The Journal of Open Source Software

mamonca: magnetic Monte Carlo code

Osamu Waseda [1*¶], **Tilmann Hickel** [1*], **and Jörg Neugebauer** [1]

1 Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, D-40237 Düsseldorf, Germany ¶ Corresponding author * These authors contributed equally.

DOI: 10.xxxxxx/draft

Software

- Review
- Repository
- Archive

Editor: Kelly Rowland

Reviewers:

- @arjunsavel
- @vipinagrawal25

Submitted: 10 November 2023
Published: unpublished

In partnership with

AMERICAN ASTRONOMICAL SOCIETY

This article and software are linked with research article DOI 10.3847/xxxxx <- update this with the DOI from AAS once you know it., published in the Astrophysical Journal <- The name of the AAS journal..

Summary

Magnetic interactions account for a significant portion of free energy in certain materials, ranging from relatively simple systems such as iron to complex magnetocaloric effects of Heusler alloys (Weiss & Piccard, 1917). More specifically, in the case of iron, the ground state would be wrongly predicted without considering magnetic interactions (Friák et al., 2001). In Heusler systems, the understanding of 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 magnetic part of 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. The Monte Carlo method has the advantage of obtaining the free energy rapidly, while spin dynamics would deliver also the kinetics of the system. `mamonca` allows for the evaluation of the Heisenberg Hamiltonian with extended terms using both Monte Carlo method and spin dynamics.

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 `mamonca` 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). A typical workflow with pyiron would consist of a general set of physical parameters (chemical element, lattice parameter etc.), which is then evaluated by the software of user's choice. The results can be straightforwardly evaluated to obtain the exchange parameters with the existing tools inside pyiron. Finally, `mamonca` can run to deliver the finite temperature effects of the magnetic part. This means, the user in principle needs only to insert physical parameters to obtain the magnetic finite temperature behaviour they are interested in. 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. It is crucial to include these features within the code, as they have to be applied at each step of the simulation and cannot be evaluated in the post-processing. To authors' knowledge, it is the only one code that is able to run Monte Carlo calculations with Metadynamics and magnetic thermodynamic integration.

Acknowledgements

We gratefully acknowledge the financial support from the German Research Foundation (DFG) under grant HI 1300/15-1 within the DFG-ANR project C-TRAM.

References

Bauer, B., Carr, L., Evertz, H. G., Feiguin, A., Freire, J., Fuchs, S., Gamper, L., Gukelberger, J., Gull, E., Guertler, S., & others. (2011). The ALPS project release 2.0: Open source software for strongly correlated systems. *Journal of Statistical Mechanics: Theory and Experiment*, *2011*(05), P05001.

Evans, R. F., Fan, W. J., Chureemart, P., Ostler, T. A., Ellis, M. O., & Chantrell, R. W. (2014). Atomistic spin model simulations of magnetic nanomaterials. *Journal of Physics: Condensed Matter*, *26*(10), 103202. https://doi.org/10.1088/0953-8984/26/10/103202

Frenkel, D., & Smit, B. (2023). *Understanding molecular simulation: From algorithms to applications*. Elsevier.

Friák, M., Šob, M., & Vitek, V. (2001). Ab initio calculation of phase boundaries in iron along the bcc-fcc transformation path and magnetism of iron overlayers. *Physical Review B*, *63*(5), 052405.

He, X., Helbig, N., Verstraete, M. J., & Bousquet, E. (2021). TB2J: A python package for computing magnetic interaction parameters. *Computer Physics Communications*, *264*, 107938. https://doi.org/10.1016/j.cpc.2021.107938

Hellsvik, J., Skubic, B., & Taroni, A. (2011). *Uppsala atomistic spin dynamics user guide*.

Janssen, J., Surendralal, S., Lysogorskiy, Y., Todorova, M., Hickel, T., Drautz, R., & Neugebauer, J. (2019). Pyiron: An integrated development environment for computational materials science. *Computational Materials Science*, *163*, 24–36. https://doi.org/10.1016/j.commatsci.2018.07.043

Kawamura, M., Yoshimi, K., Misawa, T., Yamaji, Y., Todo, S., & Kawashima, N. (2017). Quantum lattice model solver hΦ. *Computer Physics Communications*, *217*, 180–192.

Larsen, A. H., Mortensen, J. J., Blomqvist, J., Castelli, I. E., Christensen, R., Dułak, M., Friis, J., Groves, M. N., Hammer, B., Hargus, C., & others. (2017). The atomic simulation environment—a python library for working with atoms. *Journal of Physics: Condensed Matter*, *29*(27), 273002.

Schneider, A., Fu, C.-C., Waseda, O., Barreteau, C., & Hickel, T. (2021). Ab initio based models for temperature-dependent magnetochemical interplay in bcc fe-mn alloys. *Physical Review B*, *103*(2), 024421.

Theodoropoulos, C., Qian, Y.-H., & Kevrekidis, I. G. (2000). "Coarse" stability and bifurcation analysis using time-steppers: A reaction-diffusion example. *Proceedings of the National Academy of Sciences*, *97*(18), 9840–9843. https://doi.org/10.1073/pnas.97.18.9840

Weiss, P., & Piccard, A. (1917). Le phénomène magnétocalorique. *J. Phys. Theor. Appl.*, *7*(1), 103–109. https://doi.org/10.1051/jphystap:019170070010300