La2CuO4 isolator gap, AF structure and pseudogaps from spin-space entangled orbitals in the Hartree-Fock scheme

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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 $\mu_B$, a result that satisfactorily reproduces the measured value of 0.68 $\mu_B$. 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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