} and T_{FL} via the position of these kinks, as described below. (A systematic method for determining the kink positions is described in Appendix C.) When discussing finite-temperature properties in later sections, we see that the scales so obtained also serve as crossover scales separating low-, intermediate-, and high-temperature regimes.

We have computed $\chi''[O](\omega)$ for the following local cluster operators, defined in the momentum-spin basis, with indices $\alpha \in \{+, -\}$ and $\sigma \in \{\uparrow, \downarrow\}$:

$$T^a = \frac{1}{2} f_{\alpha\sigma}^\dagger \tau_{\alpha\alpha'}^a \delta_{\sigma\sigma'} f_{\alpha'\sigma'} \quad (\text{momentum}), \quad (9a)$$

$$S^b = \frac{1}{2} f_{\alpha\sigma}^\dagger \delta_{\alpha\alpha'} \sigma_{\sigma\sigma'}^b f_{\alpha'\sigma'} \quad (\text{spin}), \quad (9b)$$

$$X^{ab} = \frac{1}{2} f_{\alpha\sigma}^\dagger \tau_{\alpha\alpha'}^a \sigma_{\sigma\sigma'}^b f_{\alpha'\sigma'} \quad (\text{spin-momentum}), \quad (9c)$$

$$W^a = f_{\alpha\sigma}^\dagger \tau_{\alpha\alpha'}^a \delta_{\sigma\sigma'} c_{\alpha'\sigma'} + \text{H.c.} \quad (\text{hybridization}), \quad (9d)$$

$$P^a = \frac{1}{\sqrt{2}} f_{\alpha\sigma}^\dagger \tau_{\alpha\alpha'}^a i \sigma_{\sigma\sigma'}^y f_{\alpha'\sigma'} \quad (\text{singlet pairing}), \quad (9e)$$

$$Q^{ab} = f_{\alpha\sigma} f_{\alpha'\sigma'} \hat{\tau}_{\alpha\alpha'}^a \hat{\tau}_{\sigma\sigma'}^b \quad (\text{triplet pairing}), \quad (9f)$$

$$j = -ite(c_{1\sigma}^\dagger c_{2\sigma} - \text{H.c.}) \quad (\text{current}). \quad (9g)$$

Here, sums over repeated indices are implied, τ^a and σ^b are Pauli matrices in the momentum and spin sectors, respectively, $i\sigma^y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, and $\hat{J}^b$ are SU(2) generators in the triplet representation. These operators can also be expressed in the position spin basis via the Hadamard transformation U_H , which maps $\tau^x \rightarrow \tau^z$, $\tau^y \rightarrow -\tau^y$, and $\tau^z \rightarrow \tau^x$. For example, T^z can be expressed as

$$T^z = \sum_{\alpha, \alpha' = \pm} \frac{1}{2} f_{\alpha\sigma}^\dagger \tau_{\alpha\alpha'}^z f_{\alpha'\sigma} = \sum_{i,j=1}^2 \frac{1}{2} f_{i\sigma}^\dagger \tau_{ij}^x f_{j\sigma}, \quad (10)$$

describing f hopping between sites 1 and 2. Similarly, S^z describes the total f -electron spin, $X^{xz} = S_{f1}^z - S_{f2}^z$ the staggered magnetization, $W^z = \sum_{ij} f_{i\sigma}^\dagger \tau_{ij}^x c_{j\sigma} + \text{H.c.}$ nearest-neighbor f - c hybridization, and P^z f -electron nearest-neighbor singlet pairing.

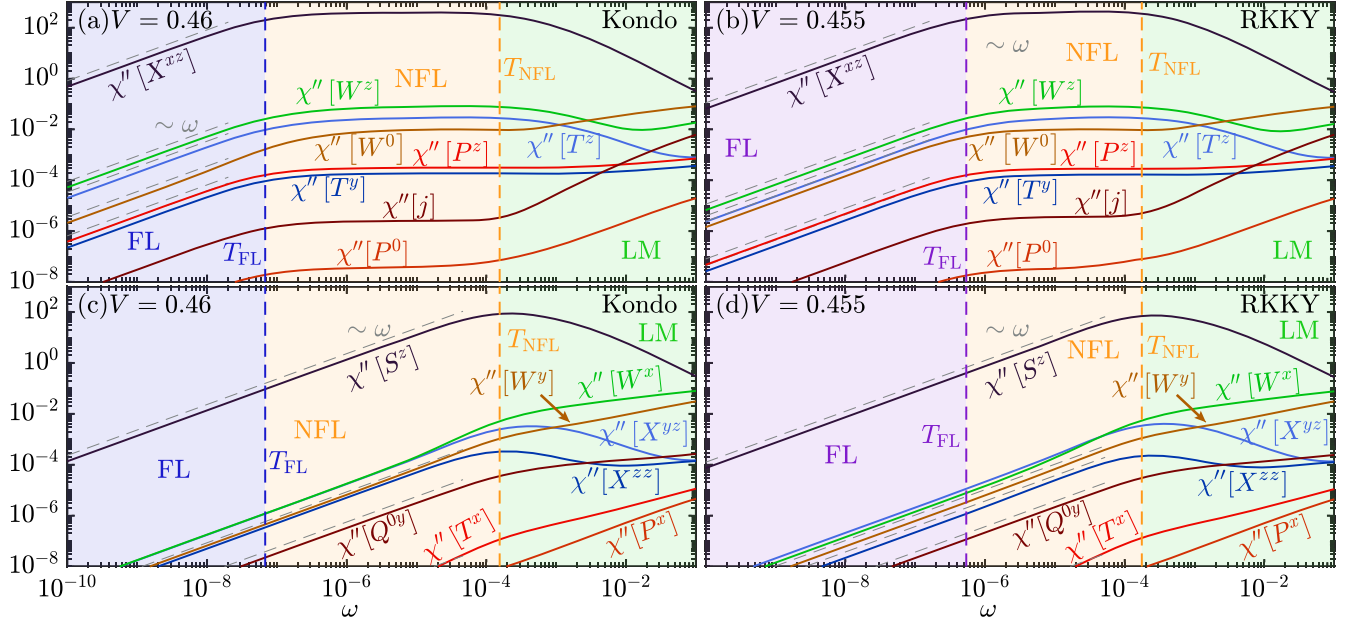


FIG. 4. Dynamical impurity susceptibilities $\chi''(\omega)$ for various operators defined in Eq. (9), computed in (a),(c) the Kondo phase, at $V = 0.46$, and (b),(d) the RKKY phase at $V = 0.455$, both at $T = 0$, close to the QCP. For the susceptibilities collected in (c),(d), the χ'' curves exhibit a maximum around T_{NFL} ; for those in (a),(b), they instead exhibit a plateau between T_{FL} and T_{NFL} . This plateau indicates that the FL is reached in a two-stage screening process, leading to the emergence of NFL behavior at intermediate-energy scales. Gray dashed lines are guides to the eye for $\sim\omega$ behavior.

Figure 4 shows various χ'' susceptibilities at $T = 0$ for the choices $V = 0.46$ [Figs. 4(a) and 4(c)] and $V = 0.455$ [Figs. 4(b) and 4(d)], in the Kondo and RKKY phases close to the QCP, respectively. For $\omega < T_{\text{FL}}$, all χ'' 's decrease linearly with decreasing ω , indicative of FL behavior. Hence, all local fluctuations are fully screened in that energy window, leading to well-defined Fermi-liquid QPs. By contrast, for $T_{\text{FL}} < \omega < T_{\text{NFL}}$ only the χ'' 's in Figs. 4(c) and 4(d) (e.g., $\chi''[S^z]$) decrease with decreasing ω , while the ones in Figs. 4(a) and 4(b) (e.g., $\chi''[T^z]$, $\chi''[X^{xz}]$, $\chi''[W^z]$, and $\chi''[P^z]$) all traverse plateaus. These plateaus are reminiscent of those found for $\chi''_{2\text{CK}}[S^z]$ of the overscreened, $S = \frac{1}{2}$ two-channel Kondo model (2CK) and for $\chi''_{2\text{IKM}}[S_1^z - S_2^z]$ of the two-impurity Kondo model (2IKM) in their respective NFL regimes (see Fig. 20 below). This implies that the total spin in the $\pm$ basis is screened, whereas the momentum, spin-momentum, pairing, and hybridization fluctuations are *overscreened*, yielding the intermediate NFL.

The χ'' curves at $T = 0$ in Fig. 4 clearly demonstrate that, when V is close to V_c , the screening process evolves through two stages, characterized by T_{NFL} and T_{FL} . Precisely at the critical point, where $T_{\text{FL}} = 0$, the plateaus would extend all the way to zero. Conversely, when V is tuned away from the QCP, T_{FL} tends toward T_{NFL} [see Fig. 2(a)]. The two scales merge for $|V - V_c| \gtrsim 0.1$, where the χ'' plateaus have shrunk to become mere peaks, shown for $\chi''[X^{xz}]$ in Fig. 5. The curves in Fig. 5 further illustrate

that the KB QCP is continuous, because $\chi''[X^{xz}]$ evolves smoothly without any discontinuities across the KB QCP. We find similar behavior for the other dynamical susceptibilities shown in Fig. 4. In a companion paper [152], we show that those χ'' which exhibit a plateau [those shown in Figs. 4(a) and 4(b)] exhibit logarithmic ω/T scaling in the NFL region while the corresponding static susceptibilities are singular at the KB QCP, where the NFL region extends down to $T = 0$. In Ref. [152], we also show that the plateau and in χ'' and ω/T scaling in the NFL are a result of strong vertex contributions (as also mentioned at the end of

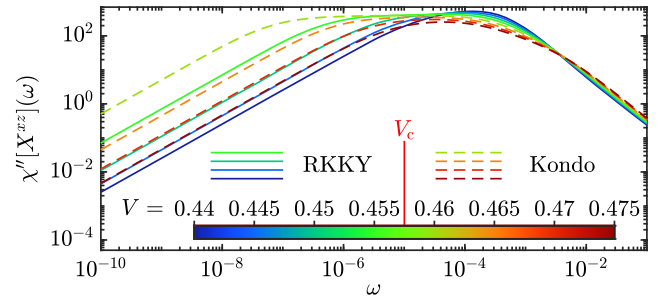


FIG. 5. Evolution of $\chi''[X^{xz}]$ with V across the QCP at $T = 0$. Solid lines, RKKY phase; dashed lines, Kondo phase. As $V \rightarrow V_c$ from either above or below such that $T_{\text{FL}} \rightarrow 0$, the dashed and dotted plateaus both extend to ever lower scales (they would coincide at V_c , where $T_{\text{FL}} = 0$), demonstrating that the KB QCP is continuous.

Sec. VID below). The fact that many static susceptibilities with different symmetries diverge at the QCP suggests that many different, possibly competing symmetry-breaking orders may be possible in the vicinity of the QCP. Which order prevails (if any) will be carefully studied in future work.

V. SINGLE-PARTICLE PROPERTIES—PRELIMINARIES

The fact that $T_{\text{FL}} \rightarrow 0$ at the QCP [Fig. 2(a)] indicates a breakdown of the FL and QP concepts at the KB QCP. Experimental evidence for such a breakdown is found in the sudden reconstruction of the FS [26,37] and the divergence of the effective mass [28] at the KB QCP. It is to date not fully settled how this should be understood [3,6]. In the next two sections, Secs. VI and VII, we revisit such questions, exploiting the ability of CDMFT-NRG to explore very low temperatures and frequencies. This allows us to clarify the behavior of spectral functions and self-energies in unprecedented detail. We discuss their cluster versions for the self-consistent 2IAM in Sec. VI and the corresponding lattice functions for the PAM in Sec. VII.

In the present section, we set the stage for this analysis by summarizing, for future reference, some well-established considerations regarding single-particle properties. We first recall standard expressions for low-frequency expansions of correlators and self-energies in the PAM and the definition of its Fermi surface (Sec. VA). Even though our focus here is on the PAM, we note that low-frequency expressions similar to those reviewed in Sec. VA can be obtained for the Kondo lattice using slave particles [3,74,110,111]. In Sec. VB, we discuss possible scenarios how the parameters appearing in the low-frequency expansions in Sec. VA behave in the vicinity of a KB QCP.

A. Fermi-liquid expansions, Fermi surface, Luttinger surface

In what follows, we often refer to the low-energy expansions, applicable in conventional FL phases, of the functions $G_{x\mathbf{k}}(z)$ and $\Sigma_{x\mathbf{k}}(z)$ ($x = f, c$) defined in Eqs. (3). We list them here for future reference.

Fermi-liquid expansions.—For z below a characteristic FL scale, $|z| \ll T_{\text{FL}}$, and for $\mathbf{k}$ close to the FS, the self-energies can be expanded as [175]

$$\Sigma_{x\mathbf{k}}(z) = \text{Re}\Sigma_{x\mathbf{k}}(0) + z\text{Re}\Sigma'_{x\mathbf{k}}(0) + \delta\Sigma_{x\mathbf{k}}(z), \quad (11)$$

where $\Sigma'(z) = \partial_z \Sigma(z)$ and $\delta\Sigma_{x\mathbf{k}}(z)$ is of the order of $\mathcal{O}(z^2/T_{\text{FL}}^2)$. Moreover, analyticity of $G_{x\mathbf{k}}(z)$ in the upper half-plane requires $\text{Im}\Sigma_{x\mathbf{k}}(z) < 0$ for $\text{Im}z > 0$. For $z = \omega^+$, this implies $\text{Im}\Sigma_{x\mathbf{k}}(\omega^+) < 0$ and $\text{Re}\Sigma'_{x\mathbf{k}}(0) \leq 0$ [the latter follows since $\delta\Sigma_{x\mathbf{k}}(z) \sim z^2$ implies $\text{Im}\Sigma_{x\mathbf{k}}(0) = 0$].

The expansion coefficients determine the so-called free QP energies, weights, and the effective hybridization:

$$\epsilon_{x\mathbf{k}}^* = Z_{x\mathbf{k}}[\epsilon_{x\mathbf{k}} + \text{Re}\Sigma_{x\mathbf{k}}(0)], \quad (12a)$$

$$Z_{x\mathbf{k}} = [1 - \text{Re}\Sigma'_{x\mathbf{k}}(0)]^{-1}, \quad (12b)$$

$$V_{\mathbf{k}}^* = \sqrt{Z_{f\mathbf{k}}}V, \quad (12c)$$

with $\epsilon_{x\mathbf{k}} = \epsilon_f$ or $\epsilon_{c\mathbf{k}}$ for $x = f, c$. Since $\text{Re}\Sigma'_{x\mathbf{k}}(0) \leq 0$, the QP weights satisfy $Z_{x\mathbf{k}} \leq 1$. The QP energies and weights, in turn, appear in the low-frequency expansions of Σ_c and G_c [cf. Eqs. (3)]:

$$\Sigma_{c\mathbf{k}}(z) = \frac{(V_{\mathbf{k}}^*)^2}{z - \epsilon_{f\mathbf{k}}^*} + \mathcal{O}(z^2/T_{\text{FL}}^2), \quad (13a)$$

$$G_{c\mathbf{k}}(z) = \frac{Z_{c\mathbf{k}}}{z - \epsilon_{c\mathbf{k}}^*} + \mathcal{O}(z^2/T_{\text{FL}}^2). \quad (13b)$$

Evidently, the low-energy expansion of Σ_c is fully determined by that of Σ_f , with

$$\text{Re}\Sigma_{c\mathbf{k}}(0) = -\frac{V_{\mathbf{k}}^{*2}}{\epsilon_{f\mathbf{k}}^*}, \quad \text{Re}\Sigma'_{c\mathbf{k}}(0) = -\frac{V_{\mathbf{k}}^{*2}}{\epsilon_{f\mathbf{k}}^{*2}}, \quad (14)$$

$$Z_{c\mathbf{k}} = \left[1 + \frac{V_{\mathbf{k}}^{*2}}{\epsilon_{f\mathbf{k}}^{*2}}\right]^{-1} = \frac{\epsilon_{f\mathbf{k}}^{*2}}{\epsilon_{f\mathbf{k}}^{*2} + V_{\mathbf{k}}^{*2}}. \quad (15)$$

These expressions make explicit how c - f hybridization effects c electrons: The sign of the energy shift $\text{Re}\Sigma_{c\mathbf{k}}(0)$ is determined by and opposite to that of $\epsilon_{f\mathbf{k}}^*$; and $\text{Re}\Sigma'_{c\mathbf{k}}(0)$ changes from zero to negative, thereby decreasing $Z_{c\mathbf{k}}$ below 1 and causing c electron mass enhancement [175]. Since $\epsilon_{f\mathbf{k}}^* \sim Z_{f\mathbf{k}}$ and $V_{\mathbf{k}}^* \sim \sqrt{Z_{f\mathbf{k}}}$, Eq. (15) implies $Z_{c\mathbf{k}} \sim Z_{f\mathbf{k}}$ when $Z_{f\mathbf{k}} \ll 1$.

Fermi surface.—Next, we recall the definition of the FS. For the PAM, this is not entirely trivial, since the correlators G_c and G_f are not independent but coupled through Eqs. (3).

We focus on $T = 0$ (else the FS is not sharply defined). If there is no hybridization, $V = 0$, the situation is simple: The partially filled c band is metallic, and the half-filled f band a Mott insulator. Then, the FS comprises essentially only c electrons and is defined by the conditions [13,175]

$$\epsilon_{c\mathbf{k}}^* = 0, \quad Z_{c\mathbf{k}} > 0, \quad \text{Im}\Sigma_{c\mathbf{k}}(0) = 0. \quad (16)$$

The first condition identifies the FS as the locus of $\mathbf{k}$ points in the Brillouin zone for which the free QP energy vanishes; the second states that the QP occupation should exhibit an abrupt jump when this surface is crossed ($Z_{c\mathbf{k}}$ governs the size of this jump); and the third requires the QP scattering

rate to vanish at the FS. Together, they imply that the FS is the locus of $\mathbf{k}$ points at which $G_{c\mathbf{k}}^{-1}(0) = 0$.

More generally, for $V \neq 0$, we start from the matrix form, $G_{\mathbf{k}}(z)$, of the combined f and c correlators [Eq. (2)]. Then, the FS is defined as the locus of $\mathbf{k}$ points for which some eigenvalue of $G_{\mathbf{k}}^{-1}(0)$ vanishes. Thus, all points on the FS satisfy the condition $\det[G_{\mathbf{k}}^{-1}(0)] = 0$, or

$$\epsilon_{c\mathbf{k}}(\epsilon_f + \Sigma_{f\mathbf{k}}(0)) - V^2 = 0. \quad (17)$$

For $V \rightarrow 0$, either the first or second factor on the left must vanish, implying $\epsilon_{c\mathbf{k}} = 0$ or $\epsilon_f + \Sigma_{f\mathbf{k}}(0) = 0$, respectively. The first condition defines the bare FS for the c band; the second condition is never satisfied for the case of present interest, where the bare f electrons form a half-filled Mott insulator with μ lying within the gap.

If V is nonzero, Eq. (17) implies that *both* of the following inequalities hold on the FS [assuming that $\Sigma_{f\mathbf{k}}(0)$ does not diverge there]:

$$\epsilon_{c\mathbf{k}} \neq 0, \quad \epsilon_f + \Sigma_{f\mathbf{k}}(0) \neq 0. \quad (18)$$

Thus, the bare and actual FS do not intersect. Dividing Eq. (17) by the first or second factor, we obtain [131,132]

$$G_{f\mathbf{k}}^{-1}(0) = 0, \quad G_{c\mathbf{k}}^{-1}(0) = 0. \quad (19)$$

These two conditions are equivalent, in that one implies the other, via Eq. (17). Moreover, the second inequality in Eq. (18) ensures that $\Sigma_{c\mathbf{k}}(0)$ does not diverge; hence, the second condition in Eq. (19) implies Eqs. (16). We thus conclude that Eqs. (16) define the FS also for nonzero V .

Luttinger surface.—A second surface of importance is the *Luttinger surface* (LS) [11,176,177]. For the PAM, it is defined [131] as the locus of $\mathbf{k}$ points for which $\Sigma_{f\mathbf{k}}(z)$ has a pole at $z = 0$. This definition, together with Eqs. (3a) and (3e), implies that the following relations hold on the LS:

$$|\Sigma_{f\mathbf{k}}(0)| = \infty, \quad G_{f\mathbf{k}}(0) = 0, \quad \Sigma_{c\mathbf{k}}(0) = 0. \quad (20)$$

The first relation just restates the definition of the LS; the second should be contrasted with the relation $G_{f\mathbf{k}}(0) = \infty$ holding on the FS; and the third implies, via Eq. (12a), that $\epsilon_{c\mathbf{k}}^* = Z_{c\mathbf{k}}\epsilon_{c\mathbf{k}}$; i.e., on the LS, the renormalized dispersion is obtained from the bare one purely by rescaling, without any shift. If the LS coincides with the bare FS, then the FS, too, coincides with the bare c -electron FS ($\epsilon_{c\mathbf{k}} = 0$).

Note that $|\Sigma_{f\mathbf{k}}(\omega)|$ can diverge only at isolated frequency values, not on extended frequency intervals, since the frequency integral over its spectral function must be finite. Therefore, when $|\Sigma_{f\mathbf{k}}(0)|$ diverges, $|\Sigma'_{f\mathbf{k}}(0)|$ diverges, too. By Eq. (12b), it follows that $Z_{f\mathbf{k}} = 0$ on the LS.

The behavior of $Z_{c\mathbf{k}}$ depends on how strongly $\Sigma_{f\mathbf{k}}(z)$ diverges for $z \rightarrow 0$. For example, suppose $\Sigma_{f\mathbf{k}}(z) \sim z^{-\alpha}$ for some $\alpha > 0$. Then, Eq. (3e) implies $\Sigma_{c\mathbf{k}} \sim z^{\alpha}$, $\Sigma'_{c\mathbf{k}} \sim z^{\alpha-1}$. Thus, we obtain $Z_{c\mathbf{k}} \sim z^{1-\alpha} \rightarrow 0$ or ∞ or $= 1$ for $\alpha < 1$ or $\alpha = 1$ or $\alpha > 1$, respectively; i.e., the c -QP weight may or may not be renormalized.

We show results for the FS and LS in Sec. VII and discuss their volumes together with Luttinger's sum rule in Sec. VIII.

B. Kondo breakdown

In the introduction, we have qualitatively described the Kondo breakdown scenarios that have been proposed to characterize the KB QCP. For future reference, we here distinguish KB scenarios of two types: (i) a KB QCP *with* Kondo destruction (KD), defined below, and (ii) a KB QCP *without* KD. In both scenarios, the f electron quasiparticle weight Z_f decreases to zero when approaching the KB QCP from the Kondo side. However, in (i), Z_f remains zero on the RKKY side (i.e., all Kondo correlations have been destroyed, hence the moniker “KD”), whereas, in (ii), Z_f is nonzero on the RKKY side, too (i.e., some Kondo correlations survive there). [Thus, our nomenclature distinguishes between KB, which happens only *at* the critical point, and KD, which, in a type (i) scenario, happens throughout the RKKY phase.] We emphasize that (ii) is different from the Hertz-Millis-type SDW QCP, where the QP weight is also nonzero at the QCP. Figure 6 sketches the different scenarios. Most of the scenarios for the KB QCP proposed in the literature are of type (i), with KD. By contrast, we find a KB QCP of type (ii), without KD. We summarize below the concepts used to describe the HF problem and, in particular, how type (i) and (ii) scenarios differ.

1. Hybridization gap

The hybridization of c and f electrons leads to a well-developed pole in $\Sigma_{c\mathbf{k}}(z)$, called hybridization pole

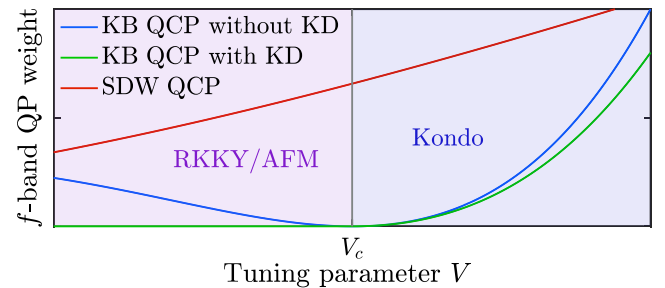


FIG. 6. Sketch of the generic f -band QP weight in different scenarios for quantum criticality. In the conventional SDW QCP (red), the QP weight is finite at the QCP. At a KB QCP, it is zero at the QCP. In a type (i) scenario with KD (green), it remains zero in the RKKY phase; in a type (ii) scenario without KD (blue), it is finite there.

(h pole), lying at energies well above the FL scale T_{FL} . It manifests itself as a strong peak in $-\text{Im}\Sigma_{c\mathbf{k}}(z)$, causing the corresponding c -electron spectral functions to exhibit distinctive gaps or pseudogaps, called hybridization gaps (h gaps). It occurs irrespective of whether the $T = 0$ phase is Kondo or RKKY correlated and is present for temperatures both above and below T_{FL} . The formation of a h gap has been observed in many experiments, as reviewed in the introduction. Note that, while in the noninteracting PAM ($U = 0$), the h gap is positioned at $\epsilon_{f\mathbf{k}}^*$, this is not the case in the interacting case: The h gap forms at scales which can much larger than the FL scale (in our case, it forms at T_{NFL} ; see the next section); i.e., $\epsilon_{f\mathbf{k}}^*$ and the position of the h gap are renormalized differently by interactions.

2. Kondo phase

In the Kondo phase, $Z_{f\mathbf{k}}$ is nonzero for all $\mathbf{k}$. The presence of Kondo correlations is phenomenologically described [3,74] by Eq. (13a). This situation can phenomenologically be interpreted as arising through an effective hybridization with strength $V_{\mathbf{k}}^*$ (sometimes referred to as “amplitude of static Kondo correlations” [3,74]) of c electrons with an effective f band with dispersion $\epsilon_{f\mathbf{k}}^*$. This effective hybridization shifts the c -electron Fermi surface from its $V = 0$ form, defined by $\epsilon_{c\mathbf{k}} = 0$, to a form defined by $\epsilon_{c\mathbf{k}}^* = 0$, i.e.,

$$\epsilon_{c\mathbf{k}} - \frac{V_{\mathbf{k}}^{*2}}{\epsilon_{f\mathbf{k}}^*} = 0. \quad (21)$$

Therefore, the FS volume changes, reflecting the influence of f orbitals. Within the Kondo phase, $V_{\mathbf{k}}^*$ remains nonzero but continuously approaches zero as the KB QCP is approached. Moreover, in the Kondo phase, the ratio $(V_{\mathbf{k}}^*)^2/\epsilon_{f\mathbf{k}}^*$ remains essentially constant as long as $V_{\mathbf{k}}^*$ is finite, because both $(V_{\mathbf{k}}^*)^2 \sim Z_{f\mathbf{k}}$ and $\epsilon_{f\mathbf{k}}^* \sim Z_{f\mathbf{k}}$ [cf. Eq. (12a)]. Therefore, the FS will remain basically unchanged in the Kondo phase, even very close to the KB QCP.

Two comments are in order. First, in general, the first term in Eq. (13a) usually does not represent an actual pole of $\Sigma_{c\mathbf{k}}$: It was derived assuming $|z| \ll T_{\text{FL}}$ and $\mathbf{k}$ close to the FS, whereas $\epsilon_{f\mathbf{k}}^*$ typically lies outside that window [i.e., for $z \rightarrow \epsilon_{f\mathbf{k}}^*$, Eqs. (11) and (13a) no longer apply]. Second, $\epsilon_{f\mathbf{k}}^*$ is not directly related to the hybridization gaps, as already mentioned in point (i) above: The latter are determined by pseudogaps of $G_{c\mathbf{k}}$ of Eq. (3b), and since these lie at high energies of the order of $\pm T_{\text{NFL}}$, their positions are not governed by Eq. (13a) but rather by the general form (3e) of $\Sigma_{c\mathbf{k}}$ (see Sec. VII below).

3. Kondo breakdown

As summarized in Refs. [3,74], the following behavior is expected when approaching the KB QCP from the Kondo

phase: $V_{\mathbf{k}}^*$, or equivalently $Z_{f\mathbf{k}}$, decreases continuously to zero; hence, the low-energy hybridization becomes weaker, while the ratio $(V_{\mathbf{k}}^*)^2/\epsilon_{f\mathbf{k}}^*$ and, thus, the FS remain constant and different from the bare c -electron FS. Since $Z_{c\mathbf{k}} \sim Z_{f\mathbf{k}}$ if $Z_{f\mathbf{k}} \ll 1$ [cf. Eq. (15) and its discussion], e.g., close to the KB QCP, both QP weights are expected to continuously decrease to zero when approaching the KB QCP. At the KB QCP, V^* vanishes; i.e., low-energy hybridization and, thus, Kondo correlations break down.

4. RKKY with Kondo destruction

In the type (i) KD scenario [3,74], $V_{\mathbf{k}}^*$, or equivalently $Z_{f\mathbf{k}}$, remains zero in the RKKY phase; i.e., Kondo correlations remain absent—i.e., they have been destroyed. By Eq. (21), that implies the FS reduces to the bare c -electron one, accounting for c electrons only. All in all, the FS jumps across the KB QCP due to Kondo destruction. Since $Z_{f\mathbf{k}} = 0$ in this scenario, Eq. (11) for the f electrons and, therefore, also Eq. (13a) do not apply anymore. Equation (11) may, however, still apply for the c electrons [see also the discussion below Eq. (20)], leading to QP mass enhancement due to the existence of c - f hybridization at finite frequencies. This is sometimes referred to as “dynamical Kondo correlations” [27,178]. The type (i) KD scenario emerges from the Kondo lattice model in both a slave-particle [110,111] or an EDMFT treatment [5,135–137].

5. RKKY without Kondo destruction

Here, we describe the type (ii) scenario of a Kondo breakdown without Kondo destruction in the RKKY phase. We emphasize that, also in this scenario, the QP weights become zero at the KB QCP and the FS is small in the RKKY phase. Nevertheless, in the RKKY phase, the f -electron QP weight is nonzero at the FS. In the type (ii) scenario, $Z_{f\mathbf{k}}$ becomes zero only at a LS [see Eq. (20)], where the f -electron self-energy diverges. If the LS does not coincide with the FS (the converse would require significant fine-tuning), this implies non-zero $Z_{f\mathbf{k}}$ at the FS and c - f hybridized QPs also in the RKKY phase.

The type (ii) scenario described above is not so unusual: There is growing evidence that Mott insulators described beyond the single-site DMFT approximation generically feature momentum-dependent Mott poles [179–181], with a singular part of the f self-energy of the form [181]

$$\Sigma_{f,\text{singular}} \sim \frac{1}{z - \epsilon_{\Sigma\mathbf{k}}^*}. \quad (22)$$

Here, $\epsilon_{\Sigma\mathbf{k}}^*$ is related to the free dispersion with renormalized parameters and opposite sign of the hopping amplitudes [181]. Such a self-energy, therefore, features a LS, defined by $\epsilon_{\Sigma\mathbf{k}}^* = 0$. It has been suggested that the LS is the defining

feature of Mott phases and that this feature is stable to perturbations [182–184]. The LS of a Mott phase should, therefore, in principle, be stable to small hybridization with a metal, provided the hybridization strength is not too large, resulting in an orbital-selective Mott phase (OSMP). $Z_{f\mathbf{k}}$ is zero only at the LS where Σ_f diverges. If the LS and the FS do not coincide, it follows that $Z_{f\mathbf{k}}$ is nonzero at the FS.

A comment is in order regarding single-site DMFT or EDMFT, where the Mott pole is not momentum dependent and the QP weight is zero throughout the whole BZ. In single-site DMFT, this phase is not stable to interorbital hybridization [125,185]. As a result, single-site DMFT will always describe a Kondo phase at $T = 0$ [125]. By contrast, OSMPs described by EDMFT seem to be stable to interorbital hybridization [186], leading to the type (i) scenario described above.

In our own CDMFT-NRG studies of the PAM, we find a KB scenario of type (ii). In Sec. VI, we establish this by a detailed study the low-energy behavior of the self-consistent effective 2IAM. There, the role of $\mathbf{k}$ is taken by $\alpha = \pm$; i.e., we show that

$$\Sigma_{c\alpha}(z) = \frac{V_\alpha^{*2}}{z - \epsilon_{f\alpha}^*} + \mathcal{O}(z^2/T_{\text{FL}}^2) \quad (23)$$

is valid, with $V_\alpha^* \neq 0$ on both sides of the QCP. When V approaches V_c from either side, V_α^* approaches 0, leading to a breakdown of Kondo correlations at the KB QCP. We find that the FS reconstruction at V_c is caused by a sign change of ϵ_{f+}^* , as explained in Sec. VI. The consequences for the lattice model are established in Sec. VII and for the Luttinger sum rule in Sec. VIII.

VI. SINGLE-PARTICLE PROPERTIES—CLUSTER

In this section, we discuss the single-particle properties of the self-consistent 2IAM, focusing on the spectral functions and retarded self-energies of both c and f orbitals. A discussion of the corresponding momentum-dependent lattice properties follows in Sec. VII. We argue that the KB quantum phase transition is a continuous OSMT at $T = 0$. The Kondo phase is a normal metallic phase, while in the RKKY phase, the f electrons are in a Mott phase; i.e. this phase is an OSMP. The defining feature of the OSMP is a momentum-dependent pole in the f -electron self-energy, *not* a single-particle gap. The RKKY phase is, thus, *not* an orbital-selective Mott *insulator*. Indeed, we find that, even in the OSMP, the f electrons exhibit a finite QP weight due to finite hybridization with the c electrons.

In Secs. VIA and VIB, we discuss spectral functions and self-energies at $T = 0$ on the real-frequency axis, exploiting the capabilities of NRG to resolve exponentially small energy scales. We then investigate QP properties in more detail in Sec. VIC: We clearly show that both the c - and f -electron QP weights are finite in both the Kondo

and RKKY phases but vanish at the KB QCP. Finally, in Sec. VID, we discuss finite-temperature properties, showing that c - f hybridization is already fully developed around T_{NFL} , whereas QP coherence and self-energy poles are fully formed only at T_{FL} .

A. Cluster spectral functions at $T = 0$: Overview

In this subsection, we provide a phenomenological overview over the cluster spectral properties of the self-consistent 2IAM at $T = 0$ as functions of V ; details and physical insights follow in Sec. VIB. We adopt the $\pm$ basis, where G_f and G_c from Eq. (6) are both diagonal, and study $A(\omega) = -(1/\pi)\text{Im}G(\omega^+)$ for both f and c orbitals. (When referring to A_f below, we mean both components $A_{f\pm}$, and likewise for A_c .) Our results for A_f and A_c are shown in Fig. 7 on a linear frequency scale to provide a coarse overview. We enumerate some of their characteristic features, proceeding from high- to low-frequency features.

1. Hubbard peaks, band structure

Figures 7(a), 7(b), 7(e), and 7(f) and Figs. 7(c), 7(d), 7(g), and 7(h) show the spectral functions $A_f(\omega)$ and $A_c(\omega)$ for different V on a linear frequency scale, for the ranges $\omega \in [-10, 10]$ and $\omega \in [-1.25, 1.25]$, respectively, containing all significant spectral weight. A_f has two Hubbard bands around $\omega \simeq \pm 5 = \pm U/2$. They are almost independent of V . Moreover, they show the same structure for A_{f+} and A_{f-} , implying that these high-energy features are momentum independent. By contrast, A_c has no Hubbard bands, since the c electrons do not interact, with spectral weight only in the range of the noninteracting bandwidth, $\omega \in [-1.2, 0.8]$. Its shape mimics that obtained for $V = 0$ [insets in Figs. 7(c) and 7(d)], reflecting the bare c -electron band structure, except for some sharp structures at intermediate and low frequencies, discussed below.

2. Center of c band

For A_c , the highest-frequency sharp feature furthest from $\omega = 0$ lies at $\omega \simeq -0.2$, the middle of the bare c -electron band. This feature is prominently developed deep in the RKKY phase at $V = 0.4$ [Figs. 7(g) and 7(h)] but almost invisible deep in the Kondo phase at $V = 0.6$ [Figs. 7(c) and 7(d)]. It is due to scattering of c electrons by antiferromagnetic fluctuations and reflects a tendency toward antiferromagnetic order in the RKKY phase. Though our CDMFT setup excludes such order, it does find strong antiferromagnetic correlations in the RKKY phase [see $\langle S_{f1} \cdot S_{f2} \rangle$ in Fig. 2(b)], causing enhanced scattering of c electrons at the band center.

3. Kondo peaks, hybridization gaps

Deep in the Kondo phase at $V = 0.6$ (red lines), A_f shows a sharp Kondo peak near $\omega \simeq 0$, while A_c has a

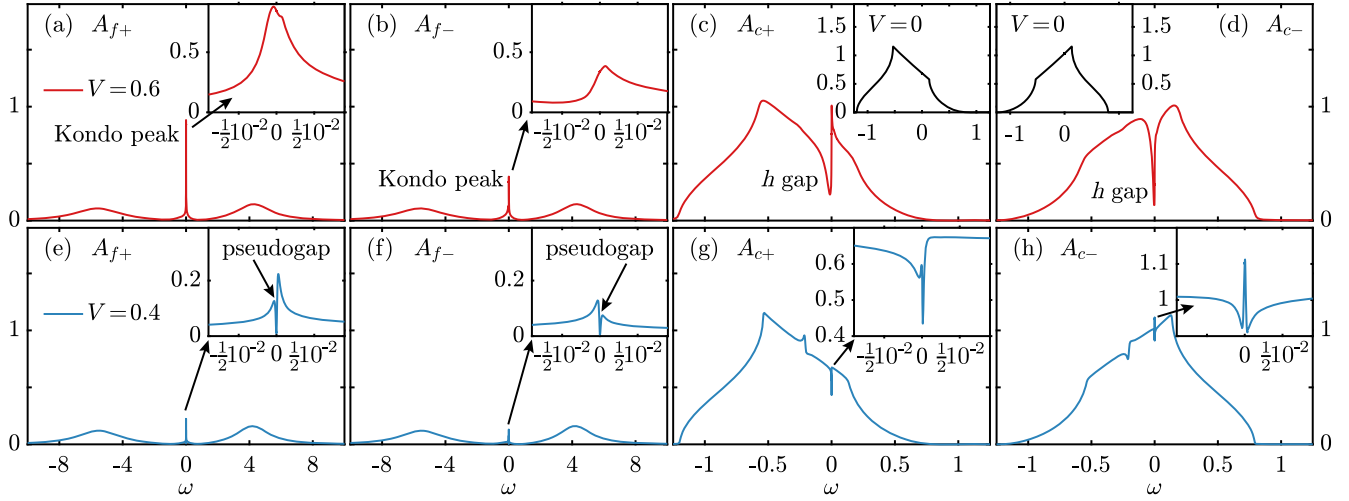


FIG. 7. Cluster spectral functions at $T = 0$, for $V = 0.6$ (top row, deep in the Kondo phase) and for $V = 0.4$ (bottom row, deep in the RKKY phase). (a),(b),(e),(f) and (c),(d),(g),(h) show the f - and c -electron spectral functions, respectively. The insets in (c),(d) show the c -electron spectral functions at $V = 0$; the insets in all other panels show an enlargement into the low-frequency region.

distinct dip, known as the hybridization gap (h gap; see also Sec. V), at a small, negative value of ω . Both these features are indicative of strong c - f hybridization and coherent QPs. By contrast, deep in the RKKY phase at $V = 0.4$ (blue lines), the Kondo peak in A_f has disappeared, giving rise to a pseudogap [see the insets in Figs. 7(e) and 7(f)], and the h gap in A_c has become very weak. Nevertheless, we see in Sec. VIB that, even deep in the RKKY phase, c - f hybridization is present even at low energies and the f -electron QP weight is finite in this phase. This leads to a sharp peak inside the h gaps of A_c [see the insets in Figs. 7(g) and 7(h)]. As discussed in more detail in Sec. VII, this sharp feature reflects a narrow QP band with a FS close to $\Pi = (\pi, \pi, \pi)$.

4. Momentum dependence

The spectral functions and self-energies show several qualitative and/or quantitative differences between the $+$ and $-$ channels (different Kondo peak heights, different h gap shapes, etc.). Such channel asymmetries reflect the fact that our system is electron doped—the Fermi surface lies closer to the Γ point than the Π point, causing a stronger c - f hybridization (encoded in $\Sigma_{c\pm}$) for bonding than antibonding orbitals. This asymmetry leads to different behavior for momenta near $\Gamma = (0, 0, 0)$ and $\Pi = (\pi, \pi, \pi)$. However, these asymmetries in the *spectral functions* are not necessarily indicative of nonlocal correlations. Especially deep in the Kondo phase, the channel asymmetries are mostly due to the single-particle dispersion and are not nonlocal *self-energy* effects. We discuss this in more detail in Sec. VIB.

B. Cluster spectral functions and self-energies at $T = 0$: Details

Next, we discuss the main spectral features relevant to KB physics, referring to Fig. 8. It shows both the spectral

functions $A_{\alpha\alpha}(\omega)$ and retarded self-energies $\Sigma_{\alpha\alpha}(\omega^+)$ using a symmetric logarithmic frequency scale with $|\omega| > 10^{-10}$. Figures 8(a)–8(d) show this evolution for A_f and A_c , while Figs. 8(e)–8(h) show the corresponding self-energies.

1. Self-energy poles for Σ_f

The most important feature is the pole in Σ_f (denoted as fs pole), which is present in the RKKY phase but not in the Kondo phase, see Fig. 8(e) and 8(f). This fs pole in the RKKY phase is indicative of Mott physics [131,132] present in the f band but not in the c band (see also the discussion in Sec. VB). This brings us to one of our main conclusions: *The RKKY phase is an OSMP, and the KB quantum phase transition is an OSMT.* Moreover, the fs pole continuously disappears when approaching the KB QCP from the RKKY phase. This further shows that the KB quantum phase transition is a *continuous* OSMT (see also Fig. 5 and its discussion). We also note that we found no coexistence region, which further underpins our conclusion of a continuous quantum phase transition (QPT).

Our conclusion that the KB is an OSMT matches the conclusion of previous CDMFT plus ED studies of the PAM using the same parameters [131,132]. Nevertheless, the considerably improved accuracy of our NRG impurity solver compared to the ED impurity solver used there yields new conceptional insights and reveals new emergent physics.

The fs pole in the RKKY phase is positioned at a negative frequency for Σ_{f+} (at $\omega \simeq -T_{\text{FL}}$) and at a positive frequency for Σ_{f-} (at $\omega \simeq T_{\text{FL}}$). Therefore, its position depends on momentum; i.e., it is *dispersive*. A dispersive fs pole is a generic feature of Mott phases in finite dimensions $d < \infty$ [179,181] (see also Sec. VB). By contrast, in the $d \rightarrow \infty$ limit (or, equivalently, in the single-site DMFT approximation) where the self-energy and, thus, also the fs

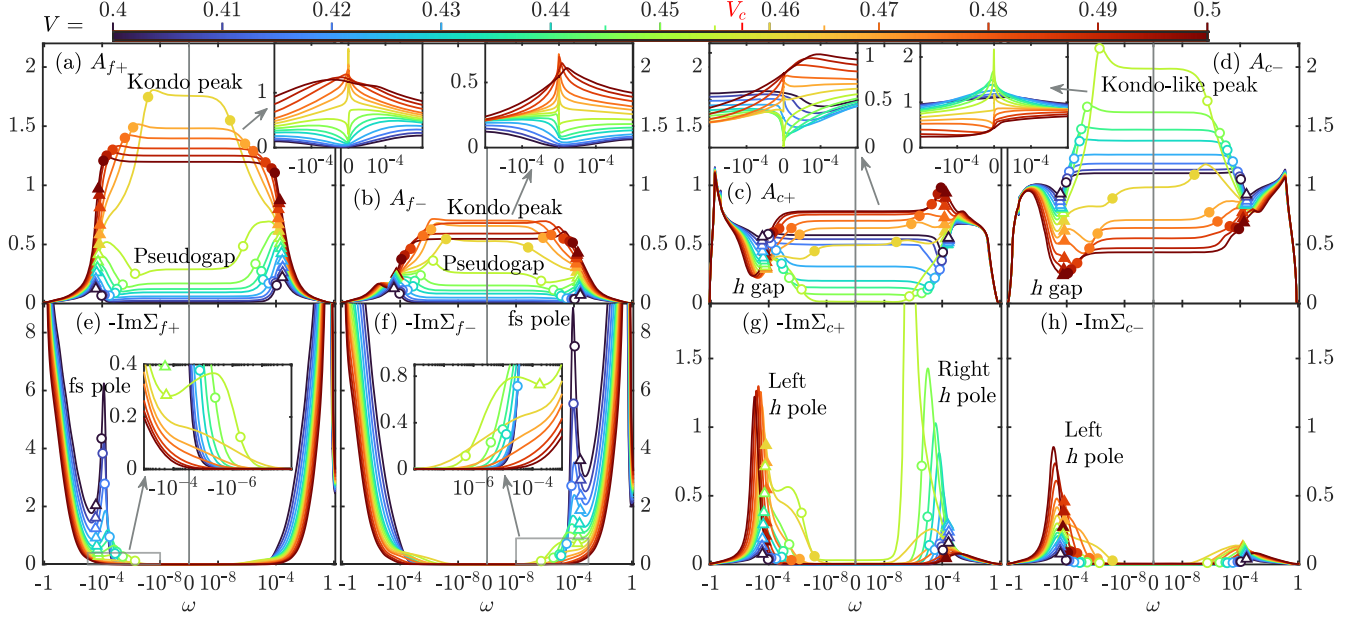


FIG. 8. Evolution of cluster spectral functions $A_{\alpha\alpha}(\omega)$ and retarded self-energies $\Sigma_{\alpha\alpha}(\omega^+)$ at $T = 0$ as V is tuned across the QCP. Colored curves correspond to V values marked by ticks on the color bar. A symmetric log scale with $10^{-10} < |\omega| < 1.25$ is used. On such a scale, the plateaus seen for all curves for very low frequencies, $|\omega| < 10^{-8}$, demonstrate that no new features arise in that range. Triangles and circles mark the crossover scales $\pm T_{\text{NFL}}$ and $\pm T_{\text{FL}}$, respectively, with filled (open) symbols identifying curves in the Kondo (RKKY) phase. The insets in (a)–(d) show the spectral functions on a linear frequency scale for $|\omega| < 2 \times 10^{-4}$.

pole are momentum independent, the OSMF is *not* stable against interorbital hopping [185] (i.e., against finite c - f hybridization V in the present context). The momentum resolution provided by two-site CDMFT, though coarse, is therefore a crucial ingredient to stabilize the OSMF. We show in Sec. VII that, after reperiodization of the CDMFT self-energy, the dispersive nature of the fs pole leads to a reperiodized self-energy with a continuous $\mathbf{k}$ dependence of the form of Eq. (22). Based on the results in Ref. [151], the fs pole can be associated with emergent spinon excitations; its emergence, therefore, suggests a fractionalization of the f electron. Since the position of the sf pole is momentum dependent, the emergent spinon is dispersive.

Even though the dispersive fs pole is the most pronounced momentum-dependent feature of Σ_f , more subtle momentum-dependent features are responsible for the NFL physics close to the QCP: In the Kondo phase, shoulderlike structures show up in Σ_f below $T_{\text{FL}} < |\omega| < 10^{-4}$ [see insets in Figs. 8(e) and 8(f)]. These are more pronounced for Σ_{f-} than for Σ_{f+} , leading to momentum-dependent scattering rates at the corresponding energy scales.

The features of A_f [Figs. 8(a) and 8(b)], A_c [Figs. 8(c) and 8(d)], and Σ_c [Figs. 8(g) and 8(h)] can largely be understood in terms of a continuous OSMF. In the following, we enumerate and describe the main spectral and self-energy features and discuss their connection to the presence or absence of fs poles in Σ_f . We follow the evolution, with decreasing V , from the Kondo phase through the QCP into the RKKY phase, noting the following salient features.

2. From Kondo peak to pseudogap for $A_{f\pm}$

In the Kondo phase, the Kondo peak of A_{f+} lies slightly below $-T_{\text{FL}}$ and that of A_{f-} slightly below T_{FL} . As V decreases toward V_c , the Kondo peaks of both A_{f+} and A_{f-} shift toward zero and become higher and narrower [Figs. 8(a) and 8(b)], leaving behind shoulderlike structures at $\pm T_{\text{NFL}}$ (marked by triangles). The Kondo peak of A_{f+} is higher than that of A_{f-} , reflecting the fact that in the Kondo phase the FS is positioned closer to the Γ point than to the Π point. When V crosses V_c , the Kondo peak abruptly changes into a pseudogap, flanked by the two shoulders. The emergence of the pseudogap in A_f is caused by the appearance of fs poles in Σ_f in the RKKY phase. A further decrease of V deepens the pseudogap, because the poles in Σ_f become stronger. The pseudogap never becomes a true gap (except for $V = 0$), because the poles of Σ_f are positioned away from $\omega = 0$. Thus, the QP weight of the f electrons is finite even in the RKKY phase (see also Sec. VI C). This is one of the crucial differences to the findings of Refs. [131,132]; there, a charge gap in A_f was found due to the poor energy resolution of the ED impurity solver used in these studies.

3. Pseudogap for A_{c+} , Kondo-like peak for A_{c-}

Once V drops below V_c , A_{c+} rapidly develops a pronounced pseudogap around $\omega = 0$, which weakens (becomes less pronounced) when V is decreased further. This pseudogap emerges because ϵ_{f+}^* [see Eq. (23)]

continuously changes sign at the KB QCP, from $\epsilon_{f+}^* < 0$ in the Kondo phase to $\epsilon_{f+}^* > 0$ in the RKKY phase [see Fig. 9(b) below]. Because of the low-energy form of Σ_{c+} shown in Eq. (23), this leads to a h pole in Σ_{c+} which is close to $\omega = 0$ in the vicinity of the KB QCP and whose position changes sign across the QCP, in the same way as ϵ_{f+}^* . This h pole is clearly visible in Fig. 8(g), where we show $-\text{Im}\Sigma_{c+}$. We discuss the sign change of ϵ_{f+}^* in more detail in Sec. VIC, where we also show that this sign change is intricately connected to the emergence of the f pole in Σ_{f+} . The sign change of ϵ_{f+}^* and, therefore, also the pseudogap in A_{c+} is, therefore, an integral part of the OSMT. We further show in Sec. VIII that the sign change of ϵ_{f+}^* is ultimately tied to a reconstruction of the FS.

In striking contrast, A_{c-} develops a Kondo-like peak around $\omega = 0$, whose peak height increases rapidly as V drops below V_c and then decreases when V is decreased further. The emergence of such a peak for *delocalized* electrons is rather unexpected, which is why we call it “Kondo-like” (in contrast to “Kondo peak” for localized electrons). This sharp peak suggests that, close to the KB QCP, the c electrons become more localized, i.e., that their Fermi velocity is strongly renormalized downward due to the momentum dependence of Σ_c .

4. Hybridization poles for $\text{Im}\Sigma_c$

The h gap at negative frequencies for A_c is caused by a corresponding peak in $\text{Im}\Sigma_c$ [Figs. 8(g) and 8(h)]. It reflects a c self-energy pole, to be called left hybridization pole (left h pole). The frequency location of the h gap and left h pole is comparable in magnitude to the NFL scale. When V is reduced toward and past V_c into the RKKY phase, the left h pole in $\text{Im}\Sigma_c$ weakens and almost disappears, causing the same for the h gap in A_c . At the same time, for the bonding channel, a peak in $-\text{Im}\Sigma_{c+}$ at positive frequencies emerges in the RKKY phase. It corresponds to an additional pole of Σ_{c+} , to be called right h pole, located at $\approx T_{\text{FL}}$. It causes the h gap in A_{c+} around $\omega = 0$ close to the KB QCP. By contrast, for the antibonding channel, $\text{Im}\Sigma_{c-}$ does not have a second pole—its very weak peak on the right, in fact, is the tail of its left h pole. (This becomes more clear from the temperature dependence of Σ_c and is explained in more detail in Sec. VID.)

5. Low-energy Fermi liquid

For all considered values of V , the $\omega = 0$ quantities $\text{Im}\Sigma_f(i0^+)$ and $\text{Im}\Sigma_c(i0^+)$ all vanish. This implies FL behavior at the lowest energy scales for all $V \neq V_c$ (consistent with the results in Sec. IVA). Moreover, $A_f(0)$ and $A_c(0)$ never vanish, even in the RKKY phase. Thus, the pseudogap in A_f never becomes a true gap, implying that f electrons keep contributing to the QPs constituting the low-energy FL.

C. Quasiparticle properties

In this subsection, we substantiate our claims made in the previous subsection regarding QP weights and ϵ_f^* . In particular, we seek to show that the low-frequency form Eq. (23) applies to Σ_c on both sides of the KB QCP. Note that Eq. (23) is meaningful only if the low-energy physics shows FL behavior; our study of finite-size spectra in Sec. IVA confirms that this is the case.

We define cluster QP weights and effective level positions for both f and c electrons by replacing $\mathbf{k} \rightarrow \alpha$ in Eqs. (12a):

$$\epsilon_{x\alpha}^* = Z_{x\alpha}[\epsilon_{x\alpha} + \text{Re}\Sigma_{x\alpha}(0)], \quad (24a)$$

$$Z_{x\alpha} = [1 - \text{Re}\Sigma'_{x\alpha}(0)]^{-1} \quad (x = f, c) \quad (24b)$$

with $\epsilon_{f\alpha} = \epsilon_f - \mu$ and $\epsilon_{c\alpha} = -\alpha t - \mu$. The f -electron QP weight is nonzero as long as $\Sigma'_{f\alpha}(0)$ is not infinite, i.e., as long as $\Sigma_{f\alpha}$ has no pole at $z = 0$. In the Kondo phase, there are no low-frequency poles in $\Sigma_{f\alpha}$ at all, while the poles appearing in the RKKY phase are shifted away from $z = 0$.

The QP weights $Z_{f\alpha}$ and effective level positions $\epsilon_{f\alpha}^*$ can be extracted directly from NRG finite-size spectra [187,188], which avoids fitting frequency-dependent data; $Z_{c\alpha}$ and $\epsilon_{c\alpha}^*$ are obtained via Eqs. (14) and (15). Figure 9 shows them all. We see that both Z_f and Z_c vanish at the KB QCP, as expected. However, Z_f is finite not only in the Kondo phase, *but also in the RKKY phase*. This further substantiates our claim that the f electrons contribute to the low-energy QP even for $V < V_c$.

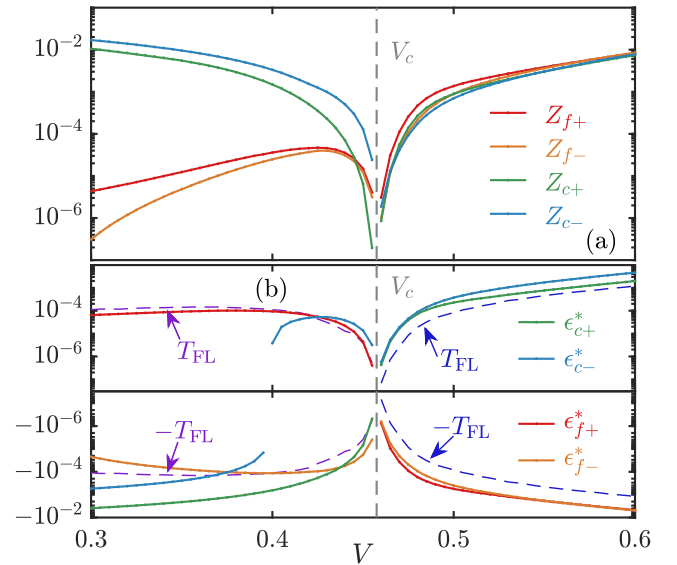


FIG. 9. (a) QP weights and (b) effective level positions of the self-consistent effective 2IAM, computed directly from the NRG finite-size spectra at $T = 0$. Blue and purple dashed lines in (b) mark $\pm T_{\text{FL}}$ and $\pm T_{\text{FL}}^*$ for reference, respectively.

The key difference between the RKKY and Kondo phases, therefore, is *not* zero versus nonzero Z_f —instead, the key difference turns out to be the sign of ϵ_{f+}^* . Note that our discussion below is applicable for the *electron-doped* case considered in this work; a corresponding discussion of the hole-doped case would follow along the same lines, but with the signs of $\epsilon_{f\alpha}^*$ flipped and the role of bonding and antibonding cluster orbitals interchanged. Both ϵ_{f+}^* and ϵ_{f-}^* are negative in the Kondo phase; see Fig. 9(b). The same is true for $U = 0$, and in this sense the noninteracting limit is adiabatically connected to the Kondo phase. However, while ϵ_{f-}^* remains negative in the RKKY phase, ϵ_{f+}^* changes sign at the KB QCP and becomes positive. Now, Eqs. (6e) and (24a) imply

$$V^2\text{Re}\Sigma_{c\alpha}^{-1}(z) = z - \epsilon_f - \Sigma_{f\alpha}(z), \quad (25a)$$

$$\text{sgn}\epsilon_{f\alpha}^* = -\text{sgn}\text{Re}\Sigma_{c\alpha}^{-1}(0). \quad (25b)$$

Thus, the sign change in ϵ_{f+}^* is also visible in Fig. 10(a) as a sign change of $V^2\text{Re}\Sigma_{c+}^{-1}(0)$. In Sec. VIII, where we perform a careful analysis of the Luttinger sum rule for the PAM, we show explicitly that this sign change of ϵ_{f+}^* leads to a jump of the FS volume corresponding to exactly one electron per site.

Figure 10(a) also reveals how the sign change of ϵ_{f+}^* is connected to the fs pole in $\Sigma_{f+}(\omega^+)$. Close to the KB QCP, in both the Kondo and RKKY phases, when ω is increased (starting from large negative), $V^2\text{Re}\Sigma_{c+}^{-1}(\omega^+)$ increases through zero around $\omega \simeq -T_{\text{NFL}}$. This sign change results in the left h pole in Σ_{c+} , visible in Fig. 8(g). [Deeper in the RKKY phase, $V^2\text{Re}\Sigma_{c+}^{-1}(\omega^+)$ does not actually change sign at $\omega \simeq -T_{\text{NFL}}$ but, nevertheless, becomes almost zero, again causing the left h pole of Σ_{c+} .] This feature is adiabatically connected to the $U \rightarrow 0$ case, where it is also present. It is an intermediate-energy feature which characterizes the onset of NFL behavior. (We show in Sec. VID

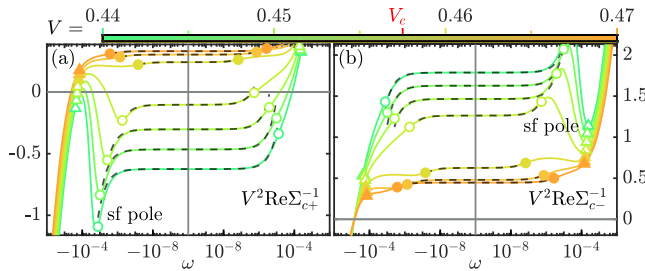


FIG. 10. Evolution of $V^2\text{Re}\Sigma_{c\pm}^{-1}(\omega^+)$ at $T = 0$ as V is tuned in a narrow range across the QCP. As V is lowered, nonmonotonic behavior emerges, whose double-wiggle structure (local maximum followed by local minimum) reflects the fs poles of $-\text{Re}\Sigma_{f\pm}$ [cf. Eq. (25a)]. Circles, triangles, and tick marks on the color bar have the same meaning as in Fig. 8. Black dashed lines indicate linear behavior around $\omega = 0$.

that the left h pole in Σ_c forms around $T \simeq T_{\text{NFL}}$, irrespective of $V > V_c$ or $V < V_c$.)

In the Kondo phase, the sign of $V^2\text{Re}\Sigma_{c+}^{-1}(\omega^+)$ changes only once with increasing ω , remaining positive for $\omega > -T_{\text{NFL}}$ and, in particular, at $\omega = 0$, so that ϵ_{f+}^* is negative. By contrast, in the RKKY phase, the initial increase with ω in $V^2\text{Re}\Sigma_{c+}^{-1}(\omega^+)$ for ω large negative is counteracted by the fs pole in $\Sigma_{f+}(\omega^+)$, which induces a double-wiggle structure in $V^2\text{Re}\Sigma_{c+}^{-1}(\omega^+)$ near $\omega \simeq -T_{\text{FL}}$. As a result, $V^2\text{Re}\Sigma_{c+}^{-1}(i0^+)$ is negative and ϵ_{f+}^* positive in the RKKY phase. The KB QCP lies in between, at $\epsilon_{f+}^* = 0$.

In summary, in the Kondo phase, the sign change of $V^2\text{Re}\Sigma_{c+}^{-1}(\omega^+)$ around $\omega \simeq -T_{\text{NFL}}$ leads to the left h pole and to $V^2\text{Re}\Sigma_{c+}^{-1}(0) > 0$, implying $\epsilon_{f+}^* < 0$. In the RKKY phase, the formation of the fs pole in $\Sigma_{f+}(\omega^+)$ at energy scales between $-T_{\text{NFL}}$ and $-T_{\text{FL}}$ results in $V^2\text{Re}\Sigma_{c+}^{-1}(0) < 0$ and, therefore, $\epsilon_{f+}^* > 0$.

D. Temperature dependence close to V_c

We next discuss the temperature dependence of cluster spectral functions and self-energies close to the QCP at $V_c = 0.4575$. We first discuss the case $V = 0.46 > V_c$ (Fig. 11) and then $V = 0.455 < V_c$ (Fig. 12), which at $T = 0$ yield the Kondo and RKKY phases, respectively. For each, we proceed from high to low temperatures.

$V = 0.46$, $T \gtrsim T_{\text{NFL}}$.—When the temperature is lowered in the LM regime from $T = 10^{-3}$ toward T_{NFL} , the onset of c - f hybridization leads to the emergence of a hybridization gap in $A_c(\omega)$ [Figs. 11(c) and 11(d)] and a left h pole in $-\text{Im}\Sigma_c(\omega^+)$ [Figs. 11(g) and 11(h)], all at $\omega \simeq -10^{-4} \simeq -T_{\text{NFL}}$. This triggers the onset of screening, signified by increased spectral weight in A_f around $\omega = 0$ [Figs. 11(a) and 11(b)] and a decrease of $-\text{Im}\Sigma_f$ at $\omega = 0$ [Figs. 11(e) and 11(f)]. However, at T_{NFL} , no coherent QPs have formed yet: Both $-\text{Im}\Sigma_f$ and $-\text{Im}\Sigma_c$ have significant spectral weight around $\omega \simeq 0$, implying strong scattering for electrons near the chemical potential.

$V = 0.46$, $T_{\text{FL}} \lesssim T \lesssim T_{\text{NFL}}$.—When the temperature is lowered further toward T_{FL} , screening becomes stronger: Both $-\text{Im}\Sigma_f$ and $-\text{Im}\Sigma_c$ at $\omega \simeq 0$ decrease, albeit slowly, as $\sim \ln(T)$. [In Figs. 11(e)–11(h), T values equally spaced on logarithmic scale yield $-\text{Im}\Sigma(i0^+)$ values equally spaced on a linear scale.] At the same time, coherent QPs begin to form: A sharp Kondo peak gradually forms in A_f , and narrow structures A_c emerge.

$V = 0.46$, $T \lesssim T_{\text{FL}}$.—Below T_{FL} , coherent QPs have formed [$\Sigma_f(i0^+)$ and $\Sigma_c(i0^+)$ approach zero], and the T dependence of the spectral functions becomes weak.

We next consider the case $V < V_c$.

$V = 0.455$, $T \gtrsim T_{\text{NFL}}$.—In the LM regime, the behavior for $V < V_c$ is similar to that for $V > V_c$: As T is lowered from 10^{-3} toward T_{NFL} , a hybridization gap emerges in $A_c(\omega^+)$ [Figs. 12(c) and 12(d)] and a left h pole in $-\text{Im}\Sigma_c$

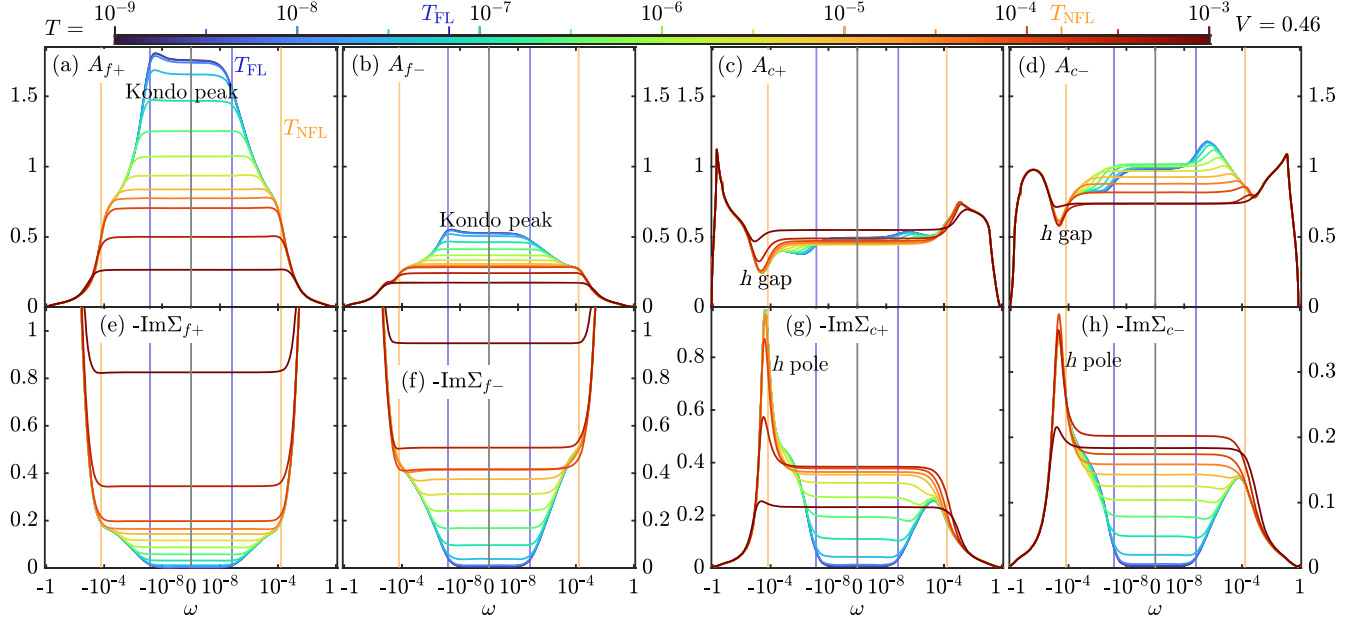


FIG. 11. Evolution of cluster spectral functions and retarded cluster self-energies $\Sigma_{\alpha\alpha}(\omega^+)$ at $V = 0.46 > V_c$ (Kondo phase at $T = 0$) as temperature is increased. Colored curves correspond to T values marked by ticks on the color bar. A symmetric log scale with $10^{-10} < |\omega| < 1.25$ is used. Vertical blue and orange lines mark $\pm T_{FL}$ and $\pm T_{NFL}$, respectively.

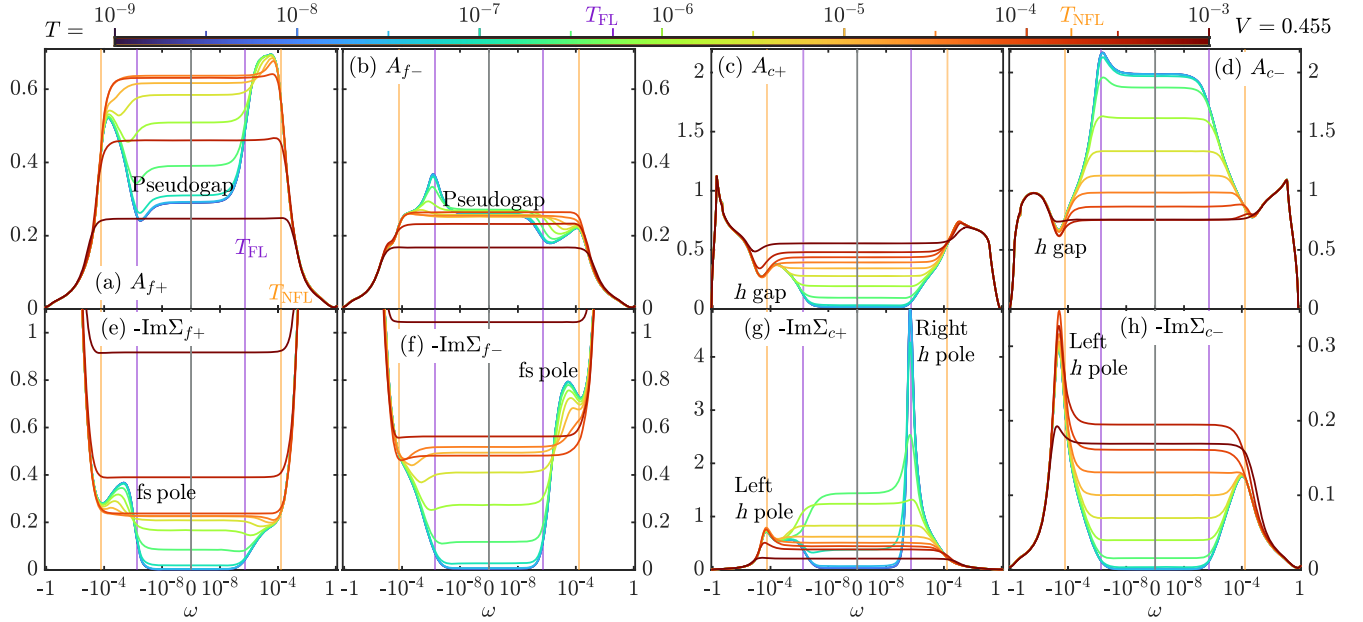


FIG. 12. The same as Fig. 11, but for $V = 0.455 < V_c$ (RKKY phase at $T = 0$).

[Figs. 12(g) and 12(h)], all at $\omega \simeq -10^{-4}$. Correspondingly, A_f increases for frequencies near $\omega = 0$; the temperature dependence at $T > T_{NFL}$ is, thus, similar to $V > V_c$, as expected.

$V = 0.455$, $T_{FL} \lesssim T \lesssim T_{NFL}$.—By contrast, below T_{NFL} the temperature dependence is quite different from $V > V_c$. When T is lowered within the NFL regime from T_{NFL}

toward T_{FL} , $\text{Im}\Sigma_f$ develops fs poles [Figs. 12(e) and 12(f)]. At the same time, $-\text{Im}\Sigma_{c+}$ develops a right h pole at a small positive frequency, $\omega \gtrsim T_{FL}$ [Fig. 12(g)], causing a strong increase of $-\text{Im}\Sigma_{c+}(0)$. The formation of the right h pole is associated with the formation of the fs poles in Σ_f , as discussed in Sec. VIC. On the other hand, $-\text{Im}\Sigma_{c-}$ behaves quite similar to its counterpart at $V = 0.46$ in the NFL

region, decreasing logarithmically around $\omega = 0$. The appearance of fs poles in the f -electron self-energies is accompanied by the formation of (somewhat asymmetric) pseudogaps in A_f around $\omega = 0$ [Figs. 12(a) and 12(b)]. Moreover, the right h pole in $-\text{Im}\Sigma_{c+}$ in the NFL region causes a pseudogap in A_{c+} in the same temperature window [Fig. 12(c)]. A_{c-} , on the other hand, develops a sharp peak around $\omega = 0$ in the NFL region, similarly to the behavior of A_{f+} for $V > V_c$ [Fig. 12(d)].

$V = 0.455$, $T \lesssim T_{\text{FL}}$.—When T is lowered below T_{FL} , the imaginary parts of all self-energies quickly tend to zero at $\omega = 0$, as expected in a FL. [Thus, the overall behavior of $-\text{Im}\Sigma_{c+}(i0^+)$ with decreasing temperature is nonmonotonic, first increasing in the NFL regime, then decreasing down to zero in the FL regime.]

No marginal FL phenomenology.—In the NFL regime, neither the f - nor the c -electron self-energies show marginal FL phenomenology. The latter would require $-\text{Im}\Sigma(\omega^+, T) \sim \max(|\omega|, T)$ [69]. Instead, the imaginary parts of the self-energies have a much weaker, namely logarithmic frequency and temperature dependence. Nonetheless, the spectral parts of various susceptibilities all show the same phenomenological frequency dependence [69] in the NFL region, namely, a plateau for $T \lesssim |\omega| \lesssim T_{\text{NFL}}$ and a $\sim\omega$ dependence for $\omega < T$ [69]. This frequency dependence has already been shown above in Fig. 4; we discuss the temperature dependence in a companion paper [152]. There, we also emphasize that the susceptibilities are not governed by the self-energy alone, as would be the case, in diagrammatic parlance, when evaluating only the bubble contribution—instead, vertex contributions play a crucial role. This especially also concerns the conductivity, which shows an $\sim 1/T$ dependence in the NFL region despite the $\sim \ln(T)$ dependence of $\text{Im}\Sigma(i0^+)$ [152].

VII. SINGLE-PARTICLE PROPERTIES—LATTICE

Having focused on the single-particle properties of the effective 2IAM in the previous section, we now discuss how these translate to the lattice model. Our analysis builds on that of De Leo, Civelli, and Kotliar [131,132], but with our better energy resolution, we uncover much additional detail and new emergent physics at low energies. In particular, we obtain a detailed understanding of the Fermi surface reconstruction occurring when traversing the KB QCP.

A. Reperiodization

Since the CDMFT artificially breaks translation invariance, the c - and f -electron self-energies have to be reperiodized before computing lattice spectral functions. To this end, we reperiodize the cluster cumulant [157,158]

$$M(z) = [z + \mu - \Sigma_c(z)]^{-1}. \quad (26)$$

It may be viewed as a c -electron propagator excluding bare nearest-neighbor hopping and in an expansion around the $t = 0$ limit [189] takes the role of the cluster self-energy. Its reperiodized version $M_{\mathbf{k}}(z)$ is defined as

$$M_{\mathbf{k}}(z) = M_{11}(z) + M_{12}(z) \sum_{a=x,y,z} \frac{1}{3} \cos(k_a). \quad (27)$$

Here, M_{11} and M_{12} are the local and nearest-neighbor cluster cumulants, respectively, and the latter is accompanied by the cosine factors arising when diagonalizing a noninteracting hopping Hamiltonian. At the points $\Gamma = (0, 0, 0)$ and $\Pi = (\pi, \pi, \pi)$, the lattice cumulants reduce to the cluster ones, $M_+ = M_{11} + M_{12} = M_{\Gamma}$ and $M_- = M_{11} - M_{12} = M_{\Pi}$. This reflects the correspondence, mentioned in Sec. II, of the BZ points Γ and Π and the bonding and antibonding cluster orbitals. The $\mathbf{k}$ -dependent self-energies are then defined via the relations

$$M_{\mathbf{k}}(z) = [z + \mu - \Sigma_{c\mathbf{k}}(z)]^{-1}, \quad (28a)$$

$$\Sigma_{c\mathbf{k}}(z) = V^2 [z - \epsilon_f^0 + \mu - \Sigma_{f\mathbf{k}}(z)]^{-1}. \quad (28b)$$

We see in Sec. VIII that the CDMFT solution to the PAM must fulfill a generalized version of the Luttinger sum rule—this sum rule is verifiable via cluster quantities only, i.e., without reperiodization. The reperiodization scheme above is, however, not guaranteed to preserve this property. We, therefore, slightly modify the above scheme by adjusting μ in Eqs. (26) and (28a) during the reperiodization only, such that the reperiodized self-energies fulfill this generalized Luttinger sum rule in the same way as the corresponding cluster quantities. We describe our reperiodization procedure and evaluate its validity in detail in Appendix A 3.

B. Lattice spectral functions

Figure 13 (top row) shows the evolution with V of the ($T = 0$) momentum-dependent spectral function $A_{\mathbf{k}}(\omega) = A_{f\mathbf{k}}(\omega) + A_{c\mathbf{k}}(\omega)$ and of the FS. [Corresponding retarded self-energies $\text{Im}\Sigma_{f\mathbf{k}}(\omega^+)$ and $\text{Im}\Sigma_{c\mathbf{k}}(\omega^+)$ are shown in Fig. 14 below.] To highlight all relevant energy scales and the changes of $A_{\mathbf{k}}(\omega)$ at low frequencies close to the QCP, we use a logarithmic frequency grid for $|\omega| > 10^{-9}$ and a linear grid for $|\omega| < 10^{-9}$ (gray shaded region) to cross $\omega = 0$.

Figure 13 (bottom row) shows three different surfaces, defined in Sec. VA: the free Fermi surface $V = 0$ (FS0, green), where $\epsilon_{c\mathbf{k}} = 0$; the actual Fermi surface (FS, red), where $\text{Re}G_{x\mathbf{k}}^{-1}(i0^+) = 0$ for both $x = f, c$ [numerically, we use $\text{Re}G_{c\mathbf{k}}^{-1}(i0^+) = 0$]; and the Luttinger surface (LS, blue), where $|\Sigma_{f\mathbf{k}}(0)| = \infty$, $G_{f\mathbf{k}}(0) = 0$, and $\Sigma_{c\mathbf{k}}(0) = 0$ [numerically, we use $\text{Re}\Sigma_{c\mathbf{k}}(i0^+) = 0$]. In summary,

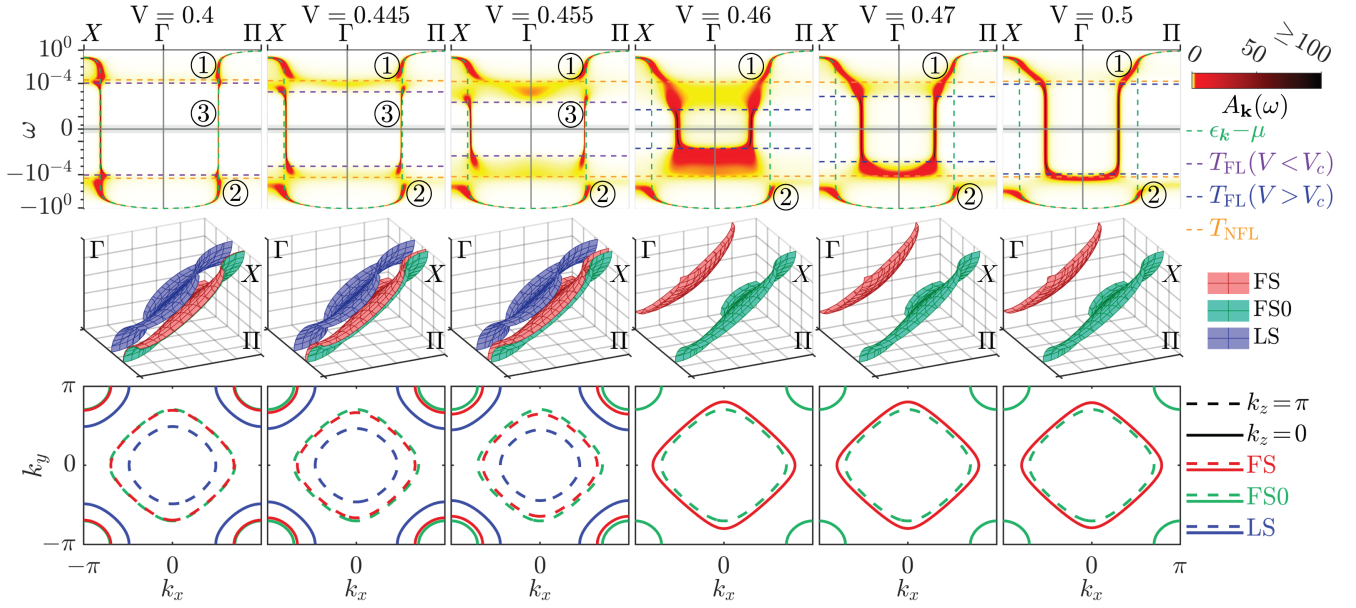


FIG. 13. Top row: momentum resolved total spectral function $A_{\mathbf{k}}(\omega) = A_{c\mathbf{k}}(\omega) + A_{f\mathbf{k}}(\omega)$ at $T = 0$, for various V crossing the QCP at $V_c = 0.4575(25)$, plotted from $X = (\pi, \pi, 0)$ over $\Gamma = (0, 0, 0)$ to $\Pi = (\pi, \pi, \pi)$. $A_{\mathbf{k}}(\omega)$ is shown on a logarithmic frequency scale for $|\omega| > 10^{-9}$ and on a linear scale for $|\omega| < 10^{-9}$ (gray shaded region). The green dashed line marks the c -electron dispersion at $V = 0$. On the Kondo side ($V > V_c$), $A_{\mathbf{k}}(\omega)$ shows a two-band structure, marked ① and ②, as expected from adiabatic continuation from the $U = 0$, with the upper band intersecting $\omega = 0$ close to Γ . On the RKKY side ($V < V_c$), $A_{\mathbf{k}}(\omega)$ shows a three-band structure, marked ①, ②, and ③, with the narrow middle band intersecting $\omega = 0$ close to Π . Middle row: corresponding FS (red) where $\epsilon_{c\mathbf{k}}^* = 0$, FS at $V = 0$ (green, FS0) where $\epsilon_{c\mathbf{k}} = 0$, and LS where $\Sigma_{f\mathbf{k}}(0) = \infty$ (blue), in an octant of the first Brillouin zone. For $V > V_c$, the FS is centered around Γ . Crossing the QCP toward $V < V_c$, the FS center point jumps to Π and a LS emerges. Bottom row: Brillouin zone cuts showing the FS (red lines), FS0 (green lines), and LS (blue lines) at constant $k_z = 0$ (solid) or $k_z = \pi$ (dashed) versus k_x and k_y .

$$\text{FS0: } \epsilon_{c\mathbf{k}} = 0, \quad (29a)$$

$$\text{FS: } \text{Re} G_{x\mathbf{k}}^{-1}(i0^+) = 0 \Leftrightarrow \left\{ \begin{array}{l} \det G_{\mathbf{k}}^{-1}(i0^+) \\ \epsilon_{c\mathbf{k}}^* \\ \epsilon_{f\mathbf{k}}^* - \frac{(V_{\mathbf{k}}^*)^2}{\epsilon_{c\mathbf{k}}} \end{array} \right\} = 0, \quad (29b)$$

$$\text{LS: } |\Sigma_{f\mathbf{k}}(0)| = \infty \Leftrightarrow \Sigma_{c\mathbf{k}}(i0^+) = 0. \quad (29c)$$

Next, we discuss some salient features of Fig. 13.

Band structures.—In the Kondo phase, $A_{\mathbf{k}}(\omega)$ has a two-band structure [190] (marked ① and ② in Fig. 13) with a well-defined QP peak in band ①, as expected in this phase. The dispersion around $\omega = 0$ is clearly shifted away from the $V = 0$ dispersion (indicated by a dashed green line in Fig. 13). As V is lowered toward the QCP at V_c , the upper band develops a broad region of incoherent spectral weight in the NFL energy window $T_{\text{FL}} < |\omega| < T_{\text{NFL}}$.

Interestingly, in the RKKY phase, the spectral function shows a three-band structure (marked ①, ②, and ③ in Fig. 13): The top and bottom bands (① and ②) do not cross $\omega = 0$. In addition, there is a third, narrow middle band (③) of width $\sim T_{\text{FL}}$ crossing $\omega = 0$ near Π . The dispersion around $\omega = 0$ of band ③ almost matches the $V = 0$ dispersion. Band ③ is separated from the other two bands by a region of incoherent spectral weight in the NFL

window $T_{\text{FL}} < |\omega| < T_{\text{NFL}}$. The additional band gap in the RKKY phase comes from a dispersive fs pole in Σ_f (see Figs. 8 and 14 and their discussions), associated with orbital-selective Mott physics. Reference [151] suggests that the fs pole may be interpreted as an emergent coherent spinon excitation [151]. This suggests that the f electron is fractionalized and the RKKY phase is a fractionalized FL [110,111]. We will clarify this view in future work. As discussed in Sec. VB, for non-single-site DMFT (as here, where we use two-site CDMFT), it is natural for a Mott insulator (the f band in the present case) to hybridize with a metal (the c band) and contribute nonzero weight to the low-energy QP, resulting in an OSMP. Because the f band, which is in a (strongly correlated) Mott phase, contributes nonzero QP weight, the QP dispersion is strongly renormalized, leading to the narrow middle band. Its narrow width ($\sim T_{\text{FL}}$) for $V < V_c$ indicates a large effective mass m^* , as observed experimentally, e.g., in Refs. [33,191] and discussed in detail in Sec. IX below. Note that this strong-correlation effect occurs even though the actual FS lies very close to the free c -electron Fermi surface FS0, for reasons discussed below.

Fermi surface reconstruction.—In the Kondo phase, the FS (red) is electronlike and centered around the $\Gamma = (0, 0, 0)$ point, in contrast to the holelike free FS0 (green) of the c electrons, centered at $\Pi = (\pi, \pi, \pi)$. The FS

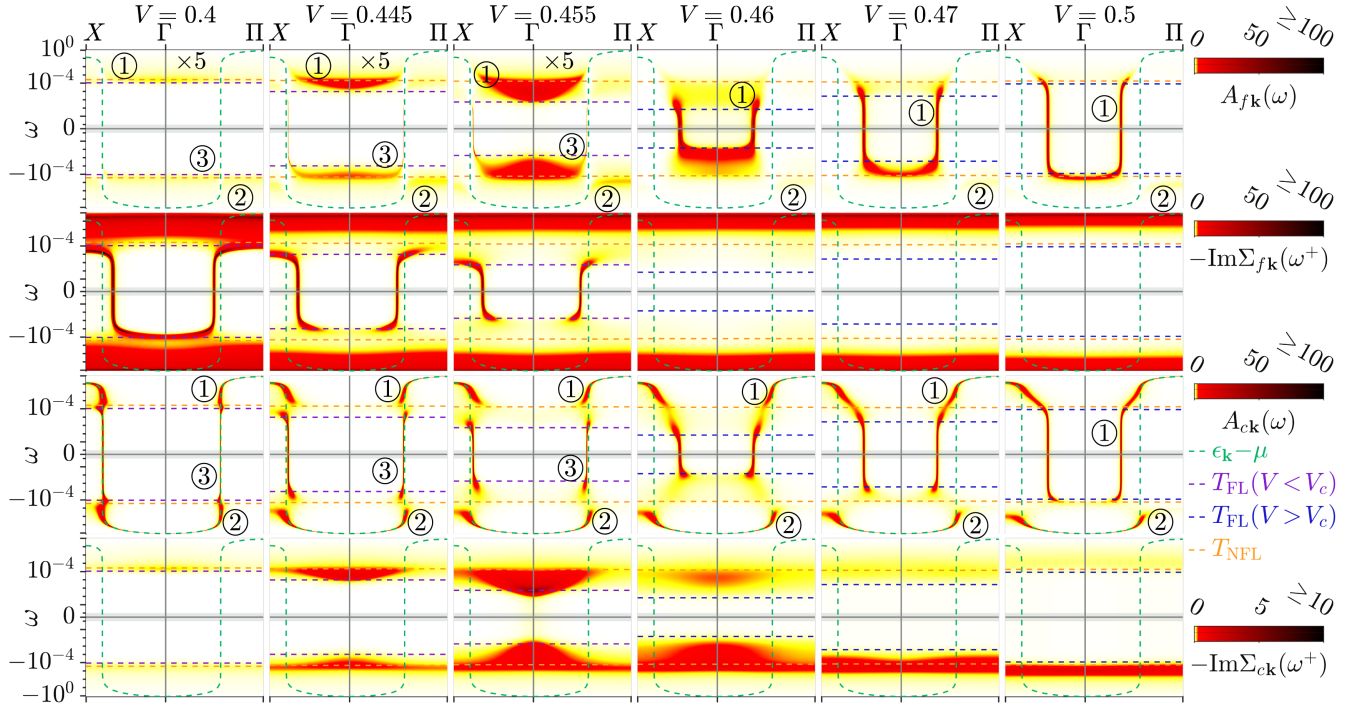


FIG. 14. Momentum resolved f and c spectral functions and imaginary parts of retarded self-energies, $A_{f\mathbf{k}}(\omega)$ (top row), $-\text{Im}\Sigma_{f\mathbf{k}}(\omega^+)$ (second row), $A_{c\mathbf{k}}(\omega)$ (third row), and $-\text{Im}\Sigma_{c\mathbf{k}}(\omega^+)$ (bottom row) at $T = 0$, corresponding to the spectral functions shown in Fig. 13. The three leftmost panels ($V < V_c$) in the top row show $5 \times A_{f\mathbf{k}}(\omega)$ to improve the visibility of f -electron spectral features in the OSMP. Note that, in the RKKY phase, the spectral weight of $A_{f\mathbf{k}}(\omega)$ close to $\omega = 0$ is underestimated by our reperiodization scheme, as discussed in Appendix A 3. We have scaled it by a factor of 5 to improve visibility. As discussed in Sec. VI, there is a nonzero f -electron contribution to the FS throughout the RKKY phase. The markers ①, ②, and ③ mirror those in Fig. 13.

depends only very weakly on V , because it is constrained by the Luttinger sum rule: The latter relates the density $n_f + n_c$ to the FS volume (see Sec. VIII for details), which depends only very weakly on V (see Fig. 17). As the QCP is crossed, the FS undergoes a sudden reconstruction and becomes centered around Π , positioned close to FS0. This leads to a jump of the Hall coefficient, as discussed with Fig. 18. The FS reconstruction is accompanied by the emergence of a LS (blue), which accounts for the change in the FS volume (see Sec. VIII). The emergence of a LS is the hallmark property of a Mott phase, and it has been shown that the LS is stable to small perturbations [182]. This emphasizes again our claim that the RKKY phase is an OSMP. In the RKKY phase, the FS again depends only very weakly on V due to the Luttinger sum rule constraint (the weak V dependence is again due to a weak V dependence of the filling).

C. Lattice self-energies

To get a better understanding how the features of the spectral functions in Fig. 13 emerge, Fig. 14 shows the imaginary parts of the momentum-dependent c - and f -electron self-energies. In the Kondo phase at $V > V_c$, $-\text{Im}\Sigma_{f\mathbf{k}}(\omega^+)$ shows only weak momentum dependence. It is large at high frequencies but vanishes toward $\omega = 0$,

consistent with the presence of coherent QP. Interestingly, its structure is almost independent of V in the Kondo regime. However, as we have seen in Sec. VI, the f -electron self-energy becomes slightly nonlocal in the Kondo regime close to the QCP (though this is not easily visible in Fig. 14).

Crossing the QCP to the RKKY phase at $V < V_c$, the nondispersive high-frequency structure remains essentially the same as in the Kondo phase. However, additionally a sharp dispersing pole emerges in $\Sigma_{f\mathbf{k}}$ at low frequencies for $|\omega| < T_{\text{FL}}$. As discussed in Secs. VB and VI, this dispersive pole in $\Sigma_{f\mathbf{k}}$ in the RKKY phase is a clear sign of Mott physics present in the f band. Importantly, the fact that the pole is dispersive [cf. Eq. (22)] results from employing cluster DMFT instead of single-site DMFT. We are, therefore, not in the $d \rightarrow \infty$ limit where the OSMP (i.e., the RKKY phase) would be unstable to finite c - f hybridization V [185].

The c self-energy, shown in the bottom row in Fig. 14, has most of its spectral weight at $\omega \simeq -T_{\text{NFL}}$ deep in the Kondo phase. It is mostly momentum independent and signals the position of the hybridization gap. As V is decreased toward V_c , $-\text{Im}\Sigma_{c\mathbf{k}}(\omega^+)$ becomes increasingly momentum dependent, with more spectral weight at Γ than at Π . Furthermore, at $V = 0.46$ close to the QCP on the Kondo side, spectral weight starts to smear out significantly

over the NFL region, and significant weight appears at positive frequencies. This suggests that f and c begin to hybridize more strongly at positive frequencies. When the QCP is crossed to $V < V_c$, the spectral weight of Σ_{ck} is now stronger at $\omega > 0$ than at $\omega < 0$, showing that c and f now hybridize more strongly at positive frequencies than in the Kondo regime. However, significant spectral weight does also remain at $\omega < 0$, reflecting the presence of a left and right h pole, as discussed already in the previous section. This suggests that, in the RKKY regime, the f band is split apart by the pole in Σ_{fk} and the c electrons then hybridize with both of the resulting two f bands, leading to a three-band structure. Thus, the f electrons still hybridize significantly with the c electrons in the RKKY phase close to the QCP, explaining intuitively the strong renormalization of m^* in the RKKY regime mentioned earlier and observed in experiments [192]. Finally, as V is lowered further toward $V = 0$, the overall magnitude of $-\text{Im}\Sigma_{ck}(\omega^+)$ decreases rapidly, suggesting that f and c bands continuously decouple when $V \rightarrow 0$.

D. Finite temperature

In Fig. 15, we show the temperature dependence of $A_{\mathbf{k}}(\omega)$ at both $V = 0.46 > V_c$ and $V = 0.455 < V_c$. For $T < T_{\text{FL}}$, the spectral functions are mostly independent of temperature as expected. As T crosses T_{FL} into the NFL region, the incoherent features at $T_{\text{FL}} < |\omega| < T_{\text{NFL}}$ are thermally broadened, and the sharp QP features at $\omega = 0$ are smeared out, indicating a thermal destruction of the QP. Deep in the NFL region at $T \simeq 10^{-5}$, spectral weight around $\omega = 0$ is completely incoherent, and no FS with sharp QP excitations can be made out. At $T = 10^{-2} > T_{\text{NFL}}$ in the LM region, the features of $A_{\mathbf{k}}(\omega)$ become sharp again around $\omega = 0$, and a single band forms which coincides with the $V = 0$ c -electron dispersion. In this temperature regime, the f electrons can be viewed as free local moments decoupled from the free c electrons. The interaction between c electrons and f moments then leads to scattering, slightly smearing out the features in the spectral function while leaving the qualitative picture of the LM region unaltered.

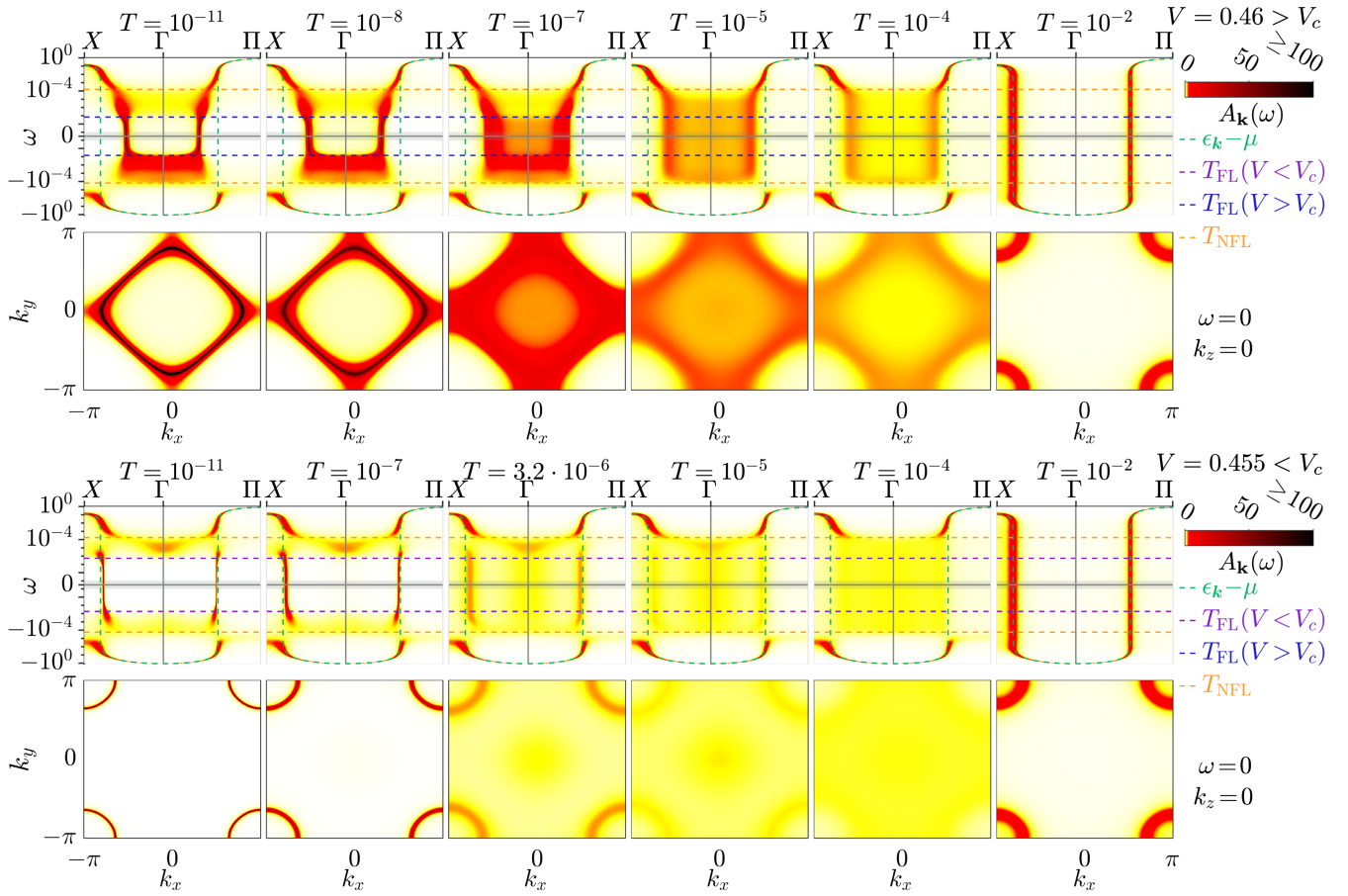


FIG. 15. Temperature dependence of $A_{\mathbf{k}}(\omega)$ at $V = 0.46 > V_c = 0.4575$ (rows 1 and 2) and $V = 0.455 < V_c$ (rows 3 and 4). The layout of rows 1 and 3 mirrors that of the top row in Fig. 13. Rows 2 and 4 show cuts at $\omega = 0$ and $k_z = 0$. These illustrate how the sharp FS at $T = 0$, large for $V > V_c$ and small for $V < V_c$, dissolves as T increases into the NFL regime and finally evolves to a (temperature-broadened) small FS in the LM regime at high T .

VIII. GENERALIZED LUTTINGER SUM RULE

In this section, we discuss the FS reconstruction of the previous section from the perspective of the generalized Luttinger sum rule [9–14,177,193,194]. It states that if a Fermi surface exists, the density n of electrons in partially filled bands can be expressed as $n = 2v_{\text{FS}} + 2I_{\text{L}}$, where v_{FS} is the FS volume and I_{L} is an integral known as the Luttinger integral. In case of a FL, the generalized Luttinger sum rule as stated above can be derived from a simple, exact decomposition of the Green's function based on Dyson's equation (we review this decomposition below). The sum rule becomes useful when it is possible to formulate constraints on I_{L} .

For instance, if the interacting and noninteracting ground states are adiabatically connected [9,195], perturbative arguments can be used to show that $I_{\text{L}} = 0$, leading to the celebrated Luttinger sum rule $n = 2v_{\text{FS}}$ (also called Luttinger's theorem). Subsequent work [193,194] has shown that $I_{\text{L}} = 0$ is a consequence of U(1) charge conservation in case Σ is Φ -derivable, i.e., if $\Sigma = \delta\Phi/\delta G$, where Φ is the Luttinger-Ward (LW) functional.

Explicitly, consider a multiband model with a U(1) total charge symmetry (we assume every band has the same gauge charge). The Green's function $G_{\mathbf{k}}(z)$ is matrix valued, with entries $G_{\alpha\beta\mathbf{k}}(z)$, where α and β label the bands. If the matrix-valued self-energy is Φ -derivable, i.e., $\Sigma_{\mathbf{k}}(z) = \delta\Phi/\delta G_{\mathbf{k}}(z)$, then the Luttinger integral

$$I_{\text{L}} = \frac{-1}{\pi} \text{Im} \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \int_{-\infty}^0 d\omega \text{Tr}[G_{\mathbf{k}}(\omega^+) \partial_{\omega} \Sigma_{\mathbf{k}}(\omega^+)] \quad (30)$$

equals zero, $I_{\text{L}} = 0$. Note that $I_{\text{L}} = 0$ holds *only* in the $T \rightarrow 0$ limit.

This extends the applicability of Luttinger's theorem beyond the perturbative regime (see also Ref. [10] for a different approach) but requires the existence of the LW functional $\Phi[G]$, at least in the vicinity of the physical Green's function G (note that Φ can be constructed non-perturbatively [196]). However, it has been established that, in general, the LW functional is multivalued [197–199] and does not exist for certain physically relevant Green's functions [14,200], which can lead to $I_{\text{L}} \neq 0$ [14,177,200].

A very instructive analysis of a situation where $I_{\text{L}} = 0$ breaks down is provided in Refs. [12,13] in terms of a fermionic two-impurity model, where the role of the Luttinger sum rule is taken by the Friedel sum rule [190]. This model exhibits a QPT from a Kondo-type to an RKKY-type phase, with the local density remaining constant while the free QP density changes abruptly. This violates the Friedel sum rule, and the violation was traced to a Luttinger integral abruptly becoming nonzero.

In this section, we perform a similar analysis for the KB QPT of the PAM. We find that the Luttinger integral is numerically zero in both the RKKY and Kondo phases; the FS reconstruction is due to the appearance of a LS in the

RKKY phase and not due to a failure of Luttinger's theorem as formulated in Ref. [193]. As a warm-up, we first consider a single partially filled band of conduction electrons and briefly recall the origin of the generalized Luttinger sum rule. Then, we focus on the PAM and derive a generalized Luttinger sum rule for $n_c + n_f$ (there are no useful separate sum rules for only n_c or only n_f , as these are not conserved quantities). It involves not only the FS, comprising all $\mathbf{k}$ points in the Brillouin zone at which $G_{f\mathbf{k}}(i0^+)$ and $G_{c\mathbf{k}}(i0^+)$ have poles, but also the LS, at which $\Sigma_{f\mathbf{k}}(i0^+)$ diverges [11]. We then express our results purely through cluster quantities that are directly available from cellular DMFT calculations without requiring reperiodization or interpolation. Thereafter, we show that the discontinuous jump of the FS volume when crossing the QCP into the RKKY phase is accompanied by the emergence of a LS while I_{L} remains zero throughout. Finally, we discuss this finding together with the Hall coefficient calculated from our data and relate it to experimental findings on YbRh₂Si₂ and CeCoIn₅.

A. Luttinger's theorem for a single band

We begin by recalling standard arguments leading to Luttinger's theorem, following Refs. [9,13,175,193]. We consider a one-band model at $T = 0$, with propagator $G_{\mathbf{k}}(z) = [z - \epsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(z)]^{-1}$. The average electron density can be expressed as

$$n = \frac{-2}{\pi} \text{Im} \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \int d\omega G_{\mathbf{k}}(\omega^+) \theta(-\omega), \quad (31)$$

where the prefactor 2 accounts for spin, $\mathcal{V}_{\text{BZ}}$ is the volume of the Brillouin zone, and the step function $\theta(-\omega)$ is the zero-temperature limit of the Fermi function.

For the next step, we need the identity

$$G_{\mathbf{k}} = \partial_z \ln G_{\mathbf{k}}^{-1} + G_{\mathbf{k}} \partial_z \Sigma_{\mathbf{k}}, \quad (32)$$

expressing the correlator through derivatives. Using the latter in Eq. (31), together with $\text{Im} \ln G_{\mathbf{k}}^{-1} = \arg G_{\mathbf{k}}^{-1}$, we obtain

$$n = 2v_{\text{FS}} + 2I_{\text{L}}, \quad (33)$$

$$v_{\text{FS}} = \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \frac{\delta_{\mathbf{k}}}{\pi},$$

$$\delta_{\mathbf{k}} = -\text{Im} \int_{-\infty}^0 d\omega \partial_{\omega} \ln G_{\mathbf{k}}^{-1}(\omega^+) = -\left[\arg G_{\mathbf{k}}^{-1}(\omega^+)\right]_{-\infty}^0, \quad (34)$$

$$I_{\text{L}} = \frac{-1}{\pi} \text{Im} \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \int_{-\infty}^0 d\omega G_{\mathbf{k}}(\omega^+) \partial_{\omega} \Sigma_{\mathbf{k}}(\omega^+). \quad (35)$$

Here, $\delta_{\mathbf{k}}$ is the phase shift of $G_{\mathbf{k}}^{-1}(\omega^+)$ $\omega = -\infty$ and 0; v_{FS} is a shorthand for its integral over the BZ; and I_{L} is the

Luttinger integral [cf. Eq. (30)]. Equation (33) is the generalized Luttinger sum rule. It is an exact expression of the electron density n ; no assumptions on FL behavior have been made yet. We show below that, in a FL, the average phase shift Eq. (34) is given by the FS volume.

As mentioned above, it can be argued on rather general grounds that $I_L = 0$ in many cases [193]. Conditions are that (i) the interaction preserves the U(1) charge symmetry and (ii) Σ is Φ -derivable, i.e., $\Sigma = \delta\Phi/\delta G$, where Φ is the LW functional. Condition (ii) breaks down if Σ is sufficiently singular, i.e., if no functional Φ exists whose variation with respect to G produces Σ [14,200]; in that case, I_L can become nonzero.

Now, if a sharp FS exists, i.e., if the imaginary part of the retarded self-energy vanishes at $\omega = 0$ [cf. Eq. (16)],

$$\text{Im}\Sigma_{\mathbf{k}}(i0^+) = -0^+, \quad (36)$$

then the integral v_{FS} defined in Eq. (34) gives the FS volume. Let us recapitulate why this is the case. Condition (36) holds for regular Fermi liquids and, more generally, in the perturbative regime considered by Luttinger and Ward [9,195]. Now, Eq. (36) implies $\arg G_{\mathbf{k}}^{-1}(i0^+) = \pi\theta(-\text{Re}G_{\mathbf{k}}^{-1}(i0^+))$, while $\text{Im}\Sigma_{\mathbf{k}}(\omega^+) < 0$ implies $\arg G_{\mathbf{k}}^{-1}(-\infty + i0^+) = \pi$. Therefore, the phase shift is

$$\begin{aligned} \delta_{\mathbf{k}} &= \pi - \pi\theta(-\text{Re}G_{\mathbf{k}}^{-1}(i0^+)) \\ &= \pi\theta(-\epsilon_{\mathbf{k}} - \text{Re}\Sigma_{\mathbf{k}}(i0^+)) = \pi\theta(-\epsilon_{\mathbf{k}}^*). \end{aligned} \quad (37)$$

By definition, the Fermi surface encloses all $\mathbf{k}$ points in the Brillouin zone having $\epsilon_{\mathbf{k}}^* < 0$. For these, $\delta_{\mathbf{k}}/\pi$ equals 1; for all others, it vanishes. Hence, Eq. (34) reduces to

$$v_{\text{FS}} = \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \theta(-\epsilon_{\mathbf{k}}^*), \quad (38)$$

which is the FS volume measured in units of $\mathcal{V}_{\text{BZ}}$ (hence, dimensionless). Moreover, in a normal FL, Σ is not singular; hence, $I_L = 0$ holds, and, hence, the generalized Luttinger sum rule (33) reduces to the Luttinger sum rule for a FL, $n = 2v_{\text{FS}}$, relating the density to the FS volume.

B. Generalized Luttinger theorem for the PAM

The PAM describes hybridized f and c electrons, the former with local interactions, the latter without. Their correlators G_f and G_c are coupled through Eqs. (3). Importantly, because Φ does not depend on propagators involving noninteracting orbitals [175], the LW functional for the PAM depends only on G_f , not on G_c or G_{fc} . Therefore, $\Sigma_f = \delta\Phi/\delta G_f$ is the only Φ -derivable, proper (i.e., one-particle irreducible) self-energy in the PAM. Σ_c knows about interactions only via its dependence on Σ_f and, hence, is not a proper self-energy; in particular,

$\delta\Phi/\delta G_c = \delta\Phi/\delta G_{fc} = 0$. Analogous to the previous subsection, we first derive general formulas for the phase shifts. We then make assumptions on the self-energies compatible with our observations in Secs. VI and VII. These allow us to write down expressions in terms of the FS and LS volumes.

Our starting point again is an identity expressing correlators through derivatives. Equation (2) implies

$$\begin{aligned} \text{Tr}G_{\mathbf{k}} &= G_{f\mathbf{k}} + G_{c\mathbf{k}} = \text{Tr}G_{\mathbf{k}}\partial_z G_{\mathbf{k}}^{-1} + G_{f\mathbf{k}}\partial_z \Sigma_{f\mathbf{k}} \\ &= \partial_z \text{Tr} \ln G_{\mathbf{k}}^{-1} + G_{f\mathbf{k}}\partial_z \Sigma_{f\mathbf{k}} \\ &= \partial_z \ln G_{c\mathbf{k}}^{-1} + \partial_z \ln \Sigma_{c\mathbf{k}}^{-1} + G_{f\mathbf{k}}\partial_z \Sigma_{f\mathbf{k}}. \end{aligned} \quad (39)$$

To derive the last equality, note that the definitions (2) and (3) for the lattice correlators imply the relation

$$\begin{aligned} \det G_{\mathbf{k}}^{-1} &= (z - \epsilon_{c\mathbf{k}})(z - \epsilon_f - \Sigma_{f\mathbf{k}}) - V^2 \\ &= \left(z - \epsilon_{c\mathbf{k}} - \frac{V^2}{z - \epsilon_f - \Sigma_{f\mathbf{k}}}\right)(z - \epsilon_f - \Sigma_{f\mathbf{k}}) \\ &= G_{c\mathbf{k}}^{-1}\Sigma_{c\mathbf{k}}^{-1}/V^2, \end{aligned} \quad (40)$$

which, together with $\text{Tr} \ln G_{\mathbf{k}}^{-1} = \ln \det G_{\mathbf{k}}^{-1}$, yields Eq. (39). Integrating $G_f + G_c$ as in Eq. (31),

$$n_f + n_c = \frac{-2}{\pi} \text{Im} \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \int_{-\infty}^0 d\omega [G_{f\mathbf{k}}(\omega^+) + G_{c\mathbf{k}}(\omega^+)],$$

and using Eq. (39), we obtain

$$n_f + n_c = 2v_{\text{FS}} + 2v_{\text{LS}} + 2I_L, \quad (41)$$

with ingredients defined in analogy to Eqs. (34) and (35):

$$v_{\text{FS}} = \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \frac{\delta_{c\mathbf{k}}}{\pi}, \quad v_{\text{LS}} = \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \frac{\delta_{\Sigma\mathbf{k}}}{\pi}, \quad (42)$$

$$\begin{aligned} \delta_{c\mathbf{k}} &= -\text{Im} \int_{-\infty}^0 d\omega \partial_{\omega} \ln G_{c\mathbf{k}}^{-1}(\omega^+) = -[\arg G_{c\mathbf{k}}^{-1}(\omega^+)]_{-\infty}^0, \\ \delta_{\Sigma\mathbf{k}} &= -\text{Im} \int_{-\infty}^0 d\omega \partial_{\omega} \ln \Sigma_{c\mathbf{k}}^{-1}(\omega^+) = +[\arg \Sigma_{c\mathbf{k}}^{-1}(\omega^+)]_{-\infty}^0, \\ I_L &= \frac{-1}{\pi} \text{Im} \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \int_{-\infty}^0 d\omega G_{f\mathbf{k}}(\omega^+) \partial_{\omega} \Sigma_{f\mathbf{k}}(\omega^+). \end{aligned} \quad (43)$$

Here, $\delta_{c\mathbf{k}}$ and $\delta_{\Sigma\mathbf{k}}$ describe the phase shifts of $G_{c\mathbf{k}}^{-1}$ and $\Sigma_{c\mathbf{k}}^{-1}$ between $\omega = -\infty$ and 0; v_{FS} and v_{LS} are shorthand for their integrals over the BZ; and I_L is the Luttinger integral, now involving only f (no c) functions. Equations (41)–(43) are exact, and, in the spirit of Refs. [12,13], we refer to Eq. (41) as the generalized Luttinger sum rule for the PAM, or Luttinger-PAM sum rule, for short. To the best of our knowledge, the existence of such a relation, involving the phase shifts not only of $G_{c\mathbf{k}}^{-1}$, but also of $\Sigma_{c\mathbf{k}}^{-1}$, has so far not

been appreciated in the literature. The form (41) is specific to the PAM. For other multiband models, the arguments presented here have to be suitably adapted.

Now, if a sharp FS exists, i.e., if

$$\text{Im}\Sigma_{c\mathbf{k}}(i0^+) = -0^+, \quad (44)$$

then the integrals v_{FS} and v_{LS} defined in Eqs. (42) give the FS and LS volumes, respectively. The argument proceeds as in the previous subsection. Equation (44) implies $\arg G_{c\mathbf{k}}^{-1}(i0^+) = \pi\theta(-\text{Re}G_{c\mathbf{k}}^{-1}(i0^+))$ and $\arg \Sigma_{c\mathbf{k}}(i0^+) = -\pi\theta(-\text{Re}\Sigma_{c\mathbf{k}}(i0^+))$, while $\text{Im}\Sigma_{c\mathbf{k}}(\omega^+) < 0$ implies $\arg G_{c\mathbf{k}}^{-1}(-\infty + i0^+) = \pi$ and $\arg \Sigma_{c\mathbf{k}}(-\infty + i0^+) = -\pi$. Therefore, the phase shifts in Eq. (43) yield

$$\begin{aligned} \delta_{c\mathbf{k}} &= \pi - \pi\theta(-\text{Re}G_{c\mathbf{k}}^{-1}(i0^+)) \\ &= \pi\theta(-\epsilon_{c\mathbf{k}} - \text{Re}\Sigma_{c\mathbf{k}}(i0^+)) = \pi\theta(-\epsilon_{c\mathbf{k}}^*), \end{aligned} \quad (45a)$$

$$\delta_{\Sigma\mathbf{k}} = \pi - \pi\theta(-\text{Re}\Sigma_{c\mathbf{k}}(i0^+)) = \pi\theta(\text{Re}\Sigma_{c\mathbf{k}}(i0^+)). \quad (45b)$$

The phase shifts $\delta_{c\mathbf{k}}$ and $\delta_{\Sigma\mathbf{k}}$ are either 0 or π . The jump between these values occurs at the FS, defined by $\text{Re}G_{c\mathbf{k}}^{-1}(i0^+) = 0$ and the LS, defined by $\text{Re}\Sigma_{c\mathbf{k}}(i0^+) = 0$, respectively [see Eqs. (29b) and Fig. 16]. Thus, Eqs. (42) reduce to

$$v_{\text{FS}} = \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \theta(-\epsilon_{c\mathbf{k}}^*), \quad v_{\text{LS}} = \int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \theta(\text{Re}\Sigma_{c\mathbf{k}}(i0^+)), \quad (46)$$

giving the FS and LS volumes in units of $\mathcal{V}_{\text{BZ}}$. Thus, if a sharp FS exists, the Luttinger-PAM sum rule (41) relates the density of c and f electrons to the FS and LS volumes v_{FS} and v_{LS} and the Luttinger integral I_L .

The above arguments are directly applicable to our CDMFT + NRG results for the PAM, since the condition (44) is consistent with our results for $0 < V \neq V_c$: indeed, we find that the imaginary part of Σ_c vanishes at $\omega = 0$, both in the effective impurity model (see Sec. VI) and after reperiodization (see Sec. VII).

Since Φ depends only on G_f , so that $\delta\Phi/\delta G_c = 0$ and $\delta\Phi/\delta G_{fc} = 0$, I_L as defined in Eq. (43) has the same form as Eq. (30). We, therefore, expect $I_L = 0$ if the functional Φ exists in the vicinity of G_f , but we do not concern ourselves here with general considerations about the existence of the LW functional. We have, however, checked numerically that $I_L = 0$ holds in our study of the PAM, for all considered values of V at $T = 0$, i.e., in both the Kondo and RKKY regimes. Thus, we henceforth assume that $I_L = 0$ throughout.

While n_c and n_f evolve smoothly with V , sudden jumps can occur for v_{FS} and v_{LS} , which must compensate each other appropriately if I_L remains zero. In particular, by

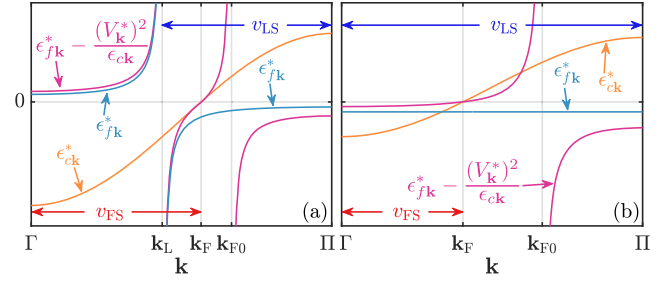


FIG. 16. Sketch of the qualitative behavior of $\epsilon_{f\mathbf{k}}^*$, $\epsilon_{c\mathbf{k}}^*$, and $\epsilon_{f\mathbf{k}}^* - (V_{\mathbf{k}}^*)^2/\epsilon_{c\mathbf{k}}^*$ in (a) the RKKY phase and (b) the Kondo phase. They are related to the Green's functions and the c -electron self-energy via $\text{Re}G_{c\mathbf{k}}^{-1}(0) = -\epsilon_{c\mathbf{k}}^*/Z_{c\mathbf{k}}$, $\text{Re}G_{f\mathbf{k}}^{-1}(0) = -[\epsilon_{f\mathbf{k}}^* - (V_{\mathbf{k}}^*)^2/\epsilon_{c\mathbf{k}}^*]/Z_{f\mathbf{k}}$, and $\text{Re}\Sigma_{c\mathbf{k}}(0) = -(V_{\mathbf{k}}^*)^2/\epsilon_{f\mathbf{k}}^*$, respectively. The FS (marked by $\mathbf{k}_F$) is defined by $\epsilon_{c\mathbf{k}}^* = \epsilon_{f\mathbf{k}}^* - (V_{\mathbf{k}}^*)^2/\epsilon_{c\mathbf{k}}^* = 0$; its inside is defined by $\epsilon_{c\mathbf{k}}^* < 0$. $|\epsilon_{f\mathbf{k}}^*| = \infty$ [$\text{Re}\Sigma_{c\mathbf{k}}(0) = 0$] defines the LS (marked by $\mathbf{k}_L$), with its inside defined by $\epsilon_{f\mathbf{k}}^* < 0$. The function $\epsilon_{f\mathbf{k}}^* - (V_{\mathbf{k}}^*)^2/\epsilon_{c\mathbf{k}}^*$ changes sign via a pole both at the LS (due to $\epsilon_{f\mathbf{k}}^*$) and at the free FS (marked by $\mathbf{k}_{F0}$) due to $\epsilon_{c\mathbf{k}} = 0$. In the Kondo phase, $\epsilon_{f\mathbf{k}}^*$ remains negative everywhere in the BZ, while in the RKKY phase, $\epsilon_{f\mathbf{k}}^*$ changes sign between Γ and Π (cf. Fig. 9) via a pole at the LS. As a result, $\epsilon_{f\mathbf{k}}^* - (V_{\mathbf{k}}^*)^2/\epsilon_{c\mathbf{k}}^*$ changes sign twice in the Kondo phase (via a zero at $\mathbf{k}_F$ and a pole at $\mathbf{k}_{F0}$) and three times in the RKKY phase (via a pole at $\mathbf{k}_L$, a zero at $\mathbf{k}_F$, and a pole at $\mathbf{k}_{F0}$). The pole at $\mathbf{k}_L$ shifts the position of $\mathbf{k}_F$ in the RKKY phase compared to its position in the Kondo phase. Note that the distance between $\mathbf{k}_F$ and $\mathbf{k}_{F0}$ in (a) is exaggerated in the sketch above.

Eq. (41), a jump in v_{LS} induces a jump in v_{FS} , implying a FS reconstruction, even though $I_L = 0$ remains unchanged.

C. Luttinger's theorem in CDMFT: Computing v_{FS} , v_{LS} , and I_L without reperiodization

The formulas derived in Sec. VIII A require explicit knowledge of the $\mathbf{k}$ dependence of Σ_f to compute v_{FS} , v_{LS} , and I_L . As CDMFT artificially breaks translation invariance, we have to reperiodize Σ_f if we want to acquire knowledge on its $\mathbf{k}$ dependence. Reperiodization is, however, a postprocessing step which is to some extent *ad hoc*. The specific choice of reperiodization affects the values of the aforementioned quantities. In particular, the question whether $I_L = 0$ holds can, therefore, not be answered conclusively when relying on some reperiodization scheme. In the following, we therefore provide and motivate formulas for v_{FS} , v_{LS} , and I_L which do not require reperiodization.

First, we note that the momentum integrals in the preceding part of this section represent a trace over all quantum numbers. In the case of translational invariance, it is convenient to use the momentum basis to perform this trace, as the Green's functions and self-energies are diagonal in this basis. In the two-site CDMFT approach,

it is, however, more convenient to represent them as 2×2 matrices depending on momenta $\mathbf{K}$ in the cluster BZ (cBZ). This leads to the replacement

$$\int_{\text{BZ}} \frac{d\mathbf{k}}{\mathcal{V}_{\text{BZ}}} \rightarrow \frac{1}{2} \text{Tr} \int_{\text{cBZ}} \frac{d\mathbf{K}}{\mathcal{V}_{\text{cBZ}}} \quad (47)$$

in the formulas presented in Sec. VIII B. Here, $\mathcal{V}_{\text{cBZ}} = \mathcal{V}_{\text{BZ}}/2$ the volume of the cBZ, and Tr is the trace of the $\mathbf{K}$ -dependent 2×2 matrices.

Now, within the CDMFT approximation, Σ_f and, therefore, also Σ_c are independent of $\mathbf{K}$:

$$\Sigma_{x\mathbf{K}}(z) = \Sigma_x(z) \quad (x = f, c). \quad (48)$$

(This $\mathbf{K}$ independence breaks the translation invariance.) Moreover, the cluster propagators in Eq. (6), defined as $\mathbf{K}$ -integrated objects, are likewise $\mathbf{K}$ independent:

$$G_x(z) \equiv \int_{\text{cBZ}} \frac{d\mathbf{K}}{\mathcal{V}_{\text{cBZ}}} G_{x\mathbf{K}}(z) \quad (x = f, c). \quad (49)$$

Using Eqs. (47)–(49), the ingredients (42) and (43) of the Luttinger-PAM sum rule (41) can now readily be transcribed to obtain the following expressions:

$$\begin{aligned} v_{\text{FS}} &= \text{Tr} \int_{\text{cBZ}} \frac{d\mathbf{K}}{\mathcal{V}_{\text{cBZ}}} \frac{\delta_{c\mathbf{K}}}{2\pi}, \quad v_{\text{LS}} = \text{Tr} \int_{\text{cBZ}} \frac{d\mathbf{K}}{\mathcal{V}_{\text{cBZ}}} \frac{\delta_{\Sigma}}{2\pi}, \\ \delta_{c\mathbf{K}} &= -\text{Im} \int_{-\infty}^0 d\omega \partial_{\omega} \ln G_{c\mathbf{K}}^{-1}(\omega^+), \\ \delta_{\Sigma} &= -\text{Im} \int_{-\infty}^0 d\omega \partial_{\omega} \ln \Sigma_c^{-1}(\omega^+) = + \left[\arg \Sigma_c^{-1}(\omega^+) \right]_{-\infty}^0, \\ I_L &= \frac{-1}{2\pi} \text{Im} \int_{-\infty}^0 d\omega \text{Tr} [G_f(\omega^+) \partial_{\omega} \Sigma_f(\omega^+)]. \end{aligned} \quad (50)$$

Here, v_{FS} and v_{LS} are expressed as traces of the cBZ integrals of the matrix-valued phase shifts $\delta_{c\mathbf{K}}$ and δ_{Σ} , respectively. For the latter, which is $\mathbf{K}$ -independent δ_{Σ} , the integral is trivial. For the $\mathbf{K}$ -dependent, we use

$$\partial_z \ln G_{c\mathbf{K}}^{-1}(z) = G_{c\mathbf{K}}(z) [1 - \partial_z \Sigma_c(z)], \quad (52)$$

such that the $\mathbf{K}$ integral yields a local cluster quantity:

$$\delta_c = \int_{\text{cBZ}} \frac{d\mathbf{K}}{\mathcal{V}_{\text{cBZ}}} \delta_{c\mathbf{K}} = -\text{Im} \int_{-\infty}^0 d\omega G_c(\omega^+) [1 - \partial_{\omega} \Sigma_c(\omega^+)]. \quad (53)$$

Note that, in Eq. (53), $1 - \partial_z \Sigma_c(z) \neq \partial_z G_c^{-1}(z)$ because $G_c(z)$ is a $\mathbf{K}$ -integrated quantity, so that $G_c^{-1}(z)$ contains an additional hybridization term $\Delta_c(z)$; cf. Eq. (6b). Thus, Eqs. (50) reduce to

$$v_{\text{FS}} = \frac{1}{2\pi} \text{Tr} \delta_c, \quad v_{\text{LS}} = \frac{1}{2\pi} \text{Tr} \delta_{\Sigma}. \quad (54)$$

Equations (54), (53), and (51) achieve our stated goal of expressing v_{FS} , v_{LS} , and I_L purely through the local Green's functions and self-energies of the effective 2IAM. They can, hence, be computed without using reperiodization.

D. Results

Our CDMFT results for v_{FS} , v_{LS} , and I_L (obtained with the formulas from Sec. VIII C) are shown in Fig. 17, together with the particle numbers n_c and n_f . As mentioned before, we find $I_L = 0$ for all considered values of V . We note that $I_L = 0$ is an empirical numerical finding and may not hold if, e.g., different fillings are considered [201,202]; this will be explored in more detail in future work. Furthermore, we find that the particle numbers n_c and n_f evolve smoothly across the KB QCP, in contrast to v_{FS} and v_{LS} , which exhibit a jump when crossing the KB QCP. The jumps are such that $2v_{\text{FS}} + 2v_{\text{LS}} = n_f + n_c$ evolves smoothly across the KB QCP; i.e., the jumps of v_{FS} and v_{LS} compensate each other.

In the Kondo phase, $v_{\text{LS}} = 1$ and v_{FS} is such that, together, v_{LS} and v_{FS} account for the total particle number. Note that $v_{\text{LS}} = 1$ means that the LS volume fills the whole BZ; i.e., there is no LS in the Kondo phase. In the RKKY phase, on the other hand, $v_{\text{LS}} = \frac{1}{2} \simeq \frac{1}{2} n_f$ while $v_{\text{FS}} \simeq \frac{1}{2} n_c$. v_{LS} takes a fractional value in the RKKY phase, which means the LS volume fills a fraction of the BZ and there is a LS. The presence of a LS can be linked to an emergent spinon FS [151], suggesting that the RKKY phase is a fractionalized FL [110,111]. We will provide a more detailed analysis of this in future work.

In the Kondo phase, v_{FS} is the same as in the $U = 0$ limit at the same filling (the same is true for v_{LS}). The FS in the Kondo phase is, therefore, as expected in a normal FL in the PAM. v_{FS} “trivially” (in the sense that one can infer it from the $U = 0$ limit) accounts for both the f and c electrons, which is why it is called a “large” FS, even though the value of v_{FS} is smaller than in the RKKY phase. In the RKKY phase, by contrast, $v_{\text{FS}} \simeq \frac{1}{2} n_c$ takes almost the value expected for $V = 0$ with $U \neq 0$. The FS seems to account

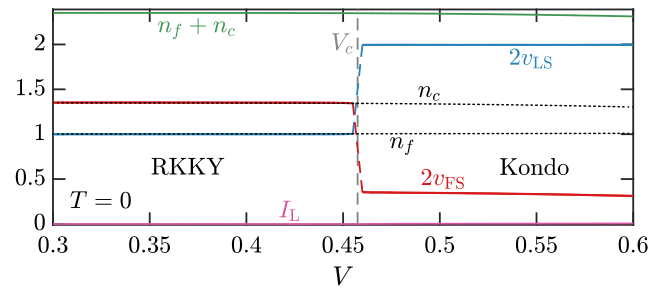


FIG. 17. FS and LS volumes v_{FS} (red line) and v_{LS} (blue line) and the Luttinger integral I_L (pink line), together with the particle numbers n_f and n_c (black dotted line) and their sum (green line), plotted as functions of V at $T = 0$.

only for the c electrons and, hence, is called a “small” FS. Based on the shape and volume of the FS in the RKKY phase, one may be tempted to conclude that c and f electrons have decoupled. However, this is not the case, as elaborated in Secs. VI and VII above.

We now elaborate how the jump in v_{FS} and v_{LS} is connected to the sign change of ϵ_{f+}^* across the KB QCP, which we have discussed in Sec. VIC. To make this connection, we examine Eq. (54) for v_{LS} (computed without reperiodization) in more detail, while assuming $\text{Im}\Sigma_c(0) = -0^+$ [Eq. (44)], consistent with our results. Analogously to our discussion of $\delta_{\Sigma\mathbf{k}}$ under the aforementioned assumption [see Eq. (45b)], the corresponding phase shift of the effective 2IAM [see Eq. (51)] [is given by $\delta_{\Sigma} = \pi\theta(\text{Re}\Sigma_c(i0^+))$] [note that both δ_{Σ} and $\Sigma_c(i0^+)$ are 2×2 matrices which are in our case diagonal in the $\pm$ basis]. We can identify three different cases, which lead to distinct values of v_{LS} : Both eigenvalues of $\text{Re}\Sigma_c(i0^+)$ are (i) positive or (ii) negative, or (iii) the eigenvalues of $\text{Re}\Sigma_c(i0^+)$ have opposite signs—i.e., one is positive, the other negative. Inserting these into $v_{\text{LS}} = \text{Tr}\delta_{\Sigma}/(2\pi)$ [see Eq. (54)], we find (i) $v_{\text{LS}} = 1$, (ii) $v_{\text{LS}} = 0$, or (iii) $v_{\text{LS}} = \frac{1}{2}$. The value of v_{LS} is, therefore, connected to the *signs* of the *eigenvalues* of $\text{Re}\Sigma_c(i0^+)$, which in our case are $\text{Re}\Sigma_{c\pm}(i0^+)$. The signs are related to those of $\epsilon_{f\pm}^*$ via Eq. (25b), namely, $\text{sgnRe}\Sigma_{c\pm}(i0^+) = -\text{sgn}\epsilon_{f\pm}^*$. Thus, we find (i) $v_{\text{LS}} = 1$ if $\epsilon_{f\pm}^*$ are both negative, (ii) $v_{\text{LS}} = 0$ if $\epsilon_{f\pm}^*$ are both positive, and (iii) $v_{\text{LS}} = \frac{1}{2}$ if $\epsilon_{f\pm}^*$ come with opposite signs.

In the Kondo phase, both $\epsilon_{f\pm}^*$ are negative (cf. Fig. 9), just as in the $U \rightarrow 0$ limit for the parameters we have chosen, which leads to $v_{\text{LS}} = 1$ in the Kondo phase. As discussed in more detail in Sec. VIC, when the KB QCP is crossed from the Kondo to the RKKY phase, ϵ_{f+}^* changes sign and becomes positive while ϵ_{f-}^* remains negative, which leads to $v_{\text{LS}} = \frac{1}{2}$ in the RKKY phase. Since v_{LS} jumps due to the sign change of ϵ_{f+}^* , v_{FS} exhibits a corresponding jump.

Therefore, the crucial ingredient for the emergence of a LS resulting in a FS reconstruction is momentum differentiation in $\epsilon_{f\mathbf{k}}^*$. The two-site cluster is the smallest unit where momentum differentiation can occur, and our results and analysis show that this momentum differentiation is sufficient to stabilize the small FS of the RKKY phase. Figure 9(b) also shows that $|\epsilon_{f+}^* - \epsilon_{f-}^*| \sim T_{\text{FL}}$; i.e., the momentum differentiation is weak and occurs on the order of the low-energy scale T_{FL} .

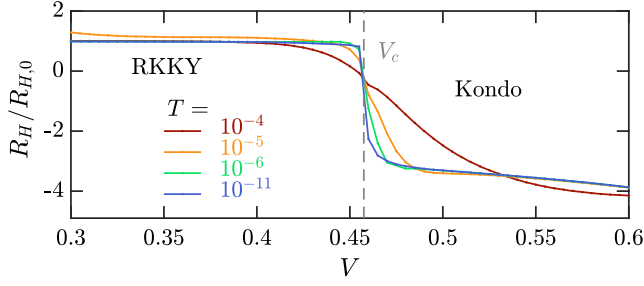
We note that a jump of v_{LS} and v_{FS} is not at odds with a continuous QPT. Indeed, ϵ_{f+}^* changes smoothly across the KB QCP. The reason why v_{LS} jumps is because it is not sensitive to the absolute value of $\epsilon_{f\pm}^*$, but only to the signs. Signs are, by definition, discrete quantities, and changes can occur only via jumps, which is why both v_{LS} and v_{FS}

change via a jump, even though the QPT is continuous. We emphasize that a prerequisite for this sign sensitivity is that $\text{Im}\Sigma_c(i0^+) = 0^-$, i.e., that the $T \rightarrow 0$ phase is a FL. If $\text{Im}\Sigma_c(i0^+)$ were finite, v_{LS} and v_{FS} could change continuously. Because finite $\text{Im}\Sigma_c(i0^+)$ would imply that the $T \rightarrow 0$ phase is not a FL, v_{LS} and v_{FS} then would not have the interpretations of being volumes in the BZ bounded by sharply defined Fermi or Luttinger surfaces.

Furthermore, our analysis shows that the FS reconstruction is *a priori* independent of possible translation symmetry breaking like antiferromagnetic or charge density wave order. Translation symmetry breaking increases the size of the unit cell and, thus, reduces the size of the BZ. While this may change the FS volume measured in units of the smaller BZ, it does *not* change the average phase shifts v_{LS} and v_{FS} as they appear in Eqs. (42) and (50). For instance, the onset of antiferromagnetic order without jumps in the phase shifts v_{LS} and v_{FS} marks a SDW QCP, while jumps in the phase shifts v_{LS} and v_{FS} mark a KB QCP, regardless of whether it is or is not accompanied by the onset of, e.g., AFM order.

The generalized Luttinger’s theorem also offers a possible explanation why the QCP in the 2IAM is stabilized by the CDMFT self-consistency condition. Without self-consistency, the QCP in the 2IAM is stable only if the scattering phase shifts are constrained by symmetry [87,89,174]. The symmetry constraint then prevents a smooth change of the phase shifts, resulting in a QCP where the phase shifts jump between allowed values [87,89]. However, if such symmetry constraints are *absent*, the phase shifts will simply change without a QCP [89]. In the self-consistent 2IAM, the phase shifts *are* constrained, not by symmetry, but by the Luttinger sum rule, as we have seen in the previous discussions in this section. We conjecture that this Luttinger sum rule constraint is the reason why the self-consistent 2IAM does have a QCP. A more detailed analysis will be presented in future work.

One of the experimental hallmarks of a FS reconstruction at a KB QCP is a sharp crossover of the Hall coefficient $R_{\text{H}} \sim 1/n_{\text{H}}$ and, thus, of the Hall carrier density n_{H} [6,26,32]. This has been observed in experiments on YbRh_2Si_2 [26,37,203] and CeCoIn_5 [32]. A sign change of R_{H} has also been observed in $\text{CeCu}_{6-x}\text{Au}_x$ when increasing x from 0 to 0.1 [204]. To make contact to these experiments, we show the Hall coefficient calculated from our data in Fig. 18, as a function of V at different temperatures. It is calculated using reperiodized self-energies with the formulas shown in Appendix A 5. At all considered temperatures, we find two qualitatively distinct values of R_{H} deep in the Kondo regime (high V) and deep in the RKKY regime (low V). It shows a sign change across V_c , reflecting a reconstruction from a particlelike FS in the Kondo regime to a holelike FS in the RKKY regime. These are connected by a smooth crossover at high temperatures, which becomes sharper as temperature is lowered and

FIG. 18. Hall coefficient versus V for different temperatures.

almost steplike at the lowest temperature. This is qualitatively very similar to the experimental findings on YbRh_2Si_2 [26,37,203] and CeCoIn_5 [32].

The analysis of generalized Luttinger sum rules for coupled c and f bands presented in this section makes no claims for generality—it focuses solely on the PAM and is based on assumptions consistent with our numerical results for this model. Nevertheless, similar analyses are likely possible for related models hosting QPTs with FS reconstruction, and we expect the LS to play a crucial role there, too.

IX. SOMMERFELD COEFFICIENT AND ENTROPY

A further quantity showing interesting behavior at a heavy-fermion QCP is the lattice Sommerfeld coefficient

$$\gamma_{\text{latt}} = C_{\text{latt}}/T = \partial S_{\text{latt}}/\partial T. \quad (55)$$

Here, C_{latt} and S_{latt} are the lattice specific heat and entropy per two-site cluster (*not* just the impurity contribution), respectively. S_{latt} can be computed from the f -electron contribution to the entropy S_f of the effective 2IAM and a correction term S_{corr} [119,205], as follows:

$$S_{\text{latt}} = S_f + S_{\text{corr}}, \quad (56a)$$

$$S_f = -\left. \frac{\partial \Omega_f}{\partial T} \right|_{\Delta_f = \text{const}}, \quad (56b)$$

$$\Omega_f = \Phi[G_f] - \frac{2}{\pi} \text{Tr} \int_{\omega} f_T(\omega) (\delta_f - \text{Im}[\Sigma_f G_f]), \quad (56c)$$

$$S_{\text{corr}} = \frac{2}{\pi} \text{Tr} \int_{\omega} \frac{\partial f_T(\omega)}{\partial T} (\delta_c + \delta_{\Sigma} - \delta_f), \quad (56d)$$

$$\delta_f(\omega^+) = -\text{Im} \ln G_f^{-1}(\omega^+), \quad (56e)$$

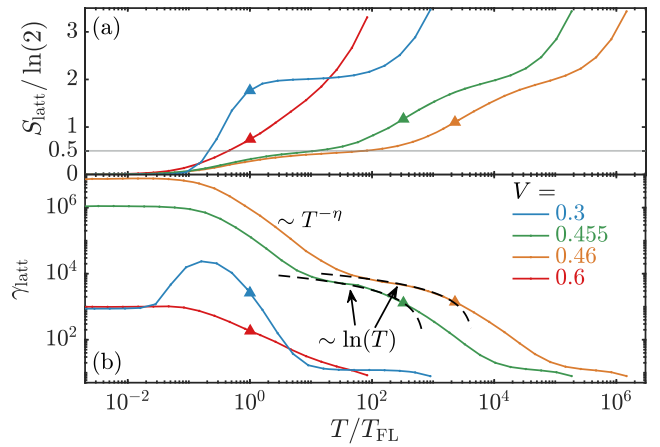
$$\delta_{\Sigma}(\omega^+) = -\text{Im} \ln \Sigma_c^{-1}(\omega^+), \quad (56f)$$

$$\delta_c(\omega^+) = -\text{Im} \int_{\text{cBZ}} \frac{d\mathbf{K}}{\mathcal{V}_{\text{cBZ}}} \ln G_{c\mathbf{K}}^{-1}(\omega^+). \quad (56g)$$

Here, Φ is the Luttinger-Ward functional of the 2IAM, $f_T(\omega) = 1/[\exp(\omega/T) + 1]$ is the Fermi-Dirac distribution, Tr is a trace over the cluster indices, and δ_f , δ_{Σ} , and δ_c are matrix-valued phase shifts. The derivative in Eq. (56b), which is evaluated while keeping the hybridization function Δ_f fixed, is accessible via NRG [206]. The correction S_{corr} accounts for the fact that $\Delta_f(T)$ actually depends on temperature [205]. To compute the Sommerfeld coefficient $\gamma_{\text{latt}} = \partial S_{\text{latt}}/\partial T$, we numerically differentiate $S_{\text{latt}}(T)$.

The Sommerfeld coefficient is a measure of the density of states. In a FL, it is proportional to the QP mass (m^*) and QP weight (Z), $\gamma \sim m^* \sim Z^{-1}$ [15] and, hence, is expected to be independent of temperature. By contrast, a $\gamma_{\text{latt}} \sim \ln(T)$ dependence, indicating NFL behavior, has been observed almost universally for numerous compounds in strange-metallic regimes at finite temperatures above QCPs [4,7,207,208], e.g., for YbRh_2Si_2 [25,28,192,209], $\text{CeCu}_{6-x}\text{Au}_x$ [29,64], and CeCoIn_5 [67]. Furthermore, γ_{latt} has been observed to diverge when approaching the KB QCP from either side [28,191]; this implies a divergent effective mass m^* at the QCP. A divergence of m^* when approaching the KB QCP from either side has been observed in many HF materials using different measurement techniques [28–30,33]. This is direct evidence for a breakdown of the FL at the QCP [28].

Our results for $S_{\text{latt}}(T)$ and $\gamma_{\text{latt}}(T)$ are shown Figs. 19(a) and 19(b). At very high temperatures ($T \gg T_{\text{NFL}}$), S_{latt} decreases from some high- T value and, for $V < 0.6$, exhibits a shoulder around $2\ln(2)$ (the entropy of two local moments). This shoulder becomes more pronounced for lower V (and is not visible for $V = 0.6$). In the same high-temperature range, γ_{latt} shows a shoulder which is also more pronounced for lower V (and again not visible for $V = 0.6$). Thus, the entropy in this high-temperature regime has a linear T dependence, $S_{\text{latt}}(T) \simeq 2\ln(2) + a \cdot T$,

FIG. 19. Temperature dependence of (a) the lattice entropy and (b) the specific heat coefficient per two-site cluster. Triangles mark the position of $T_{\text{NFL}}/T_{\text{FL}}$.

with a slope a which is almost independent of V (since $\gamma_{\text{latt}} = \partial_T S_{\text{latt}}$ is roughly independent of V in the high- T shoulder region). This behavior can be understood in terms of thermally fluctuating f moments (leading to the shoulder of S_{latt}) and unrenormalized thermally excited c electrons, leading to the V -independent linear-in- T dependence and, hence, a V -independent shoulder in γ_{latt} . Such a temperature dependence is characteristic for the LM regime, which is also expected to be more pronounced for lower V .

As T is lowered, the free moments begin to hybridize with the c electrons. This leads to screening of the moments, by forming both Kondo singlets and interimpurity singlets, thus reducing the entropy. Far away from V_c (blue and red curves), where $T_{\text{FL}} \simeq T_{\text{NFL}}$, the entropy drops to zero as $T \rightarrow 0$ without notable features at intermediate temperatures. Deep in the RKKY regime ($V = 0.3$), this entropy decrease reflects the formation of f -electron singlets and is very rapid, leading to a pronounced hump of γ_{latt} around $T \simeq T_{\text{FL}} \simeq T_{\text{NFL}}$.

However, close to V_c (green and orange curves), $S_{\text{latt}}(T)$ flattens considerably in the intermediate range $T_{\text{FL}} \lesssim T \lesssim T_{\text{NFL}}$, resulting in a second shoulder near $\ln \sqrt{2}$. Concurrently, $\gamma_{\text{latt}}(T)$ shows a logarithmic T dependence (black dashed lines), implying a $T \ln T$ behavior for the specific heat. As mentioned above, this is an almost universal feature of heavy-fermion compounds with KB QCPs.

The shoulder at $\ln \sqrt{2}$ for the lattice entropy suggests that at the QCP, where $T_{\text{FL}} = 0$, the zero-temperature entropy would be nonzero, $S_{\text{latt}}(T \rightarrow 0) = \ln \sqrt{2}$. This value is also found for the zero-temperature impurity entropy of the two-channel Kondo model and the two-impurity Kondo model, where it can be attributed to an unscreened Majorana zero mode at the QCP [79,166,210] (see also the next section). For the PAM, this means that two-site CDMFT predicts a nonzero, extensive entropy at $T = 0$ at the QCP. This suggests that the KB QCP in two-site CDMFT would be highly unstable to symmetry-breaking orders tending to get rid of the nonzero entropy. It remains to be checked in future work (by studying larger cluster sizes) whether this extensive entropy is due to the finite cluster size, i.e., whether the entropy per lattice site at the KB QCP scales to zero with increasing the cluster size or whether the nonzero $T \rightarrow 0$ entropy per lattice site is robust, independent of cluster size.

When T is decreased to about 1–2 orders of magnitude below T_{NFL} , the $\ln T$ dependence of γ_{latt} turns to a $T^{-\eta}$ dependence, with $\eta \simeq 4/3$, before becoming constant below T_{FL} . A somewhat similar power-law T dependence, with an onset temperature of less than 1 order of magnitude below T_{NFL} , has also been found in YbRh_2Si_2 [28,192,209], albeit with different exponent of $\eta = 1/3 < 1$ [28]. Reference [28] suggested that, for YbRh_2Si_2 , the $T^{-\eta}$ dependence is a property of the NFL. For our PAM, however, this cannot be the case: Since at V_c the NFL

regime reaches down $T \rightarrow 0$, it cannot support $T^{-\eta}$ behavior with $\eta > 1$, since its specific heat $C_{\text{latt}} = T\gamma_{\text{latt}} \sim T^{1-\eta}$ would diverge, which is thermodynamically impossible. Furthermore, since $\gamma_{\text{latt}} = \partial_T S_{\text{latt}}$, the $T^{-\eta}$ behavior of γ_{latt} implies $S_{\text{latt}}(T) \sim T^{1-\eta}/(1-\eta) + \text{const}$ in this regime. If the power-law dependence would extend all the way down to $T = 0$, $\eta > 1$ would imply $S_{\text{latt}}(T = 0) = -\infty$, which is clearly nonsense. Therefore, we view the $T^{-\eta}$ power law of γ_{latt} to be a property of the NFL-FL *crossover* rather than of the NFL regime itself. Since $\gamma_{\text{latt}} \sim \ln T$ in the NFL region is a much weaker singularity than the $T^{-\eta}$ crossover behavior, the latter takes over at a relatively high temperature compared to T_{FL} .

For $T < T_{\text{FL}}$, $\gamma_{\text{latt}}(T)$ is constant for all V values shown, as expected in a FL. It is orders of magnitude larger close to the QCP on either side (green and orange curves) than further away from it (blue and red curves), reflecting the divergence of the QP mass $m^* \sim \gamma_{\text{latt}}(T = 0) \sim Z^{-1}$ at the QCP. It is noteworthy that, far from the QCP, the value of $\gamma_{\text{latt}}(T = 0)$ for the RKKY phase is comparable to that in the Kondo phase. This suggests that in the RKKY phase the localized spins, though tending to lock into nearest-neighbor singlets, nevertheless contribute quite significantly to the density of states. Understanding this aspect in more detail is left as an interesting task for future work.

X. RELATION TO OTHER MODELS

The NFL regime in the PAM shares several similarities with the NFL in the two-impurity Kondo model [87–89,155,156] and the two-channel Kondo model [77,78,167–171]: (i) The Sommerfeld coefficient γ shows a region of $\ln(T)$ dependence [cf. Fig. 19(b)]; (ii) the entropy takes the value of $\ln \sqrt{2}$; and (iii) plateaus in dynamical susceptibilities imply overscreening.

In this section, we compare the features of the effective 2IAM describing the PAM at $V = 0.46$ close to the QCP to known features of the 2IKM close to its QCP. We also include data on the 2CKM close to its QCP [77,78,167–171], since its critical behavior is known to be closely related to that of the 2IKM [155,156].

The Hamiltonian describing the 2IKM is given by

$$H = \sum_{i=1,2} \left[\sum_{k\sigma} \epsilon_k c_{ik\sigma}^\dagger c_{ik\sigma} + JS_i \cdot s_i \right] + KS_1 \cdot S_2. \quad (57)$$

Here, $c_{ik\sigma}$ destroys an electron in channel $i = 1, 2$ with energy ϵ_k and spin σ , $s_i = \frac{1}{2} \sum_{kk'\sigma\sigma'} c_{ik\sigma}^\dagger \hat{\sigma}_{\sigma\sigma'} c_{ik'\sigma'}$ describes the local spin of channel i at the origin, and S_i describe two impurity-spin-1/2 degrees of freedom at the origin. The impurity spins are coupled antiferromagnetically to the corresponding conduction electrons with coupling strengths $J > 0$. S_1 and S_2 are further coupled antiferromagnetically with coupling strength $K > 0$. The 2IKM can be tuned through a QCP from a Kondo regime at $K < K_c$,

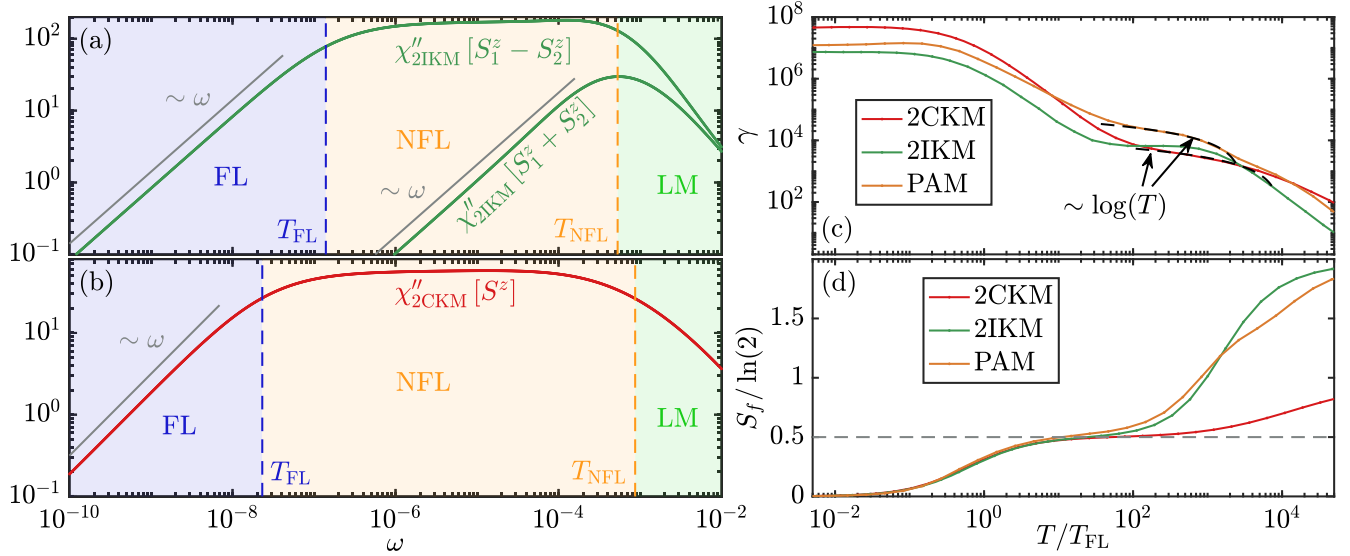


FIG. 20. (a),(b) Spectral part of the spin susceptibility of (a) a 2IKM and (b) a 2CKM close to their QCPs. $\chi''_{2IKM}[S_1^z - S_2^z]$ and $\chi''_{2CKM}[S^z]$ show similar features as $\chi''[X^{zx}]$ in the PAM close to the KB QCP (cf. Fig. 4). (c) Sommerfeld coefficient and (d) impurity contribution to the entropy of the 2IKM, 2CKM, and PAM close to their QCPs. The data for the PAM are taken at $V = 0.46$. Most notable, in the NFL region, γ shows a $\ln(T)$ behavior for the 2CKM and the PAM, and $S_f \simeq \frac{1}{2} \cdot \ln(2)$ for all three models.

where S_i is screened by its corresponding bath, to an RKKY regime at $K > K_c$, where S_1 and S_2 form a singlet. At the QCP, T_{FL} vanishes and an intermediate NFL region emerges, similar to the case of the PAM discussed in the main text.

The NFL in the 2IKM is closely related to the NFL found in the 2CKM, described by the Hamiltonian

$$H = \sum_{i=1,2} \left[\sum_{k\sigma} \epsilon_k c_{ik\sigma}^\dagger c_{ik\sigma} + J_i \mathbf{S} \cdot \mathbf{s}_i \right]. \quad (58)$$

Here, there is only one impurity spin, coupled antiferromagnetically to two channels, $i = 1, 2$, with coupling strengths $J_i > 0$. The 2CKM has a QCP at $J_1 = J_2$, where the impurity changes from being screened by channel 1 at $J_1 > J_2$ to being screened by channel 2 at $J_1 < J_2$. Close to its QCP, a NFL fixed point is found which extends to $T = 0$ at the QCP and shows features similar to these of the NFL in the 2IKM and in the PAM as presented in the main part.

In the following, we consider a 2IKM and a 2CKM tuned close to their respective QCPs. We compare their Sommerfeld coefficients, impurity contributions to the entropy and dynamical correlation functions to the f electron contribution to the entropy and Sommerfeld coefficient of the self-consistent 2IAM describing the PAM close to its QCP, shown in Fig. 20. For both the 2IKM and the 2CKM, a box-shaped, particle-hole symmetric density of states with width 2 and height $1/2$ is used for both channels. As parameters, $J = 0.256$ and $K = 7.2 \times 10^{-4}$ were used for the 2IKM, and $J_1 = 0.29$ and $J_2 = 0.2894$ were chosen for the 2CKM. Both

models are solved with NRG using $\Lambda = 3$ and keeping $N_{\text{keep}} = 2000$ $\text{SU}(2)_{\text{charge}} \times \text{SU}(2)_{\text{charge}} \times \text{SU}(2)_{\text{spin}}$ multiplets at every NRG iteration.

Figure 20(a) shows $\chi''_{2IKM}[S_1^z + S_2^z]$ and $\chi''_{2IKM}[S_1^z - S_2^z]$, together with the NFL and FL scales extracted from the kinks of $\chi''_{2IKM}[S_1^z + S_2^z]$ and $\chi''_{2IKM}[S_1^z - S_2^z]$ on the $\ln$ - $\ln$ scale, respectively, similar as described for the PAM before. In Fig. 20(b), we show the impurity spin susceptibility of the considered 2CKM, $\chi''_{2CKM}[S^z]$, with the corresponding NFL and FL scales both extracted from $\chi''_{2CKM}[S^z]$. The similarity of $\chi''_{2IKM}[S_1^z - S_2^z]$ in Fig. 20(a), $\chi''_{2CKM}[S^z]$ in Fig. 20(b), and $\chi''[X^{zx}]$ in Fig. 4 is evident.

The Sommerfeld coefficient $\gamma = dS_f/dT$ and the impurity contribution to the entropy S_f are shown in Figs. 20(c) and 20(d), respectively, for the 2IKM, the 2CKM, and the PAM at $V = 0.46$. Qualitatively similar behavior is found, most notably, a plateau in S_f with $S_f \simeq \frac{1}{2} \ln(2)$ for all three models and a $\ln(T)$ dependence of γ at intermediate temperatures for the 2CKM and the PAM [the 2IKM shows similar behavior, though without a clean $\ln(T)$ dependence]. A further elucidation of the nature of the NFL in the PAM will require an impurity model analysis as done in Refs. [211,212]. We leave this for future work.

XI. CONCLUSION AND OUTLOOK

We have presented an extensive two-site CDMFT plus NRG study of the PAM, following up on and considerably extending and refining previous work done with an ED impurity solver [131,132]. Leveraging the capabilities of NRG to resolve exponentially small energy scales on the

real-frequency axis, we confirmed the existence of the KB QCP found in Refs. [131,132], which can be understood in terms of a continuous OSMT at $T = 0$.

Beyond that, we unambiguously showed that the KB QCP marks a second-order transition between two FL phases (Fig. 3) which differ in their FS volumes (Sec. VIII), leading to a sharp jump of the FS volume (Fig. 17) and the Hall coefficient (Fig. 18). We found that, in contrast to widespread belief [3], the f -electron QP weight is nonzero in both the Kondo and the RKKY phases (Sec. VI, in particular Fig. 9) and becomes zero only at the QCP itself. We showed that the FS reconstruction across the KB QCP can be understood in terms of a sign change of the effective level position ϵ_{f+}^* (Fig. 9 and Sec. VIII), which is connected to the emergence of a dispersive pole in the RKKY phase (Fig. 10). An interesting consequence of the nonzero f -electron QP weight is that, in the RKKY phase, the band structure consists of *three* bands, with a very narrow band crossing the Fermi level (Sec. VII). We also showed that, in both the Kondo and RKKY phases, the specific heat is linear in T , as expected from a FL; we find that the Sommerfeld coefficient diverges when the KB QCP is approached from either side (Sec. IX).

We find that the physics at the KB QCP and at nonzero temperatures in its vicinity is governed by a NFL fixed point (Sec. IV), which has some resemblance to the NFL fixed points in the two-impurity and two-channel Kondo models (Sec. X). In this paper, we reported a strange-metal-like $\sim T \ln T$ specific heat in the NFL region (Sec. IX). A more detailed analysis of the NFL regime is provided in a companion paper [152], where we show data regarding ω/T of the optical conductivity closely resembling experimental data [63] and evidence for linear-in- T resistivity.

We should, however, also mention some caveats in our work, which may be addressed in future work. For instance, while we provided some extensive formal treatment of Luttinger's theorem (Sec. VIII), we refrained from offering any physical interpretation on how and why the FS in the RKKY phase can be small. Indeed, Oshikawa's nonperturbative treatment of Luttinger's theorem [10] implies that, in the case of a violation of Luttinger's theorem, additional low-energy degrees of freedom must be present [110,116]. We leave their identification within the context of the PAM to future work. We expect that this could also lead to a connection to slave-particle theories [110,115]. Further insights could possibly be pursued along the lines of recent work by Fabrizio [151,176,213]. As we have pointed out repeatedly in this paper, the work cited above draws a connection between Luttinger surfaces and fractionalized spinon excitations. Our work paves the way to explore this connection in detail in terms of a concrete example.

An obvious limitation of our CDMFT study is the small cluster size of only two sites—which very likely overestimates the tendency for f singlet formation in the RKKY phase. Therefore, an important line of future work should be to check the cluster-size dependence of our results. However, the two-site cluster is already sufficient to capture momentum differentiation in $\epsilon_{f\mathbf{k}}^*$, which is crucial for the occurrence of a LS and a FS reconstruction, as shown in Sec. VIII. We expect that further improving the momentum resolution via larger cluster sizes will mainly have a quantitative impact and will not alter the qualitative picture drawn by the two-site approximation.

Another unsatisfactory aspect of our two-site CDMFT treatment is that it yields a nonzero entropy at the KB QCP at $T = 0$; see Sec. IX. As mentioned in that section, such a nonzero entropy would render the KB QCP highly unstable to symmetry breaking. Whether this is a finite cluster size effect or continues to be the case also for larger cluster sizes needs to be checked in future work.

Lastly, our CDMFT treatment requires reperiodization of self-energies to obtain a periodic self-energy with $\mathbf{k}$ dependence. Reperiodization is an *ad hoc* postprocessing procedure. We have checked that our most important claims are consistent with our nonreperiodized bare data. Nevertheless, in our view, it would be important to cross-check our results in future studies, for instance, with numerically exact methods. Such studies will be very useful for establishing the range of applicability of CDMFT for describing KB physics.

Our work motivates several follow-up studies. For instance, as mentioned before, it would be interesting to explore the interplay between KB physics and potential symmetry-breaking orders of all kinds, e.g., antiferromagnetic or superconducting orders. Similar studies could also be done for models appropriate to other classes of strongly correlated materials. Obvious candidate material classes, which experimentally show quantum critical behavior quite similar to heavy fermions, are cuprates [214–219] or twisted bilayer graphene [220–222].

ACKNOWLEDGMENTS

We thank Assa Auerbach, Silke Bühler-Paschen, Andrey Chubukov, Piers Coleman, Dominic Else, Fabian Kugler, Antoine Georges, Sean Hartnoll, Andy Millis, Marcin Raczkowski, Achim Rosch, Subir Sachdev, Qimiao Si, Katharina Stadler, Senthil Todadri, Matthias Vojta, Andreas Weichselbaum, and Krzysztof Wójcik for helpful discussions. This work was funded in part by the Deutsche Forschungsgemeinschaft under Germany's Excellence Strategy EXC-2111 (Project No. 390814868). It is part of the Munich Quantum Valley, supported by the Bavarian state government with funds from the Hightech Agenda Bayern Plus. This work was further supported by Grant No. INST 86/1885-1 FUGG of the German Research

Foundation (DFG). S.-S. B. L. was supported by Samsung Electronics Co., Ltd. (No. IO220817-02066-01), the Global-LAMP Program of the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education (No. RS-2023-00301976), and by the National Research Foundation of Korea (NRF) grant funded by the Korean government (MSIT) (No. RS-2023-00214464). G. K. was supported by the National Science Foundation Grant No. DMR-1733071 and J. v. D. in part under PHY-1748958.

APPENDIX A: CDMFT FOR THE PAM

In the two-site CDMFT treatment of the PAM, the three-dimensional lattice is tiled into a superlattice of two-site clusters [121,130,132]. An effective action can then be constructed via the cavity method [119]. It takes the form of a 2IAM coupled to an effective bath, describing the rest of the lattice from the point of view of the two-site cluster in the CDMFT approximation. The c electrons can either be treated explicitly, or they can be integrated out and merged with the effective bath, as they are noninteracting. We decided to treat the c electrons explicitly, as this enables us to directly calculate dynamical susceptibilities involving c -electron degrees of freedom. Additional calculations, treating the c electrons together with the bath, confirmed that both methods give the same results. Note that both methods have roughly the same amount of computational complexity for the NRG impurity solver. Since the f electrons couple to the bath only via the c electrons as they do not have any nonlocal hopping term, one obtains two bands of spinful bath electrons in both cases. For a detailed description of two-site CDMFT for the PAM, see Ref. [130].

1. Self-consistency

In the CDMFT approximation, the cluster Green's function is given by

$$G_{\text{loc}}(z) = \int_{\mathbf{k}} \begin{pmatrix} z - \epsilon_f - \Sigma_f(z) & -V \\ -V & \mathcal{G}_{0,c\mathbf{k}}^{-1}(z) \end{pmatrix}^{-1} \quad (\text{A1a})$$

$$= \begin{pmatrix} G_{\text{loc},f}(z) & G_{\text{loc},fc}(z) \\ G_{\text{loc},fc}(z) & G_{\text{loc},c}(z) \end{pmatrix}, \quad (\text{A1b})$$

where $\mathcal{G}_{0,c\mathbf{k}}$ is the c -band Green's functions at $V = 0$,

$$\mathcal{G}_{0,c\mathbf{k}}(z) = \frac{1}{(z + \mu)^2 - (\epsilon_{c\mathbf{k}}^0)^2} \begin{pmatrix} z + \mu & e^{ik_x} \epsilon_{c\mathbf{k}}^0 \\ e^{-ik_x} \epsilon_{c\mathbf{k}}^0 & z + \mu \end{pmatrix}, \quad (\text{A2})$$

and $\Sigma_f(z)$ is the cluster f -electron self-energy (which is a proper, single-particle irreducible self-energy),

$$\Sigma_f(z) = \begin{pmatrix} \Sigma_{f11}(z) & \Sigma_{f12}(z) \\ \Sigma_{f21}(z) & \Sigma_{f22}(z) \end{pmatrix}, \quad (\text{A3})$$

which is $\mathbf{k}$ independent in CDMFT. $G_{\text{loc},c}(z)$ can be computed by performing a momentum integral (cf. Sec. A 2):

$$G_{\text{loc},c}(z) = \int_{\mathbf{k}} [\mathcal{G}_{0,c\mathbf{k}}^{-1}(z) - \Sigma_c(zv)]^{-1}, \quad (\text{A4})$$

while $G_{\text{loc},f}(z)$ and $G_{\text{loc},fc}(z)$ are related to $G_{\text{loc},c}(z)$ via Eq. (6c). $\Sigma_c(z)$ is the cluster c -electron self-energy (which is not single-particle irreducible), related to $\Sigma_f(z)$ via Eq. (6e). $\Sigma_f(z)$ can be computed from an auxiliary self-consistent 2IAM [cf. Eq. (4)] with $G_{\text{loc}}(z) = G_{2\text{IAM}}(z)$, with the corresponding Green's functions of the 2IAM given in Eq. (6).

The self-consistent solution is not known *a priori* and has to be computed via a self-consistency cycle. For that, the hybridization function of the 2IAM Eq. (5) is initialized with some guess. Then, (i) the self-energies are computed via NRG, (ii) $G_{\text{loc},c}(z)$ is computed via Eq. (A4), and (iii) the hybridization function is updated via

$$\Delta_c(z) = z + \mu + t \cdot \tau^x - \Sigma_c(z) - G_{\text{loc},c}^{-1}(z). \quad (\text{A5})$$

This cycle is repeated until convergence is reached.

2. Momentum integration

To achieve accurate results, a method for precise momentum integration of propagators is needed in the CDMFT. For this, we employ the tetrahedron method [223,224], which is applicable for integrals of the form

$$\int_{1,\text{BZ}} d\mathbf{k} \frac{f_{\mathbf{k}}}{g_{\mathbf{k}}}, \quad (\text{A6})$$

where $f_{\mathbf{k}}$ and $g_{\mathbf{k}}$ are smooth functions of $\mathbf{k}$. The Brillouin zone is tiled into tetrahedra, and both f and g are interpolated linearly on this tetrahedron. The integral can then be performed analytically, yielding

$$I_{\text{tetra}} = \sum_i f_i w_i(\{g_i\}). \quad (\text{A7})$$

Here, f_i and g_i are the functions f and g evaluated at the corners of the tetrahedron, and $w_i(\{g_i\})$ are integration weights which depend on g only. Formulas for these weights are quite lengthy and can be found in Ref. [224] for one-, two-, and three-dimensional integration. We further use an adaptive momentum grid to reduce computational effort, adjusting the grid size according to the degree of difficulty of the integral in a certain region. This enables us to evaluate all our integrals with an absolute error less than 5×10^{-4} . For this, the integration domain is tiled into a coarse and a fine grid, and the grid is iteratively refined in regions where the error bound is not fulfilled, until convergence is reached within the error bounds. Using the tetrahedron method, we

then calculate $G_{\text{loc},c}(\omega)$ via Eq. (A4). The computational effort for this integral can be reduced by treating the integral over k_y and k_z as a density of states integration, thereby mapping Eq. (A4) to a two-dimensional integral:

$$\begin{aligned}\epsilon(k_x, E) &= -2t(\cos(k_x) + E), \\ \mathcal{G}_{0,c}^{-1}(z, k_x, E) &= \begin{pmatrix} z + \mu & -e^{ik_x}\epsilon(k_x, E) \\ -e^{-ik_x}\epsilon(k_x, E) & z + \mu \end{pmatrix}, \\ G_{\text{loc},c}(z) &= \int_{k_x} \int_E \rho_{2D}(E) [\mathcal{G}_{0,c}^{-1}(z, k_x, E) - \Sigma_c(z)]^{-1}, \\ \rho_{2D}(E) &= \int_{k_y} \int_{k_z} \delta[E - \cos(k_y) - \cos(k_z)], \quad (\text{A8})\end{aligned}$$

where ρ_{2D} is the density of states of a square lattice.

3. Reperiodization of the self-energy

To determine transport properties such as the resistivity, the Hall coefficient, or the FS, the lattice symmetries have to be restored by reperiodizing the cluster self-energy. We accomplish this via a modified periodization of the cumulant $M(z) = [z + \mu - \Sigma_c(z)]^{-1}$ (M periodization) [157,158]. As we discuss in Sec. VIII, the Luttinger integral (at $T = 0$) *without reperiodization*, i.e., Eq. (51), is zero (cf. Fig. 17). This property is not respected by conventional M periodization; the Luttinger integral *with reperiodization*, i.e., Eq. (43), is generically nonzero. To ensure that the Luttinger integral vanishes also after reperiodization, we therefore modify the cumulant by a V -dependent shift of the chemical potential in the denominator *only for reperiodization purposes*:

$$\tilde{M}(z) = [z + \mu + \delta\mu(V) - \Sigma_c(z)]^{-1}, \quad (\text{A9a})$$

$$\tilde{M}_{\mathbf{k}}(z) = \tilde{M}_{11}(z) + \tilde{M}_{12}(z) \sum_{\alpha=1}^3 \frac{1}{3} \cos(k_\alpha) \quad (\text{A9b})$$

$$= [z + \mu + \delta\mu(V) - \Sigma_{\mathbf{k}}(z)]^{-1}. \quad (\text{A9c})$$

Here, Eq. (A9a) defines the modified cumulant used for reperiodization, Eq. (A9b) defines the reperiodization of $\tilde{M}(z)$, and Eq. (A9c) relates it to $\Sigma_{\mathbf{k}}$, thereby defining $\Sigma_{\mathbf{k}}$; quantities like $\Sigma_{f\mathbf{k}}$ or $G_{x\mathbf{k}}$ are obtained from $\Sigma_{\mathbf{k}}$ using the relations Eqs. (3). Note that the shift $\delta\mu(V)$ appears both in Eq. (A9a) and in Eq. (A9c); it, therefore, does not constitute an *actual* shift in the chemical potential but rather slightly redefines the quantity used for reperiodization (i.e., $\tilde{M}$ instead of M is reperiodized). The shift $\delta\mu(V)$ is chosen such that the Luttinger integral after reperiodization [Eq. (43)] coincides with that before reperiodization [Eq. (51)] at $T = 0$. The same shift $\delta\mu(V)$ is then used at $T > 0$ for the same V . After reperiodization, we have $\tilde{M}_\Gamma = \tilde{M}_{11} + \tilde{M}_{12} = \tilde{M}_+$ and $\tilde{M}_\Pi = \tilde{M}_{11} - \tilde{M}_{12} = \tilde{M}_-$;

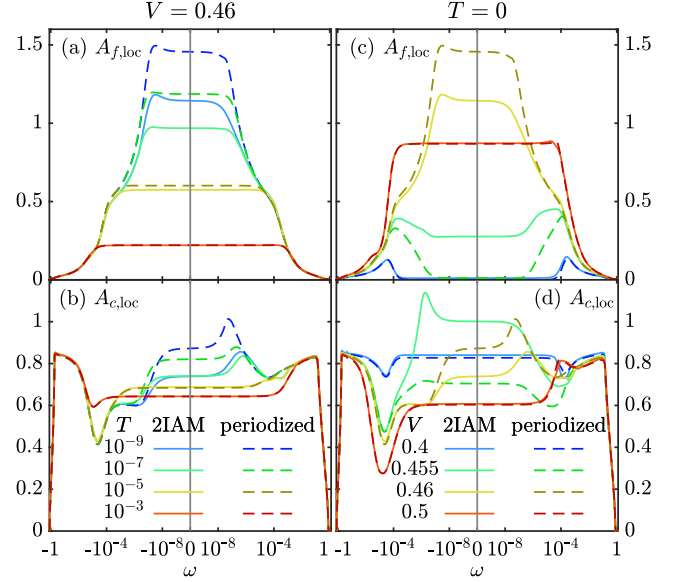


FIG. 21. Comparison of local cluster spectral functions (solid lines) and local lattice spectral function (dashed lines) after periodization of the self-energies. The upper and lower rows show the f - and c -electron spectral function, respectively. The left show data for four different temperatures at fixed $V = 0.46$, close to V_c . The right show data for four different V at $T = 0$. The layout mirrors that in Fig. 8.

the same relation also holds between $\Sigma_{x\mathbf{k}}$ and $\Sigma_{x\alpha}$. This establishes a correspondence between the Γ (Π) point in the lattice model and $+$ ($-$) orbital in the effective cluster model.

To benchmark our reperiodization scheme, we compare the local spectral functions with and without reperiodization, shown in Fig. 21. For V not too close to $V_c = 0.4575$ and at elevated temperatures, these two functions agree, implying that reperiodization works well here. Close to the QCP (low temperatures, $V \simeq V_c$), however, reperiodized and cluster results show differences. These differences are mostly quantitative, while most of the qualitative features remain similar. For instance, for A_f at $T = 0$, both the Kondo peak height at $V = 0.46$ and the pseudogap at $V = 0.455$ are more pronounced after periodization, but the qualitative behavior is the same before and after periodization [Fig. 21(c)]. The most severe qualitative mismatch is the $A_{c,\text{loc}}(0)$ for $V < V_c$ [Fig. 21(d)]: At $T = 0$ in the RKKY phase, as V is increased toward V_c , a Kondo-like peak develops in $A_{c,\text{loc}}$ before periodization (see our discussion in Sec. VIB)—i.e., $A_{c,\text{loc}}(0)$ increases as V approaches V_c (solid green curve lies above solid blue curve at $\omega = 0$); after periodization, the converse happens—i.e., $A_{c,\text{loc}}(0)$ decreases as V approaches V_c (dashed green curve lies below dashed blue curve at $\omega = 0$). Our periodization procedure, thus, misses the development of the Kondo-like peak in $A_{c,\text{loc}}$.

We emphasize that reperiodization is an *ad hoc* post-processing procedure. Features in reperiodized data should

always be substantiated by analyzing the raw data before reperiodization. We have done so repeatedly in the main text, for instance, for the FS and LS volumes, the dispersive pole in Σ_f , or the two- and three-band structures in the Kondo and RKKY phases, respectively.

4. Self-consistent hybridization function versus V

In the main text, we emphasize the importance of self-consistency to access the KB QCP in two-site CDMFT. Here, we elaborate this aspect by showing that the self-consistent hybridization functions in the vicinity of the KB QCP show (i) a strong ω dependence and (ii) a strong V dependence. This implies that self-consistency is of high importance if one wants to capture the KB QCP.

Figure 22 shows the hybridization functions at $T = 0$ on a logarithmic frequency scale, plotted for several different values of V close to the KB QCP. As seen from the insets, showing the same data on a linear frequency scale, the hybridization functions have sharp features at low frequencies. The sharp features appear stretched out on the log scale of the main panels, which reveal that, for V very close to V_c (green and yellow), they occur at frequencies as low as $|\omega| \simeq 10^{-8}$. This shows that the hybridization functions of the effective 2IAM describing the self-consistent PAM depend strongly on frequency. For a non-self-consistent 2IKM with weakly frequency-dependent hybridization functions, it has been shown that the NFL fixed point and, thus, the QCP are unstable to the breaking of symmetries which are indeed broken in our effective 2IAM [82,83,86,89]. Our work implies that this conclusion

does not generalize to the case of hybridization functions displaying a strong frequency dependence.

Figure 22 shows that the hybridization functions are also strongly V dependent, especially close to $\omega = 0$. A change of V by 5×10^{-3} in the vicinity of the KB QCP induces comparably large changes in the hybridization functions, of the order of 10^{-1} at some frequencies. Thus, close to the KB QCP, a tiny change in V leads to a considerable readjustment of the self-consistent hybridization function by iterating the CDMFT self-consistency cycle. This shows that self-consistency is of high importance to capture the KB QCP.

In Fig. 23, we plot the absolute value of the derivative of the hybridization functions at $\omega = 0$, $|\partial_\omega \Delta_{\alpha\alpha}(\omega^+)|_{\omega=0}$, at $T = 0$ as functions of V . The zero-frequency derivative of the hybridization functions has a peak at the KB QCP at V_c , indicative of a divergence. This suggests that the self-consistent hybridization functions become singular at $\omega = 0$ at the KB QCP. This further emphasizes that (i) results obtained on the 2IAM with weakly frequency-dependent hybridization functions are not straightforwardly applicable to the self-consistent 2IAM arising in our CDMFT solution of the PAM, and (ii) self-consistency is important to capture this singular behavior at the KB QCP. A more detailed study investigating how the self-consistency equations manage to drive the 2IAM to a stable QCP will be subject to future work.

5. Transport properties

For the calculation of the resistivity and the Hall coefficient, the M -reperiodized self-energy is used. The

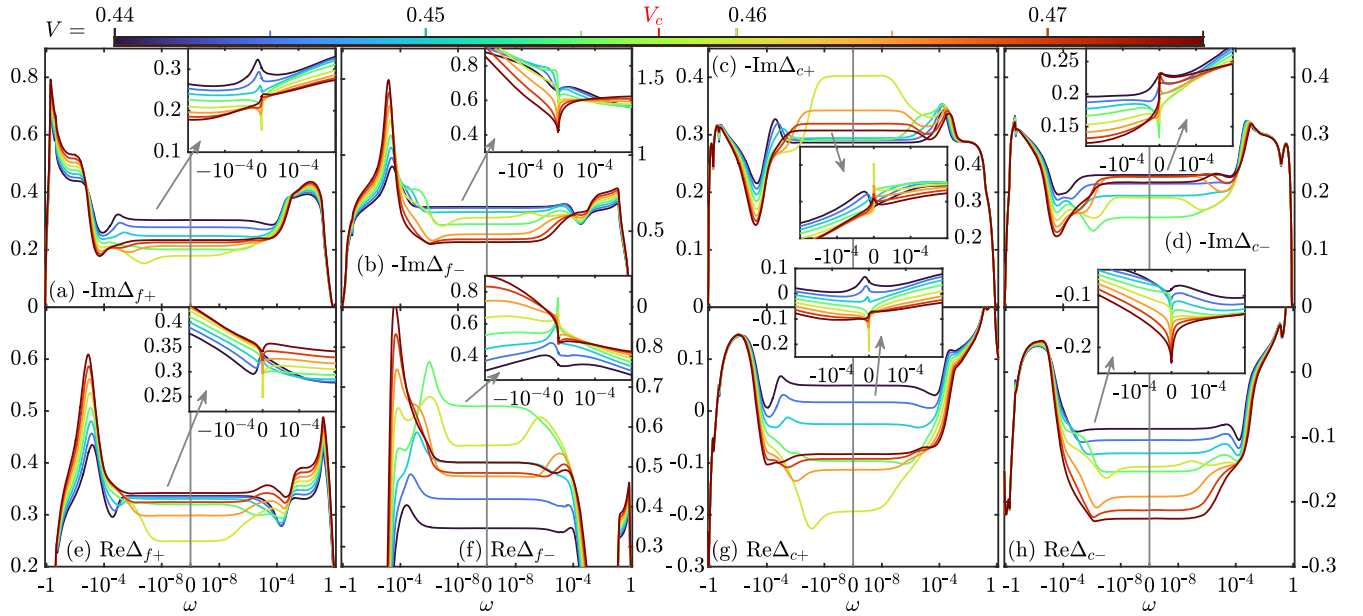


FIG. 22. Evolution of the self-consistent hybridization functions $\Delta_{\alpha\alpha}(\omega^+)$ at $T = 0$ as V is tuned across the QCP. Colored curves correspond to V values marked by ticks on the color bar. The layout mirrors that in Fig. 8 in the main text. Top row: imaginary parts; bottom row: real parts. The insets show the hybridization functions on a linear frequency scale for $|\omega| < 2 \times 10^{-4}$.

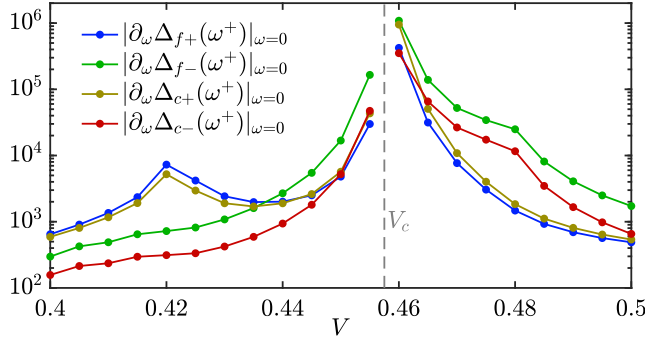


FIG. 23. Absolute value of the derivative of the hybridization function as zero frequency, $|\partial_\omega \Delta_{f\alpha}(\omega^+)|_{\omega=0}$ at $T = 0$, plotted as a function of V .

formulas for the optical conductivity $\sigma(\omega)$ ignoring vertex contributions, resistivity $\rho_{xx} = 1/\sigma_{xx}$, and the Hall coefficient $R_H = \sigma_{xy}/(\sigma_{xx}^2 H)$ are given by [225,226]

$$\begin{aligned}\sigma(\omega) &= 2\pi e^2 \int d\epsilon \Phi_{xx}(\epsilon) \tilde{\sigma}(\epsilon, \omega), \\ \tilde{\sigma}(\epsilon, \omega) &= \int d\tilde{\omega} \frac{f(\tilde{\omega}) - f(\tilde{\omega} + \omega)}{\omega} A_c(\epsilon, \tilde{\omega}) A_c(\epsilon, \tilde{\omega} + \omega), \\ \sigma_{xx} &= \lim_{\omega \rightarrow 0} \sigma(\omega), \\ \sigma_{xy} &= \frac{4}{3} \pi^2 e^3 H \int d\epsilon \Phi_{xy}(\epsilon) \int d\omega \left[-\frac{\partial f}{\partial \omega} \right] A_c^3(\epsilon, \omega), \\ \Phi_{xx}(\epsilon) &= \int_{1.BZ} \frac{d\mathbf{k}}{(2\pi)^3} (\epsilon_{\mathbf{k}}^x)^2 \delta(\epsilon - \epsilon_{c\mathbf{k}}), \\ \Phi_{xy}(\epsilon) &= \int_{1.BZ} \frac{d\mathbf{k}}{(2\pi)^3} \begin{vmatrix} \epsilon_{\mathbf{k}}^x \epsilon_{\mathbf{k}}^x & \epsilon_{\mathbf{k}}^{xy} \\ \epsilon_{\mathbf{k}}^y \epsilon_{\mathbf{k}}^x & \epsilon_{\mathbf{k}}^{yy} \end{vmatrix} \delta(\epsilon - \epsilon_{c\mathbf{k}}),\end{aligned}\quad (\text{A10})$$

where H denotes the magnetic field, $e < 0$ the charge of the electrons, $f(\omega)$ the Fermi function, $\epsilon_{\mathbf{k}}^x = \partial_{k_x} \epsilon_{c\mathbf{k}}$ the derivative of the dispersion by k_x (and, correspondingly, for, e.g., $\epsilon_{\mathbf{k}}^{xy}$), and $|\cdot|$ the determinant. In the above formulas, only the c -electron spectral function appears, as there are no terms involving the f electrons which do not conserve local charge. Note also that the $\mathbf{k}$ -dependent spectral function depends on $\mathbf{k}$ only through $\epsilon_{c\mathbf{k}}$ after reperiodization via Eq. (A9).

Equations (A10) include only the bubble contribution to the conductivities and ignore vertex contributions. In a companion paper [152], we show that vertex contributions to the conductivity are qualitatively important in order to capture the correct scaling of the optical conductivity in the NFL region. A full treatment of vertex contributions is currently computationally unfeasible with our NRG impurity solver, because the computation of four-point correlation functions for the 2IAM at hand is too expensive. To compute the Hall coefficient shown in Fig. 18, we therefore do *not* consider vertex contributions but just use the formulas presented in Eqs. (A10).

APPENDIX B: CONVERGENCE OF NRG

In this section, we provide details on the reliability of our NRG data. For that, we first show in Appendix B 1 that our data are converged with the number of kept SU(2) multiplets. In Appendix B 2, we then discuss how we broaden our discrete spectral data. Appendix B 3 shortly discusses how our results depend on the NRG discretization parameter Λ .

1. Convergence with N_{keep}

To obtain the data in the main text, we use $\Lambda = 3$ as our NRG discretization parameter and keep $N_{\text{keep}} = 25\,000$ SU(2) multiplets. For the most challenging Wilson shell (typically $\ell = 3$, the first shell where truncation occurs; $\ell = 0$ is the impurity), this results in a truncation energy $E_{\text{trunc}} \simeq 9E_\ell$, where $E_\ell \propto \Lambda^{-\ell/2}$ is the energy scale of shell ℓ , which is normalized so that $\lim_{\ell \rightarrow \infty} E_\ell/t_\ell = 1$, and t_ℓ is the hopping matrix element between sites $\ell - 1$ and ℓ .

From experience, $E_{\text{trunc}} > 7E_\ell$ usually leads to reliable data. Therefore, our results with $E_{\text{trunc}} \simeq 9E_\ell$ are expected to be reasonably converged in N_{keep} . To explicitly check the convergence in the challenging region close to the QCP, we check that $N_{\text{keep}} = 8000$, i.e., less than 1/3 of the N_{keep} we use, is sufficient to obtain qualitatively correct data. This is shown in Fig. 24, where we compare the f -electron spectral function [Figs. B4(a) and B4(b)] and self-energy

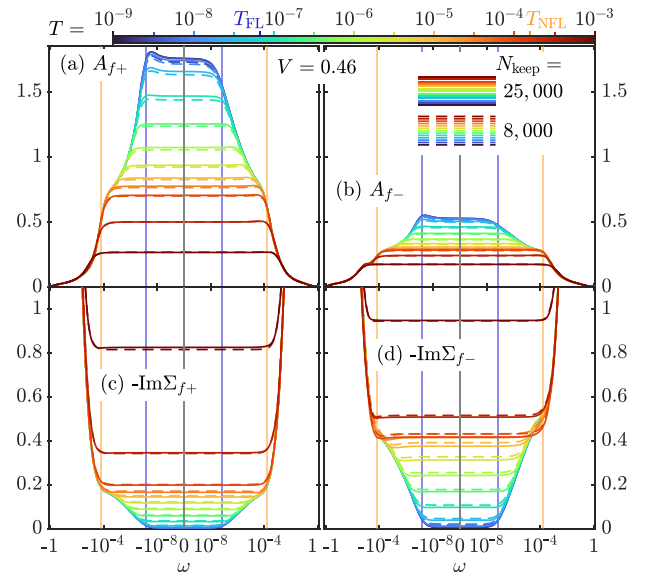


FIG. 24. (a),(b) f -electron spectral function and (c),(d) f -electron self-energy at $V = 0.46$ and different temperatures for $N_{\text{keep}} = 25000$ (solid lines) and $N_{\text{keep}} = 8000$ (dashed lines). (a)–(d) mirror the layout in Figs. 15(a), 15(b), 15(e), and 15(f), respectively. Both $N_{\text{keep}} = 25000$ and $N_{\text{keep}} = 8000$ capture the same qualitative behavior. Visible differences are small and occur at low frequencies and temperatures, $|\omega| < T_{\text{NFL}}$ and $T < T_{\text{NFL}}$. For the spectral functions in (a) and (b), visible differences ($\lesssim 2\%$) occur at low frequencies $|\omega| \ll T_{\text{NFL}}$ and $T < T_{\text{NFL}}$.

[Figs. B4(c) and B4(d)] at $V = 0.46$ and different temperatures for $N_{\text{keep}} = 25000$ (solid lines) versus $N_{\text{keep}} = 8000$ (dashed lines). Small differences of $\lesssim 2\%$ are visible in the spectral functions at low frequencies $|\omega| < T_{\text{NFL}}$ and temperatures $T < T_{\text{NFL}}$. Similar small visible differences of $\lesssim 5\%$ are visible in $\Sigma_{f\pm}(\omega)$ for $|\omega| < T_{\text{NFL}}$ in the NFL region, $T_{\text{FL}} < T < T_{\text{NFL}}$.

2. Broadening

We broaden the discrete spectral functions obtained from fdm-NRG using the scheme described in Ref. [161]. There, a log-Gaussian broadening kernel [cf. Eq. (17) in Ref. [161]] is applied first, followed by a linear broadening kernel; cf. Eq. (21) in Ref. [161]. The adaptive log-Gaussian broadening width introduced in Ref. [161] is not used in this work.

Fermionic spectral functions.—For fermionic spectral functions, we use a symmetric log-Gaussian kernel [161]:

$$\delta_{\sigma}^s(\omega, \omega_k) = \frac{\theta(\omega\omega_k)}{\sqrt{\pi\sigma}|\omega_k|} e^{-(\ln|\omega/\omega_k|/\sigma - \sigma/4)^2}, \quad (\text{B1})$$

which preserves the height of spectral peaks. The spectral peak heights are crucial to obtain correct scattering phase shifts, which, at low temperatures, are usually tied to the filling via the Friedel sum rule in impurity models or the Luttinger sum rule in a lattice model; cf. Sec. VIII B. Because of that, the $\delta_{\sigma}^s(\omega, \omega_k)$ is our kernel of choice for fermionic spectra. For the data shown in the main text, we use $\sigma = 0.75 \ln \Lambda$, which is chosen just large enough to avoid visible broadening artifacts. As a linear broadening kernel, we use the derivative of the Fermi-Dirac distribution, Eq. (21) in Ref. [161], with broadening width $\gamma = T/5$.

Bosonic spectral functions.—For bosonic spectra, shown, for instance, in Fig. 4, we use a centered log-Gaussian kernel:

$$\delta_{\sigma}^c(\omega, \omega_k) = \frac{\theta(\omega\omega_k)}{\sqrt{\pi\sigma}|\omega_k|} e^{-(\ln|\omega/\omega_k|/\sigma)^2} e^{\sigma^2/4}, \quad (\text{B2})$$

which preserves the positions of peaks. Since we determine the energy scales T_{FL} and T_{NFL} from the positions where power laws of bosonic spectra change (cf. Appendix C) and since $\delta_{\sigma}^c(\omega, \omega_k)$ preserves these positions, our kernel of choice for bosonic spectra is $\delta_{\sigma}^c(\omega, \omega_k)$. As broadening widths, we chose $\sigma = \ln \Lambda$ and $\gamma = T/10$ for bosonic spectra.

We have checked that the main qualitative features discussed in the main text, for both fermionic and bosonic spectra, do not depend on the specific (reasonable) choices of σ (of the order of $\ln \Lambda$) and γ ($\lesssim T$).

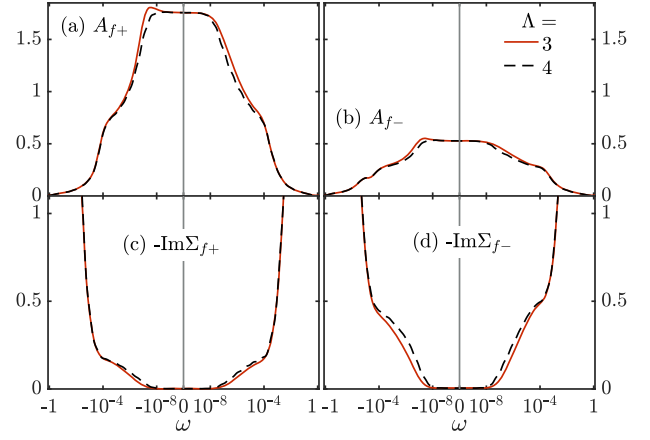


FIG. 25. (a),(b) f -electron spectral function and (c),(d) f -electron self-energy at $V = 0.46$ and $T = 0$ for $\Lambda = 3$ (red solid lines) and $\Lambda = 4$ (black dashed lines). Both $\Lambda = 3$ and $\Lambda = 4$ capture the same qualitative behavior.

3. Λ dependence

To illustrate how the choice of discretization parameter Λ influences our results, Fig. 25 shows the f -electron spectral functions [Figs. B5(a) and B5(b)] and self-energies [Figs. B5(c) and B5(d)] at $V = 0.46$ and $T = 0$ (our data point closest to the QCP), computed for $\Lambda = 3$ (our choice in the main text) and, for comparison, for $\Lambda = 4$. The results for $\Lambda = 4$ are obtained by a “single-shot” NRG calculation using the converged $\Lambda = 3$ hybridization function as input. Both choices of Λ produce the same qualitative results, albeit with small quantitative differences. For example, $\Lambda = 4$ yields somewhat narrower Kondo peaks in A_f and narrower gaps in Σ_f compared to $\Lambda = 3$.

APPENDIX C: DETERMINATION OF ENERGY SCALES

To determine the crossover scales T_{FL} and T_{NFL} , we exploit the fact that the spectral functions of particular susceptibilities show a well-defined power-law dependence in the fixed point regions, which changes when traversing the crossover regions. On a log-log scale, this leads to straight lines with kinks in the crossover regions, as can be seen in Fig. 4 in the main text. The second derivative of $\chi''[O](\omega)$ on the log-log scale,

$$\tilde{\chi}[O](\omega) = \frac{\partial^2 \ln_{10}\{\chi''[O](\omega)\}}{\partial \ln_{10}(\omega)^2}, \quad (\text{C1})$$

tracks the change in slope at the crossover, enabling us to determine the corresponding scale. We use $\chi''[S^z]$ to determine the NFL scale and $\chi''[X^{xz}]$, $\chi''[T^z]$, $\chi''[T^y]$, and $\chi''[P^z]$ to determine the FL scale. The corresponding operators are defined in Eq. (9) in the main text. $\chi''[X^{xz}]$, $\chi''[T^z]$, $\chi''[T^y]$, and $\chi''[P^z]$ are shown in Fig. 2.

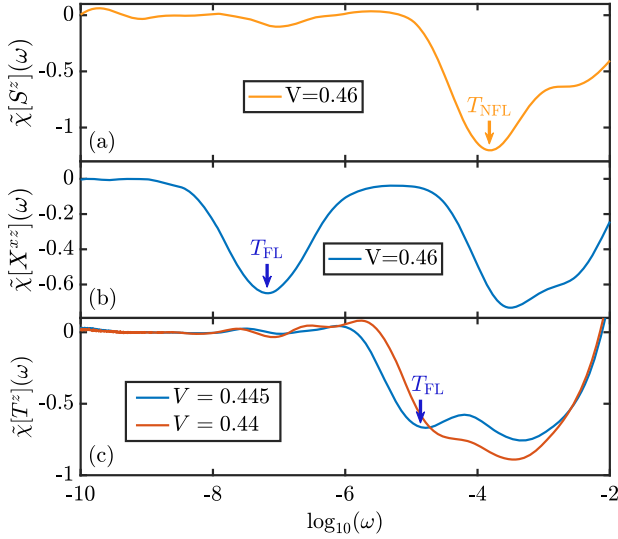


FIG. 26. (a) $\tilde{\chi}[S^z](\omega)$ plotted versus $\ln_{10}(\omega)$ at $V = 0.46$ and $T = 0$. We extract the NFL scale from the position of the minimum marked by the orange arrow. (b) $\tilde{\chi}[X^{xz}](\omega)$ plotted versus $\ln_{10}(\omega)$ at $V = 0.46$ and $T = 0$. The FL scale is extracted from the position of the minimum marked by the blue arrow. Note that, while the other minimum is associated with T_{NFL} , it is not used to extract this scale. (c) $\tilde{\chi}[T^z](\omega)$ plotted versus $\ln_{10}(\omega)$ at $V = 0.445$ and $V = 0.44$ at $T = 0$. While the FL scale can still be extracted from $\tilde{\chi}[T^z](\omega)$ at $V = 0.445$ because both minima in $\tilde{\chi}[T^z](\omega)$ are still clearly distinguishable, it is not possible any more for $V = 0.44$ as the minima have merged.

Examples for the determination of the NFL scale via $\chi''[S^z]$ and of the FL scale via $\chi''[X^{xz}]$ are shown in Figs. 26(a) and 26(b), respectively. While $\chi''[T^y]$ and $\chi''[P^z]$ are much smaller than $\chi''[T^z]$ and $\chi''[X^{xz}]$, they are more suitable than the latter two far away from the QCP, especially for $V < V_c$. The reason for this is shown in Fig. 26(c) for $\chi''[T^z]$: The second derivative on the ln-ln scale shows two minima, the first related to T_{FL} and the

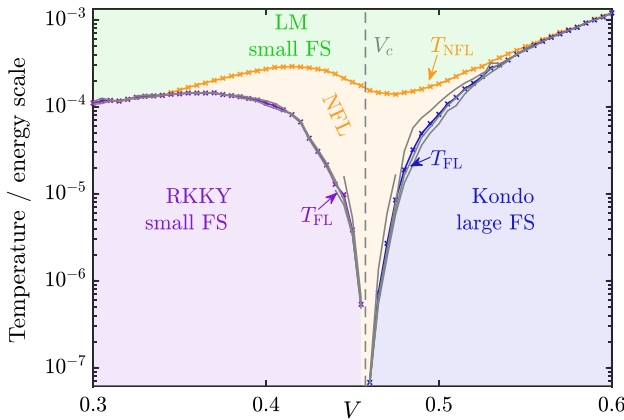


FIG. 27. FL scales, extracted from different correlators (gray lines). For more information on the energy scales, see Fig. 2 in the main text and the corresponding discussion there.

second related to T_{NFL} . The same is true for $\chi''[X^{xz}]$ (not shown). These two minima merge away from the QCP, preventing the determination of T_{FL} . The determination via $\chi''[T^y]$ and $\chi''[P^z]$ is not faced with these difficulties, as they have only one minimum, associated with T_{FL} .

We note that the determination of T_{FL} via $\chi''[X^{xz}]$ works well in the Kondo regime for all V but in the RKKY regime only close to the QCP, while $\chi''[T^z]$ works only close to the QCP in both the Kondo and the RKKY regimes. As the FL scale extracted from different correlators in are generally not exactly equal, we define T_{FL} as their geometric mean as shown in Fig. 27. Each gray line there shows a FL scale extracted from a different correlator, while the blue and purple lines show their geometric mean. The gray lines do not exactly lie on top of each other, but they are sufficiently similar to justify the averaging described above.

APPENDIX D: DETERMINATION OF T_{Hall}

Figure 2 includes data points (red dots) marked $T_{\text{Hall}}(V)$, showing how the crossover from a large FS in the Kondo phase to a small FS in the RKKY phase evolves with temperature. Here, we describe how T_{Hall} was determined.

We closely follow the procedure used in Ref. [26]. We fit our numerical V -dependent Hall coefficient data (see Fig. 18) at $T = 10^{-4}$, 10^{-5} , and 10^{-6} to the form

$$\frac{R_H(V)}{R_{H,0}} \stackrel{\text{fit}}{\simeq} a + \frac{b}{1 + (V/V_{\text{Hall}})^p}, \quad (\text{D1})$$

with fit parameters a , b , p , and V_{Hall} ; i.e., we impose the same functional form as used in Ref. [26] (except for the different tuning parameter, V in our case and B field in Ref. [26]). To closely mirror the procedure used in Ref. [26], we constrain our fit for a given, fixed T to the crossover region from Kondo to RKKY regime by fitting only in a V region determined by $T > 0.1 \cdot T_{\text{FL}}(V)$ (i.e., we omit data points deep in the FL regions). This yields $V_{\text{Hall}}(T)$, and inverting this function yields $T_{\text{Hall}}(V)$. Figure 28 shows our Hall effect data with the corresponding fits.

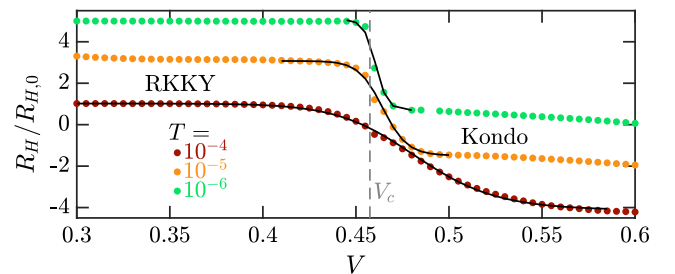


FIG. 28. Hall coefficient data from Fig. 18 (symbols) and corresponding fits via Eq. (D1) (black lines). To improve visibility, the data for $T = 10^{-5}$ and $T = 10^{-6}$ are offset by 2 and 4, respectively.

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