Lattice dynamics with broken time reversal symmetry

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The dynamics of atoms in molecules and solids are conventionally formulated in terms of forces which are a function of nuclear positions; this results in equations of motion which are symmetric under time reversal symmetry. In magnetically ordered systems such a formulation will not correctly reflect the physical vibration mode degeneracies which are determined by the magnetic symmetry group. The absence of time reversal symmetry can lead to chiral phonon modes where excitations involving "clockwise" and "counterclockwise" atomic trajectories occur at distinct energies. In this talk I will present and compare first principles methods for computing phonon spectra which go beyond the conventional interatomic force matrix approach to incorporate time reversal symmetry breaking effects. The first method, based on an adiabatic separation between electronic and nuclear degrees of freedom, includes the first order changes in forces with atomic velocities[1]. The second method goes beyond this adiabatic assumption and treats phonons and spin excitations on the same footing [2]. While both approaches yield vibration modes which correctly reflect the degeneracies of the magnetic symmetry group, we demonstrate that in systems such as the ferromagnetic insulator CrI_3 the adiabatic approach yields qualitatively incorrect spectra as the relevant spin degrees of freedom are not "fast" with respect to phonon excitations.

References

[1] Daniyar Saparov, Bangguo Xiong, Yafei Ren, and Qian Niu. Lattice dynamics with molecular berry curvature: Chiral optical phonons. *Phys. Rev. B*, 105:064303, Feb 2022.

[2] John Bonini, Shang Ren, David Vanderbilt, Massimiliano Stengel, Cyrus E. Dreyer, and Sinisa Coh. Frequency splitting of chiral phonons from broken time-reversal symmetry in CrI_3. *Phys. Rev. Lett.*, 130:086701, Feb 2023.