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

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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.
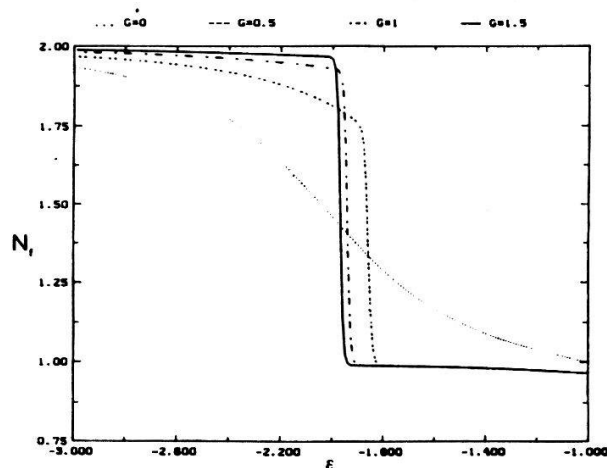
We see that the electronic transition is driven by the strength of the Coulomb interaction between c and f-electrons: increasing the value of G from 0 to 1.5 eV the transition passes continuously from second order to first order.

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. <u>References</u>

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