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mamonca: magnetic Monte Carlo code

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Summary

Magnetic interactions account for a significant portion of free energy in certain materials, ranging from iron, whose ground state would be wrongly predicted without considering magnetic interactions (Friák et al., 2001), to the magnetocaloric effects of Heusler alloys (Weiss & Piccard, 1917), whose magnetic properties could allow for the development of highly efficient refrgiration systems. In materials science, the Heisenberg model is frequently employed to heuristically compute the potential energy. There are two main methods to make use of the Heisenberg model at finite temperature: one is the Monte Carlo method for an efficient free energy minimization, the other is spin dynamics for the calculation of spin configuration evolution.

Statement of need

`mamonca` is a C++-based python software package for the computation of magnetic interactions in solid materials. All inputs and outputs are given by setters (starting with `set_`) and getters (starting with `get_`), in order for `mamonca` to spare file-reading and writing, in strong contrast to other existing software packages (Bauer et al., 2011; Evans et al., 2014; Hellsvik et al., 2011; Kawamura et al., 2017). As a result, it has excellent interactivity, as the parameters can be changed on-the-fly, as well as the outputs can be retrieved at any interval chosen by the user. With `mamonca`, the user can analyse any structure that can be defined by other software packages such as Atomic Structure Environment (ASE) (Larsen et al., 2017) or pyiron (Janssen et al., 2019), as it takes only the exchange parameters and does not require the knowledge of the structure, which is a strong contrast to existing software packages (Bauer et al., 2011; Kawamura et al., 2017). `mamonca` has also high flexibility in defining the Hamiltonian, as it allows the user to define not only the classical Heisenberg model, but higher order components including the longitudinal variation, as it has been employed for Fe-Mn systems (Schneider et al., 2021). The input parameters for the Hamiltonian can be straightforwardly obtained using a workflow tool such as pyiron, or other calculation software packages such as TB2J (He et al., 2021). In addition to the classical Monte Carlo and spin-dynamics, `mamonca` allows also for an addition of Metadynamics (Theodoropoulos et al., 2000) and magnetic thermodynamic integration (Frenkel & Smit, 2023), which can deliver the free energy variation. To authors' knowledge, it is the only one code that is able to run Monte Carlo calculations with Metadynamics and magnetic thermodynamic integration.

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