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Spin-space entangled orbitals in a Hartree-Fock scheme predicting the AF and insulator properties of La2CuO4 ALEJANDRO CABO MONTES DE OCA, Departamento de Fisica Teorica, Instituto de Cibernetica, Matematica y Fisica, La Habana, Cuba, ALEJANDRO CABO-BIZET, Centro de Estudios Aplicados al Desarrollo Nuclear, La Habana, Cuba — Its is argued that spin-orbit entangled single particle states in a Hartree-Fock scheme can describe the insulator and antiferromagnetic nature of La2CuO4, as independent particle properties. Therefore, a currently considered as a Mott insulator material, is represented as a Slater one. This curious outcome is not strange if we consider that, strictly speaking, correlation quantities should be defined by the differences between the exact result and the "best" Hartree-Fock one. The discussion opens a road for understanding the connections between the successful phenomenological Mott picture and the First Principle (Slater) schemes of calculations. The results also furnish a simple framework for further studying the normal state properties of HTc superconductors. In particular, the microscopic structure of the antiferromagnetic order and the isolator size of the gap in La2CuO4 are both explained as coherent effects coming from the entangled "spin-orbit" structure of the single particle Hartree-Fock states. The possibility of the stability of the isolator gap when temperature rises up to the experimental Neel value is argued to be allowed by the same entanglement effect.

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