

Abstract template for Conference and Advanced School on Low-Dimensional Quantum Systems I (smr 3820)

Paula Mellado¹

¹ *Universidad Adolfo Ibañez, Chile*

In the Vander Waals antiferromagnet NiPS₃, Ni atoms have spin $S=1$ and realize a honeycomb lattice. Six sulfur atoms surround the Ni, and in monolayers, the crystal field of the sulfurs splits their d manifold into three filled and two unfilled sets of bands. Aimed to determine the effective spin hamiltonian of NiPS₃, we study the exchange mechanism of the minimal two-band half-filled Hubbard model. Hopping between Ni atoms is mediated by sulfur atoms, and therefore, a superexchange mechanism becomes relevant to determine the effective exchange couplings in the system. In the limit of strong electronic correlations, we compute first, second, and third neighbor bilinear exchange couplings and find that the biquadratic spin interaction is relevant in this system. Using variational approximation, we study the magnetic ground states phase diagram of the effective XXZ spin model with biquadratic interactions on the honeycomb lattice and find some of the magnetic states reported in bulk samples of NiPS₃ at low temperatures.

- [1] R. Basnet, A. Wegner, K. Pandey, S. Storment, and J. Hu, Physical Review Materials 5, 064413 (2021).
- [2] C. Autieri, G. Cuono, C. Noce, M. Rybak, K. M. Kotur, C. E. Agrapdis, K. Wohlfeld, and M. Birowska, The Journal of Physical Chemistry C 126, 6791 (2022).
- [3] C. Lane and J.-X. Zhu, Physical Review B 102, 075124 (2020).
- [4] K. Kim, S. Y. Lim, J.-U. Lee, S. Lee, T. Y. Kim, K. Park, G. S. Jeon, C.-H. Park, J.-G. Park, and H. Cheong, Nature Communications 10, 1 (2019).