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Magnetic pair distribution function analysis: introduction and applications

B. Frandsen[1], X. Yang[2], S. Billinge[2,3]
[1]Columbia University, Department of Physics, New York, United States, [2]Columbia University, Department of Applied Physics and Applied Mathematics, New York, United States, [3]Brookhaven National Laboratory, Condensed Matter Physics and Materials Science Department, Upton, United States

Short-range magnetic correlations play a crucial role in a variety of condensed matter phenomena, yet they remain notoriously difficult to investigate experimentally. Quantitative analysis of the diffuse scattering of neutrons from local magnetic correlations represents a viable but challenging route toward revealing short-range magnetic order in complex materials. Reverse Monte Carlo techniques that iteratively fit randomly generated structural models in momentum space have been used successfully [1], demonstrating that diffuse magnetic scattering can be rich in information. Recently [2], we developed a real-space approach to investigating local magnetic correlations, which we call magnetic pair distribution function (mPDF) analysis in analogy to the more familiar atomic pair distribution function. This experimentally accessible quantity reveals magnetic correlations directly in real space and places diffuse and Bragg scattering on equal footing, thereby gaining sensitivity to both short- and long-range magnetic order. Here we present the basic theory behind mPDF analysis and provide several examples of its utility using both simulated and experimentally measured data on several interesting magnetic systems, including a canonical antiferromagnetic, a spin glass, and a spin ice. We discuss the potential impact that mPDF methods may have on current and future research interests in magnetism.

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