Bachelor/Master Thesis Topic

Optimizing a Neural Network Approach for the Reverse Transformation of Spin-Wave-Theory

Motivation and Background. In collaboration with the Helmholtz-Zentrum Berlin [1], data science methods have emerged as a tool towards understanding magnetic materials and the fundamental physics arising from them. Specifically, they allow the analysis and search of interesting and useful novel quantum magnets as well as materials with strong correlated electrons [2,3,4]. The conventional procedure is to compare experimental measurements of the magnetic excitation spectrum with spin-wave calculations e.g. by using the software package SpinW [5]. Machine learning can provide more effective routes in finding the characteristic parameters responsible for their magnetic behavior.

Goals. The goal of this thesis is to optimize a neuronal network to do a reverse transformation from the measurement data to the fundamental parameters governing the physical properties. A fully-coupled neural network already exists as a proof-of-concept.

Description of the Task

The specific tasks are:

- Understand the workflow and the analysis strategy
- Model better trainings data sets
- Develop tools for model validation
- Optimize the existing neural network

Research Type

Theoretical Aspects:	*****
Industrial Relevance:	*****
Implementation	*****

Prerequisite

The student should be enrolled in the bachelor/master of computer science program, and has completed the required course modules to start a bachelor/master thesis.

Skills required

Programming skills in Python.

Contacts

Software Engineering Group, Institut für Informatik, Humboldt-Universität zu Berlin and J.-U. Hoffmann Helmholtz-Zentrum Berlin

Application

Please contact me during my office hours or send me an email with the title: "[ThesisProject]-SpinW" to hoffmann-j@helmholtz-berlin.de and se-career@informatik.hu-berlin.de

References

[1] Helholtz-Zentrum Berlin: Institute for Quantum Phenomena in Novel Materials: https://www.helmholtz-berlin.de/forschung/oe/qm/quantenphaenomene/datascience/

[2] Physical realization of a quantum spin liquid based on a complex frustration mechanism C. Balz, B. Lake, J. Reuther, H. Luetkens, R. Schönemann, T. Herrmannsdörfer, Y. Singh, A. T. M. N. Islam, E. M. Wheeler, J. A. Rodriguez-Rivera, T. Guidi, G. G. Simeoni, C. Baines, H. Ryll. Nature Physics12, 942–949 (2016) https://www.nature.com/articles/nphys3826

[3] Field-induced quantum spin-1/2 chains and disorder in Nd2Zr2O7 J. Xu, A. T. M. N. Islam, I. N. Glavatskyy, M. Reehuis, J.-U. Hoffmann, and B. Lake, Phys. Rev. B 98, 060408(R) (2018); https://link.aps.org/doi/10.1103/PhysRevB.98.060408

[4] Theory of multiple-phase competition in pyrochlore magnets with anisotropic exchange with application to Yb2Ti2O7, Er2Ti2O7, and Er2Sn2O7; H. Yan, O. Benton, L. Jaubert, N. Shannon; Phys. Rev. B 95, 094422 (2017) https://link.aps.org/doi/10.1103/PhysRevB.95.094422

[5] Linear spin wave theory for single-Q incommensurate magnetic structures; S. Toth, B. Lake; J. Phys.: Condens. Matter 27, 166002 (2015). https://doi.org/10.1088%2F0953-8984%2F27%2F16%2F166002