First-principles study of magnetoelectricity: finite magnetic field and density functional perturbation theory.

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First-principles studies of the magnetoelectric response of crystals has emerged rather recently. The first occurrence of such a calculation was performed through a finite differences technique followed by the use of finite field techniques. These techniques appeared to be successful in calculating the magnetoelectric response of magnetoelectric crystals and to give a deep insight into the underlying microscopic mechanisms. Despite these successful achievements, the use of these two techniques didn’t reach a widespread use in the community due to the cumbersome human investment that can require the finite differences technique or the CPU time consuming that can be necessary with finite field relaxations within non-collinear plus spin-orbit coupling calculations. In this talk, I will discuss the use and limits of the finite magnetic field method and, going beyond, I will also present the development of a density functional perturbation theory (DFPT) with magnetic field in order to compute the magnetoelectric response. With respect to the two previously used techniques, DFPT is code-development time consuming but once done it allows to compute the whole magnetoelectric tensor in an automated way that requires no specific human investment and thus whatever the crystal complexity or size.