Recent Advances in Magnetic PDF Analysis: A Case Study with MnTe

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Short-range magnetic correlations play an important role in numerous condensed matter systems of both fundamental and applied interest, ranging from quantum spin liquids to superconductors to technologically relevant magnetic alloys. When probed by neutron scattering, these short-range correlations give rise to diffuse magnetic scattering. Analyzing this diffuse magnetic scattering has been challenging historically, making it difficult to extract detailed information about the short-range magnetic correlations of interest. Magnetic pair distribution function (mPDF) analysis of neutron total scattering data has recently emerged as one promising method for probing short-range magnetism via Fourier transformation of the diffuse scattering, providing a real-space view of pairwise correlations between magnetic moments. Here, I will present recent advances in mPDF analysis using a comprehensive mPDF investigation of the antiferromagnetic semiconductor MnTe as a case study. These advances include improved software infrastructure, more effective methods for modeling magnetic and atomic PDF data together, tools for three-dimensional mPDF analysis of single crystals, the use of polarized neutrons, and more. Along the way, we will build a detailed and quantitatively accurate picture of the short-range magnetic correlations present above the Neel temperature in MnTe.

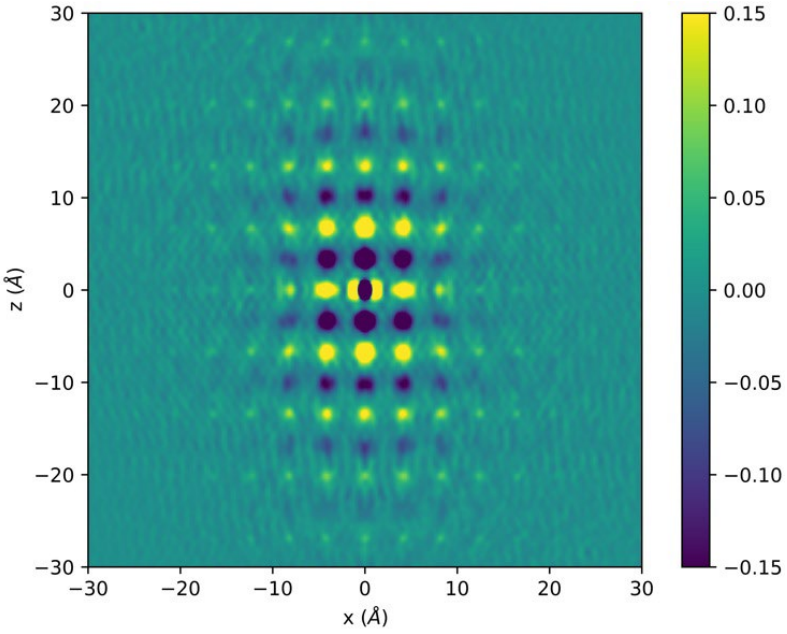

Figure 1