Abstract Submitted for the MAR15 Meeting of The American Physical Society

Spin zero-point fluctuations in d-metals VLADIMIR ANTROPOV, ANDREY KUTEPOV, Ames Laboratory, Ames, USA, KAY DEWHURST, SANGEETA SHARMA, MPI for Microstructure Physics, Halle, Germany — We analyze the structure and the strength of spin fluctuations at T=0 in pure metals: ferromagnetic 3d metals (Fe,Co,Ni) and paramagnetic Pd. The studies have been performed using obtained full tensor of generalized linear spin susceptibility in the density functional approach. Both real and imaginary frequencies integration with LAPW basis set have been implemented and tested for systems of different size. Our analysis is mainly focused on a decomposition of the fluctuating magnetic moment as a function of frequency and polarization near a point of magnetic instability. In addition we present the results when the external pressure and magnetic field applied. The obtained numbers have been incorporated into the traditional spin fluctuations theories. The spin fluctuation renormalization of mean field parameters has been found rather large and incompatible with the perturbation theory treatment. At the end we discuss the applicability of these theories for the analysis of real magnetic systems at low temperatures.

> Vladimir Antropov Ames Lab

Date submitted: 14 Nov 2014

Electronic form version 1.4