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Empirical Magnetic Structure Solution of Frustrated Spin Systems

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Frustrated spin systems can exhibit a macroscopic degeneracy of magnetic ground states which suppresses periodic magnetic order [1]. The importance of understanding these correlations lies primarily in determining the origin of exotic phenomena that emerge from frustrated spin systems, e.g. the evolution of high-temperature superconductivity from spin liquids and the ability of spin ices to support emergent magnetic charges [2]. The magnetic structures of ordered magnets can usually be determined by crystallographic analysis of the magnetic Bragg scattering observed in neutron diffraction experiments. However, the suppression of periodic magnetic order in frustrated magnets means that only magnetic diffuse scattering is observed. This has led to a consensus that single-crystal data are needed for a detailed understanding of spin correlations in frustrated systems. In my presentation, I will explore how the powder magnetic diffuse scattering pattern I(Q) can be converted robustly into a magnetic-structure model. Our approach is to consider simulated I(Q) data for a number of test cases. These data are then fitted using the reverse Monte Carlo (RMC) method. Finally, the quality of the models obtained is assessed by calculating the 3D scattering function I(Q). I will show that the extent of information loss during spherical averaging of I(Q) is surprisingly minimal, and that the full I(Q) is recoverable from powder diffraction data for each frustrated system that we explore [3]. I will go on to discuss real examples where we have used the RMC approach to obtain insight into frustrated materials. First, I will examine the interplay between geometrical frustration and low dimensionality in the paramagnetic phase of the spin-chain compound Ca3Co2O6. Finally, I will show how the RMC method can be extended for the analysis of large single-crystal diffuse scattering datasets, using as an example the canonical antiferromagnet MnO.

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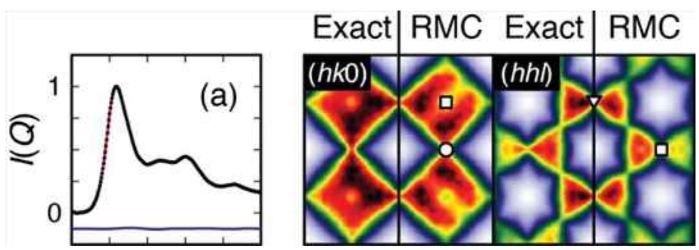

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