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ON THE IMPORTANCE OF ANISOTROPIC EXCHANGE COUPLING ON TO THE STRUCTURE OF SPIN-POLARIZED CLUSTERS IN LAYERED CUPRATES

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The low energy spectrum of spin-polarized clusters in layered cuprates is examined. Two types of clusters confining the motion of oxygen holes are discussed. The ground state of the pentanuclear copper cluster has a total spin $S = 2$, whereas the one of the tetranuclear copper cluster is characterised by $S = 3/2$. Anisotropic exchange coupling splits the magnetic ground state into a sequence of states, which in a natural way provide e.g. an explanation of EPR data for $La_2CuO_{4+\delta}$ compounds.

1. Introduction

At present there exists a large and fast increasing number of experimental data meintaining the idea [1] of the formation of spin-polarized clusters in layered cuprate superconductors [2 - 6]. The aim of this short communication is to present the results of a first rough calculation of the detailed spin-structure of clusters which appear by hole doping in the CuO_2 planes. For simpicity we only consider the CuO_2 plane with a tetragonal symmetry. There are two possibilities but basically different situations characterising the motion of a hole spreaded over oxygen positions (oxygen hole).In the first situation (a) "spin-spin" coupling confines the motion around a centralized copper site (Fig 1 a), whereas in the second case (b) the motion goes through a square with the centre beeing an intersite copper position (Fig 1 b). Their internal symmetries are different.
The wave function for the oxygen hole in case (a) can be written as

$$P_{b_{1g}}^{(a)} = \frac{\alpha_a}{2}(x_1 - y_2 - x_3 + y_4) + \frac{\beta_a}{\sqrt{8}} (y_5 - x_6 + x_7 + y_8 - y_9 + x_{10} - x_{11} - y_{12}) \quad (1)$$

where the $x_i(y_i)$ are the oxygen orbitals $p_x^i(p_y^i)$, α_a and β_b are coefficients treated as variable parameters, and b_{1g} is the symbol of the irreducible representation of the point group symmetry D_{4h}. Other oxygen orbitals transforming according to the representations b_{2g} and e_g do not hybridize with the $d_{x^2-y^2}$ copper orbital and, therefore, are of no interest in the following.

The wave function for the oxygen hole in case (b) reads as follows:

$$P_{b_{2g}}^{(b)} = \frac{\alpha_b}{2}(y_1 - x_2 - y_3 + x_4) + \frac{\beta_b}{\sqrt{8}}(x_5 - y_6 + x_7 + x_8 - x_9 + y_{10} - y_{11} - x_{12}) \quad (2)$$

where b_{2g} is the symbol of irreducible representation of the point group symmetry D_{4h}. The coefficients α_b and β_b again are treated as variable parameters.
Due to the quantum coherence effect in the motion of the oxygen hole an important energy gain δ_p appears. For the case a) δ_p is given by

$$\delta_p^a = -2t^{xy}(\alpha_a + \beta_a\sqrt{2})^2 + t_\sigma^{xx} - \sqrt{8}t_\pi^{xx}\alpha_a\beta_a \quad (3)$$

and for the case b) by

$$\delta_p^b = -2t^{xy}(\alpha_b + \beta_b/\sqrt{2})^2 + \sqrt{8}t_\sigma^{xx}\alpha_b\beta_b - t_\pi^{xx} \quad (4)$$

Here t^{xy}, t_σ^{xx} and t_π^{xx} are the transfer integrals between oxygen orbitals. They are about 0.6 eV, 0.4 eV and 0.2 eV respectively [7,8]. Spin-spin coupling between the hole an oxygen and the hole an copper influences the magnetic structure in a more complicated way. Therefore, in the following we consider this influence in detail for each of both variants separately.

2. Cluster confining oxygen hole with the state $P_{b_{1g}}$

Spin-spin coupling between oxygen and copper holes arises in second order of perturbation theory and is given by

$$H_{ex}^{(1)} = -3t_\sigma^2\alpha_a^2 Z_a[\frac{1}{2} - 2(\bar{s}_p\bar{s}_{f_0})] \quad (5)$$

and

$$H_{ex}^{(2)} = -\frac{3}{8}t_\sigma^2(\alpha_a + \sqrt{2}\beta_a)^2 Z_a[1 - 2(\bar{s}_p\bar{S}_t)] \quad (6)$$

$\bar{s}_p$ is the spin of the oxygen hole, $\bar{s}_{f_0}$ and $\bar{S}_t$ are the spin operators of copper at the centre of Fig 1 a) and four at the neighbouring plaquette copper respectively, $t_{pd} = \frac{\sqrt{3}}{2}t_\sigma$ is the copper-oxygen transfer integral which in accordance to [7,8] is about 1 eV. The energy factor Z_a is written as following

$$Z_a = \frac{1}{U_{dd} - 2V_{pd} - \Delta - \delta_p^a} + \frac{1}{U_{pp} + \Delta + \delta_p^a} \quad . \quad (1)$$

U_{dd} and U_{pp} are the parameters of Coulomb repulsion of