Field-induced phase transition in the periodic Anderson model

Takuma Ohashi *, Akihisa Koga, Sei-ichiro Suga, and Norio Kawakami
Department of Applied Physics, Osaka University, Suita, Osaka 565-0871, Japan

Abstract
We investigate the effect of magnetic fields on a Kondo insulator by using the periodic Anderson model. The analysis by dynamical mean field theory combined with quantum Monte Carlo simulations reveals that the magnetic field drives the Kondo insulator to a transverse antiferromagnetic insulator at low temperatures. We calculate the staggered spin susceptibility and find its divergence signaling the antiferromagnetic instability. Further investigation of the spin correlation functions and the magnetization process clarifies how the magnetic field suppresses the Kondo singlet formation and induces the transverse antiferromagnetic ordering.

Key words: Kondo insulator, field-induced phase transition, dynamical mean field theory

Heavy-fermion systems with various ground states have attracted continued interest. One of the interesting examples is the Kondo insulator (KI), where a small charge gap renormalized by the Coulomb interaction appears at low temperatures[1]. It is known that this insulating phase gets unstable upon introducing the magnetic field, the pressure, etc. Experiments on some KI in high magnetic fields indicate closure of the Kondo-insulating gap[2], exemplifying a transition from the KI to a correlated metal[3,4]. If the KI is in the proximity of magnetic instability, the local singlet formation gets weak, and an applied field may possibly trigger a phase transition to the antiferromagnetic (AF) ordered state before it becomes a metal.

The periodic Anderson model (PAM) at half filling may be a simplified model to describe the Kondo insulating phase and the AF phase. The magnetic instability of the PAM has been investigated by a variety of methods[5,6,7,8]. Recently, the magnetic-field effects on the two-dimensional Kondo lattice model have been studied on the basis of the mean field theory and quantum Monte Carlo (QMC) simulations. It has been found that the magnetic field induces a second-order phase transition from the paramagnetic to the AF ground state[9,10].

In this paper, we investigate field-induced AF phase transitions in the PAM by using dynamical mean field theory (DMFT) [11] combined with QMC simulations [12] at finite temperatures. The model we study here is the PAM with the Zeeman splitting,

\[
H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + V \sum_i c_{i\sigma}^{\dagger} f_{i\sigma} + \text{h.c.} \\
+ U \sum_i \left[ n_i^{\uparrow} - 1/2 \right] \left[ n_i^{\downarrow} - 1/2 \right] \\
- g\mu_B B \sum_i \left[ S_i^z + S_i^c \right],
\]

where all the symbols have their usual meaning. We consider the hyper-cubic lattice with a bipartite property in infinite dimensions. The bare density of states for conduction (c) electrons is Gaussian with the width \(t^*\): \(\rho_0(\epsilon) = \exp[-(\epsilon/t^*)^2]/\sqrt{\pi t^*}\). We choose \(t^* = 1\) as the energy unit. The magnetic field \(B\) applied along the \(z\) direction is coupled to both of \(c\) and \(f\) electrons. We set \(g\mu_B = 1\) for both \(c\) and \(f\) electrons.

DMFT is a powerful framework to study strongly correlated electron systems. In DMFT, the original lattice model is mapped onto an effective impurity model.
with the self-consistently determined medium, which is solved by means of QMC simulations in our approach. We use the typical parameters $U = 2.0$ and $V = 0.6$ in the following calculation. For these parameters, the ground state at zero field is a paramagnetic KI, as shown by Jarrell et al. [7].

We first show that the magnetic field induces a KI-AF phase transition. We calculate the staggered spin susceptibility $\chi_{xx}(Q = Q_f)$, with $Q = \{x, x, \ldots\}$, where the suffix $x$ denotes the direction perpendicular to the field. In Fig. 1, we plot the inverse of the total susceptibility $\chi_{xx}^{\text{tot}}(Q)$ and the susceptibility for $f$ electrons $\chi_{xx}^f(Q)$ as a function of the magnetic field for different temperatures. At temperatures $T = 1/24$ and $T = 1/28$, the staggered susceptibilities take a maximum at the magnetic field $B \sim 0.28$. At the lowest temperature $T = 1/32$, the susceptibilities diverge at the field $0.25 < B < 0.34$. The magnetic field triggers a phase transition from the paramagnetic KI to AF ordered state. We determine two critical values of the field by extrapolating the inverse susceptibility to zero with the form $\chi_{xx}^{-1}(Q) \propto B - B_c$.

We further calculate the magnetization process and the field dependence of the spin correlation functions at $T = 1/30$, which is slightly higher than AF transition temperature. The magnetization $M$, defined as

$$M = \langle n_{\uparrow}^x n_{\downarrow}^x - n_{\uparrow}^x n_{\downarrow}^x \rangle,$$

is shown in the top panel of Fig. 2. We can see the crossover behavior from the KI with the spin gap to the paramagnetic metal around $B \sim 0.28$. Around this field, we also see the change in the character of the spin correlation functions. In the middle of Fig. 2, we show the variance of the $m$-moment in the $z$ direction $\langle |S^z_f|^2 \rangle$, and in the $x$ direction $\langle |S^x_f|^2 \rangle$. When the magnetic field is larger than $B \sim 0.28$ is applied, spin fluctuations in the $z$ direction are suppressed and the moment in the $x$ direction get large, since the Kondo singlet formation is suppressed by a magnetic field. The consistent behavior is seen in the spin correlation functions between the $c$ and $f$ electrons, $\langle S^x_c : S^x_f \rangle$ and $\langle S^z_c : S^z_f \rangle$, plotted in the bottom of Fig. 2. AF correlations between the $c$ and $f$ electrons are suppressed by a magnetic field. We can see that the correlations in the $z$ direction are more suppressed than those in the $x$ direction. The above behavior explains why the transverse rather than longitudinal antiferromagnetic ordering is favored in finite magnetic fields.

The authors thank T. Saso for valuable discussions. A part of computations was done at the Supercomputer Center at the Institute for Solid State Physics, University of Tokyo. This work was partly supported by a Grant-in-Aid from the Ministry of Education, Science, Sports and Culture of Japan.

References

[1] P. S. Riseborough, Adv. Phys. 49, 257 (2000).
[2] K. Sugiyama, et al., J. Phys. Soc. Jpn. 57, 3946 (1988); J. C. Cooley, et al., J. Supercond. 12, 171 (1999); M. Jaime, et al., Nature 405, 160 (2000).
[3] T. Saso, J. Phys. Soc. Jpn. 66, 1175 (1995); T. Saso, et al., Phys. Rev. B 53, 6877 (1996).
[4] T. Mutou, Phys. Rev. B 62, 15589 (2000).
[5] V. Dorin et al., Phys. Rev. B 46, 10800 (1992).
[6] R. Doradziński et al., Phys. Rev. B 58, 3293 (1998).
[7] M. Jarrell, et al., Phys. Rev. Lett. 70, 1670 (1993); M. Jarrell Phys. Rev. B 51, 7429 (1995).
[8] M. J. Rozenberg, Phys. Rev. B 52, 7369 (1995).
[9] K. S. D. Beach, et al., Phys. Rev. Lett. 92, 26401 (2004).
[10] I. Milat, et al., cond-mat/0312450.
[11] A. Georges, et al., Rev. Mod. Phys. 68, 13 (1996).
[12] J. E. Hirsch et al., Phys. Rev. Lett. 56, 2521 (1986).