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Spin fluctuations in 3d paramagnetic metals ALEKSANDER WYSOCKI, ANDREY KUTEPOV, VLADIMIR ANTROPOV, Ames Laboratory, U.S. Department of Energy, Ames, Iowa 50011, USA — Spin fluctuations (SFs) in 3d paramagnetic metals were investigated using the linear response formalism within the time dependent density functional theory. An efficient scheme of frequency integration using the Matsubara technique has been implemented and tested. The SFs spectrum in 3d paramagnets is analyzed in real and reciprocal spaces as a function of frequency and temperature. For all materials the SFs are characterized by the coexistence of low and high energy branches which originate from different regions of the Brillouin zone. The low-energy ones can be measured by neutron scattering experiments while the high-energy SFs appear to be more localized. Further, we studied the nature of square of fluctuating magnetic moment in these materials. This work was supported, in part, by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy (DOE), and by the Office of Basic Energy Science, Division of Materials Science and Engineering. The research was performed at Ames Laboratory, which is operated for the U.S. DOE by Iowa State University under contract # DE-AC02-07CH11358.

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