

Magnetism, non-Fermi-liquid behavior and deconfinement in Kondo lattices

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Anomalous f -systems, which are usually described as Kondo lattices, show unusual behavior of thermodynamic and transport properties, e.g., large electron specific heat, $\gamma = C/T \sim 1/T_K$ (T_K the Kondo temperature) or even a non-Fermi-liquid behavior. At the same time, a number of such systems with frustrated magnetic structures demonstrate spin-liquid features with $\gamma \sim 1/J$ where J is the Heisenberg exchange interaction.

A scaling theory of the Kondo lattices [1, 2] demonstrates that during the scaling procedure the process of magnetic moment compensation terminates somewhere at the boundary of the strong coupling region, which can result in the formation of a finite (although possibly small) saturation moment. Thus a unified energy scale is established, both the effective spin-fluctuation frequency (i.e., J) and T_K being strongly renormalized, as well as frustration parameters [3].

In Ref. [4], a mean-field description of the magnetic ground state of the Kondo lattices was proposed. Here we generalize this approach and formulate the effective hybridization model describing the competition of magnetic and non-magnetic Kondo and spin-liquid states. We also go beyond the mean-field theory by taking into account fluctuations contribution, including gauge field ones.

Unlike previous works [5], we use the formulation by Coleman and Andrei [6] which reduces the $s - f$ exchange coupling to the effective hybridization V and yields the correct value of the Kondo temperature T_K . As for Heisenberg term, we use the representation of pseudofermions $f_{i\sigma}^\dagger$. In the spin-liquid state, they are essentially operators of spinons – neutral fermions which have dispersion on the scale J , so that the spinon Fermi surface is formed. The single-occupancy constraint can be enforced by a gauge field. The presence of hybridization results in the formation of a unified “large” Fermi surface including both conduction electrons and f -states.

To take into account fluctuations effects, we use the slave-particle representation $f_{i\sigma} \rightarrow f_{i\sigma} b_i$, the effective hybridization being determined by the boson condensate $b_0 = \langle b \rangle$. Fluctuations can destroy the condensate picture, so that b_0 vanishes. Then we obtain a spin-liquid-like state where spinon and electron Fermi surfaces are distinct, i.e., a “small” Fermi surface. This state was called fractionalized Fermi-liquid (FL*) [7].

In the quantum critical regime, a topological transformation from large Fermi surface (Kondo lattice state) to small Fermi surface is possible, which can be accompanied by magnetic-order instability. A topological “Kondo breakdown” transition can occur between FL* and “usual” heavy Fermi liquid (FL) states. In the spin-liquid state, gauge field fluctuations can play a role in thermodynamics and heat transport even in the insulating phase (in the absence of conduction electrons, but in the presence of the spinon Fermi surface). In particular, there occurs a spinon contribution to specific heat. This contribution retains in FL* state and in FL state near the topological transition. As demonstrate the calculation [7], the specific heat coefficient $\gamma = C/T$ diverges logarithmically at $T \rightarrow 0$ in the FL* phase, which means the non-Fermi-liquid behavior (in the $2d$ case, $C(T) \sim T^{2/3}$). At approaching the transition from the FL side, we have $\gamma \sim \ln(1/b_0)$.

In the quantum critical regime, the fluctuations of order parameter field b yield additional contributions to thermodynamic properties. Unlike gauge field (neutral spinon) ones, they contribute also to electronic transport. Due to mismatch of electron and spinon Fermi surfaces, the decay of bosons into particle-hole pairs becomes possible above an energy E^* , which can be small if the distance between the two Fermi surfaces is small. Then at $T > E^*$ one obtains a $T \ln T$ contribution to specific heat. Besides that, the fluctuation scattering results in the $T \ln T$ dependence of resistivity $R(T)$ in this regime [8]. For $T < E^*$, the behavior of thermodynamic and transport properties depends on that the Fermi surfaces intersect or not [9]. In the first case we have $R(T) \sim T^{3/2}$ and $R(T) \sim T \ln T$ in $3d$ and $2d$

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cases, respectively. In the FL states, this contribution is cut at the Kondo gap of order of T_K , which is related to the boson condensate, $T_K \simeq \pi\rho V^2 b_0^2$ in the vicinity of the critical point.

The FL* state with the spinon Fermi surface should be unstable with to a broken-symmetry antiferromagnetic (AFM) ordering (spin-density wave, SDW state) with the wavevector $\mathbf{Q}$ [7]. The exotic AFM order on the spinon Fermi surface is called AFM* or SDW* phase. The presence of an SDW* condensate does not cause a radical change in the structure of the gauge fluctuation in comparison with the FL* state: the spinons remain deconfined and coupled to a gapless U(1) gauge field. The gauge field excitations coexist with the gapless Goldstone magnon mode and with a Fermi surface of conduction electrons. Because of the broken translational symmetry, there is no clear difference between small and large Fermi surfaces now [7].

With increasing $s - d(f)$ exchange coupling, the deconfined phase with small Fermi surface can pass first into usual itinerant AFM state with a large Fermi surface volume, and then into FL state. The spinon Fermi surface of the FL*-phase is expected to evolve smoothly into the FL region in some vicinity of the topological transition, so that the SDW order can continue to FL in the ground state, as discussed in [1]. Thus there is no sharp transition between the FL and FL* regions, and there is instead expected to be a large intermediate quantum-critical region [7].

The contribution of transverse spin fluctuation to conduction-electron self-energy reads

$$\Sigma_{\mathbf{k}}^{(2)}(E) = V^2 \bar{S} \sum_{\mathbf{q}} (u_{\mathbf{q}} - v_{\mathbf{q}})^2 \times \\ \times \left(\frac{1 - n_{\mathbf{k}+\mathbf{q}} + N_{\mathbf{q}}}{E - \epsilon_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{q}}} + \frac{n_{\mathbf{k}+\mathbf{q}} + N_{\mathbf{q}}}{E - \epsilon_{\mathbf{k}+\mathbf{q}} + \omega_{\mathbf{q}}} \right), \quad (1)$$

where $n_{\mathbf{k}} = \langle f_{\mathbf{k}}^\dagger f_{\mathbf{k}} \rangle$ and $N_{\mathbf{q}} = \langle \beta_{\mathbf{q}}^\dagger \beta_{\mathbf{q}} \rangle$ are Fermi and Bose functions of spinons and magnons, $\epsilon_{\mathbf{k}}$ the spinon spectrum, $u_{\mathbf{q}}, v_{\mathbf{q}}$ the Bogoliubov transformation factors.

The contribution (1) is similar to that of the usual perturbation theory in the $s - d(f)$ exchange model [10], but works on the scale of the spinon bandwidth. In the FL* state the hybridization V plays the role of the $s - f$ exchange parameter and mediates the RKKY (Ruderman–Kittel–Kasuya–Yosida) type interaction between f -states. The contribution (1) survives in the FL state where a unified electron-spinon Fermi surface arises and a correlated $s - f$ band with narrow density-of-states peaks is formed. However, in such a situation the spectrum $\epsilon_{\mathbf{k}}$ and prefactor in (1) change.

In the case of weak antiferromagnetism we have an energy scale $T^* = (\Delta/v_F)J$ (Δ is the AFM splitting of the spectrum), so that for $T^* < T < J$ the transitions between AFM subbands become singular. It should be

noted that the splitting and magnon frequency are, generally speaking, renormalized in a different way – both in scaling equations [1] and due to frustrations. This favors formation the scale T^* even in the absence of the small parameter of the $s - f$ exchange coupling I .

In the general $d = 3$ case we have $\text{Im}\Sigma^{(2)}(E) \propto E^2$ for $T^* < T < J$. For $d = 2$ $\text{Im}\Sigma(E)$ is linear in $|E|$. The corresponding intersubband correction to specific heat can be derived similar to [10]. In the $2d$ (or “nesting” $3d$) case the integral in (1) is logarithmically divergent at $\mathbf{q} \rightarrow \mathbf{Q}$ and the divergence is cut at $\max(T, T^*)$, so that

$$\delta C_{\text{inter}}(T) \propto T \ln \frac{\bar{\omega}}{\max(T, T^*)}. \quad (2)$$

Thus for $T > T^*$ we obtain the $T \ln T$ -dependence. The result (2) holds also in the case of frustrated ($2d$ -like) magnon spectrum. For the $2d$ magnon spectrum or “nested” $3d$ situation one obtains for spin-wave resistivity

$$R(T) \propto T \ln(1 - \exp(-T^*/T)) \simeq T \ln(T/T^*).$$

The role of magnetic fluctuations depends on the relation between J and T_K (in frustrated and low-dimensional systems with strong short-range order the scale J can be considerably larger than T_N). Similar to [4], we can find singular corrections to sublattice magnetization owing to spin-wave damping, which may be of order of unity.

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