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# Simultaneous ferromagnetic and semiconductor-metal transition in EuO

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## Abstract

We develop a theory for the simultaneous para-to-ferromagnetic and semiconductor to metal transition in O-depleted EuO. An analysis of the total charge conservation across the transition indicates that strong Coulomb correlations in the localized O-defect states must play a crucial role. This leads to a generalized Anderson impurity model with Stoner-like magnetic correlations in the conduction band and a dilute concentration of Anderson impurities in the semiconducting gap. We solve this model using the Non-Crossing Approximation and can explain the simultaneous phase transitions in a natural way. © 2001 Elsevier Science. All rights reserved

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## 1. Introduction and model

Europium oxide (EuO) is a paramagnetic semiconductor with a wide band gap of 1.2 eV, which becomes a ferromagnetic metal below the critical temperature  $T_c = 69K$  [1,2,3]. In the metallic phase the polarization of the charge carriers is found to be nearly 100 per cent. In the O-depleted compound EuO of trivalent EuO and bivalent O, the stoichiometry implies the existence of excess charge carriers. In the high temperature phase they are bound in localized oxygen defect states lying in the semiconducting gap. These features, known since the early 1970s, and the concomitant, colossal magnetoresistance have recently raised considerable interest in EuO because of possible spintronics applications. Previous theoretical studies [4] assume phenomenologically a T-dependent Stoner-like splitting of the conduction band, induced by the Eu 4f moments and motivated by band structure calculations [5], which causes the metallic phase transition when the majority band overlaps with the O defect band. However, a theoretical understanding of the nature and the simultaneity of the magnetic and the metallic transition is lacking up to the present day.

The local 4f moments of Eu induce magnetic correlations in the conduction band via an exchange interaction, as soon as the conduction band is occupied. Since the O-defect concentration,  $n_{imp}$ , and hence the possible conduction band filling are small, the Fermi wavelength is much larger than the lattice spacing, so that the RKKY-induced coupling between the conduction electrons is ferromagnetic. We model this coupling by an effective mean-field Stoner coupling  $U$ . The O-defect levels are at an energy  $E_d$  below the conduction band edge. The conservation of the total charge above and below the transition,  $\sum_{\sigma}(n_{d\sigma} + n_{c\sigma}) = n_{imp}$  (with  $n_{d\sigma}$ ,  $n_{c\sigma}$  the defect electron and conduction electron density, respectively), implies that in the metallic phase the majority conduction band can shift below the chemical potential  $\mu$  only if at the same time sufficient spectral weight is transferred from the impurities to energies above  $\mu$ . Since this is a dynamical process, we conclude that the Coulomb repulsion in the O-defect states,  $U_d$ , must be significant. In this way one obtains the model Hamiltonian for EuO as,

$$H = \sum_{\vec{k}\sigma} (\epsilon_{\vec{k}} - \mu) c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}\sigma} + (E_d - \mu) \sum_{i\sigma} d_{i\sigma}^{\dagger} d_{i\sigma} + U_d \sum_i \hat{n}_{d i \uparrow} \hat{n}_{d i \downarrow} + V \sum_{\vec{i}\vec{k}\sigma} (c_{\vec{k}\sigma}^{\dagger} d_{i\sigma} + h.c.) + U \sum_{\vec{k}\vec{k}'\sigma} \langle \hat{n}_{c \vec{k}'\sigma} \rangle \hat{n}_{c \vec{k}-\sigma} \quad (1)$$

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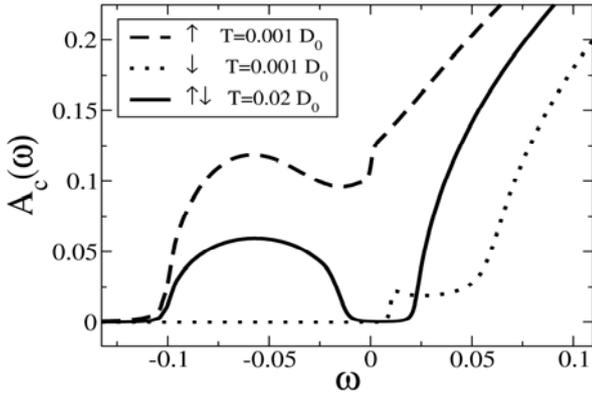


Fig. 1. The conduction electron spectral density for  $T > T_c$  (solid line) and for  $T < T_c$  (broken lines). The gap of the semiconductor and the almost complete spin polarization in the metallic phase are clearly seen.  $D_0$  denotes the half bandwidth of the bare conduction band.

where the first term represents the conduction band, the second and third terms the O-defects at sites  $i$ , including the local Coulomb repulsion  $U_d$ , the fourth term describes the defect-conduction band hybridization, and the last one is the Stoner term with the conduction electron number operator for momentum  $k$  and spin  $\sigma$ ,  $n_{c\bar{\sigma}}$ .  $\mu$  is the common chemical potential of the defect and conduction electrons.

## 2. Results and discussion

We have calculated the spin dependent spectral density of conduction electrons,  $A_c(\omega) = -\int dk \text{Im} G_c(\omega) / \pi$ , where the retarded conduction electron propagator reads,

$$G_{c\sigma}(\omega) = [\omega + \mu - \varepsilon_k - \Sigma_{c\sigma}(\omega)]^{-1} \quad (2)$$

$$\Sigma_{c\sigma}(\omega) = U(\hat{n}_{c-\sigma} + n_{imp})|V|^2 G_{d\sigma}(\omega) \quad (3)$$

where the c-electron selfenergy  $\Sigma_{c\sigma}(\omega)$  is local and consists of the Stoner and the impurity scattering contributions. We treat the local Coulomb correlations on

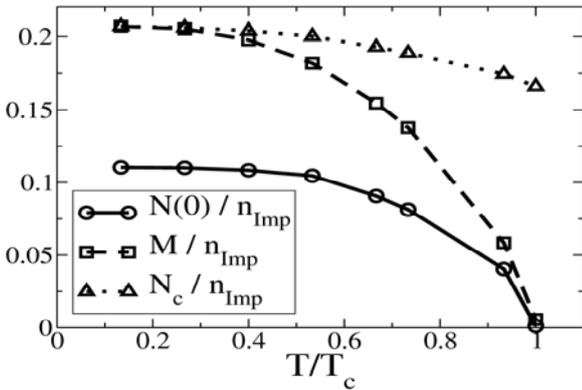


Fig. 2. Simultaneous metallic and ferromagnetic phase transition in the model Eq. (1): the  $T$ -dependent density of states  $N(0)$  at the chemical potential and the magnetization  $M = n_{c\uparrow} - n_{c\downarrow}$ . The electron number in the conduction band,  $N_c$ , remains finite across the transition, c.f. Fig. 1.

the O-defects by means of an auxiliary boson representation in the limit  $U_d \rightarrow \infty$ , using the well-known non-crossing approximation (NCA) [6,7]. The defect electron propagator  $G_{d\sigma}(\omega)$  is then given in terms of the auxiliary fermion and boson propagators  $G_{f\sigma}$ ,  $G_b$  and their selfenergies  $\Sigma_{f\sigma}$ ,  $\Sigma_b$  by the set of equations,

$$\Sigma_{f\sigma}(\omega) = \Gamma \int \frac{d\varepsilon}{\pi} [1 - f(\varepsilon)] A_{c\sigma}(\varepsilon) G_b(\omega - \varepsilon) \quad (4)$$

$$\Sigma_b(\omega) = \Gamma \sum_{\sigma} \int \frac{d\varepsilon}{\pi} f(\varepsilon) A_{c\sigma}(\varepsilon) G_{f\sigma}(\omega + \varepsilon) \quad (5)$$

$$G_{d\sigma}(\omega) = \int d\varepsilon e^{-\beta\varepsilon} [G_{f\sigma}(\omega + \varepsilon) A_b(\varepsilon) - A_{f\sigma}(\varepsilon) G_b^*(\varepsilon - \omega)] \quad (6)$$

with  $\Gamma = \pi V^2$ . For details of the NCA and its efficient evaluation see [8]. The equations (2)-(6) are solved selfconsistently, fixing the total electron number by the chemical potential  $\mu$ .

The results obtained in this way exhibit the following features. Even above  $T_c$  the hybridization  $V$  induces conduction electron spectral weight around  $E_d$ , however a gap the chemical potential remains (Fig. 1). Two scenarios for the formation of a metallic low- $T$  phase, signaled by finite spectral density at  $\mu$ , are possible. (1) Weak Stoner coupling  $U$ ; no magnetic solution [9]. The generation of a finite spectral density at  $\mu$  is driven by the formation of a Kondo resonance (spin fluctuations) in the defect spectrum, with the Kondo temperature  $T_K \approx T_c$ . (2) Strong Stoner coupling  $U$ ; see Figs. 1, 2 for  $E_d - \mu = -.05 D_0$ ,  $\Gamma = .2 D_0^2$ ,  $U = 4.0 D_0$ ,  $n_{imp} = 0.05$ . Low-lying spin fluctuations are suppressed by either the gap ( $T > T_c$ ) or the complete polarization of the conduction electrons ( $T < T_c$ ). The metallic phase transition is driven by c-d charge fluctuations on the scale  $\Gamma$ , with spin polarization induced by the Stoner coupling in the conduction band.

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## References

- [1] M. Oliver *et al.*, Phys. Rev. B 5 (1972) 1078.
- [2] Y. Shapira, T. Foner, and S. B. Reed, Phys. Rev. B 8 (1973) 2299; 8, (1973) 2316.
- [3] P. B. Steeneken *et al.*, Phys. Rev. Lett. 88 (2002) 047201.
- [4] P. Sinjukov and W. Nolting, Phys. Rev. B 68 (2003) 125107.
- [5] R. Schiller, W. Müller, and W. Nolting, Phys. Rev. B 64 (2001) 134409.
- [6] N. Grewe and H. Keiter, Phys. Rev. B 24 (1981) 4420.
- [7] Y. Kuramoto and H. Kojima, Z. Phys. B 57 (1984) 95; Y. Kuramoto, Z. Phys. B 65 (1986) 29.
- [8] T. A. Costi, J. Kroha, and P. Wölfle, Phys. Rev. B (1996).
- [9] M. Arnold and J. Kroha, to be published.

