

Understanding the Heavy Fermion Phenomenology from a Microscopic Model

Ping Sun¹ and Gabriel Kotliar¹

¹*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-8019, USA*
(Received 23 January 2005; published 29 June 2005)

We solve the 3D periodic Anderson model using a two impurity cluster dynamical mean field theory. We obtain the temperature versus hybridization phase diagram. Approaching the quantum critical point (QCP) both the Néel and lattice Kondo temperatures decrease and they do not cross at the lowest temperature we reached. While strong ferromagnetic spin fluctuation on the Kondo side is observed, our result suggests the critical static spin susceptibility is local in space at the QCP. We observe in the crossover region a logarithmic temperature dependence in the specific heat coefficient and spin susceptibility.

DOI: [10.1103/PhysRevLett.95.016402](https://doi.org/10.1103/PhysRevLett.95.016402)

PACS numbers: 71.27.+a, 71.10.Hf, 72.15.Qm, 75.20.Hr

The heavy fermion phenomenon is among the most intensively studied subjects in condensed matter physics [1]. Experimental information accumulated over the past 30 years has revealed many unconventional aspects of heavy fermion physics [1,2].

Heavy fermion physics is derived from a local moment band hybridizing with an extended conduction band. The hybridization induces the competing Kondo (J_K) and RKKY interactions [3]. At $J_K \ll T$, the physics is dominated by those of the two bands separately with the hybridization as a perturbation. As the temperature is lowered, depending on the strength of J_K , different physics may develop. In the region where $J_K \ll W$ (the conduction bandwidth), the RKKY interaction prevails. The RKKY is a long range exchange mediated by the conduction electrons near the Fermi surface and oscillates with $k = 2k_F$ asymptotically. At $T \lesssim J_K^2/W$, the RKKY interaction can induce a transition to a magnetically ordered phase. In the crossover regime on this side, the Kondo behavior, though subdominant, would still show up in various measurables due to its nonanalyticity in terms of the energy cutoff, e.g., temperature. As J_K is increased, the Kondo effect becomes more important and eventually dominates. Here the Kondo screening begins at high temperatures $T \sim J_K$ where the conduction electrons near the Fermi energy starts to screen the local f moments. If this remains so as the temperature is lowered, there would not be enough conduction electrons to completely screen the f moment lattice [4]. Actually, in heavy fermions the entire conduction Fermi sea gets involved in screening. As the temperature is lowered, conduction electrons farther away from the Fermi surface participate in the Kondo screening. The system may then be described, to the leading order, as a band of local moments whose magnitude is progressively reduced. These reduced local moments still hybridize with the conduction electrons which have not participated in the Kondo screening and live near the conduction band bottom. Hence, on the Kondo side, the RKKY correlation, as T is lowered, becomes more ferromagnetic (FM). The FM spin correlation remains at further lower temperatures when the heavy Fermi liquid is formed. Macroscopically, the FM behavior

is related to the lattice Kondo energy, T_0 , which is proportional to the Fermi energy. T_0 can be defined in terms of the saturated homogeneous spin susceptibility in the Fermi liquid phase, $\chi_{\vec{k}=0} = C/T_0$, where C is the Curie constant. Should T_0 approach zero, strong FM spin fluctuation would be observed.

It turns out that the thermodynamics related to the continuous condensation of the local moments into the heavy fermion fluid is quite universal [5], as contrasted with that more material specific in the low temperature region. At low temperatures, various phases may develop, including a superconducting phase [1]. One interesting possibility is that the competing Kondo and RKKY interactions result in a quantum phase transition (QPT) without the interference of any other phases. Such a situation is observed experimentally in $\text{CeCu}_{1-x}\text{Au}_x$ [6,7] and YbRh_2Si_2 [8].

Two different scenarios have been proposed for the heavy fermion QPT. One is the Hertz-Millis-Moriya theory [9], which is applicable when the energy scale of the Kondo screening is much higher than that of the magnetic ordering near the quantum critical point (QCP). As a result, the local moments are fully screened in the quantum critical regime. However, by comparing the predicted critical exponents with the experiments, the theory is found to be inapplicable in many cases [1,2,7,8]. In the second scenario, one expects the magnetic ordering (T_N) and lattice Kondo screening (T_0) energies vanish simultaneously at the QCP [2,7] (see also [10]). Since the critical spin fluctuations at $k = 2k_F$ and $k = 0$ are associated with the T_N and vanishing T_0 , respectively, it is interesting to know what kind of critical magnetic mode may develop in the neighborhood of the QCP. We will show later that near the QCP the two critical modes strongly interact with each other and the critical spin fluctuation becomes local in space (see also [2]). In this scenario, the local moments survive at the QCP.

It is important that the heavy fermion physics as we understand be obtained from a microscopic model. To this end the main theoretical difficulty lies in treating on equal footing the Kondo and RKKY interactions. Many bosonic

mean field theories, like the Hertz-Millis-Moriya [9] and slave-boson [11] theories, fail because they rely on the order parameter of either the magnetic or Kondo phase and miss the properties of the other. On the other hand, a fermionic mean field theory, like the dynamical mean field theory (DMFT) [12], would allow the possible orders to develop and compete and is more desirable.

The DMFT extends the Weiss mean field theory to describe fermions. The single impurity DMFT was applied to both the Kondo and magnetically ordered phases in heavy fermions [13] (see also Ref. [14]). Besides the over estimation of the Neel temperature due to the lack of the magnetic fluctuation, this approach cannot capture properly the renormalization of the RKKY interaction. A partial solution to this problem is to add an RKKY interaction to the model and allow the renormalization of the RKKY by extending the Weiss approximation to the interaction [15]. The resulted formalism, the so-called extended DMFT (EDMFT), is able to describe qualitatively the heavy fermions [16] in both the Kondo and antiferromagnetic (AFM) phases. However, it predicts a first order phase transition due to the local mean field treatment of the RKKY interaction [16,17].

A parallel path in studying the heavy fermions is through the two impurity problem. This model contains the dynamics of both the Kondo and RKKY interactions and is solvable [18,19]. It was shown, at the particle-hole symmetry, there was a non-Fermi liquid fixed point separating the Kondo and magnetic phases. However, it is difficult to extend the properties of a multi-impurity model to a lattice of impurities.

In this Letter, we combine the two impurity model with DMFT so that a lattice of impurities can be described. This overcomes the difficulties of both the single impurity DMFT and multi-impurity approaches. It handles the Kondo and RKKY interactions in a more balanced way.

We consider the periodic Anderson model in 3D

$$H = \sum_{\vec{k}, \sigma} (\epsilon_{\vec{k}} - \mu) c_{\vec{k}, \sigma}^\dagger c_{\vec{k}, \sigma} + (E_f - \mu) \sum_{j, \sigma} n_{j, \sigma}^f + U \sum_j \left(n_{j, \uparrow}^f - \frac{1}{2} \right) \left(n_{j, \downarrow}^f - \frac{1}{2} \right) + V \sum_{j, \sigma} (f_{j, \sigma}^\dagger c_{j, \sigma} + c_{j, \sigma}^\dagger f_{j, \sigma}) \quad (1)$$

with $\epsilon_{\vec{k}} = -\frac{1}{3} \sum_{i=1}^3 \cos k_i$. We divide the lattice into two interpenetrating sublattices, *A* and *B*. The unit cell is then doubled. Applying the cavity method [12], we obtain an effective local action:

$$S^0 = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\sigma} \sum_{X, Y=A, B} f_{X, 0\sigma}^\dagger(\tau) [\mathcal{G}_{0\sigma}^f]_{XY}^{-1}(\tau - \tau') f_{Y, 0\sigma}(\tau') + U \int_0^\beta d\tau \sum_{X=A, B} \left(n_{X, 0\uparrow}^f - \frac{1}{2} \right) \left(n_{X, 0\downarrow}^f - \frac{1}{2} \right) \quad (2)$$

The Weiss function $\mathcal{G}_{0\sigma}^f$ is determined self-consistently as follows. First, we use the quantum Monte Carlo method (QMC) [20] and obtain the impurity Green's function. Then, from the Dyson equation for the impurities, we get the impurity self-energy $[\Sigma_\sigma^{\text{imp}}]_{XY}$. The lattice self-energy is constructed to be:

$$\Sigma_\sigma^{ff}(\vec{k}, ip_n) = \begin{pmatrix} \Sigma_{AA, \sigma}^{\text{imp}}(ip_n) & -2d\epsilon_{\vec{k}} f(\vec{k}) \Sigma_{AB, \sigma}^{\text{imp}}(ip_n) \\ -2d\epsilon_{\vec{k}} f^*(\vec{k}) \Sigma_{AB, \sigma}^{\text{imp}}(ip_n) & \Sigma_{BB, \sigma}^{\text{imp}}(ip_n) \end{pmatrix} \quad (3)$$

from which we obtain the local Green's function:

$$G_{\text{loc}, \sigma}^{ff}(ip_n) = \sum_{\vec{k}} \left[\begin{pmatrix} ip_n + \mu - E_f & 0 \\ 0 & ip_n + \mu - E_f \end{pmatrix} - \frac{V^2}{(ip_n + \mu)^2 - \epsilon_{\vec{k}}^2} \begin{pmatrix} ip_n + \mu & \epsilon_{\vec{k}} f(\vec{k}) \\ \epsilon_{\vec{k}} f^*(\vec{k}) & ip_n + \mu \end{pmatrix} - \Sigma_\sigma^{ff}(\vec{k}, ip_n) \right]^{-1}, \quad (4)$$

with $f(\vec{k}) = \exp(ik_x)$. By identifying the local (within a unit cell) Green's function on the lattice with that of the impurity model, we form a self-consistent loop [12,21]. While solving the impurity model we can measure the *z*-direction spin susceptibility $\chi_{XY}(\tau) = \langle T_\tau S_Z^f(X, \tau) S_Z^f(Y, 0) \rangle$, with $S_Z^f(X) = n_{X, \uparrow}^f - n_{X, \downarrow}^f$. The lattice susceptibility is obtained in the same way as the lattice self-energy given in Eq. (3).

We study the phase diagram of temperature versus *V* at fixed $U = 1.2$ and $E_f = -0.15$. To avoid crossing the band gap, we change the chemical potential μ along with *V* so that the free ($U = 0$) particle density per site at $T = 0$ is fixed at $N_{\text{tot}}^{\text{free}} = 2.5423$. The resulting physical density changes slightly as *V* increases and is always greater than

and close to the half-filling [22]. We study the AFM and paramagnetic (PM) phases and the transition between them. In solving the two impurity problem we use the QMC. We always use $U\Delta\tau \approx 1$ where $\Delta\tau = \beta/L$ and *L* is the number of time slices in QMC. In each DMFT iteration, we perform QMC sweeps $\sim 10^5$. Away from the phase transitions around 10 DMFT iterations are usually enough to converge the results. Near the phase transition a lot more are needed due to the critical slowing down.

Figure 1 is the phase diagram we obtained. Two technical remarks are in place. First, to exam if the AFM to PM transition is continuous, we checked the inverse static spin susceptibilities at $\vec{k} = (\pi, \pi, \pi)$ which becomes very critical at the corresponding transition values of *V* [22].

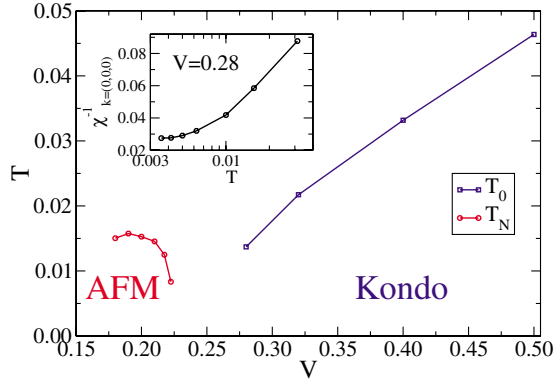


FIG. 1 (color online). The calculated phase diagram. The two lines, $T_N(V)$ and $T_0(V)$, do not cross at the lowest temperatures we reached. The inset shows the low temperature saturation of the static homogeneous spin susceptibility at $V = 0.28$.

Second, the crossover temperature T_0 is obtained using the saturated static homogeneous spin susceptibility $\chi(\vec{k} = 0, i0) \rightarrow C/T_0$ at low temperatures. [We used Curie constant $C = 1/2$ which is obtained in the high temperature limit.] An example of the saturation behavior is shown in the inset of Fig. 1. Note that T_0 being small means the FM spin fluctuation becomes very strong.

To study the critical magnetic fluctuation around the QPT, we plot in Fig. 2 $\chi_{AA}(i0)$ and $\chi_{AB}(i0)$. From the result we see that $\chi_{AB}(i0)$ changes sign when V increases. This sign change is actually a special manifestation of a more general evolution of the RKKY correlation from being AFM to FM as hybridization is increased, due to the conduction electrons mediating the RKKY change from those near the Fermi surface to around the band bottom. Meanwhile, $\chi_{AA}(i0)$ is always positive and becomes very strong in the crossover regime. This scenario should extend to $T = 0$ and there would be a point at which

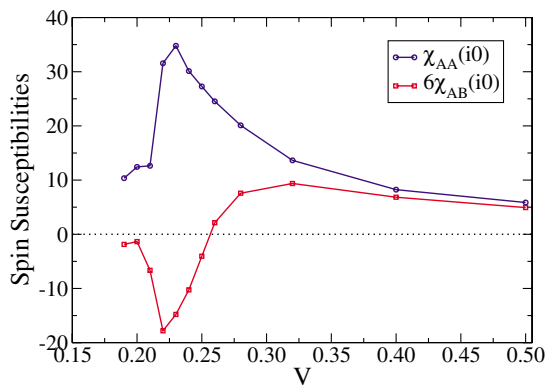


FIG. 2 (color online). The local, $\chi_{AA}(i0)$, and nearest-neighbor, $\chi_{AB}(i0)$, spin susceptibilities at $\beta = 120$ versus V . $\chi_{AA}(i0)$ is always positive and shows a peak in the crossover region. $\chi_{AB}(i0)$ changes from negative in the AFM phase to positive in the Kondo phase. We multiplied χ_{AB} by the coordination number which reflects its contribution to the lattice spin susceptibility.

$\chi_{AB}(i0) = 0$ and $\chi_{AA}(i0)$ becomes critical. This point would be the heavy fermion QCP. Note that the static spin response being local does not mean a local electron self-energy. Actually, the nonlocal self-energy becomes stronger at lower temperatures [22].

An important question is how the Kondo screening, which is local in space, becomes coherent in heavy fermions. To this end, we study the evolution of the spatial correlation in the spin responses in Fig. 3. It shows that spin fluctuations are quite local in space down to $T \sim 0.1$ for $V = 0.26$ and $T \sim 0.2$ for $V = 0.50$. At lower temperatures, the FM spin susceptibility becomes dominant. This is similar to that observed experimentally in YbRh_2Si_2 [23]. Two remarks are in place. (1) the nonlocality in χ develops at lower temperature for $V = 0.26$ than that for $V = 0.50$. This reflects the local nature of the spin fluctuation in the quantum critical region which extends to lower temperature as the QCP is approached and is consistent with Fig. 2. (2) The logarithmic temperature dependence of χ as shown in Fig. 3 is similar to those observed in many heavy

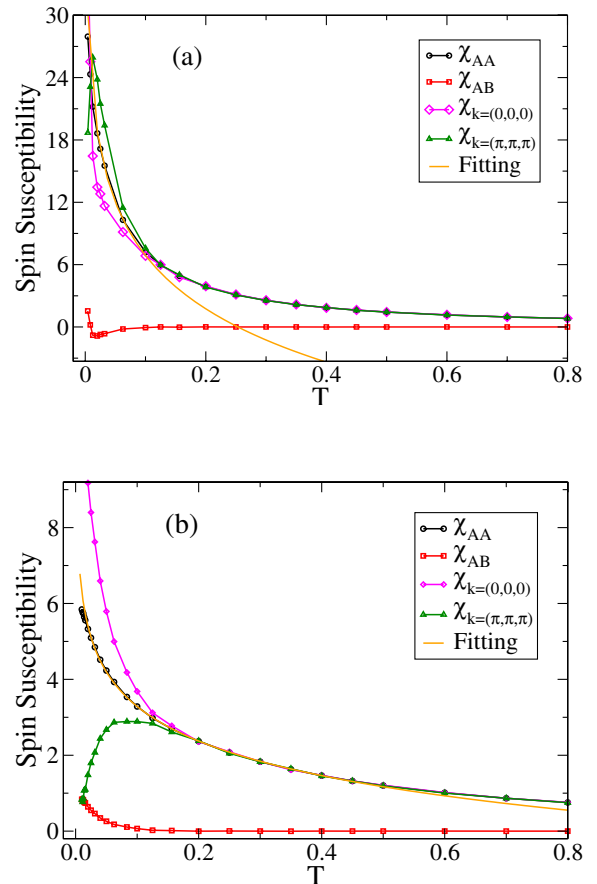


FIG. 3 (color online). The static spin susceptibilities as functions of the temperature at (a) $V = 0.26$ and (b) $V = 0.5$. The fittings are given by $\chi(T) = 7.399 \ln(0.253/T)$ in (a) and $\chi(T) = 1.314 \ln(1.218/T)$ in (b). Note that according to Fig. 1 $V = 0.26$ is close to the QCP on the Kondo side.

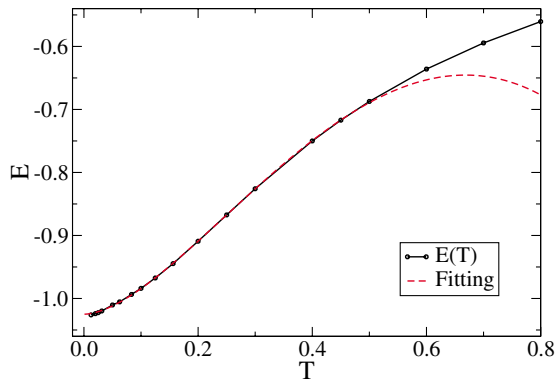


FIG. 4 (color online). The total energy at $V = 0.26$. We fitted $E(T) = -1.025 + 1.700T^2 \ln(1.102/T)$. The corresponding specific heat coefficient is $\gamma(T) = 3.400 \ln(0.6682/T)$.

fermion compounds [1]. A logarithmic temperature dependence is also found in the total energy shown in Fig. 4.

To conclude, using a two impurity DMFT, we studied the periodic Anderson model on cubic lattice at finite temperatures. We obtained the phase diagram which is consistent with the picture that both the Neel and Kondo temperatures vanish at the QCP. As the QCP was approached from the Kondo side, we found strong ferromagnetic spin fluctuations. From the sign change of the static nearest-neighbor spin susceptibility, we conjectured that the critical static spin fluctuation become local at the heavy fermion QCP. We explored the crossover region and observed logarithmic temperature dependences in the specific heat coefficient and spin susceptibility.

Our results presented in this Letter imply that a two impurity Anderson model combined with DMFT might serve as a minimal model in describing most of the thermodynamics of the heavy fermions. However, we should also keep in mind that there could exist other phases, like the superconducting phase [24], whose existence may require mechanisms which are more spatially extended than those describable in a two impurity model.

Since the $4f$ or $5f$ orbital contributes to the local moment physics in most heavy fermion compounds, there are inevitably many physical properties oversimplified by the periodic Anderson model, like the orbital degeneracy and the subsequent crystalline field splitting. These are further complicated by the spin-orbital coupling, lattice frustration, disorder, hybridization with other bands, etc. Actually all these contribute to a much richer physics observed in experiments [1] than we have obtained. To this end, our current work can be considered as a useful guide to distinguish the “universal” heavy fermion features from those specific to individual materials.

The authors would like to acknowledge helpful discussions with E. Abrahams, P. Coleman, A. Georges, O. Parcollet, C. Pepin, A. Schiller, and Q. Si. This research was supported by NSF under No. DMR-0096462, the Center for Materials Theory at Rutgers University, and

(P. S.) 12CAM.

-
- [1] G. R. Stewart, *Rev. Mod. Phys.* **73**, 797 (2001).
 - [2] P. Coleman, C. Pepin, Q. Si, and R. Ramazashvili, *J. Phys. Condens. Matter* **13**, R723 (2001).
 - [3] C. M. Varma, *Rev. Mod. Phys.* **48**, 219 (1976); S. Doniach, *Physica (Amsterdam)* **91B**, 231 (1977); P. A. Lee *et al.*, *Comments Condens. Matter Phys.* **12**, 99 (1986).
 - [4] P. Nozieres, *Ann. Phys. (Paris)* **10**, 19 (1985).
 - [5] N. J. Curro *et al.*, *Phys. Rev. B* **70**, 235117 (2004); S. Nakatsuji, D. Pines, and Z. Fisk, *Phys. Rev. Lett.* **92**, 16401 (2004).
 - [6] H. von Lohneysen, *J. Phys. Condens. Matter* **8**, 9689 (1996).
 - [7] A. Schröder *et al.*, *Nature (London)* **407**, 351 (2000).
 - [8] J. Custers *et al.*, *Nature (London)* **424**, 524 (2003); P. Gegenwart *et al.*, *Phys. Rev. Lett.* **89**, 56402 (2002).
 - [9] J. A. Hertz, *Phys. Rev. B* **14**, 1165 (1976); A. J. Millis, *Phys. Rev. B* **48**, 7183 (1993); T. Moriya and T. Takimoto, *J. Phys. Soc. Jpn.* **64**, 960 (1995); S. Kambe *et al.*, *ibid.* **65**, 3294 (1996).
 - [10] T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003); T. Senthil, M. Vojta, and S. Sachdev, *Phys. Rev. B* **69**, 035111 (2004).
 - [11] See, for example, A. J. Millis and P. A. Lee, *Phys. Rev. B* **35**, 3394 (1987); P. Coleman, *Phys. Rev. B* **35**, 5072 (1987); D. M. Newns and N. Read, *Adv. Phys.* **36**, 799 (1987); M. Grilli, B. G. Kotliar, and A. J. Millis, *Phys. Rev. B* **42**, 329 (1990); A. M. Sengupta and A. Georges, *Phys. Rev. B* **52**, 10295 (1995).
 - [12] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).
 - [13] M. Jarrell, H. Akhlaghpour, and Th. Pruschke, *Phys. Rev. Lett.* **70**, 1670 (1993); M. Jarrell, *Phys. Rev. B* **51**, 7429 (1995); M. Rozenberg, *Phys. Rev. B* **52**, 7369 (1995).
 - [14] DMFT results in a local electron self-energy. A similar idea was explored in studying the heavy fermion phenomenology by C. M. Varma, *Phys. Rev. Lett.* **55**, 2723 (1985).
 - [15] Q. Si, S. Rabello, K. Ingersent, and J. L. Smith, *Nature (London)* **413**, 804 (2001).
 - [16] P. Sun and G. Kotliar, *Phys. Rev. Lett.* **91**, 037209 (2003).
 - [17] P. Sun and G. Kotliar, *Phys. Rev. B* **71**, 245104 (2005).
 - [18] B. A. Jones and C. M. Varma, *Phys. Rev. B* **40**, 324 (1989).
 - [19] I. Affleck, A. W. W. Ludwig, and B. A. Jones, *Phys. Rev. B* **52**, 9528 (1995).
 - [20] J. E. Hirsch and R. M. Fye, *Phys. Rev. Lett.* **56**, 2521 (1986).
 - [21] G. Kotliar, S. Y. Savrasov, G. Palsson, and G. Biroli, *Phys. Rev. Lett.* **87**, 186401 (2001); O. Parcollet, G. Biroli, and G. Kotliar, *Phys. Rev. Lett.* **92**, 226402 (2004); G. Biroli, O. Parcollet, and G. Kotliar, *Phys. Rev. B* **69**, 205108 (2004).
 - [22] P. Sun and G. Kotliar (unpublished).
 - [23] K. Ishida *et al.*, *Phys. Rev. Lett.* **89**, 107202 (2002); P. Gegenwart *et al.*, *Phys. Rev. Lett.* **94**, 076402 (2005).
 - [24] See, e.g., M. Lavagna, A. J. Millis, and P. A. Lee, *Phys. Rev. Lett.* **58**, 266 (1987).