Non-collinear treatment within DFPT and magnetic field perturbation

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In this talk we will first briefly present the status of the non-collinear magnetism in ABINIT for ground state calculations and related capabilities (convergence, applied Zeeman magnetic field, constrained magnetic moments).
Then we will discuss our developments regarding the extension of DFPT for non-collinear magnetism [1]. We will see that the main problem comes with the exchange-correlation (XC) potential derivatives, which are the only ones that are affected by the non-collinearity of the system. Most of the present XC functionals are, however, constructed at the collinear level such that the off-diagonal derivatives coming from the non-collinearity are absent. We will show that a good solution is to perform the non-collinear derivatives through a local collinear basis where the z axis is aligned with the magnetization. We will present the results of our implementation on phonons and electric field perturbation for LDA functional and norm-conserving pseudopotential scheme.
At last, we will discuss the development of a DFPT extension treating magnetic field perturbation acting on the spins (Zeeman field perturbation). Our implementation has been done for LDA and norm-conserving case and works for any wave-vector q, giving access to the q-dependent magnetic susceptibility or magnon spectra.

References

[1] F. Ricci, S. Prokhorenko, M. Torrent, M. J. Verstraete, E. Bousquet, arXiv:1901.04323 (2019).