Ecole Polytechnique Fédéral de Lausanne (EPFL, Switzerland), Paul Scherrer Institute (PSI, Switzerland) and Institut Laue-Langevin (ILL, France) jointly invite applications for a three-year PhD program focusing on

Physics informed machine learning on quantum magnetic systems

The PhD project is part of a three-year collaboration between the three institutes. The student will be based in Grenoble, France, with several prolonged visits at PSI and EPFL. She or he will be affiliated with the Laboratory of Theoretical and Computational Physics at EPFL under the supervision of Prof. Dr. Andreas Martin Läuchli Herzig.

In this project we propose to develop a fundamental new concept to efficiently measure the spin-spin correlations of quantum magnetic systems with inelastic neutron scattering. Notably, we intend to combine prior physical available information, such as the form of theoretically predicted spin Hamiltonians, with machine-learning algorithms to optimize the number of experimentally required data points. This approach is opposite to so-called data-driven methods which aim to maximize the amount of experimental data, or methods that extract data patterns and physical information with the help of neural networks or similar AI techniques.

Our goal is to determine the most accurate model Hamiltonian of a material, and to determine the relevant model parameters up to a user defined precision. This should be accomplished during the experiment, in contrary to traditional methods where a detailed data analysis is usually done after the experiment. Our proposal will be achieved via two key steps, a *probabilistic evaluation* (predicted mean, uncertainty estimates) of the model parameters after every newly acquired data point, and the development of *decision policies* to determine the most promising location of the next data point in a higher dimensional data space. Using a complete autonomous feed-back loop, the algorithms will train themselves via reinforcement (active) learning, thereby assisting the scientists with statistically founded predictions during the course of the experiments.

The central task of the successful candidate will involve the development and test of various algorithms, and to benchmark them against established acquisition strategies. Thereby the student will build on existing concepts of autonomous experiments, including the ones recently developed by us and by other groups. The student will also participate in on-going research projects in the field of quantum magnetism, and will thereby test the developed methods via cutting edge research problems.

We are looking for a highly motivated candidate with a MSc in physics, applied mathematics or material science. Applications (including brief motivation letter, CV and a contact person for a reference) should be sent to Andreas Martin Läuchli Herzig (andreas.laeuchli@psi.ch), Daniel Mazzone (daniel.mazzone@psi.ch) and Martin Boehm (boehm@ill.fr).

Deadline: 24 September 2023.