Local spin Hamiltonians in ab initio spin dynamics

S. Streib,[1] A. Szilva,[1] V. Borisov,[1] M. Pereiro,[1] A. Bergman,[1] E. Sjöqvist,[1] A. Delin,[2,3] M. I. Katsnelson,[4] O. Eriksson,[1,5] and D. Thonig[5,1]

[1] *Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden*
[2] *Department of Applied Physics, School of Engineering Sciences, KTH Royal Institute of Technology, Kista, Sweden*
[3] *Swedish e-Science Research Center (SeRC), KTH Royal Institute of Technology, Stockholm, Sweden*
[4] *Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands*
[5] *School of Science and Technology, Örebro University, Sweden*

The derivation of effective spin Hamiltonians from ab initio electronic structure calculations is an important tool for modeling the spin dynamics of magnetic materials since a full electronic description of the dynamics is numerically very challenging. We contrast two different approaches that we label as "local" and "global". The global approach aims at describing arbitrary spin configurations, whereas the local approach is only valid for small magnetic fluctuations locally around a given spin configuration. We argue that global symmetry requirements, such as time-reversal symmetry, do not necessarily restrict local spin Hamiltonians if the dependence of the effective exchange parameters on the magnetic state is taken into account. We present a general formalism to map tight-binding electronic structure theory to a local spin Hamiltonian and we check our formalism by means of numerical calculations for iron dimers and chains [1].

References:

[1] S. Streib et al., "Exchange constants for local spin Hamiltonians from tight-binding models", arXiv:2103.04726.