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Objekttyp: **Article**

Zeitschrift: **Helvetica Physica Acta**

Band (Jahr): **65 (1992)**

Heft 2-3

PDF erstellt am: **21.07.2024**

Persistenter Link: https://doi.org/10.5169/seals-116472

Ground State Phase Diagram of the Two-Dimensional Kondo Lattice

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Abstract. The variational method is used to map out the phase diagram of the Kondo lattice hamiltonian where the conduction band is given by the tight binding model on a square lattice. Particular attention is paid to the competition of magnetic and non-magnetic behaviour. It is found that a wide range of collective Kondo state separates the regime of RKKY-magnetism at weak couplings from a region of Nagaoka-type ferromagnetism at strong coupling.

Recent experiments have uncovered a rich variety of low-temperature behaviour in heavy fermionic systems, which is thought to arise from the competition between magnetic ordering, and the tendency to form a heavy, non-magnetic Fermi liquid. It is generally accepted that these systems should be describable by the nearly integral valent limit of the periodic Anderson model which can be transformed to the Kondo lattice model. Here we choose to study the square lattice Kondo model, both for its inherent interest, and also because of its potential relevance for Kondo systems with a quasi-two-dimensional structure [1]. The hamiltonian for a tight-binding band of d-electrons, and localized $S = 1/2$ f-spins at each lattice site is

$$H_{KL} = -2t\sum_{\mathbf{k}\sigma}(\cos k_x + \cos k_y)d^+_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma} + J\sum_{\mathbf{g}}\vec{S}^f_{\mathbf{g}}\cdot\vec{S}^d_{\mathbf{g}} \tag{1}$$

where $\mathbf{k}$ are Bloch-vectors, $\mathbf{g}$ site indices, $J > 0$ the Kondo coupling, and $\vec{S}^d_{\mathbf{g}}$ is the conduction electron spin at site $\mathbf{g}$. The number of lattice sites is L.

Conventional criteria [2] based on comparing the single ion Kondo energy to the RKKY energy scale J^2/t would lead us to expect that the transition from RKKY magnetism to collective Kondo behaviour sets in at $J \sim (4-6)t$. However, recent experiments indicate that RKKY magnetism becomes unstable when J is about a factor of 5 smaller than the above estimate. We suggest that this can be explained by taking into account the lattice coherence enhancement of the Kondo effect which is predicted by Gutzwiller-type variational theories, based either on the Anderson lattice [3], or the Kondo lattice model [4]. The trial state for the heavy Fermi liquid is constructed as the Bloch-coherent superposition of Kondo singlets centered at each lattice site

$$|\Psi\rangle = \prod_{\mathbf{k}\sigma}^{L-N} d_{\mathbf{k}\sigma} \prod_{\mathbf{g}}[f^+_{\mathbf{g}\uparrow}\chi^+_{\mathbf{g}\downarrow} - f^+_{\mathbf{g}\downarrow}\chi^+_{\mathbf{g}\uparrow}]|0\rangle \tag{2}$$

where the $\mathbf{k}$-product keeps the total number of f- and d-electrons at a prescribed $2N$ (the conduction electron number/site will thus be $n_c = 2n-1$, where $n = N/L$). The operator

$$\chi^+_{\mathbf{g}\sigma} = \sum_{\mathbf{k}}\frac{e^{i\mathbf{kg}}}{\sqrt{L}}a(\mathbf{k})d^+_{\mathbf{k}\sigma} \tag{3}$$

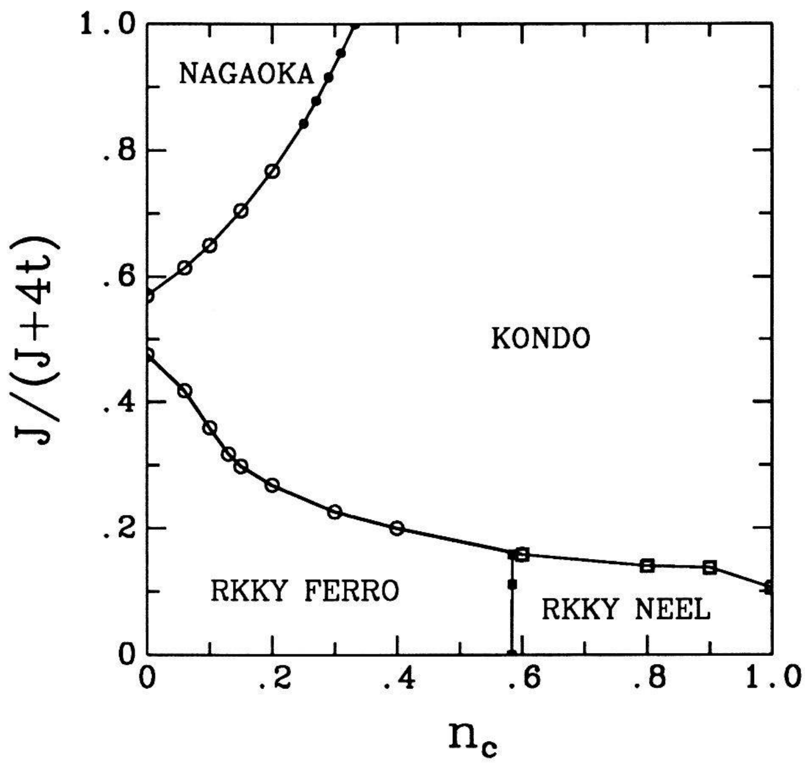

Figure 1: Phase diagram of the square lattice Kondo model in the conduction electron density – Kondo-coupling plane, between zero and half-filling. The RKKY and Nagaoka states are magnetic, the Kondo state is a heavy Fermi liquid with a Luttinger Fermi surface.

creates the d-component of the Kondo clouds; the $a(\mathbf{k})$ are independent variational parameters. The collective Kondo state $|\Psi\rangle$ has a Luttinger Fermi surface containing N $\mathbf{k}$-vectors, in contrast to the RKKY magnetic states, whose Fermi volume corresponds to the number of conduction electrons. A general discussion of the Ansatz (2) was given by Shiba and one of us [4]. Here we carry out the detailed evaluation for the hamiltonian (1), and compare the Fermi liquid energy with the energies obtained from using simple RKKY-, and Nagaoka-type trial states. The resulting phase diagram is shown above. Salient features are: 1) a very significant shrinking of the RKKY regime, which we ascribe to the lattice enhancement of the Kondo effect, and 2) the appearance of a Nagaoka-type ferromagnetic state at very high couplings.

The details of this investigation will be published elsewhere [5].

This work was supported by the Sonderforschungsbereich 341.

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