

Stabilization of valence fluctuations in the cerium solid by the time-dependent collision approach

RATAN LAL

Physics Department, Regional Engineering College, Silchar 788 010, India

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Abstract. The collision-generated hybridization which has been found responsible for the on-site mixing of the atomic-like f -state and the band-like d states in mixed valence solids has been studied for the cerium solid. A practical expression which depends on the lattice constant and temperature has been obtained for the collision-generated hybridization. Numerical calculations show that the valence varies continuously with lattice constant and that temperature makes the transition smoother. The collision-generated hybridization is found to be of significant strength in the intermediate valence regime; but over a wide range of the valence near 3.5 it varies rather slowly without preferring a particular valence. Factors which can assist the collision-generated hybridization in stabilizing the mixed valence phase at a particular lattice constant are discussed.

Keywords. Mixed valence; intermediate valence; valence fluctuations; cerium solid; time-dependent collision.

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1. Introduction

A class of rare earth solids show anomalous physical properties (Khomskii 1979; Robinson 1979; Lawrence *et al* 1981; Lee *et al* 1986). Experimental findings suggest that the state of such solid systems belongs to the non-integer valence. The origin of non-integer valence lies in the coexistence of two configurations, f^n and f^{n-1} , with similar energies. Except at very low temperatures, the fluctuations of the f electron between these two configurations are mainly local in character (Schlottmann 1980; Gunnarsson and Schonhammer 1983; Barnes 1985). To understand the behaviour of mixed valence solids many theoretical efforts have been made in recent years (Kasuya and Saso 1985; Lee *et al* 1986). However, almost all the existing theories work in terms of pre-assumed mixed valence conditions by taking parametric forms of relevant interactions. Development of a microscopic theory which can provide a method for the estimation of the various interaction parameters is at its initial stage only (Lal 1983, 1986). In our previous papers (Lal 1983, 1984, 1986) we have seen that the use of the time-dependent collision theory provides us a way for the estimation of the strength of the on-site hybridization interaction, the so-called "collision-generated hybridization (CGH)". The CGH does not suffer from the objections caused by the symmetry as in the case of Anderson hybridization (Lal 1984). Moreover, the fact that the two-site hybridization of Kaplan and Mahanti (1975) is neither based on the interactions which exist in the system, nor does it find any experimental support (Robinson 1979) makes the CGH