

Magnons from first principles using time-dependent density-functional perturbation theory

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Understanding and predicting collective spin excitations from first principles remains challenging, particularly in materials with localized electronic states, strong spin-orbit coupling, or noncollinear magnetic order. In this talk, I will present a first-principles framework for calculating magnon spectra based on time-dependent density-functional perturbation theory (TDDFPT) and the Liouville-Lanczos approach [1]. The method avoids explicit sums over empty states and frequency-by-frequency solutions of the linear-response equations, while naturally accounting for the coupling between spin and charge fluctuations. Magnon spectra are obtained efficiently from the dynamical spin susceptibility using a single Lanczos chain for each wave vector and polarization.

I will first discuss the implementation of this approach in the turboMagnon code [2], an open-source component of Quantum ESPRESSO [3], and its validation for bulk Fe and Ni. The framework is formulated in a general noncollinear setting and includes spin-orbit coupling self-consistently, enabling the study of complex magnetic systems. I will then show how TDDFPT can be combined with self-consistent, *ab initio* Hubbard U corrections [4], providing a parameter-free description of spin excitations in materials with localized electronic states [5]. Applications to NiO and MnO demonstrate excellent agreement with neutron-scattering experiments and highlight the importance of treating the dynamical response and Hubbard contributions consistently [6].

The versatility of the approach will be illustrated through two-dimensional and unconventional magnetic systems. For monolayer CrI₃, TDDFPT reveals the role of spin-orbit coupling and interlayer interactions in the zone-border magnon gap [7] and, together with lattice-dynamical calculations, points to magnon-phonon coupling as an important additional mechanism [8]. Finally, I will present recent results for the prototypical altermagnet MnTe, where TDDFPT+ U reproduces both the magnon dispersion and the experimentally observed chiral magnon splitting, and predicts its evolution under pressure.

Overall, these results establish TDDFPT and Liouville-Lanczos methods as an efficient and broadly applicable route to quantitative first-principles modeling of magnons, providing access to magnetic excitations beyond conventional mappings onto model spin Hamiltonians.

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