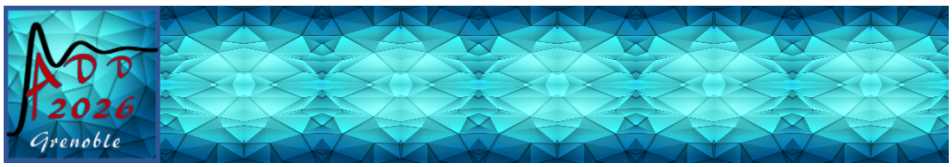

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Using mPDF to probe magnetic exchange interactions

Content

Determining magnetic exchange interactions is vital for understanding the magnetic behavior of materials. The standard method for exchange interaction determination involves performing inelastic neutron scattering experiments on single crystals to measure spin wave dispersions from a long-range-ordered magnetic ground state. However, the influence of exchange interactions is not limited exclusively to spin waves in ordered states but also governs the system's physics in all magnetic states, including the short-range correlations that persist into the paramagnetic regime. Exchange parameters have been successfully recovered in the past from energy-integrated diffuse neutron scattering data from paramagnets, indicating that the diffuse scattering and underlying short-range magnetic correlations are rich in information. Consequently, magnetic pair distribution function (mPDF) analysis, which directly probes short-range magnetic correlations, is expected to be well suited for extracting exchange parameters from correlated paramagnets. Here, we demonstrate two approaches for determination of exchange parameters from mPDF data, including Monte Carlo mPDF simulations and a robust mean-field theory approach. In the latter case, we incorporate the Onsager reaction field to develop an analytical model for exchange interaction determination from the mPDF. We showcase several materials where we use real-space magnetic correlation data to successfully recover exchange interaction values comparable to literature values.

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