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Singular Fermi liquid behavior in the underscreened Kondo model

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Using the Schwinger boson spin representation, we reveal a new aspect to the physics of a partially screened magnetic moment in a metal, as described by the spin-S Kondo model. We show that the residual ferromagnetic interaction between a partially screened spin and the electron sea destabilizes the Landau Fermi liquid, forming a singular Fermi liquid with a $1/[T \ln^4(T_K/T)]$ divergence in the low-temperature specific heat coefficient C_V/T. A magnetic field B tunes this system back into Landau Fermi liquid with a Fermi temperature proportional to $B \ln^2(T_K/B)$. We discuss a possible link with field-tuned quantum criticality in heavy-electron materials.

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Heavy-electron materials are the focus of renewed attention because of the opportunity[1–4] they present to understand the physics of matter near a quantum critical point. One of the unexplained properties of these materials is that the characteristic temperature scale of heavy-electron Fermi liquid is driven to zero at quantum critical point.[5–9] When either the paramagnet or antiferromagnetic heavy-electron phase is warmed above this temperature scale, it enters a "non-Fermi-liquid" phase. These results suggest that insight into the non-Fermi-liquid behavior of heavy-electron systems might be obtained by studying the breakup of the antiferromagnetic state.

Traditionally, ordered moment antiferromagnetism is described using a bosonic representation of the ordered moments. In this paper we examine the underscreened Kondo impurity model (UKM) and we demonstrate that the essential physics of the underscreened Kondo effect is captured by a Schwinger boson representation of the local moments. In the course of our study we obtained an unexpected new insight. The UKM describes the screening of a local moment from spin S to spin $S^* = S - \frac{1}{2}$.[12] At low temperatures, this residual moment ultimately decouples from the surrounding Fermi sea. The UKM has been studied using the strong-coupling expansion,[13] numerical renormalization group,[14] and diagonalized using the Bethe ansatz,[15,16] but the possibility of a breakdown of Landau Fermi liquid behavior was not addressed. In this paper, we show that a field-polarized underscreened moment forms a Fermi liquid with a the Fermi temperature that is proportional to the magnetic field, going to zero when the field is removed. At zero field, the residual coupling of the electron fluid to the degenerate states of the underscreened moment violates the strict phase space restrictions required for formation of a Landau Fermi liquid, leading to a strongly divergent specific heat coefficient (Fig. 1):

$$\frac{C_V}{T} \sim \frac{1}{T \ln^4(T_K/T)}. \tag{1}$$

The UKM is model is written

$$H = \sum_{k\alpha} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \vec{S} \cdot \psi^\dagger_\alpha \vec{\sigma}_{\alpha\beta} \psi_\beta, \tag{2}$$

where S denotes a spin $S > \frac{1}{2}$, $c^\dagger_{k\alpha}$ creates a conduction electron with wave vector k, spin component α, and $\psi^\dagger_\alpha = \Sigma_k c^\dagger_{k\alpha}$ creates a conduction electron at the impurity site.

We begin by reformulating the UKM as an SU(N)-invariant Coqblin-Schrieffer model, which enables us to carry out a large-N expansion of the physics. We write

$$H = \sum_{k\alpha} \epsilon_k c^\dagger_{k\alpha} c_{k\alpha} + \frac{J}{N} \sum_{\alpha\beta} (\psi^\dagger_\beta b_\beta)(b^\dagger_\alpha \psi_\alpha) - MB, \tag{3}$$

where the spin indices run over N independent values $\alpha, \beta \in (1,N)$ and the constraint $n_b = 2S$ is imposed to represent spin S. Here $M = g_N[b^\dagger_\uparrow b_\uparrow - \tilde{S}]$ is the local moment magnetization, where we denote the first spin component by $\sigma = 1 \equiv \uparrow$, and $\tilde{S} = 2S/N$. The prefactor $g_N = N/2(N-1)$ is chosen so that at maximum polarization, when $n_\uparrow = 2S$, $M = S$. A multichannel formulation of the above model has previously been treated within an integral equation formalism.[17]

Next, we cast the partition function as a path integral and factorize the interaction

$$H_I \to [\bar{\phi} b^\dagger_\sigma \psi_\sigma + \psi^\dagger_\sigma b_\sigma \phi] - \frac{N}{J} \bar{\phi} \phi. \tag{4}$$

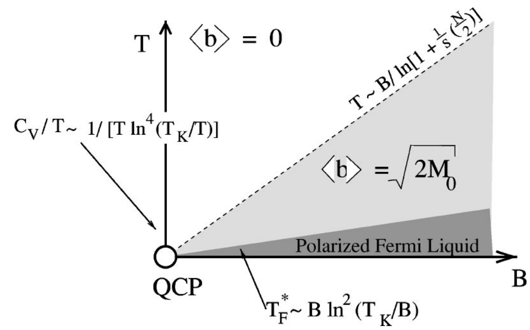

FIG. 1. Schematic phase diagram of the large-N limit of the underscreened Kondo model.

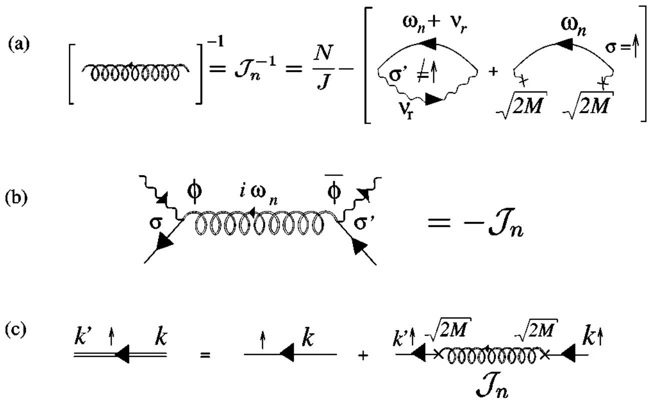

FIG. 2. Feynman diagrams for the large-N limit. (a) Feynman diagrams for the ϕ propagator, where solid and wavy lines represent conduction electron and Schwinger boson propagators, respectively. The bubble diagram involves a sum over all $\sigma' \neq \uparrow$ and the crosses in the second diagram denote the Schwinger boson condensate $\langle b_\uparrow \rangle = \sqrt{2M}$. (b) Effective Kondo interaction is mediated by the ϕ propagator $\mathcal{J}_n$. (c) In the polarized phase, the t matrix of the $\uparrow$ electrons is determined by the ϕ propagator.

We shall show how the physics of the underscreened Kondo model is obtained by examining the Gaussian fluctuations of the field ϕ about the mean-field theory obtained by taking $N\to\infty$ at fixed $\tilde{S}$. This mean-field theory describes a free moment, with free energy

$$F_{LM}=\sum_{\sigma=1}^{N} T\ln[1-e^{-\beta(\lambda-\delta_{\sigma\uparrow}\overline{B})}]-2\left(\lambda-\frac{\tilde{B}}{N}\right)S. \qquad (5)$$

where $\tilde{B}=g_N B$. The mean-field constraint $\langle n_b\rangle=2S$ becomes

$$\langle n_b\rangle = n[\lambda-\tilde{B}]+(N-1)n[\lambda]=2S, \qquad (6)$$

where $n[x]=[e^{\beta x}-1]^{-1}$ is the Bose-Einstein distribution function. There are then two types of mean-field solution: (i) "paramagnet" where $\langle b_1\rangle=0$ and $n(\lambda)=\tilde{S}$ and (ii) "polarized" moment where $\langle b_1\rangle=\sqrt{2M}$ condenses to produce magnetization M. The second phase develops at temperatures below $T=T_c=B/\zeta$, $\zeta=\ln[1+1/\tilde{S}]$ (Fig. 1). The mean-field value of λ in these two phases is given by $\lambda=\lambda_0=\max(T\zeta,\tilde{B})$.

To examine the fluctuations around the mean-field theory, we integrate out the electrons and bosons, and write the effective action so obtained in terms of the Fourier coefficients $\phi_n=\beta^{-1/2}\int_0^\beta d\tau\,\phi(\tau)e^{i\omega_n\tau}$. To quadratic order, the effective action is given by

$$S[\overline{\phi},\phi]=-\sum_{\omega_n}\overline{\phi}_n\mathcal{J}_n^{-1}\phi_n. \qquad (7)$$

The propagator $\mathcal{J}_n$ for the ϕ field is determined by the Feynman diagrams shown in Fig. 2(a). When we compute these Feynman diagrams, we find that $\mathcal{J}_n=N^{-1}\mathcal{J}(i\omega_n+\lambda_0)$, where

$$\rho\mathcal{J}(z)=\left[\psi\left(\frac{1}{2}+\frac{z}{2\pi iT}\right)-\ln\frac{T_K}{2\pi iT}+i\pi\tilde{S}\right]^{-1}. \qquad (8)$$

Here $T_K=De^{-1/\rho J}$ is the Kondo temperature, expressed in terms of the bandwidth D and density of states ρ. This propagator mediates the interaction between the spin bosons and electrons [Fig. 2(b)] and describes the frequency-dependent Kondo coupling constant. The asymptotic behavior of this function,

$$\rho\mathcal{J}(\omega,T)\sim\frac{1}{\ln\left(\frac{\max(\omega,2\pi T)}{T_K}\right)},$$

describes a coupling constant which is small and antiferromagnetic (positive) at high energies, while small and ferromagnetic (negative) at low energies. The crossover from antiferromagnetic behavior at high energies to ferromagnetic behavior at low energies is a well-known feature of this model.[2,13–16]

By carrying out the Gaussian integral over the fluctuations of the ϕ field, we are able to compute the correction to the free energy F_{LM} due to the Kondo effect,

$$F_i=F_{LM}(T,B)+\int\frac{d\omega}{\pi}f(\omega)\alpha[\omega+\max(T\zeta,\tilde{B})], \qquad (9)$$

where the phase shift $\alpha(\omega)=\mathrm{Im}\ln[\mathcal{J}^{-1}(\omega+i\delta)]$. In zero field $F_{LM}=-TS_0$, where

$$S_0[\tilde{S}]=N[(1+\tilde{S})\ln(1+\tilde{S})-\tilde{S}\ln\tilde{S}]-\frac{1}{2}\ln[2\pi N\tilde{S}(1+\tilde{S})]$$
$$+O(1/N) \qquad (10)$$

is the entropy of a free SU(N) spin. In the polarized phase,

$$F_{LM}=(N-1)T\ln(1-e^{-\beta\tilde{B}})-SB. \qquad (11)$$

We now use these results to characterize the nature of the excitation spectrum.

At zero field, the second term in Eq. (9) can be expanded at low temperatures as a power series in the small parameter $g=\rho\mathcal{J}=1/\ln(2\pi T/T_K)$. We find that the leading order contribution to the entropy is given by

$$\begin{aligned}S_{T=0}&=S_0[\tilde{S}]-\zeta-2\pi^2\tilde{S}(\tilde{S}+1)g(T)^3+O(g^4)\\&=S_0\left[\tilde{S}-\frac{1}{N}\right]+\frac{2\pi^2\tilde{S}(\tilde{S}+1)}{\ln^3\left(\frac{T_K}{2\pi T}\right)}+O(g^4).\end{aligned} \qquad (12)$$

From this result, we see that the entropy at low temperatures is that of a spin $S^*=(N/2)(\tilde{S}-1/N)=S-\frac{1}{2}$, quenched by one half unit. The g^3 term is the leading perturbative correction to the entropy of a Kondo problem, but with the bare antiferromagnetic coupling constant ρJ replaced by the running (ferromagnetic) coupling constant $\rho\mathcal{J}$. We alse see that the logarithm in $\rho\mathcal{J}$ also generates a divergent low-temperature specific heat coefficient (Fig. 3)

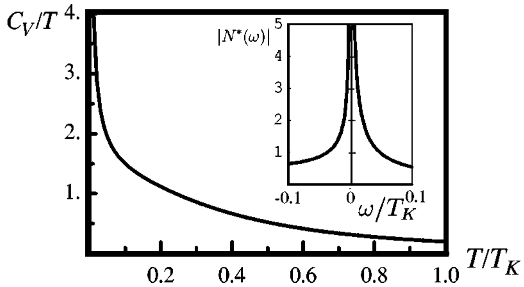

FIG. 3. Zero-field specific heat capacity of the underscreened Kondo model for the case $\tilde{S}=1/2$, showing the $1/T\ \ln^4(T_K/T)$ divergence at low temperatures. Inset: the singular density of states $N^*(\omega)$.

$$\frac{C_V}{T}=\frac{\partial S}{\partial T}=6\pi^2\frac{\tilde{S}(\tilde{S}+1)}{T\ln^4\dfrac{T_K}{2\pi T}}. \tag{13}$$

This observation of a singular specific heat coefficient is new, and it indicates that the fluid of excitations in zero field has a singular density of states: it cannot be a Landau Fermi liquid. These singularities are not a consequence of the large-N limit, but are a generic consequence of the singular energy and temperature dependence of the coupling constant.

Let us now examine the effects of a magnetic field. When we differentiate the free energy (9) to obtain the magnetization, the combination of frequency and magnetic field in the phase shift $\alpha(\omega+g_NB)$ enables us to replace the field derivative with a frequency derivative inside the integral, so that, at $T=0$,

$$\begin{aligned}M&=-\frac{\partial F}{\partial B}=S-\frac{g_N}{\pi}\alpha(\tilde{B})\\&=S-\frac{1}{2\pi}\left[\frac{\pi}{2}-\tan^{-1}\left(\frac{\ln[B/2T_K]}{\pi\tilde{S}}\right)\right],\end{aligned} \tag{14}$$

where we have replaced $g_N\rightarrow\frac{1}{2}$ in the large-N limit. $M(B)$ evolves from S at high fields to $S-\frac{1}{2}$ at low fields (Fig. 4), with a weak ferromagnetic correction $\Delta M\sim\tilde{S}/\ln(T_K/B)$ at low fields.

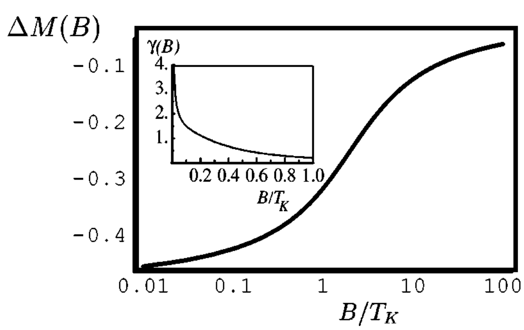

FIG. 4. Ground-state magnetization $\Delta M=S-M$ of the underscreened Kondo model for the case $\tilde{S}=0.5$. Inset: the field-dependent linear specific heat capacity $\gamma(B)$.

Once the local moment becomes polarized, the specific heat becomes linear at low temperatures, and a Landau Fermi liquid is formed. In a field at absolute zero, the Bose field is condensed with $\langle b_\uparrow\rangle=\sqrt{2S}$ so that now

$$H_I\rightarrow\sum_{\sigma\neq\uparrow}[\bar{\phi}b_\sigma^\dagger\psi_\sigma+\text{H.c.}]+\sqrt{2S}(\bar{\phi}\psi_\uparrow+\text{H.c.})-\frac{N}{J}\bar{\phi}\phi,$$

thereby giving rise to a *resonant elastic coupling* between the ϕ field and the conduction electrons, so that the t matrix $t_\uparrow(\omega)$ for the "up" electrons is now [Fig. 2(c)]

$$t_\uparrow(\omega)=\frac{2S}{N}\mathcal{J}(\omega+\tilde{B}). \tag{15}$$

Now since $\mathcal{J}=|\mathcal{J}|e^{-i\alpha(\omega)}$, we can identify $\delta_\uparrow=-\alpha(B)$ as the elastic scattering phase shift of the "up" electron at the Fermi surface. By linearizing around $\omega=0$ at zero temperature, we obtain

$$t_\uparrow(\omega-i\delta)=\frac{Z\tilde{S}}{\omega-\xi}, \tag{16}$$

where $Z=1/[\partial_\omega\mathcal{J}^{-1}(\omega)]|_{\omega=\tilde{B}}=\tilde{B}/\rho$ and

$$\xi=-Z\mathcal{J}^{-1}(\tilde{B}-i\delta)=\tilde{B}\ln\frac{T_K}{\tilde{B}}+i\pi\tilde{S}\tilde{B}. \tag{17}$$

In other words, the polarized spin generates a resonant scattering pole of strength $Z=\tilde{B}/\rho$, with phase shift $\delta_\uparrow=-\alpha(\tilde{B})$ and a width $\Delta=\pi\tilde{S}\tilde{B}$, which defines the characteristic energy scale of the field-tuned Fermi liquid. We may associate a density of states $N^*(\omega+\tilde{B})$ with the resonance that is formed, where

$$N^*(\omega)=\frac{1}{\pi}\alpha'(\omega)=\frac{1}{\pi\omega}\frac{\pi\tilde{S}}{\left[\ln\left(\dfrac{T_K}{\omega}\right)\right]^2+(\pi\tilde{S})^2}. \tag{18}$$

Notice how, in a finite field, the density of states $N*(\tilde{B})$ is nonsingular at zero energy and we can identify

$$T_F^*\sim N^*(B)^{-1}=B\ln^2\left(\frac{T_K}{\tilde{B}}\right) \tag{19}$$

as the Fermi temperature, showing that in a finite field the characteristic temperature of the Fermi liquid is the field itself. At temperatures $T\lesssim\tilde{B}$, the specific heat capacity will become linear, $C_V=\gamma(\tilde{B})T$, where $\gamma=(\pi^2k_B^2/3)N^*(B)$ (Fig. 4). As the field is reduced to zero, the temperature window for Fermi liquid behavior narrows to zero. At zero field $N^*(\omega)$ is singular, and a Fermi liquid expansion of the thermodynamics is no longer possible: the fluid is best described as a singular Fermi liquid.

Certain aspects of these results will change at finite N. One of the most important changes concerns the values of the phase shifts. In the large-N limit, the asymptotic low-field limit of the $\delta_\uparrow$ phase shift is $-\pi$. At finite N, by relating the change in magnetization to the phase shift, $\Delta M = g_N \delta_\uparrow/\pi = 1/2$, we deduce that the asymptotic low-field phase shift for the "up" electrons at finite N is $\delta_\uparrow = -\pi(1-1/N)$. Since the sum of all the phase shifts for elastic spin scattering must equal zero, this implies that $\delta_\uparrow + (N-1)\delta_\downarrow = 0$ or $\delta_\downarrow = \pi/N$ $(\sigma' \neq \uparrow)$. We see that modulo the π shift, when $B \to 0$, $\delta_\sigma \mathrm{mod}(\pi) = \pi/N$, the same phase shift as found in the fully screened Kondo model.[13]

The singular Fermi liquid behavior of the underscreened Kondo model follows quite generally from the singular energy dependence of the Kondo coupling constant. For SU(2), we expect that at a finite, but small energy, the phase shifts will have the form $\delta_\sigma(\epsilon) \sim \pi/2 + \sigma\pi g(\epsilon)$ so that $\delta_\sigma(\epsilon) \sim \pi/2 + \sigma\pi/\ln(T_K/\epsilon)$ and the derivative of the phase shift diverges as $1/\epsilon$, preventing the normal Landau expansion of the phase shift in terms of quasiparticle occupancies. In a field we must replace $\epsilon \to \epsilon + \sigma B$, so that

$$\delta_\sigma(\epsilon) = \frac{\pi}{2} + \sigma \frac{\pi}{\ln(T_K/B)} + \epsilon \frac{\pi}{B \ln^2(T_K/B)} + O(\epsilon^2) \tag{20}$$

can now be expanded in a power series in energy and quasiparticle occupancies. It follows that, quite generally,

$$\chi(B) \sim 2\gamma^*(B) \sim \frac{1}{B \ln^2(T_K/B)}. \tag{21}$$

This type of singular behavior can also occur in the ferromagnetic Kondo model,[18] but here the effective Kondo temperature $T_K \to D e^{+1/\rho J} \gg D$ is exponentially larger than the bandwidth, driving the effect to weak coupling.

Our results do not yet give us a precise understanding of the nature of the singular Fermi liquid that forms for temperatures $T > B$. The large-N treatment suggests the intriguing possibility that the fermionic resonance associated with the binding of the spin to conduction electron degrees of freedom breaks up at energy scales above $T \sim B$, as if the heavy quasiparticle splits up into a "spinon" b and a charged spinless "holon" ϕ.

In conclusion, we have shown how the treatment of the underscreened Kondo model using Schwinger bosons enables us to recover the well-known properties of this model, in the course of which our results reveal a hitherto unnoticed singular Fermi liquid state at zero field. The model provides an elementary example of a field-tuned Fermi liquid with a characteristic scale which grows linearly with the applied magnetic field. Intriguingly, the low-temperature upturn in the specific heat and the appearance of B as the only scale in the problem are both features observed in quantum critical heavy-electron systems,[6,10,11] leading us to speculate that this model may provide a useful starting point for future understanding of these systems.

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