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Magnetic-field-induced valence transition in rare-earth systems

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Abstract. The magnetic-field-induced valence transition in rare-earth systems has been investigated using the periodic Anderson model supplemented by the Falicov–Kimball term. This model has been solved by first decoupling the Falicov–Kimball term as proposed by Khomskii and Koharjan and then taking the limit of infinite intra-site Coulomb repulsion. The valence transition both in the absence and in the presence of magnetic field as a function of temperature is studied. It has been found that the system makes transition from non-magnetic to magnetic state when the magnetic field increases beyond a critical value H_c. The phase boundary defined in terms of reduced field $H_c(T)/H_c(0)$ and reduced temperature T/T_v (T_v being the valence transition temperature in the absence of field) is almost independent of the position of the localized level. The results are in qualitative agreement with experimental observations in Yb- and Eu-compounds.

Keywords. Magnetic field; valence transition; rare-earths.

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1. Introduction

The valence instabilities that are extensively observed in rare-earth compounds and/or alloys are induced by pressure, temperature or chemical alloying. The change in the valence state of rare-earth ion is found to be either continuous or discontinuous. One of the common features of all the systems which show valence instabilities is that, in the intermediate valence phase, the system fluctuates between a magnetic ($J \neq 0$) and a non-magnetic ($J = 0$) state. It is, therefore, expected that an external magnetic field may induce valence transition. In the recent past, some experimental investigations have shown such a field-induced valence transition [1,2]. It was found that the system in the intermediate valence phase makes a transition to a magnetic phase when the magnetic field increases beyond a critical value H_c. This critical field is maximum at $T = 0$ and is a decreasing function of temperature and vanishes at T_v, the valence transition temperature. The phase diagram in the H–T plane when plotted in terms of the reduced critical field $H_c(T)/H_c(0)$ and the reduced temperature T/T_v, the experimetal data for different compositions of the compound collapse into a single curve [3,4] for Yb- and Eu-based systems. This type of universal behavior has been studied qualitatively based on phenomenological models [2,5]. However, there have been some efforts to explain the field-induced valence transition based on

the electronic models [6,7] also. In the present work we investigate the scaling behavior observed experimentally based on an electronic model which has not yet been attempted.

2. The model and approximation

The Hamiltonian of the periodic Anderson model (PAM) with Falicov–Kimball term used to describe both continuous and discontinuous valence transition [8,9] in the presence of external magnetic field is given by

$$\mathcal{H} = \sum_{i,j,\sigma} \left(T_{ij} - z_\sigma H\right) d^\dagger_{i\sigma} d_{j\sigma} + \sum_{i,\sigma} \left(e_f - z_\sigma H\right) f^\dagger_{i\sigma} f_{i\sigma} + \mathcal{V} \sum_{i,\sigma} \left(f^\dagger_{i\sigma} d_{i\sigma} + \text{h.c.}\right) + \frac{U}{2} \sum_{i,\sigma} n_{fi\sigma} n_{fi-\sigma} + G \sum_{i,\sigma,\sigma'} n_{fi\sigma} n_{di\sigma'} \,. \tag{1}$$

The notation is conventional. The parameters of the model are the conduction bandwidth W, the location of the f-level e_f, the strengths of the hybridization V, the intra-atomic Coulomb repulsion U and the local repulsion between conduction- and localized-electrons G. For an approximate solution of the model, we first decouple the Falicov–Kimball term as proposed by Khomskii and Koharjan [10] which makes it a PAM with renormalized model parameters. Since the systems displaying valence instabilities have quite large U, it is realistic to take the limit of $U \longrightarrow \infty$. One can obtain [9] the self-consistent equations for the occupancy of conduction band and localized level up to terms V^2 and in the limit $U \longrightarrow \infty$ as

$$n_{d\sigma} = \int_{-\infty}^{\infty} \mathrm{d}E \; f(E) \rho_0(E - R_\sigma(E)) \,, \tag{2}$$

$$n_{f\sigma} = \left[(V + G\gamma_\sigma)(1 - n_{f-\sigma})\right]^2 \int_{-\infty}^{\infty} \frac{\mathrm{d}E \; f(E) \rho_0(E - R_\sigma(E))}{(E - e_f + z_\sigma H - G n_d)^2} \,, \tag{3}$$

where

$$\gamma_\sigma = -(V + G\gamma_\sigma)(1 - n_{f-\sigma}) \int_{-\infty}^{\infty} \frac{\mathrm{d}E \; f(E) \rho_0(E - R_\sigma(E))}{(E - e_f + z_\sigma H - G n_d)} \tag{4}$$

is the valence fluctuation function, and

$$R_\sigma(E) = -z_\sigma H + G n_f + \frac{(V + G\gamma_\sigma)^2 (1 - n_{f-\sigma})}{(E - e_f + z_\sigma H - G n_d)} \tag{5}$$

is the conduction electron self-energy. $\rho_0(E)$ is the free Bloch density of states which we take as semi-elliptic for numerical evaluation and $f(E)$ is the Fermi function. The chemical potential is fixed from the requirement

$$n = n_f + n_d - \sum_\sigma (n_{f\sigma} + n_{d\sigma}) = \text{constant.} \tag{6}$$

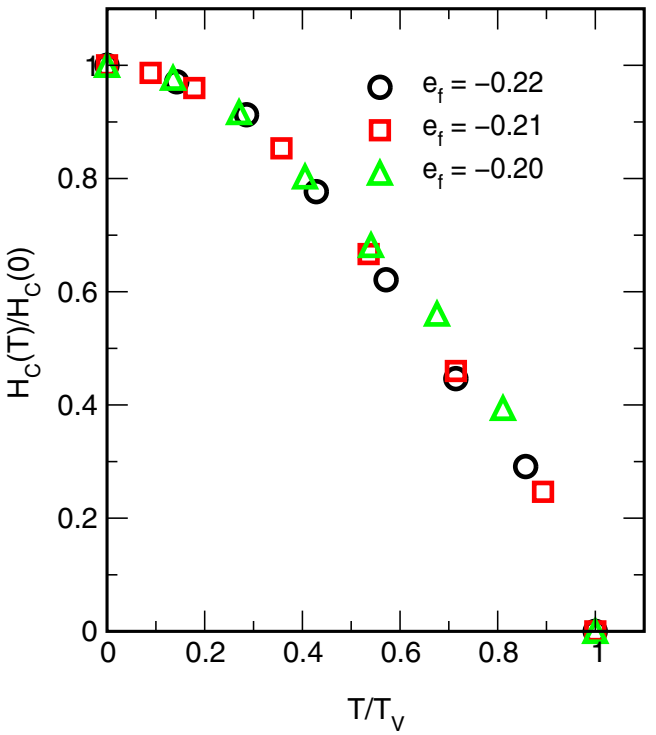

Figure 1. Phase diagram in terms of reduced critical field $H_c(T)/H_c(0)$ and reduced temperature T/T_v for $W = 1$, $V = 0.1$, $G = 0.4$ and $n = 1$.

3. Results and discussion

Equations (2)–(4) together with (6) constitute a set of self-consistent equations and have been solved numerically for various sets of the model parameters both in the absence and in the presence of magnetic field. In the absence of the field, it has been found that for a particular choice of the model parameters, n_f changes discontinuously when the temperature exceeds a critical value, which has been defined as the valence transition temperature T_v. At $T = 0$, the field dependent magnetization $M(H) = \sum_\sigma z_\sigma (n_{f\sigma} + n_{d\sigma})$ is evaluated. It is observed that $M(H)$ changes abruptly when the magnetic field increases beyond a critical value H_c. This field is maximum at $T = 0$, and decreases with T ultimately going to zero by the time $T \longrightarrow T_v$. The phase diagram in H–T plane is constructed in figure 1 in terms of reduced field $H_c(T)/H_c(0)$ and reduced temperature T/T_v for various values of the f-level position by keeping all other model parameters fixed. It has been noted that the phase boundary is independent of f-level position. If we simulate the process of change in the chemical composition with the shift in f-level position, the results shown in the figure qualitatively agree with experimental observations [3,4] in Yb- and Eu-compounds.

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