Towards Kitaev Spin Liquid in 3d Transition Metal Compounds

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The idea of realizing the Kitaev honeycomb model in iridates and ruthenates with d^5 electronic configuration [1] attracted a lot of interest in the last decade. In these materials the large spin-orbit coupling (SOC) combines the spin and orbital moments into pseudospins-1/2 forming the basis for the magnetic model. Due to the orbital component, the superexchange interactions among pseudospins acquire strong bond-selective anisotropy. Evidence is mounting that the dominant pseudospin interaction is indeed of the predicted Kitaev type but the main attraction – the quantum spin-liquid phase – is hampered by the presence of subdominant interactions stabilizing long-range zigzag magnetic order.

An interesting alternative was proposed recently – 3d honeycomb systems with d^7 ions such as Co^{2+} were suggested to host Kitaev physics as well [2,3]. A natural question is raised: Is the SOC in 3d compounds strong enough to overcome the orbital moment quenching by crystal fields? To address this, we study in detail the exchange interactions derived for honeycomb cobaltates including trigonal crystal field Δ and construct the corresponding phase diagram using the numerical method introduced in [4]. We find that the pseudospin-1/2 Hamiltonian is dominated by Kitaev interaction for a broad range of Δ values and the non-Kitaev terms nearly vanish at small Δ, resulting in spin liquid ground state. Considering $Na_3Co_2SbO_6$ as an example, we find that this compound is proximate to a Kitaev spin liquid phase, and can be driven into it by slightly reducing Δ by about 20 meV. Here the smaller SOC of 3d compounds actually comes as an advantage – it enables to easily tune the interactions, e.g., via strain or pressure control. We thus argue that cobaltates may offer the most promising search area for Kitaev model physics.

References:

[1] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009)
[2] H. Liu and G. Khaliullin, Phys. Rev. B **97**, 014407 (2018)
[3] R. Sano, Y. Kato, and Y. Motome, Phys. Rev. B **97**, 014408 (2018)
[4] J. Chaloupka and G. Khaliullin, Phys. Rev. B **94**, 064435 (2016)
[5] H. Liu, J. Chaloupka, and G. Khaliullin, Phys. Rev. Lett. **125**, 047201 (2020)