Lattice dynamics in systems with broken time-reversal symmetry

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Ab initio calculations of phonon frequencies and eigenvectors traditionally rely on the knowledge of the static force constants, defined as the second derivative of the total energy with respect to atomic displacements. Such an approach rests on the Born-Oppenheimer approximation, which is generally accurate in nonmagnetic insulators, but requires special care whenever time-reversal symmetry (TRS) is broken. In such cases, additional terms need to be incorporated in the dynamical equations of motion, which couple the atomic displacements to velocities. Moreover, low-frequency magnon modes may break adiabaticity, thus requiring the treatment of spin and phonon degrees of freedom on the same footing. In this talk I will present our recent progress in addressing these methodological challenges. I will focus on examples where TRS is broken either by an external magnetic field [1] or via spontaneous ordering of the spins. [2,3] I will also discuss strategies to accelerate the convergence of linear-response calculations in noncollinear spin systems.

[1] Asier Zabalo, Cyrus E. Dreyer, and Massimiliano Stengel, *Rotational g factors and Lorentz forces of molecules and solids from density functional perturbation theory*, Phys. Rev. B 105, 094305 (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 (2023).

[3] 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).