Exploring phonon-magnon band structures for CrI_3: Fundamental calculations, topological properties, and thermal Hall effect implications

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While phonon and magnon bands can traditionally be calculated by diagonalizing the dynamical matrix and solving the Landau-Lifshitz equation, respectively, the study of band structures that incorporate phonon-magnon interactions is still in its infancy. In our recent work [1,2], we have developed a method that treats phonons and magnons on an equal footing, focusing on zone-center modes. We are currently extending this approach to finite momenta, utilizing both the finite-difference method and a recently developed density-functional perturbation theory approach [3].

In this presentation, we will showcase the phonon-magnon band structures for both bulk and monolayer CrI_3, highlighting numerous anti-crossing points. We will demonstrate the calculation of the Chern number and confirm the existence of non-trivial topology in the magnon bands. Additionally, we will address the puzzle of the magnon Dirac gap observed in inelastic neutron scattering experiments and provide our insights into this phenomenon. Finally, we will discuss the implications of our method for understanding the thermal Hall effect.

Reference:
[1] Shang Ren, John Bonini, Massimiliano Stengel, Cyrus E. Dreyer, and David Vanderbilt, Adiabatic Dynamics of Coupled Spins and Phonons in Magnetic Insulators, Phys. Rev. X 14,011041 (2024)
[2] John Bonini, Shang Ren, David Vanderbilt, Massimiliano Stengel, Cyrus E Dreyer, Sinisa Coh, Frequency Splitting of Chiral Phonons from Broken Time-Reversal Symmetry in CrI_3, Phys. Rev. Lett. 130, 086701 (2023)
[3] Miquel Royo and Massimiliano Stengel, unpublished