Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Non-integral spin moment and electron correlation effects in magnetite P. A. MONTANO, U. of Illinois Chicago and USDOE, YINWAN LI, U. of Illinois Chicago and Argonne National Lab., B. BARBIELLINI, Northeastern U., P. E. MIJNARENDS, Delft U. of Tech. and Northeastern U., S. KAPRZYK, AGH (Poland) and Northeastern U., HSIN LIN, Northeastern U., A. BANSIL, Northeastern U. — In order to directly probe the electronic ground state of magnetic electrons, we have carried out temperature dependent magnetic Compton scattering experiments on an oriented single crystal of magnetite (Fe_3O_4). First principles band theory computations using the conventional local density approximation (LDA) as well as computations treating correlation effects beyond the LDA are used to gain insight into these measurements. The magnetic moment associated with unpaired spins in magnetite is found to be insensitive to temperature over the range of 10-300K with a value of about 3.6 μ_B/formula unit, including the region of the Verwey transition. The non-integral value of the spin moment implies that some majority spin states must be present at the Fermi energy (E_F) at all temperatures so that the polarization of electrons at the E_F cannot be 100%. Our analysis emphasizes the role of Fe^{2+} ions on the octahedral sites in producing a correlated ground state of magnetite and gives insight into the nature of the order parameter for Verwey transition and the lack of quenching of the orbital magnetic moment in the system. Work supported by the USDOE.

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Date submitted: 01 Dec 2004 Electronic form version 1.4