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Spin excitations in solids from first principles ARNO SCHINDLMAYR, Department Physik, Universitaet Paderborn, Germany, ERSOY SASIOGLU, MANFRED NIESERT, CHRISTOPH FRIEDRICH, STEFAN BLÜGEL, Forschungszentrum Juelich, Germany — The long-range order of the electron spins in magnetic solids gives rise to additional excitation modes that preserve the charge density but change the total spin of the electron system. While Stoner excitations, which correspond to spin-flip transitions between the majority and minority channels, can be described within a single-particle picture, spin waves are collective modes that result from the spin-dependent exchange interaction between the electrons. Here we discuss different approaches that we have explored for material-specific spin-wave calculations from first principles. All of these methods focus on the non-local and dynamic transverse spin susceptibility, whose spectral function can be directly related to experimental spectroscopies, but employ either time-dependent density-functional theory or many-body perturbation theory to treat exchange and correlation. In the latter case, maximally localized Wannier orbitals are used to efficiently obtain the electron-hole vertex of the multiple-scattering T matrix, which is constructed with full frequency and wave-vector dependence. The implementation uses the full-potential linearized augmented-plane-wave (FLAPW) method. For ferromagnetic transition metals like Fe, Co or Ni our results are in good agreement with experimental data and reproduce all important spectral features.

Arno Schindlmayr
Universitaet Paderborn

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