NMR CHEMICAL SHIELDING TENSORS IN HIGH TEMPERATURE CUPRATE SUPERCONDUCTORS

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Some theoretical approaches to explain the microscopic origin of high temperature superconductivity assume that antiferromagnetic correlations play a crucial role. A large amount of NMR Knight shift data has been accumulated mainly for copper and oxygen nuclei in the CuO_2 planes, which are the basic structural elements in the cuprate superconductors.

Experimental information about static and dynamic spin susceptibilities is available by NMR measurements. To determine this quantity it is essential to know the chemical shifts. Experimentally, these are extracted from the Knight shifts at very low temperature, where, however, field inhomogeneities due to the vortex lattice impede precise measurements. Theoretically, the chemical shifts have so far only been estimated by very crude models. Improved theoretical values would strongly help to understand both static and dynamic spin susceptibilities.

Both, the ADF 2000 and Gaussian 98 packages provide tools for NMR calculations of open-shell systems. On this poster, we discuss preliminary results for NMR shielding tensors for copper and oxygen nuclei in CuO_2 layered materials.