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First-principles calculations of noncollinear magnetization densities in quantum materials

Neutron scattering is an established workhorse for detecting signatures of quantum spin liquids (QSLs) including fractionalized excitations. However, this depends on having accurate magnetic form factors to analyze signals. These are commonly treated in an isolated, isotropic ion approximation, but the local magnetic degrees of freedom in QSL candidate materials are $j_{eff}=\frac{1}{2}$ moments which are anisotropic [1] and hybridize with nearby anions. We have developed a Wannier function-based method to simulate both the spin and orbital contributions to the magnetic interaction vector. We show that the associated real-space magnetization densities exhibit intra-atomic noncollinearity. These facets will notably affect neutron scattering measurements and advance beyond the basic magnetic form factor. Using α-$RuCl_3$ as an example, we identify specific scattering directions for neutron experiments to optimally detect the unique quality of the noncollinear magnetization density.

[1] Colin L. Sarkis et al, Phys. Rev. B 109, 104432 (2024).

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