Heavy Fermion Quantum Criticality

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During the last few years, investigations of Rare-Earth materials have made clear that not only the heavy fermion phase in these systems provides interesting physics, but the quantum criticality where such a phase dies exhibits novel phase transition physics not fully understood. Moreover, attempts to study the critical point numerically face the infamous fermion sign problem, which limits their accuracy. Renormalization group and effective action techniques have been very popular in high energy physics, where they enjoy a good record of success. Yet, they have been little exploited for fermionic systems in condensed matter physics. In this work, we apply the RG to the heavy fermion problem. We write for the first time the effective action which describes the low energy physics of the system. The f-fermions are replaced by a dynamical scalar field whose nonzero expected value corresponds to the heavy fermion phase. This removes the fermion sign problem, making the effective action amenable to numerical studies as the effective theory is bosonic. Renormalization group studies of the effective action can be performed to extract approximations to nonperturbative effects at the transition. By performing one-loop renormalizations, resummed via Callan-Symanzik methods, we describe the heavy fermion criticality and predict the heavy fermion critical dynamical susceptibility and critical specific heat. The specific heat coefficient exponent we obtain (0.39) is in excellent agreement with the experimental result at low temperatures (0.4).

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For a couple of decades, heavy fermion materials have attracted the focus of a large part of the experimental and theoretical condensed matter community[1, 2]. There are many reasons for such a spotlight on these materials. They exhibit exotic superconductivity, interesting magnetism, but most importantly heavy quasiparticles with an enlarged Fermi surface. This heavy quasiparticle phase perishes into a quantum critical point with interesting, puzzling and not yet understood nature[3, 4].

It is quite striking to see the fermionic quasiparticle with masses from tenths to about thousandths of an elementary electron mass. This has been understood as arising from Kondo-like physics of the almost localized $f-$electrons when they hybridize with the lower atomic angular momentum bands of the material[2, 5]. This hybridization gives rise to an enlarged Fermi surface as the $f-$electrons now contribute to the Fermi volume, and to the large quasiparticle mass and large specific heat coefficient, through enhanced collective Kondo-like low energy scattering. Of course, the $f-$electrons have a strong tendecy to localize due to their large U which fights the hybridization V.

Some of these materials can be tuned (by applying pressure, etc.) so that a critical value $(U/V)_c$ is reached such that, for values larger than the critical value, the $f-$electrons localize and there is no heavy fermion phase. Instead, there is a small Fermi surface metal that usually exhibits magnetic order mediated via RKKY interactions[6, 7]. For subcritical values of U/V, the system is in the heavy fermion phase with large Fermi surface and no magnetism.

At the critical value, a continous quantum phase transition occurs as corroborated via scaling experiments. This transition is not understood. The lack of understanding is a barrier to the full characterization of the physical properties, phase diagram and experimental response features of these materials. In this work, we turn our attention to understanding this heavy fermion quantum criticality[3, 8].

We start from the partition function for $f-$electron hybridizing with metallic $c-$electrons

$$
\mathcal{Z} = \int \mathcal{D}c^\dagger \mathcal{D}c \mathcal{D}f^\dagger \mathcal{D}f \; e^{-\mathcal{S}}
$$

$$
\mathcal{S} = \sum_M \int \frac{d\omega}{(2\pi)} \frac{d^3\vec{k}}{(2\pi)^3} \left[-\omega \left(f^\dagger_M(\omega,\vec{k}) f_M(\omega,\vec{k}) + c^\dagger_M(\omega,\vec{k}) c_M(\omega,\vec{k}) \right) + \frac{(\epsilon_{\vec{k}} - \mu)}{\hbar} c^\dagger_M(\omega,\vec{k}) c_M(\omega,\vec{k}) \right]
$$

$$
+ \sum_M \int \frac{d\omega}{(2\pi)} \frac{d^3\vec{k}}{(2\pi)^3} \frac{E_0 - U}{\hbar} f^\dagger_M(\omega,\vec{k}) f_M(\omega,\vec{k}) - \frac{V}{\hbar} \sum_M \int \frac{d\omega}{(2\pi)} \frac{d^3\vec{k}}{(2\pi)^3} \left(f^\dagger_M(\omega,\vec{k}) c_M(\omega,\vec{k}) + \text{h. c.} \right)
$$

$$
+ \frac{U}{\hbar} \sum_{ML} \int \frac{d\omega d\omega_2 d\omega_3}{(2\pi)^3} \frac{d^3\vec{k} d^3\vec{k}_2 d^3\vec{k}_3}{(2\pi)^9} f^\dagger_M(\omega,\vec{k}) f_M(\omega_2,\vec{k}_2) f^\dagger_L(\omega_3,\vec{k}_3) f_L(\omega - \omega_2 + \omega_3, \vec{k} - \vec{k}_2 + \vec{k}_3) \tag{1}
$$

where the subscripts M, L (and all capital letters subscripts for that matter) indicate the angular momentum degeneracy of the ground state ($j = 5/2$), U is the Hubbard repulsion and V represents the strength of mixing of f-electrons with the conduction band.

If we write $n_i = \sum_M f^\dagger_{iM} f_{iM}$, the Hubbard interaction term then takes the form (in Euclidean time and real space) $\frac{U}{\hbar} \sum_i \int d\tau \left[n_i^2 - n_i \right]$. We can decouple this interaction term by using the Hubbard-Stratonovich identity $e^{-\int d\tau \sum_i \frac{U}{\hbar} n_i^2} = \int \mathcal{D}\varphi e^{-\int d\tau \sum_i \frac{U}{\hbar} \left[\varphi_i^2 + 2i\varphi_i n_i \right]}$ which in Euclidean time and momentum space reads $\int \mathcal{D}\varphi e^{-\int d\tau \frac{d^3\vec{k}}{(2\pi)^3} \frac{U}{\hbar} \left[\varphi_{\vec{k}} \varphi_{-\vec{k}} + 2i n_{\vec{k}} \varphi_{-\vec{k}} \right]}$. Using $n_{\vec{k}} = \int \frac{d^3\vec{k}}{(2\pi)^3} f^\dagger_{\vec{q}} f_{\vec{q}-\vec{k}}$, this decoupling gives[5]

$$
\begin{aligned}
\mathcal{Z} &= \int \mathcal{D}c^\dagger \mathcal{D}c \mathcal{D}f^\dagger \mathcal{D}f \mathcal{D}\varphi \; e^{-\mathcal{S}} \\
\mathcal{S} &= \sum_M \int d\tau \frac{d^3\vec{k}}{(2\pi)^3} \left\{ f^\dagger_{\vec{k}M} \frac{\partial}{\partial\tau} f_{\vec{k}M} + \frac{E_0 - U}{\hbar} f^\dagger_{\vec{k}M} f_{\vec{k}M} \right. \\
&\left. + \frac{U}{N\hbar} \varphi_{\vec{k}} \varphi_{-\vec{k}} + c^\dagger_{\vec{k}M} \frac{\partial}{\partial\tau} c_{\vec{k}M} + \frac{(\epsilon_{\vec{k}} - \mu)}{\hbar} c^\dagger_{\vec{k}M} c_{\vec{k}M} \right\} \\
&- \sum_M \int d\tau \frac{d^3\vec{k}}{(2\pi)^3} \frac{V}{\hbar} \left(f^\dagger_{\vec{k}M} c_{\vec{k}M} + c^\dagger_{\vec{k}M} f_{\vec{k},M} \right) \\
&+ 2i \frac{U}{\hbar} \sum_M \int d\tau \frac{d^3\vec{k} d^3\vec{q}}{(2\pi)^6} \varphi_{-\vec{k}} f^\dagger_{\vec{q},M} f_{\vec{q}-\vec{k},M}
\end{aligned} \tag{2}
$$

In order to have f levels occupied we choose $E_0 < \mu$.

This last action is what quantum field theorists would call the bare action. It embodies the essential physics of the heavy fermion phase and the heavy fermion criticality. Unfortunately, it is very hard to solve the bare action exactly or numerically to high accuracy in order to extract the desired information from it. The famous fermion sign problem thwarts numerics, and exact solutions are normally impossible in many body problems just as this one. Fortunately, there is a way forward that can help extract some, and perhaps a lot of the physics. The renormalization group[9], and in particular effective action techniques[10–12], popular in particle physics, provide room for progress.

One of the lessons of the renormalization group is that as we concentrate on longer wavelength, lower energy degrees of freedom, the short distance and high energy fluctuations do two things. These fluctuations renormalize the strength of the terms in the original action and they generate new terms in the action which in turn change as they get renormalized. The end result is that some terms in the action become larger while others become smaller, thus not contributing to the to the universal low energy physics of the system. We will thus analyze the action for heavy fermion materials above, and obtain the effective action with terms relevant to the low energy physics of the heavy fermion phase and to the critical point where such a transition perishes.

In order to obtain the effective action, rather than obtain the renormalizations all at once, it proves advantageous to integrate out the $f-$electrons and get those terms they contribute to the effective action which are relevant for the low energy universal physics of the critical point and heavy fermion phase. After the calculations are performed, the $f-$electrons disappear from the theory. We have instead the Hubbard-Stratonovih field φ, which has acquired dynamics through the $f-$electron fluctuations. Such fluctuations also generate self-interaction terms for the φ-field, and interaction terms between the φ's and the metallic $c-$electrons.

The effective action for the heavy fermion materials comes out to be

$$Z = \int \mathcal{D}c_0^\dagger \mathcal{D}c_0 \mathcal{D}\tilde{\varphi}_0 \, e^{iS} \ , \ \text{with} \ S = \sum_M \int \frac{d\omega}{2\pi} \frac{d^3\vec{k}}{(2\pi)^3} \Big\{ \Lambda \, g_2 \, \tilde{\varphi}_0(\omega,\vec{k})\tilde{\varphi}_0(-\omega,-\vec{k}) - \omega \, \tilde{\varphi}_0(\omega,\vec{k})\tilde{\varphi}_0(-\omega,-\vec{k})$$
$$+ \left[\omega - (\epsilon_{\vec{k}} - \mu)/\hbar\right] c_{0M}^\dagger(\omega,\vec{k}) c_{0M}(\omega,\vec{k}) - \Lambda^{-1/2} \, g_3 \int \frac{d\nu}{2\pi} \frac{d^3\vec{q}}{(2\pi)^3} \, \tilde{\varphi}_0(\omega,\vec{k}) c_{0M}^\dagger(\nu,\vec{q}) c_{0M}(\omega+\nu,\vec{q}+\vec{k}) \tag{3}$$
$$+\Lambda^{-2} \, g_4 \int \frac{d\omega_2 d\omega_3}{(2\pi)^2} \frac{d^3\vec{k}_2 d^3\vec{k}_3}{(2\pi)^6} \, \tilde{\varphi}_0(\omega,\vec{k})\tilde{\varphi}_0(\omega_2,\vec{k}_2)\tilde{\varphi}_0(\omega_3,\vec{k}_3)\tilde{\varphi}_0(-\omega-\omega_2-\omega_3,-\vec{k}-\vec{k}_2-\vec{k}_3) \Big\}$$

where

$$\tilde{\varphi}_0(\omega,\vec{k}) = \sqrt{\frac{4U^2(|E_0|+U)}{\pi D^3}} \, \varphi_0(\omega,\vec{k})$$
$$g_2 = \frac{D^2}{\hbar\Lambda(|E_0|+U)} - \frac{\pi D^3}{4NU\Lambda\hbar(|E_0|+U)} g_4 = \frac{\pi D^3}{3\hbar\Lambda(|E_0|+U)^2} \ .$$

$$g_3 = \sqrt{\frac{\pi D^3 V^4}{\hbar^2\Lambda^2(E_0-U)^5}} g_4 = \frac{\pi D^3}{3\hbar\Lambda(|E_0|+U)^2} \ .$$

We see that the universal physics of the heavy fermion system is captured by an action of dynamical scalar fiels interacting with the metallic $c-$electrons. We call this action the *heavy-fermion dynamic φ^4 action.* The heavy fermion phase corresponds to g_2 being negative and φ acquiring a nonzero expected value as φ is proportional to the density of $f-$electrons that hybridizes with the metallic ones. The heavy fermion critical point occurs at $g_2 = 0$, when $\langle\varphi\rangle$ first becomes 0.

The heavy-fermion dynamic φ^4 action is a new and important result. It opens the door to accurate numerics for the fermion action, as the interacting fermions that drive the transtion have been replaced by a scalar field. This should eliminate the fermion sign problem that plagues numerics, for all the action is happening in the scalar fields and not the left-over metallic fermions.

One can apply standard order parameter RG to this action. As an example, below we do a one-loop momentum shell renormalization with the help of Callan-Symanzik equations *à la* Weinberg[12–14]to resum and thus catch some of the nonperturbative physics of the transition. This can of course be improved by going to higher orders, and there is also plenty of room to perform ϵ-expansion studies instead of momentum shell.

Since we can use the bare Fermi velocity of the metallic $c-$electrons as a standard of speed in the material, we use it as such to express our frequencies in units of momentum and work in "God-given" heavy fermion units: $v_F = 1$ and $\hbar = 1$, $k_F = m = \Lambda$. After renormalization, the heavy-fermion dynamic φ^4 action becomes

$$Z = \int \mathcal{D}c^\dagger \mathcal{D}c \mathcal{D}\tilde{\varphi} \, e^{iS} \ \text{with} \ S = \sum_M \int \frac{d\omega}{2\pi} \frac{d^3\vec{k}}{(2\pi)^3} \Big\{ \mu g_2^R \, Z_\varphi^2 \, \tilde{\varphi}(\omega,\vec{k})\tilde{\varphi}(-\omega,-\vec{k}) - Z_\varphi^2 \omega \, \tilde{\varphi}(\omega,\vec{k})\tilde{\varphi}(-\omega,-\vec{k})$$
$$+ Z_c^2 \left[\omega - (\epsilon_{\vec{k}} - \mu)\right] c_M^\dagger(\omega,\vec{k}) c_M(\omega,\vec{k}) - \mu^{-1/2} \, g_3^R \int \frac{d\nu}{2\pi} \frac{d^3\vec{q}}{(2\pi)^3} \, Z_\varphi Z_c^2 \, \tilde{\varphi}(\omega,\vec{k}) c_M^\dagger(\nu,\vec{q}) c_M(\omega+\nu,\vec{q}+\vec{k}) \tag{4}$$
$$+\mu^{-2} \, g_4^R \int \frac{d\omega_2 d\omega_3}{(2\pi)^2} \frac{d^3\vec{k}_2 d^3\vec{k}_3}{(2\pi)^6} Z_\varphi^4 \, \tilde{\varphi}(\omega,\vec{k})\tilde{\varphi}(\omega_2,\vec{k}_2)\tilde{\varphi}(\omega_3,\vec{k}_3)\tilde{\varphi}(-\omega-\omega_2-\omega_3,-\vec{k}-\vec{k}_2-\vec{k}_3) \Big\} \ .$$

We now move to consider the specific momentum shell renormalizations to determine the renormalization factors. The inverse φ propagator, $\omega - \Lambda g_2$ goes into $-\mu g_2^R \, Z_\varphi^2 + Z_\varphi^2 \omega + Z_k k_r = -\Lambda g_2 + \omega + \Sigma_\varphi$, where

$$\Sigma_\varphi = \frac{g_3^2 \Lambda}{8\pi^4} \left(1 - \mu/\Lambda\right) \left[1 - \frac{(\omega - k_r)}{4\Lambda}\right] + \frac{g_4}{2\pi} \frac{\Lambda}{} \frac{(1-\mu/\Lambda)}{(g_2 - 1)}$$

Next we tackle the renormalization of the $c-$ electron inverse propagator $\omega - (\epsilon_{\vec{k}} - \mu)$ which becomes

$Z_c^2\left[\omega-(\epsilon_{\vec{k}}-\mu)\right]=\omega-(\epsilon_{\vec{k}}-\mu)+\Sigma_c(\omega,\vec{k})$, with

$$\Sigma_c(\omega,\vec{k})=-\frac{g_3^2\,\Lambda}{(2\pi)^4}\,(1-\mu/\Lambda)\left\{\left[\frac{1}{(g_2-1)}\right]\ln\left|\frac{g_2+1}{g_2-1}\right|\right.$$
$$-\frac{4g_2}{\Lambda\,(g_2^2-1)^2}(\omega-k_r)\ln\left|\frac{\omega-k_r}{2\Lambda}\right|$$
$$\left.+\,(\omega-k_r)\left[\frac{2g_2}{\Lambda(g_2^2-1)}-\frac{1}{\Lambda(g_2-1)^2}\ln\left|\frac{g_2+1}{g_2-1}\right|\right]\right\}$$

Notice that the $c-$electron propagator does not renormalize as expected. The reason is that if g_2 is nonzero, we need to include the nonzero expected value of φ and expand around it in the heavy fermion phase in order to get the physics right. We are not interested in the heavy phase but in the critical point, where such a phase disappears. At the critical point, $g_2=0$ and things work out as expected.

We now turn our attention to vertex renormalizations, starting with the $\varphi-c$ vertex, $\Lambda^{1/2}\,g_3$. It renormalizes into $-\mu^{-1/2}\,g_3^R\,Z_\varphi Z_c^2=-\Lambda^{-1/2}\,(g_3+\Gamma_c)$, where

$$\Gamma_c=\frac{g_3^2}{(2\pi)^4}(1-\mu/\Lambda)\left\{\frac{4g_2}{(g_2^4-1)}-\frac{2\pi g_2}{(g_2^2-1)^2}\right.$$
$$\left.+\,\frac{4(g_2^2+1)}{(g_2^2-1)^2}\arctan\left(\frac{1}{g_2}\right)\right\}$$

And finally to the renormalization of the φ^4 interaction, $\mu^{-2}\,g_4^R\,Z_\varphi^4=\Lambda^{-2}g_4+\Gamma_\varphi$, with

$$\Gamma_\varphi=-\frac{g_3^4}{24\pi^4\Lambda^2}\,(1-\mu/\Lambda)+\ldots$$

$$\ldots\frac{g_4^2}{(2\pi)^4\Lambda^2}(1-\mu/\Lambda)\left\{\left[\frac{1}{g_2+1}\right]^2+\left[\frac{1}{g_2-1}\right]^2\right\}$$

The heavy fermion criticality occurs when $g_2=0$. In the $g_2=0$ critical manifold

$$Z_c=1\,,\quad Z_\varphi\simeq 1-\frac{g_3^2}{64\pi^4}\,(1-\mu/\Lambda)\,,\quad Z_k=\frac{g_3^2}{32\pi^4}$$
$$\frac{g_3^R}{\mu^{1/2}}\simeq\frac{g_3}{\Lambda^{1/2}}\left\{1+\frac{g_3}{(2\pi)^3}\left[\frac{g_3}{8\pi}-1\right](1-\mu/\Lambda)\right\}$$
$$\frac{g_4^R}{\mu^2}\simeq\frac{g_4}{\Lambda^2}+\left[\frac{2g_4^2}{(2\pi)^4\Lambda^2}-\frac{g_3^4m^2}{24\pi^4\Lambda^4}-\frac{g_3^2g_4}{(2\pi)^4\Lambda^2}\right](1-\mu/\Lambda)\,.$$

To this order of approximation

$$\beta_3=\mu\frac{\partial g_3^R}{\partial\mu}\Big|_{\mu=\Lambda}=\frac{1}{2}g_3-\frac{g_3^2}{(2\pi)^3}\left[\frac{g_3}{8\pi}-1\right]$$
$$g_3^c=4\pi\left[1+\sqrt{1+2\pi^2}\right]$$
$$\beta_4=\mu\frac{\partial g_4^R}{\partial\mu}\Big|_{\mu=\Lambda}=2g_4-\frac{6g_4^2}{(2\pi)^4}+\frac{g_3^4}{8\pi^4}+\frac{3g_3^2g_4}{(2\pi)^4}$$
$$g_4^c=\frac{g_3^{c2}}{4}+\frac{(2\pi)^4}{6}+\sqrt{\frac{19g_3^{c4}}{48}+\frac{(2\pi)^8}{36}+\frac{(2\pi)^4}{12}g_3^{c2}}$$

The φ anomalous dimension at cricitcality is

$$\gamma_\varphi=\mu\frac{\partial\ln Z_\varphi}{\partial\mu}\Big|_{\mu=\Lambda}=\frac{g_3^2}{64\pi^4}=\frac{1}{2\pi^2}\left[1+\pi^2+\sqrt{1+2\pi^2}\right]\,.$$

In the heavy fermion phase, the f-electrons contribute to the susceptibility and specific heat since they are mixed with the metallic band electrons, forming in conjunction one "Fermi liquid". The susceptibility of conduction electrons is negligible since they are nonmagnetic. The susceptibility is proportional to the number of f-electrons being "pulled" by an applied field, and hence to their density of states, which is given by the imaginary part of the $f-$electron propagator[2]. Such a propagator is proportional to $\langle\varphi\rangle$, which satisfies a Callan-Symanzik equation[12, 13]

$$0=\left[\mu\frac{\partial}{\partial\mu}+\frac{\gamma_\varphi}{2}\right]G^{(1)}\Big|_{\mu=\omega}$$
$$G^{(1)}(\omega)=\left(\frac{1}{\omega}\right)^{\gamma_\varphi/2}\sim\left(\frac{1}{\omega}\right)^{[1+\pi^2+\sqrt{1+2\pi^2}]/(4\pi^2)}$$
$$F(\omega,\vec{k}=0)\sim i\langle\varphi(\omega,\vec{k}=0)\rangle=iG^{(1)}(\omega)$$

$$\chi(\omega)=\lim_{\epsilon\rightarrow 0}Im\left[F(\omega+i\epsilon)\right]\sim\left(\frac{1}{\omega}\right)^{\gamma_\varphi/2}\,. \qquad (5)$$

The specific heat coefficient is also proportional to the density of states, which is inversely proportional to the Fermi energy[2]. The f-electrons, being quasi-localized, form a quite thin band and hence have a small E_F. Thus their density of states is so big in comparison with that of the conduction electrons, that the density of states of the "mixed Fermi liquid" can be approximated to be that of the f-electrons. We obtain

$$C_T\sim T\lim_{\epsilon\rightarrow 0}Im\left[F(\omega+i\epsilon)\right]\Big|_{\omega\sim T}\sim T\left(\frac{1}{T}\right)^{\gamma_\varphi/2} \qquad (6)$$

We obtain a specific heat coefficient exponent $\gamma_\varphi/2=0.39$. This is in excellent agreement with the exponent 0.4 found for $YbRh_2Si_2$ at low temperatures[3].

Via renormalization group studies and effective action techniques common to field theories of particle physics, we have obtained the effective field theory for heavy fermion quantum criticality. This marks important progress as the effective field theory is bosonic, vitiating the fermion sign problem and thus being amenable to numerical studies and high order ϵ expansion studies.

The critical field theory can be studied using the renormalization group. We did so via one-loop renormalization studies, improved by means of Callan-Symanzik resumations to access some of the nonpertrubative effects. We thus approximated the exponents that characterize the critical divergence of the specific heat coefficient and the critical charge susceptibility. Our specific heat coefficient exponent of 0.39 is in excellent agreement with the 0.4 found in experiments at low temperatures[3].

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