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Uncovering the peculiar 4*f* electrons in heavy fermions

Yang Liu[*]

Center for Correlated Matter and Department of Physics, Zhejiang University, Hangzhou 310058, China

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Heavy fermion (HF) compounds are prototypical strongly correlated electron systems and are prime examples to study quantum critical phenomena. The *f* electrons, which form local moments at high temperatures, can acquire itinerancy at low temperatures through quantum-mechnical coupling with the conduction electrons, a process known as the Kondo effect. This many-body process can give rise to quasiparticle bands at the Fermi level (E_F) with a very large effective mass (often >100m_e). The same spin-exchange coupling between conduction and *f* electrons can also lead to magnetically ordered states, which compete with the Kondo screening. The ground state can be easily tuned by external parameter δ (Figure 1), such as pressure, doping, and magnetic field. Near the quantum critical point (QCP) δ_c, quantum fluctuations are prominent and often lead to anomalous quantum states, including unconventional superconductivity and non-Fermi liquid behavior.

A central question for HF compounds is: are the *f* electrons localized or itinerant? Often there is no simple answer: unlike the conduction electrons, which form fully coherent Bloch waves well described by the conventional band theory, the development of heavy quasiparticles in HF compounds can be dependent on interaction strength, magnetism, and temperature. For Ce-based systems, the 4*f* spectral function consists of lower and upper Hubbard bands well below and above E_F, as well as a heavy quasiparticle band at E_F from the Kondo hybridization. Both the spectral weight and momentum dispersion of this quasiparticle band are important.

A direct method to probe heavy 4*f* bands is angle-resolved photoemission spectroscopy (ARPES). Historically, ARPES studies on HF compounds have been hampered by limited resolution, but rapid progress has been made recently thanks to technical developments. The first important question is how the heavy quasiparticles develop when lowering the temperature. A high-resolution ARPES study on $CeCoIn_5$ clearly demonstrated that the heavy quasiparticle bands start to form at a temperature (labeled by T_0 in Figure 1) much higher than that conventionally thought [1], i.e., the transport coherence temperature T*. This highlights the importance of excited crystal electric field states in the formation of heavy bands and calls for a fundamental rethinking of the lattice effect on the hybridization process. The high-temperature onset was also supported by an optical pump-probe measurement [2], which further implied that T* could be associated with the emergence of collective hybridization. For anti-ferromagnetic (AFM) $CeRhIn_5$, where local-type quantum criticality was proposed (Figure 1(b)), band-dependent hybridization is observed well above T_N (=3.8 K) [3], although the Fermi surface (FS) is still dominated by conduction bands. The band-dependent hybridization can be essential to explain the seemingly conflicting results regarding the Kondo effect in this system and demonstrates the subtlety of the localized-itinerant crossover for 4*f* electrons. These seminal studies mark an important step towards understanding the HF physics.

Another fundamental question concerns the different characteristics of 4*f* states in systems with different types of quantum criticality. For the spin-density-wave (SDW) type

*Corresponding author (email: yangliuphys@zju.edu.cn)

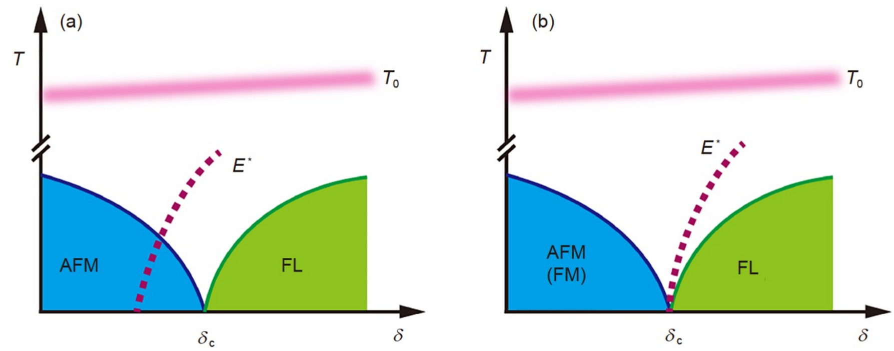

Figure 1 (Color online) Typical (T, δ) phase diagrams for HF compounds with SDW-type (a) and local-type (b) quantum criticality. E^* marks the localized-delocalized boundary for 4*f* electrons. FL indicates the Fermi liquid (FL) phase with $\rho\propto T^2$. (b) The QCP at zero temperature is accompanied by a sudden transition from a small "FS" excluding 4*f* electrons in the AFM/FM phase to a large "FS" incorporating 4*f* electrons in the FL phase.

of quantum criticality (Figure 1(a)), the 4*f* electrons play a key role in the FS-$CeCu_2Si_2$ is a canonical example. It is also the first unconventional superconductor, discovered by Frank Steglich in 1979. Its superconductivity was previously thought to be nodal *d*-wave, although recent experiments indicated a fully opened superconducting gap at ultralow temperatures [4], which sparked intense interests. Theoretical calculations predicted a warped cylindrical heavy band at E_F, as well as other lighter conduction bands [5]. Recent ARPES measurements indeed revealed the predicted heavy cylindrical band and moderately heavy conduction bands [6]. The multiband FS with orbital-dependent hybridization can be important in understanding its unconventional superconductivity.

$CeRh_6Ge_4$ is the first clean example of ferromagnetic (FM) quantum criticality, achieved by hydrostatic pressure, and possibly hosts local-type quantum criticality [7]. Quantum oscillation (QO) experiments below T_c at ambient pressure revealed oscillation frequencies in good agreement with localized 4*f* calculations [8]. Meanwhile, ARPES measurements uncovered dispersive 4*f* bands near E_F well above T_c [9]. The hybridization strength was found to be quite anisotropic in momentum space due to the Ce chains, likely an important ingredient for the FM quantum criticality. The dichotomy between QO and ARPES results suggests the possible localization of 4*f* electrons upon cooling into the FM state. It is therefore of great interest to perform ARPES measurements across T_c (=2.5 K). It is intriguing to see that similar behavior was observed in the AFM counterpart $CeRhIn_5$, where QO and ARPES measurements also revealed different 4*f* characteristics below and above T_N [3].

These studies demonstrate the complex nature of 4*f* electrons in HF systems and the importance of the momentum/orbital-dependent hybridization. The next pressing question is: how do the partially coherent 4*f* bands, which begin to develop at T_0, evolve when cooling down into the magnetically ordered phase or the FL phase? What are the spectroscopic signatures of dynamic or non-local Kondo effect? With rapid developments in the ARPES technique, particularly when combined with advanced thin film growth [10], new and important progress can be anticipated in the near future.

1 Q. Y. Chen, D. F. Xu, X. H. Niu, J. Jiang, R. Peng, H. C. Xu, C. H. P. Wen, Z. F. Ding, K. Huang, L. Shu, Y. J. Zhang, H. Lee, V. N. Strocov, M. Shi, F. Bisti, T. Schmitt, Y. B. Huang, P. Dudin, X. C. Lai, S. Kirchner, H. Q. Yuan, and D. L. Feng, Phys. Rev. B **96**, 045107 (2017), arXiv: 1610.06724.

2 Y. P. Liu, Y. J. Zhang, J. J. Dong, H. Lee, Z. X. Wei, W. L. Zhang, C. Y. Chen, H. Q. Yuan, Y. F. Yang, and J. Qi, Phys. Rev. Lett. **124**, 057404 (2020), arXiv: 1906.07990.

3 Q. Y. Chen, D. F. Xu, X. H. Niu, R. Peng, H. C. Xu, C. H. P. Wen, X. Liu, L. Shu, S. Y. Tan, X. C. Lai, Y. J. Zhang, H. Lee, V. N. Strocov, F. Bisti, P. Dudin, J. X. Zhu, H. Q. Yuan, S. Kirchner, and D. L. Feng, Phys. Rev. Lett. **120**, 066403 (2018), arXiv: 1801.07797.

4 S. Kittaka, Y. Aoki, Y. Shimura, T. Sakakibara, S. Seiro, C. Geibel, F. Steglich, H. Ikeda, and K. Machida, Phys. Rev. Lett. **112**, 067002 (2014), arXiv: 1307.3499; G. Pang, M. Smidman, J. Zhang, L. Jiao, Z. Weng, E. M. Nica, Y. Chen, W. Jiang, Y. Zhang, W. Xie, H. S. Jeevan, H. Lee, P. Gegenwart, F. Steglich, Q. Si, and H. Yuan, Proc. Natl. Acad. Sci. **115**, 5343 (2018).

5 G. Zwicknagl, Rep. Prog. Phys. **79**, 124501 (2016); X. B. Luo, Y. Zhang, Q. Y. Chen, Q. Liu, L. Z. Luo, S. Y. Tan, X. G. Zhu, and X. C. Lai, Sci. China-Phys. Mech. Astron. **63**, 287413 (2020).

6 Z. Wu, Y. Fang, H. Su, W. Xie, P. Li, Y. Wu, Y. Huang, D. Shen, B. Thiagarajan, J. Adell, C. Cao, H. Yuan, F. Steglich, and Y. Liu, Phys. Rev. Lett. **127**, 067002 (2021), arXiv: 2105.12394.

7 B. Shen, Y. Zhang, Y. Komijani, M. Nicklas, R. Borth, A. Wang, Y. Chen, Z. Nie, R. Li, X. Lu, H. Lee, M. Smidman, F. Steglich, P. Coleman, and H. Yuan, Nature **579**, 51 (2020); Y. F. Yang, Sci. China-Phys. Mech. Astron. **63**, 117431 (2020).

8 A. Wang, F. Du, Y. Zhang, D. Graf, B. Shen, Y. Chen, Y. Liu, M. Smidman, C. Cao, F. Steglich, and H. Yuan, Sci. Bull. **66**, 1389 (2021), arXiv: 2101.08972.

9 Y. Wu, Y. Zhang, F. Du, B. Shen, H. Zheng, Y. Fang, M. Smidman, C. Cao, F. Steglich, H. Yuan, J. D. Denlinger, and Y. Liu, Phys. Rev. Lett. **126**, 216406 (2021), arXiv: 2104.03600.

10 X. Y. Ji, Q. Y. Chen, X. C. Lai, L. Huang, and S. Y. Tan, Sci. China-Phys. Mech. Astron. **63**, 267411 (2020).