# PRE-CRITICAL FLUCTUATIONS IN HEAVY FERMIONS* **

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Itinerant antiferromagnetic order can gradually be suppressed by mismatching the nesting of the Fermi surfaces and a quantum critical point is obtained as $T_{\rm N} \to 0$. Within a renormalization group approach we study the instabilities to spin- and charge-density waves and superconductivity, the low-$T$ specific heat and the magnetic susceptibility. All quantities increase on a logarithmic scale when $T$ is lowered, similar to the non-Fermi-liquid behavior observed in some heavy fermion compounds.

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Non-Fermi-liquid (NFL) behavior, *e.g.* in $U_{0.2}Y_{0.8}Pd_3$, $UCu_{5-x}Pd_x$ and $CeCu_{5.9}Au_{0.1}$, manifests itself in deviations from the Fermi liquid (FL) [1] in the specific heat, the susceptibility and the resistivity, typically as a logarithmic or power-law dependence with $T$. The breakdown of the FL can be tuned by hydrostatic or chemical pressure, or a magnetic field, and usually takes place close to the onset of antiferromagnetic (AF) ordering.

Theoretical attempts to explain these properties fall into four scenarios. *(i)* The vicinity of a $T = 0$ quantum phase transition [2–5] or Griffith phase [6]. *(ii)* A disorder induced distribution of Kondo temperatures [7, 8] may lead to a $\ln(T)$-dependence in the susceptibility and the specific heat. *(iii)* The quadrupolar Kondo effect also leads to a quantum critical point (QCP) [9]. *(iv)* Two-dimensional critical ferromagnetic fluctuations coupling to the conduction electrons was proposed for $CeCu_{6-x}Au_x$ [10].

Here we adopt the point of view of a QCP arising from AF correlations (see [2]). We consider a band of heavy electrons with two nested parabolic

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pockets, one electron-like and the other hole-like, separated by a wavevector $\boldsymbol{Q}$, and a repulsive interaction between the electrons inducing itinerant AF. A nesting mismatch is introduced by varying the chemical potential, but the temperature, chemical disorder or a magnetic field lead to similar results. With increasing mismatch $T_{\rm N}$ is reduced (long-range order is suppressed) and a QCP is obtained as $T_{\rm N} \to 0$. We study the pre-critical region using a multiplicative renormalization group (RG) approach [11].

The kinetic energy for electrons in the two isotropic pockets is

$$H_0 = \sum_{l=1,2\boldsymbol{k}\sigma} \varepsilon_l(\boldsymbol{k}) c^\dagger_{l\boldsymbol{k}\sigma} c_{l\boldsymbol{k}\sigma} \,, \tag{1}$$

where $\varepsilon_1(\boldsymbol{k}) = \boldsymbol{k}^2/2m$ and $\varepsilon_2(\mathbf{k}) = E_0 - \boldsymbol{k}^2/2m$. Here $\boldsymbol{k}$ is measured from the center of the respective pocket and $E_0$ is the energy difference between the bottom of the electron and the top of the hole bands. The chemical potential $\mu$ partially fills both bands and is measured from the electron-hole symmetric situation, $|\mu| < E_0/2$, and $|\boldsymbol{k}|$ is small compared to the size of the Brillouin zone. The interaction of electrons between pockets is

$$H_{12} = \sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}\sigma\sigma'} \Big[ V c^\dagger_{1\boldsymbol{k}+\boldsymbol{q}\sigma} c_{1\boldsymbol{k}\sigma} c^\dagger_{2\boldsymbol{k}'-\boldsymbol{q}\sigma'} c_{2\boldsymbol{k}'\sigma'} + U c^\dagger_{1\boldsymbol{k}'+\boldsymbol{q}\sigma} c^\dagger_{2\boldsymbol{k}-\boldsymbol{q}\sigma'} c_{1\boldsymbol{k}\sigma'} c_{2\boldsymbol{k}'\sigma} \Big] \,. \tag{2}$$

Here $V$ and $U$ represent the interaction strength for small and large (of the order of $\boldsymbol{Q}$) momentum transfer between the pockets, respectively. The Hubbard limit is obtained for $V = U$.

The vertex corrections are logarithmic in the external energy parameter and are summed to leading order using the multiplicative RG. The leading vertex corrections are given by the zero-sound bubble diagrams (antiparallel propagator lines). We consider only one external energy variable $\omega$ and project all others onto the Fermi level. This is valid for heavy fermions where the $\omega$-dependence is more important than the $\boldsymbol{k}$-dependence, but not for transition metals. The energy $\omega$ is small compared to the cut-off energy $E_0$, and that the density of states for electrons and holes is constant, $\rho_{\rm F}$.

The notation in (2) is the same as for Luttinger liquids [12], although the physics of this three-dimensional model is very different. For a Luttinger liquid also the Cooper channel (bubble with parallel propagator lines) is logarithmically divergent [12]. The cancellations among diagrams then lead to the renormalization of the group velocities and to charge and spin separation. Hence, the present model is *very* different from a Luttinger liquid.

The logarithmic corrections to the interaction vertices yield renormalized invariant couplings (here $\xi = \ln[E_0/(|\omega| + 2|\mu|)]$ with $\mu$ (measured from $E_0/2$) being the mismatch between the Fermi surfaces) [11]

$$\tilde{V} = \frac{V\rho_{\rm F}}{1 - V\rho_{\rm F}\xi} \,, \quad 2\tilde{U} - \tilde{V} = \frac{(2U - V)\rho_{\rm F}}{1 + (2U - V)\rho_{\rm F}\xi} \,. \tag{3}$$

A divergent vertex indicates strong coupling and signals an instability.

The staggered spin susceptibility in the perturbative regime is [11]

$$\chi_{\mathrm{S}}(\boldsymbol{Q},\omega) = -2\rho_{\mathrm{F}}\xi/(1 - V\rho_{\mathrm{F}}\xi)\,. \tag{4}$$

The divergence signals the AF instability at $T_{\mathrm{N}} = E_0 \exp[-1/(\rho_{\mathrm{F}}V)] - 2|\mu|$, the condition for a QCP is $T_{\mathrm{N}} = 0$, and if $T_{\mathrm{N}} < 0$ the AF order has not yet developed. The response to a charge density wave (CDW) is

$$\chi_{\mathrm{c}}(\boldsymbol{Q},\omega) = -2\rho_{\mathrm{F}}\xi/[1 - (V - 2U)\rho_{\mathrm{F}}\xi], \tag{5}$$

such that $T_{\mathrm{c}} = E_0 \exp\{-1/[\rho_{\mathrm{F}}(V - 2U)]\} - 2|\mu|$ for $V > 2U$. The Hubbard limit, $V = U > 0$, is not unstable to CDW, but will exhibit AF if the mismatch between the Fermi surfaces is small.

Due to the spin rotational invariance of the interaction the response to singlet and triplet superconductivity is the same. Superconducting fluctuations play an important role as the AF instability is approached, but since the logarithms enter the perturbation series only two orders later than in Eq. (4), we conclude that the system is dominated by AF correlations. NFL behavior, AF order and superconductivity in the neighborhood of a QCP have been observed in $\mathrm{CePd_2Si_2}$ and $\mathrm{CeIn_3}$ under pressure [13].

The renormalization of a propagator to next leading order is [11]

$$\ln d(\omega) = -\frac{1}{4}\,\frac{(2U - V)^2\rho_{\mathrm{F}}^2\xi}{1 + (2U - V)\rho_{\mathrm{F}}\xi} - \frac{3}{4}\,\frac{V^2\rho_{\mathrm{F}}^2\xi}{1 - V\rho_{\mathrm{F}}\xi}\,. \tag{6}$$

The $\gamma$-coefficient of the specific heat is given by $[1 - \partial\Sigma/\partial i\omega]$, which when renormalized is just the inverse of $d(\omega)$, so that $\gamma/\gamma_0 = [d(T)]^{-1} = m^*(T)/m$, where $\gamma_0$ refers to the noninteracting system and $d(T)$ is (6) with $\omega = \pi T$ in $\xi$. Hence, $\gamma$ increases on a logarithmic scale as $T$ is lowered. $\gamma$ diverges at $T_{\mathrm{N}}$, but remains finite if the system does not order.

The magnetic susceptibility is obtained via FL relations [11]

$$\chi_{\mathrm{B}} = \mu_{\mathrm{B}}^2\rho_{\mathrm{F}}[m^*(T)/m]\{1 + \tilde{U}(T)[m^*(T)/m]\}\,. \tag{7}$$

The first factor are the selfenergy insertions ($T$-dependent effective mass), while the second factor represents the vertex insertion. As the critical point is approached, both $m^*$ and $\tilde{U}$ diverge, signaling the breakdown of the FL. The Wilson ratio is nonuniversal and $T$-dependent, $(\chi_{\mathrm{B}}/\chi_{\mathrm{B0}})/(\gamma/\gamma_0) = 1 + \tilde{U}[m^*(T)/m]$. At the QCP $\gamma$, $\chi_{\mathrm{B}}$ and the Wilson ratio all diverge.

The effective thermal mass and the magnetic susceptibility increase on a logarithmic scale as $T$ is reduced and diverge at the critical point, *i.e.* $T_{\mathrm{N}}$. The QCP is an unstable fixed point, *i.e.* it can only be reached by perfectly

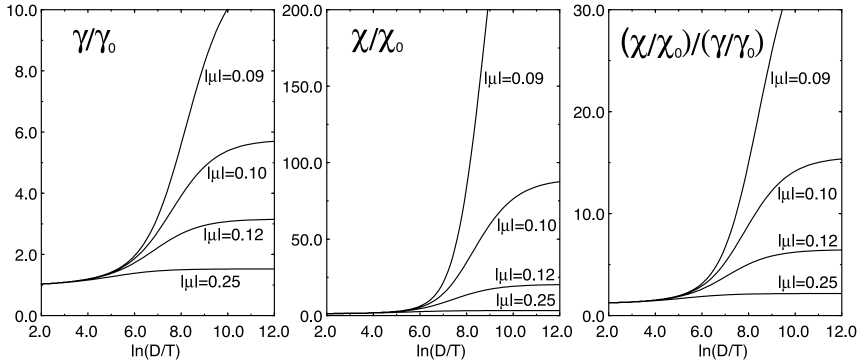


Fig. 1. $\gamma$, $\chi_{\rm B}$ and Wilson ratio normalized to their noninteracting values for $U\rho_{\rm F} = V\rho_{\rm F} = 0.2$, $D = 10$, and several values of the nesting mismatch $|\mu|$.

tuning the system (see Fig. 1). Otherwise, the RG flow will deviate to a phase with long-range order or towards the heavy electron paramagnet.

The perturbative RG is limited to the weak coupling region and cannot reach into the critical regime. As the coupling constants are renormalized to larger values, loops to all orders have to be included. In the critical regime collective bosonic modes (spinwaves) are formed, which cannot be treated perturbatively, and the Hertz–Millis approach [5], based on an effective bosonic action, should be used. In the weak and intermediate coupling regime the collective modes have a broad linewidth and are not relevant.

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