Scattering Signatures of Bond-Dependent Magnetic Interactions

Joseph Paddison[1]
[1]Oak Ridge National Laboratory
paddisonja@ornl.gov

Bond-dependent magnetic interactions can generate exotic topological states such as Kitaev spin liquids [1]. Such states have potential applications for topological quantum computation, and are of fundamental interest because they can show entangled ground states whose excitations have fractional quantum numbers [2].

Robust determination of bond-dependent interactions is key to identifying candidate quantum materials. However, such interactions are challenging to measure experimentally [3]. In this talk, I explore the extent to which bond-dependent interactions can be extracted from diffuse magnetic neutron-scattering data measured in the paramagnetic phase. I proceed by simulating such data for bond-dependent "test cases" on triangular and honeycomb lattices [4]. I show that each nearest-neighbor interaction has a distinct signature in magnetic diffuse-scattering data, and that such data contain sufficient information to determine the magnetic interactions unambiguously via unconstrained fits [5]. Remarkably, powder data also retain some sensitivity to bond-dependent interactions, and can constrain them when single-crystal samples are unavailable.

I demonstrate applications of this approach to experimental data for the triangular-lattice quantum spin-liquid candidate YbMgGaO4 [6] and the candidate Kitaev honeycomb material NaNi2BiO6–δ (δ = 0.33) [7]. I conclude by discussing its advantages and limitations in the context of crystallographic approaches to diffuse-scattering analysis such as reverse Monte Carlo and pair-distribution function refinement.

[1] Kitaev, Ann. Phys. 303, 2 (2003).
[2] Broholm et al. Science 367, eaay0668 (2020).
[3] Laurell & Okamoto, npj Quantum Mater. 5, 2 (2020).
[4] Chaloupka & Khaliullin, Phys. Rev. B 92, 024413 (2015).
[5] Paddison, Phys. Rev. Lett. 125, 247202 (2020).
[6] Paddison et al. Nat. Phys. 13, 117–122 (2017).
[7] Scheie et al. Phys. Rev. B 100, 214421 (2019).

Funding: Laboratory Directed Research and Development Program of Oak Ridge National Laboratory.

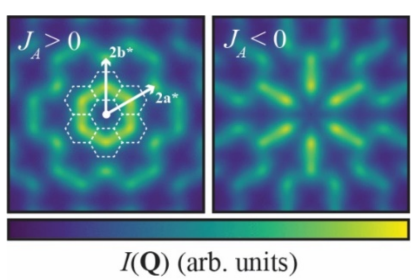

Figure 1