Zeitschrift: Helvetica Physica Acta
Band: 62 (1989)
Heft: 6-7

Artikel: Limit of zero-width conduction band for the extended Falicov-Kimball model
Autor: Marinaro, M. / Noce, C. / Romano, A.
DOI: https://doi.org/10.5169/seals-116090

LIMIT OF ZERO-WIDTH CONDUCTION BAND FOR THE EXTENDED FALICOV-KIMBALL MODEL

M.Marinaro, C.Noce, A.Romano
Dipartimento di Fisica Teorica e Unità GNSM e CISM
Università di Salerno, I-84081 Baronissi (SA), Italy

Abstract: The extended Falicov-Kimball model has been exactly solved in the limit of zero-width conduction band. Preliminary results about the occurrence of both first order and second order metal- insulator transitions are presented.

1. Introduction

The transition metal and rare earth compounds exhibit a wide variety of anomalous electronic and magnetic properties, which arise from the interaction between highly correlated and itinerant electrons. For example, under variation of external conditions (temperature, pressure, alloying) these compounds undergo first order as well as second order transitions from insulator (or semiconductor) to metal. The model proposed by Falicov and Kimball [1] and the extended version of it (EFK) [2,3] seem to be well suited to explain the behaviour of these systems.

2. Model and results

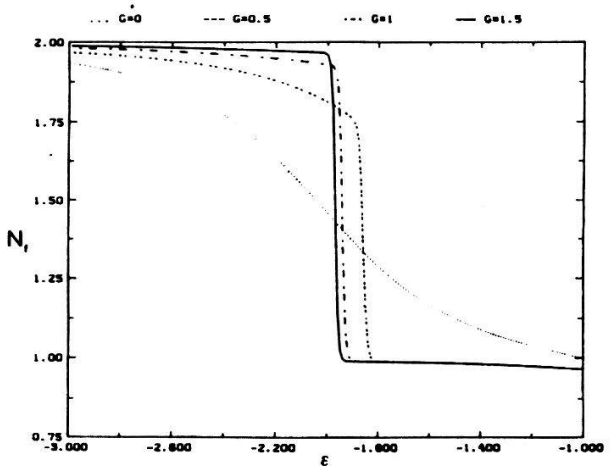
The single site EFK Hamiltonian is

$$H = \Sigma \varepsilon_k c^+_{k\sigma} c_{k\sigma} + \Sigma \varepsilon f^+_\sigma f_\sigma + U\, f^+_\uparrow f_\uparrow f^+_\downarrow f_\downarrow + G\, \Sigma f^+_\sigma f_\sigma c^+_{\sigma'} c_{\sigma'}$$

$$+ V\, \Sigma (c^+_\sigma f_\sigma + f^+_\sigma c_\sigma)$$

where standard second quantization notation is used. In the limit of vanishing conduction bandwidth the model has finite degrees of freedom and thus can be exactly solved. In a previous paper [4] the n-point Green functions have been calculated by using the path integral formalism. From two-point Green functions for localized

electrons we have calculated the number of f-electrons per site. It is reported in figure as a function of ε for T=70°K, U=2 eV V=0.2 eV, and different values of G. Due to the well known linear relation between pressure and ε, this plot shows the dependence of the valence of the f-electrons from the pressure.We see that the electronic transition is driven by the strength of the Coulomb interaction between c and f-electrons: increasing the value of G from 0 to 1.5 eV the transition passes continuously from second order to first order.



We stress that in our approach the effect of G, V and U are all included in a non-perturbative way. In this sense our results are more general than the ones reported in ref.[3] where the terms proportional to V and G are treated in mean field approximation and the limit of infinite U is considered.

Besides, we point out that the atomic limit considered here does not qualitatively affect the results about the order of the transition, as noted for example in ref.[3], and it still retains the essential features of the intermediate valence properties of some real systems [5]. More details will be presented elsewhere.

4. References

[1] L.M.Falicov, J.C.Kimball, Phys. Rev. Lett. 22, 997 (1969).

[2] M.Avignon, S.K.Ghatak, Solid State Commun. 16, 1243 (1975).

[3] C.E.T.Gonçalves da Silva, L.M.Falicov, Solid State Commun. 17, 1521 (1975).

[4] C.Noce, A.Romano, J. Phys.: Cond. Matt., in press.

[5] J.M.Coey, S.K.Ghatak, M.Avignon, F.Holtzberg, Phys. Rev. B14, 3744 (1976); S.M.Shapiro, J.D.Axe, R.J.Birgeneau,J.M.Lawrence, R.D.Parks, Phys. Rev. B16, 2225 (1977).