

THEORETICAL STUDY OF MAGNETIC IMPURITIES IN SIMPLE-METAL CLUSTERS: KONDO EFFECT AND INTERMEDIATE VALENCE BEHAVIOUR

G. M. Pastor

Laboratoire de Physique Quantique, Centre National de la Recherche Scientifique,
Université Paul Sabatier, Toulouse, France

The electronic and structural properties of simple-metal clusters containing magnetic impurities are investigated in the framework of the Anderson model by using exact diagonalization methods and variational approaches. The spin gap $\Delta E = E(S=1,3/2) - E(S=0,1/2)$ shows a remarkable dependence as a function size, structure, and conduction-band filling which can be interpreted in terms of the cluster-specific sd hybridization and conduction-electron spectrum. The magnetic susceptibility, impurity moment, cluster magnetization and specific heat are determined as a function of temperature and applied magnetic field. A finite-size equivalent of the Kondo effect is identified. The magnetic properties in the Kondo limit and in the intermediate-valence regime are contrasted. Besides electronic excitations, the effect of structural changes is quantified for $N \leq 7$ atoms by performing canonical statistical averages over all cluster topologies and impurity positions. It is shown that structural excitations play an important role in the low temperature properties of Anderson clusters. The implications of these investigations are discussed in view of cluster-beam magnetic-deflection experiments.

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