Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

La2CuO4 isolator gap, AF structure and pseudogaps from spin-space entangled orbitals in the Hartree-Fock scheme ALEJANDRO CABO MONTES DE OCA, ICIMAF, ALEJANDRO CABO BIZET, CEADEN, Havana, Cuba — It is argued that a Hartree-Fock (HF) solution of a simple model of the Cu-O planes in La2CuO4, is able to predict its insulator character and antiferromagnetic (AF) order. Pseudogap HF states are also naturally emerging from the discussion. These results follow from the deletion of symmetry restrictions usually imposed on the variational orbitals. One of them is the simplification of the spinor projection to be +1/2 or -1/2, which strongly reduces the searching space of orbitals. We also remove the demand on the orbitals to have a Bloch structure in the starting lattice. It turns out that the most stable HF solution of the problem is an AF and insulating state associated to "spin-space" entangled orbitals. The evaluated magnetic moment per cell is 0.67 μB, a result that satisfactorily reproduces the measured value of 0.68 μB. Another HF state having higher energy arises which is paramagnetic and shows a pseudogap. It follows after only requiring the Bloch structure in the original lattice. A third paramagnetic but metallic solution is received by including both of the mentioned constraints.

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Date submitted: 01 Dec 2009

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