Journal of Magnetism and Magnetic Materials 400 (2016) 47–51

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Influence of the Kondo effect on spin density waves in the Kondo lattice model

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ARTICLE INFO

Article history:
Received 11 June 2015
Received in revised form
21 July 2015
Accepted 28 July 2015
Available online 30 July 2015

Keywords:
Kondo lattice model
Spin density waves
Kondo effect
Dynamical mean field theory

ABSTRACT

We analyze the influence of the Kondo effect on the spin density wave (SDW) phase in the Kondo lattice model (KLM) for a two-dimensional square lattice. We demonstrate that in the isotropic KLM the SDW phase is divided into a small Fermi-surface region and a large Fermi-surface region and vanishes for strong interaction. On the other hand, in the Ising-spin KLM, where the Kondo effect is absent, we only find a small Fermi-surface SDW phase, which does not vanish at strong coupling. This demonstrates the importance of the Kondo effect for the large Fermi surface SDW phase as well as for the existence of the quantum critical transition between the SDW phase and the paramagnetic phase.

1. Introduction

Heavy fermion systems attract much attention because of their remarkable properties such as competing or coexisting magnetic and superconducting phases, quantum criticality accompanied by non-Fermi liquid behavior. The driving force behind all these intriguing phenomena can be found in the competition of two mechanisms, the RKKY interaction and the Kondo effect, which both try to screen local magnetic moments originating in partially filled and strongly interacting *f*-electron shells. This competition, which is described in the Doniach phase diagram [1], leads to a quantum critical transition between a magnetic and a paramagnetic state. A common model to describe this situation and thus some fundamental properties of heavy fermion systems is the Kondo lattice model (KLM) [1–3].

In our recent work [4], we have analyzed the occurrence of spin density waves (SDWs) in the Kondo lattice model away from half filling for a two-dimensional square lattice. We have found that the Fermi surface changes from small to large within this SDW phase of the Kondo lattice model. This confirms previous calculations which did not take the possibility of inhomogeneous magnetic states, such as SDWs, into account [5–9].

In this paper, we want to clarify the impact of the Kondo effect on the previously observed metallic SDW phase by comparing the isotropic KLM with the Ising-spin KLM. For this purpose we will calculate static and dynamical expectation values for both models.

This paper is organized as follows: in Section 2, we shortly describe the model and the method we use to analyze the SDW phase. This is followed by Section 3, where we discuss our findings, before concluding this paper.

2. Model and method

We analyze the Kondo lattice model, for which we explicitly allow for an anisotropic coupling between the localized spins and the conduction electrons. The model reads [1–3]

$$H = t\sum_{ij,\sigma} c^\dagger_{i\sigma}c_{j\sigma} + \frac{J^z}{2}\sum_i S^z_i(n_{i\uparrow} - n_{i\downarrow}) + \frac{J^{xy}}{2}\sum_i (S^+_i c^\dagger_{i\downarrow}c_{i\uparrow} + S^-_i c^\dagger_{i\uparrow}c_{i\downarrow}), \quad (1)$$

where $c^\dagger_{i\sigma}$ creates an electron with spin-direction σ on lattice site i. The first term in Eq. (1) describes the hopping of conduction electrons, the second and third terms describe the coupling of the conduction electrons to the localized spins. J^z (J^{xy}) describes the Ising coupling (in-plane coupling). In the isotropic case, both interaction strengths are equal. In the Ising-spin model, we set $J^{xy} = 0$, which prevents the occurrence of the Kondo effect, while the RKKY coupling exists. Throughout this paper we assume an antiferromagnetic coupling, $J^z, J^{xy} \geq 0$, and take the hopping constant t as unit of energy. All calculations are performed on a two-dimensional square lattice.

We use the real space dynamical mean field theory (DMFT) [10–12] to study these models. DMFT has been extensively used to

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http://dx.doi.org/10.1016/j.jmmm.2015.07.104
0304-8853/

study the KLM [13–35]. However, in these previous calculations, spin density waves have not been taken into account. The real space DMFT maps each lattice site of a finite cluster onto its own impurity model, from which a local self-energy is calculated. Thus, local fluctuations are exactly taken into account, while non-local fluctuations are neglected. Because the self-energy depends on the lattice site, inhomogeneous phases can be described with this method. In our calculations we have used different clusters of 400–1000 lattice sites and different geometry. We use the numerical renormalization group (NRG) [36–38] to calculate the self-energy of each lattice site. Recently, we have used similar calculations to study spin- and charge density waves in the Hubbard model [39].

3. Results

We show the phase diagram of the isotropic KLM in panel (a) of

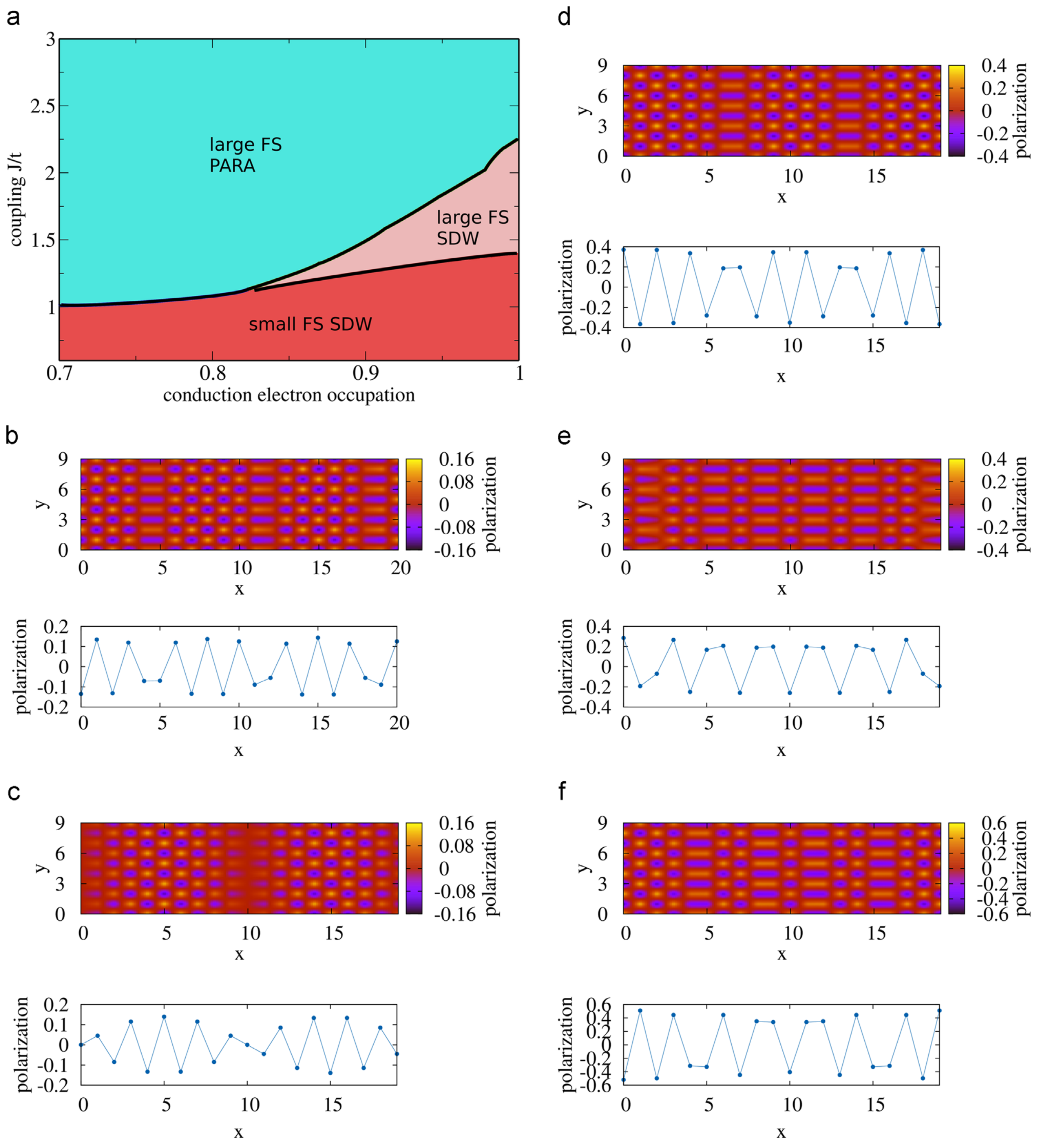

Fig. 1. (a) Phase diagram of the *isotropic* KLM as calculated by RDMFT. The SDW phase away from half filling is separated into a large Fermi-surface (FS) phase at strong coupling and a small FS phase at weak coupling. At strong coupling the paramagnetic phase with large FS is stable. (b) SDW in the *isotropic* KLM at weak coupling ($J/t = 0.6$, $\langle n\rangle = 0.9$). (c) SDW in the *isotropic* KLM at strong coupling ($J/t = 1.8$, $\langle n\rangle = 0.95$). (d) SDW in the *Ising-spin* KLM ($J/t = 1.8$, $\langle n\rangle = 0.95$). (e) SDW in the *Ising-spin* KLM ($J/t = 1.8$, $\langle n\rangle = 0.8$). (f) SDW in the *Ising-spin* KLM ($J/t = 3$, $\langle n\rangle = 0.9$). For each panel (b)–(f), we show a contour plot of the conduction electron polarization over different lattice sites of the square lattice (upper panel), and an intersection of it (lower panel).