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How to identify and resolve beyond-geometrical frustration

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In this talk, we will discuss recent theoretical developments triggered by the experimental discoveries of iridium oxides α, β, γ-Li_2IrO_3. In these polytypes, spin-orbit-coupled J=1/2 moments form 2D and 3D lattices (honeycomb, hyperhoneycomb and stripyhoneycomb) which generalize the 2D honeycomb lattice. Scattering experiments on these compounds have uncovered a peculiar non-coplanar incommensurate magnetic order, involving spirals which counter-rotate across neighboring sites. We discuss the emergence of this ordering, and the striking similarities visible across the three Li_2IrO_3 structures. The model Hamiltonians that capture the materials indicate strong magnetic frustration, which arises from spin-orbit coupling. Tuning the frustration, perhaps by just a 10% Hamiltonian perturbation, exposes a fractionalized phase: Kitaev's three-dimensional quantum spin liquid (QSL). What is its range of stability to the competing Hamiltonian terms which occur in the materials, such as antiferromagnetic Heisenberg exchange? The frustration prohibits direct computations. Instead, we demonstrate a viable approach by numerically solving the model in a fully quantum infinite-dimensional approximation, which captures both the magnetically ordered and the QSL phases. Finally, we discuss the phenomenology of the QSL phase, including the role of its emergent magnetic-like field lines in stabilizing its deconfined fermion excitations to finite temperatures. The resulting phase transition is a signature unique to three-dimensional fractionalization.