

Effect of Anisotropic Spin-Spin Coupling of Cooper and Oxygen Holes in Spin-Polarized Clusters

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Two types of spin-polarized clusters confining the motion of oxygen holes in layered cuprates are discussed. The first one containing five copper sites has a total spin $S = 2$, whereas most essential elements of the second one are four coppers and it is characterised by $S = 3/2$. Anisotropic exchange coupling splits the magnetic ground state into a sequence of state, which in a natural way provide e.g. an explanation of EPR data for $La_2CuO_{4+\delta}$ compounds.

1. INTRODUCTION

The idea of the existenz of spin-polarized clusters in cuprate superconductors find more and more experimental support [1][2]-[6] Two basically different situations characterise the motion of a hole in the CuO_2 plane. First (a) "spin-spin" coupling confines the motion around a centralized copper site (1), second (b) the motion goes through a square with the centre beeing an inter-site copper position (2).

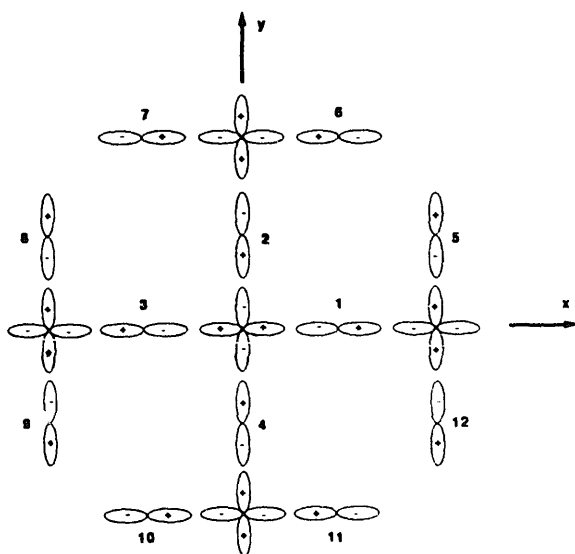


Figure 1. Schematic distribution of copper and oxygen σ -orbitals at the pentacopper cluster

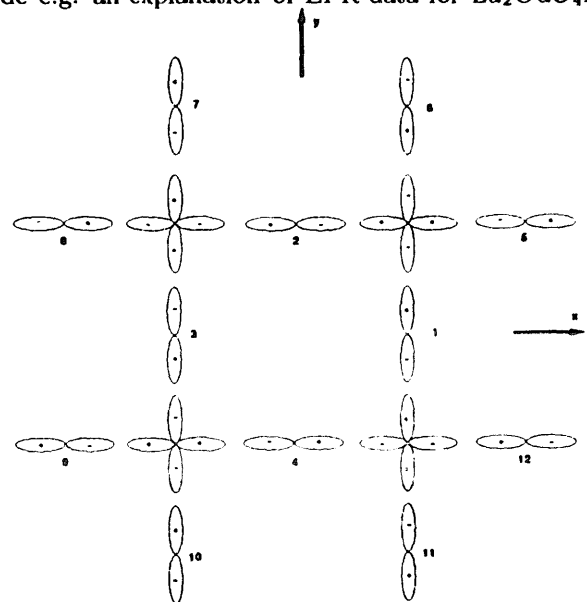


Figure 2. Tetracopper cluster confining oxygen hole into the σ -orbitals

2. CLUSTER CONFINING OXYGEN HOLE WITH THE STATE $P_{b_{1g}}$

The wave function for the oxygen hole in case (a) has b_{1g} symmetry. For the oxygen-copper spin-spin coupling one gets

$$H_{ex}^{(1)} = -3t_{\sigma}^2 \alpha_a^2 Z_a \left[\frac{1}{2} - 2(\bar{s}_p \bar{s}_{f_0}) \right] \quad (1)$$

and

$$H_{ex}^{(2)} = -\frac{3}{8} t_{\sigma}^2 (\alpha_a + \sqrt{2}\beta_a)^2 Z_a [1 - 2(\bar{s}_p \bar{S}_t)] \quad (2)$$