

Abstract Submitted
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Transverse spin susceptibility in Ni, Fe and Co LIQIN KE, TAKAO KOTANI, MARK VAN SCHILFGAARDE, School of Materials, Arizona State University, Tempe, AZ, 85287-8706, VLADIMIR ANTROPOV, Ames Laboratory, Ames, IA, 50011, USA — We calculate the full transverse spin susceptibility $\chi^\pm(\mathbf{q}, \omega)$ in the time-dependent local density approximation(TDLDA) for elemental Ni, Fe and Co. We extract the Heisenberg exchange parameters from both the energy-dependent χ^\pm and the static one. The results are compared with those given by a method assuming the rigid rotation of the magnetic moments at each site(ref.kotani2008). We observe some differences between these two methods, especially around the Brillouin zone boundaries. We also calculate χ^\pm starting from the non-interacting Hamiltonian generated from the quasiparticle self-consistent GW(QSGW) approximation (ref.Kotani2007). We analyze how the QSGW potential alter the LDA results.

Ref.

T.Kotani and M van Schilfgaarde, J. PHYS. C 20, 295214 (2008) T.Kotani, M. van Schilfgaarde, S. V. Faleev Phys. Rev. B 76, 165106 (2007)

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