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Machine learning short-range spin correlations in pyrochlore antiferromagnet Gd2Hf2O7

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Discovering new phases of condensed matter with novel properties is of vital importance for fundamental and applicational research. Classical Monte Carlo simulations are commonly employed to study phases by stochastically sampling states and evaluating physical quantities from such states. Recently, machine learning has proven useful in classifying, identifying, or interpreting datasets from Monte Carlo simulations of classical spin models [1]. In this study, we utilized machine learning to analyze spin states in real materials, in conjunction with polarized neutron diffuse neutron scattering and reverse Monte Carlo refinements.

The pyrochlore antiferromagnet serves as a prototypical model for studying frustrated magnetism, offering a fertile ground for novel states where conventional long-range orders are generally suppressed [2]. We synthesized a candidate material, Gd2Hf2O7, and investigated its magnetic properties using macroscopic and neutron scattering measurement techniques. Although ordering and spin glass transitions were indicated by AC susceptibility, polarized neutron diffuse scattering revealed a liquid-like magnetic structure factor without any magnetic Bragg peaks. Reverse Monte Carlo refinement of the scattering pattern was employed to generate spin configurations that could reproduce the observed structure factor. Principal component analysis was found to successfully identify short-range Palmer-Chalker spin correlations in Gd2Hf2O7, as predicted by theorists [2].

References

[1] J. Carrasquilla and R. G. Melko, Nature Physics 13, 431 (2017).
[2] S. E. Palmer and J. T. Chalker, Physical Review B 62, 488 (2000).

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