

Time-dependent magnons from first principles

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We propose an efficient and not perturbative scheme to compute magnetic excitations for extended systems employing the framework of time-dependent density-functional theory. Within our approach we drive the system out of equilibrium using an ultra-short magnetic kick perpendicular to ground-state magnetization of the material. The dynamical properties of the system are obtained by propagating the time-dependent Kohn-Sham equations in real time and the analysis of the time-dependent magnetization reveals the transverse magnetic excitation spectrum of the magnet. We illustrate the performance of the method by computing the magnetization dynamics, obtained from a real-time propagation, for iron, cobalt and nickel and compare them to known results obtained using the linear-response formulation of time-dependent density-functional theory. Moreover, we point out that our time-dependent approach is not limited to the linear-response regime, and we present first results for non-linear magnetic excitations from first-principles in iron.