Quantum criticality and the break-up of the Kondo pseudo-potential

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Abstract

We discuss how Anderson’s ideas of nominal and real valence can be incorporated into the current discussion of heavy electron quantum criticality. In the heavy electron phase, the nominal valence of a screened magnetic ion differs from its real valence by one unit. We identify this discrepancy with the formation of a positively charged background we call the Kondo pseudo-potential. At the quantum critical point, the sudden collapse of the heavy electron Fermi surface can be identified with the return of the nominal to the real valence. This leads to the interesting idea that the heavy electron quantum critical point may involve locally critical charge degrees of freedom. We discuss how this might come about within a large \(N\) Schwinger boson scheme.

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1. Introduction

Over the course of the development of ideas in heavy fermion physics, stretching back to the early seventies, there have been several shifts in opinion about the relative importance of charge and spin degrees of freedom in heavy electron systems. The early view was that heavy electron behavior is driven by slow valence fluctuations\textsuperscript{[1]}.

In the eighties, the discovery that most heavy electron systems lie close to integral valence, led to the community to abandon the idea mixed valence in favor of Doniach’s Kondo lattice concept \textsuperscript{[2]} in which heavy electrons form via the Kondo effect between neutral, localized moments and the surrounding conduction electrons. Yet even in this context, charge plays an important role, for the Kondo effect produces resonant scattering that enlarges the Fermi surface. Paradoxically, even though the density of quasi-particles increases, the average electronic charge density is unchanged by the Kondo effect. This paradox has assumed a new level of importance with the discovery of quantum criticality in heavy electron systems. The observation of a jump in the Hall constant \textsuperscript{[3]} and the heavy electron Fermi surface \textsuperscript{[4]} at heavy electron quantum critical points have led many \textsuperscript{[5,6,7,8,9]} to suggest that charge degrees of freedom may play an important role in heavy electron quantum criticality.

In the early eighties, Anderson introduced the idea of “nominal valence” to account for the discrepancy between the actual measured valence of a heavy electron ion, and the “nominal valence” required to account for its large Fermi surface and transport properties\textsuperscript{[10]}. For example, in Cerium heavy electron metals, such as \(CeCu_6\), the \(Ce\) ions have a real valence of three, with a localized \(4f^1\) local moment within a truly trivalent \(Ce^{3+}\) ion. However, when the Kondo effect takes place at low temperatures, each local moment liberates a mobile charged heavy fermion and the Fermi surface expands accordingly. In Anderson’s picture, \(Ce\) ions in heavy electron systems have a nominal valence.

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of four, and behave as spinless $Ce^{4+}$ ions, each donating a resonant f-electron to the Fermi sea (see Fig. 1.):

$$Ce^{3+} \rightarrow \text{Heavy } e^- + Ce^{4+}.$$  \hspace{1cm} (1)

This many-body process resembles the dissolution of a neutral atom in a polar fluid.

Fisk and Aeppli have emphasized the usefulness of Anderson’s idea for understanding the physics of Kondo insulators[11], where the “expansion” of the Fermi surface produces a completely filled band, leading to a renormalized band insulator. For example, the Kondo insulator $Ce_3Bi_4Pt_3$, containing $Ce^{3+}$ ions is iso-electronic with the band insulator $Th_3Sb_4Ni_3$, containing $Th^{4+}$ ions. The discovery of Kondo insulators and the observation of large Fermi surfaces in heavy electron systems are testament to the usefulness reality of Anderson's concept of nominal and real valence.

2. The Kondo pseudo-potential

Embodied in these early ideas, is a notion of elementary charge conservation. In this paper we examine the consequences of properly accounting for charge conservation in the Kondo effect. We argue that if a neutral spin liberates a mobile, negatively charged heavy electron, then it must leave behind a positively charged background. We call this background the “Kondo pseudo-potential”.

The key idea behind this charge book-keeping is embodied in the “Anderson Clogston” compensation theorem[12], which states that the average charge density is unchanged by the introduction of a magnetic ion into the Fermi sea. In the lattice, this leads to the following relationship between the large Fermi surface volume and the conduction electron charge density

$$n_e = \frac{2}{(2\pi)^3} \left[ \frac{V_F}{a^3} - Q \right].$$  \hspace{1cm} (2)

This kind of book-keeping emerges naturally in both the slave boson and more recent Schwinger boson descriptions of the Kondo lattice.

However, the importance of the Kondo pseudo-potential extends beyond simple book-keeping: as a real phenomenon, it has tangible, measurable consequences. At the level of a mean-field pseudo-potential, it governs the symmetries of the heavy electron Fermi surface - symmetries that are visible not just in the de Haas van Alphen measurements but are expected to manifest themselves as spatial redistributions in the local density of states, visible to STM measurements. Moreover, the Kondo pseudo-potential has specific translational, orbital and gauge symmetries, all of which can, in principle develop spontaneous broken symmetries, leading to new phases of heavy electron materials with long-range order:

- Broken translation symmetry $\rightarrow$ HF density wave
- Broken lattice symmetry $\rightarrow$ orbital order
- Broken gauge symmetry $\rightarrow$ HF superconductivity.

These are all consequences of a rigid, or classical pseudo-potential, as obtained, for example in a slave boson mean field theory, or a Korringa Kohn Rostoker (KKR) pseudo-potential approach to the Kondo lattice[13].

However, the principle focus of this paper is the idea that Kondo pseudo-potential is not just a rigid classical background, but a quantum object with its own set of excitations. This basic idea forms a common thread behind many current efforts to understand heavy electron quantum criticality. These excitations might be just bosonic fluctuations of the background pseudo-potential, as described by the Gaussian fluctuations about a slave boson mean field theory [7,9]. However, our recent calculations based on a Schwinger boson approach to the Kondo lattice[5,14] have raised the interesting possibility that the excitations of the Kondo pseudo-potential might be gapped excitations that carry either spin or charge. Closure of the gap at a quantum critical point leads to a deconfinement of these excitations and the break-down of the Kondo pseudo-potential.

3. Theoretical realization of the Kondo pseudo-potential

3.1. Slave Boson Approaches

Mean field approaches to the Kondo lattice[15,16,17,18] based on the slave boson formalism provide an elegant demonstration of the idea of the Kondo pseudo-potential, with its positively charged background. The mean field Hamiltonian is

$$\mathcal{H}_{MF} = \mathcal{H}_c + \sum_j \mathcal{H}_j(V, \lambda).$$  \hspace{1cm} (3)

where $\mathcal{H}_c$ describes the conduction electrons, and

$$\mathcal{H}_j = \frac{V}{\lambda} \sum_{\alpha} (c_{j\alpha}^\dagger f_{j\alpha} + \text{H.c.}) + \lambda(n_{fj} - Q)$$  \hspace{1cm} (4)

describes the resonant f-level within the Kondo pseudo-potential, where $c_{j\alpha}^\dagger$ and $f_{j\alpha}^\dagger$ create the conduction and composite f-electrons, while $V$ and $\lambda$ are the self-consistently determined hybridization and f-level position. In the language of field theory, the local $U(1)$ gauge invariance associated with the neutral Abrikosov fermions is broken by the development of the hybridization $V$. The associated Higgs effect “pins” the internal gauge field $\lambda$ to the external electrostatic potential, so that the f-electrons acquire a physical charge and the constraint term $Q$ becomes a positive background charge.

To see this in detail, consider the introduction of an external electric potential field $\Phi(\vec{x}, t)$ coupled to the conduction electrons. The electromagnetic gauge invariance is given by
\[ c_{j\alpha} \rightarrow e^{-i\phi_j(t)}c_{j\alpha}, \quad e\Phi_j(t) \rightarrow e\Phi_j(t) - \alpha_j(t) \]

\[ f_{j\alpha} \rightarrow e^{-i\phi_j(t)}f_{j\alpha}, \quad \lambda_j(t) \rightarrow \lambda_j(t) + \alpha_j \]

Notice that the f-electron transforms in the same way as the conduction electron, implicating its acquisition of charge. The \( \lambda \) field transforms in the same way as the external potential, implicating its new role as a physical electrostatic potential.

If we expand the action around its mean-field saddle point in the presence of a small external potential, it takes the form

\[
S = S_0 - \sum_j \eta \int dt \frac{(\delta \lambda_j(t) + e\Phi_j(t))^2}{2T_K}
\]

where \( \eta \) is a constant of order unity and \( T_K \) is the Kondo temperature. The particular combination of \( \delta \lambda_j \) and \( e\Phi_j \) is determined by the electromagnetic gauge invariance. From the saddle point condition \( \delta S/\delta \lambda_j(t) = 0 \Rightarrow (\delta \lambda_j - e\Phi_j) = 0 \), we see that in a small electrostatic field, the f-level position picks up a small time dependent component \( \delta \lambda_j(t) = -e\Phi_j(t) \). If we now look back at the original Kondo pseudo-potential, we must replace \( \lambda \rightarrow \lambda - e\Phi_j(t) \), so that it becomes

\[
\mathcal{H}_f = V \sum_{\alpha} (c_{j\alpha} f_{j\alpha} + \text{H.c.}) + (\lambda - e\Phi_j(t))(n_{fj} - Q)
\]

From this we not only see that the f-electrons have acquired a negative charge, but that the external potential has a source term of the form \( +e\Phi_j Q \), describing a positively charged background \( +Q \) in the pseudo-potential.

### 3.2. Schwinger boson approach

The Schwinger boson approach to the Kondo lattice provides a dynamical description of the Kondo pseudo-potential, which is given by

\[
H_f(j) = \sum_{\sigma \in [1,N], \nu \in [1,2S]} \left[ \bar{c}_{j\sigma\nu} (\chi_{j\nu}^\dagger b_{j\sigma}) + \text{H.c.} \right] + \frac{\chi_{j\nu}^\dagger \chi_{j\nu}}{J}
\]

where \( b_{j\sigma} \) is the “spinon” field used in the Schwinger boson description of the Kondo spin \( S_{\alpha\beta}(j) = b_{j\alpha}^\dagger b_{j\beta} \) and \( \chi_{j\nu} \) is a charged “holon” field that mediates the Kondo interaction and carries the channel index \( \nu \in [1,2S] \). The number of channels is kept precisely equal to \( 2S \), so that the spin \( S \) is perfectly screened[5,14,19]. In the limit that \( N \rightarrow \infty \) keeping \( 2S/N \) fixed, the Kondo impurity and Kondo lattice models can be solved exactly.

The Schwinger boson approach offers two advantages over its slave boson partner - for the single impurity case, the large \( N \) limit provides a smooth description of the crossover from local moment to local Fermi liquid physics, avoiding the false phase transition of the slave boson approach. More importantly however, this approach allows the inclusion of magnetism, and can be directly connected with the Arovas Auerbach[20] approach to quantum magnetism.

One of the fascinating aspects of the large \( N \) solution, is that the holon and “spinon” develop a gap in their excitation spectrum, which guarantees that the low energy excitations of system are exclusively electron quasiparticles. The positively charged holons form a filled band, providing the background charge. As the conduction electrons propagate through the Kondo pseudo-potential, they generate virtual spinon-holon pair excitations which renormalize their mass and change the Fermi surface volume (Fig. 2a). While, in the slave boson scheme, the Kondo pseudo-potential is described by the resonant scattering potential, \( \Sigma(\omega) = V^2/(\omega - \lambda) \), in the Schwinger boson scheme, this is replaced by a dynamical self energy of the form

\[
\Sigma_{sc}(\vec{r}, \tau) = G_\chi^0(-\vec{r}, -\tau)G_b(\vec{r}, \tau)
\]

Using diagrammatic means, expanding the Free energy in powers of \( 1/N \), it is now possible to extend Luttinger’s original derivation of the Fermi surface sum rule to the Schwinger boson description of the Kondo lattice[21]:

\[
\frac{n_F}{2S} = N \frac{V_{FS}}{(2\pi)^3} - \frac{V_b}{2\pi^3}
\]

where \( \frac{V_b}{2\pi^3} = 1 \), for the filled holon band, producing the background charge.

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**Fig. 2.** (a) Virtual excitation of gapped spinon/holon pair renormalizes the heavy electron mass (b) Fermi liquid parameters are generated by the exchange of gapped spinons and holons.
tion between the local susceptibility $\chi$ and the spin-spectral weight
$$\frac{\chi''(\omega)}{\omega}_{\omega=0} = \frac{\pi}{2NS}\chi^2. \quad (11)$$

These ideas are of particular interest in the context of heavy quantum criticality. In the Schwinger boson picture, magnetism is signalled by the condensation of the Schwinger bosons and provided the phase transition is second order, gauge invariance guarantees that the spinon and the holon gaps must close together. It is this process that gives rise to the break-up of the Kondo pseudo-potential and the development of non Fermi liquid behavior in the Schwinger boson scheme.

4. Deconfinement and the breakup of the Kondo Pseudo-potential

Anderson’s ideas of nominal and real valence, and the idea of the Kondo pseudo-potential acquire an interesting significance in the context of heavy electron criticality. If the heavy fermi surfaces does indeed collapse at a QCP, then it follows that the Kondo pseudo-potential must break-up at this point, and the nominal valence of each Kondo ion must revert to its real value. This is true in both the Schwinger boson and the slave boson description.

In the Schwinger boson approach however, heavy electron quantum criticality is the point where the both the spinon and the holon degrees of freedom become gapless and deconfine. We envision the following scenario: as the strength of the Kondo coupling is reduced, the spinon-holon gap shrinks to zero and the filled holon band rises to zero energy. At the quantum critical point the holons annihilate with part of the heavy electron sea to produce a spin, causing the nominal valence to revert to the real valence.

One of the simplest types of solution to seek in the large $N$ limit involves the idea of local holon quantum criticality. This provides an unexpected explanation of the local critical character of the spin fluctuations at a heavy electron quantum critical point[22,23]. In the large $N$ limit, the holon self energy is governed by a product of the conduction electron and spinon propagators
$$\Sigma^\chi(x, \tau) = G^{(0)}_c(-x,-\tau)G^\delta_b(x, \tau)$$
where $G^\delta_b(x, \tau)$ is the bare conduction propagator and $G^\delta_b(x, \tau)$ the spinon-propagator. The leading long-time singularity of $G^{(0)}_c$ is local
$$G^{(0)}_c(x, \tau) \sim \frac{1}{\tau^\alpha}\delta(x) \quad (12)$$
and this means that even though the condensing spinons have a highly non-local propagator, the leading singular behavior of the holon self energy and propagator $G^\chi$ will also be local. This suggests that that at criticality, the break-up of the Kondo pseudo-potential will lead the holon propagator to develop local criticality

$$G^\chi(x, \tau) \sim \frac{1}{\tau^\alpha}\delta(x) \quad (13)$$
The spinnor self energy is given by a similar convolution of the holon with the conduction electron,
$$\Sigma^\delta_b(x, \tau) = \frac{2S}{N}G^{(0)}_c(x, \tau)G^\chi(x, \tau)$$
and the singular part of this self-energy will also be local
$$\Sigma^\delta_b(x, \tau) \sim \delta(x) \frac{1}{\tau^\alpha}. \quad (14)$$
Thus although the spinons are not local in character, their singular critical behavior will be independent of momentum - a key element of the observed local criticality.

At this stage, it remains to be seen whether practical solution of the large $N$ equations can in practice furnish this class of solutions, but the above arguments serve to illustrate how the break-up of the Kondo pseudo-potential and the reversion of the nominal valence real valence has the potential to drive locally quantum criticality. The further investigation of these ideas is an ongoing element of our current research.

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