

Abstract Submitted
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Efficient computation of Magnon dispersions within Time Dependent Density Functional Theory Using Maximally Localized Wannier Functions BRUNO ROUSSEAU, CSIC - Centro de Física de Materiales, ASIER EIGUREN, AITOR BERGARA, Condensed Matter Physics Department, University of the Basque Country — An efficient scheme is presented to compute the transverse magnetic susceptibility within time dependent density functional theory from which magnon dispersions can be extracted. The scheme makes use of maximally localized Wannier functions in order to interpolate the band structure onto a fine k-mesh in order to converge sums on the first Brillouin zone. An optimal real space basis set containing few basis functions is shown to be sufficient to extract the magnon dispersion, making computations very efficient. The gap error in the magnon dispersion at Γ , numerically violating Goldstone's theorem, is analysed and a correction scheme is devised which can be generalized to systems where Goldstone's theorem does not apply. The method is applied to the computation of the magnon dispersion of bulk bcc iron and fcc nickel.

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