non-collinear DFPT and magnetoelectric response:

Status and perspectives in Abinit

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Status of DFPT + nspden $= 4$ + SOC

- Only implemented in Norm-conserving and LDA
- Only atom and E-field perturbations
  - Phonons
  - Permitivity tensor
  - Born effective charges
- Some works were done for PAW-LDA but not finalized (w. Marc)

Implementation Perspectives

Medium to long term (Xavier + Marc + ?):

- Add strain perturbation (NC – LDA)
- Implementation of $\alpha^{elec} = \dfrac{\partial^2 E}{\partial \mathscr{E} \partial \mathscr{B}}$ (non-variational expression)
- do the d2dkdk (w. Max, Lucas)
- Terminate works initialized for PAW-LDA+U (w. Marc):
  - atom perturbation (phonons)
  - E-field perturbation
  - strain (long term?)
- GGA ? (long term)

New properties

Dynamical magnetic effective charge:

BEC DMC

$$Z^{*e}_{\kappa,ij} = \Omega \frac{\partial P_i}{\partial \tau_{\kappa j}} = \frac{\partial^2 E}{\partial \mathscr{E}_i \partial \tau_{\kappa j}} \quad \leftrightarrow \quad Z^{*m}_{\kappa,ij} = \Omega \frac{\partial M_i}{\partial \tau_{\kappa,j}} = \frac{\partial^2 E}{\partial \mathscr{B}_i \partial \tau_{\kappa j}},$$

DMC can already be extracted (to be done, easy):

$$Z^{*m}_{\kappa,ij} = \Omega \frac{\partial M_i}{\partial \tau_{\kappa,j}} \Leftrightarrow \text{ from } m^{(1)} \text{ coming from phonon DFPT calculations!}$$

Magnetoelectric response (electronic contribution:)

$$\alpha^{elec} = \frac{\partial^2 E}{\partial \mathscr{E} \partial \mathscr{B}} \text{ (DFPT) } \quad \text{or from } m^{(1)} \text{ coming from E-field DFPT calculations!}$$

New properties

Magnetoelectric response (linear):

$$\alpha_{ij}^{\text{latt}} = \frac{\mu_0}{\Omega} \sum_{n=1}^{N_{\text{IR}}} \frac{S_{n,ij}}{\omega_n^2}$$

Magnetoelectric oscillator strength:

$$S_{n,ij} = \left(\sum_{\kappa,i'} Z^{*\text{m}}_{\kappa,ii'} u_{n,\kappa,i'} \right) \times \left(\sum_{\kappa,j'} Z^{*\text{e}}_{\kappa,j'j} u_{n,\kappa,j'} \right),$$

Mode magnetization:

$$\bar{Z}^{*\text{m}}_{n,i} = \sum_{\kappa,j} Z^{*\text{m}}_{\kappa,ij} \tilde{u}_{n,\kappa,j}.$$

New properties

Only spin contribution, what about the orbital contribution (cf Max)?

Tested first with finite differences (waiting for DFPT ;-)):

M. Braun, B. Guster, A. Urru, H. Kabbour & E. Bousquet ArXiv:2406.06298v1

TABLE IV. Linear spin ($\vec{S}$) and orbital ($\vec{L}$) dynamical magnetic effective charges ($10^{-2}\mu_B$/Å) for each inequivalent Wyckoff sites of $BiCoO_3$ as calculated with VASP and ABINIT (ABINIT values are in brackets and in italic). $\mathcal{H}_i$ refers to the magnetic field in direction i and τ_j to the atom displacement along the direction j.

Atom	Wyckoff		$\vec{S}$				$\vec{L}$		
			$\partial/\partial\mathcal{H}_x$	$\partial/\partial\mathcal{H}_y$	$\partial/\partial\mathcal{H}_z$		$\partial/\partial\mathcal{H}_x$	$\partial/\partial\mathcal{H}_y$	$\partial/\partial\mathcal{H}_z$
Bi	1a	$\partial/\partial\tau_x$	6.93 (*6.93*)	0	0	$\partial/\partial\tau_x$	9.83 (*8.32*)	0	0
		$\partial/\partial\tau_y$	0	-6.93 (*-6.93*)	0	$\partial/\partial\tau_y$	0	-9.83 (*-8.32*)	0
		$\partial/\partial\tau_z$	0	0	0	$\partial/\partial\tau_z$	0	0	0
Co	1b	$\partial/\partial\tau_x$	7.25 (*8.49*)	0	0	$\partial/\partial\tau_x$	24.63 (*22.57*)	0	0
		$\partial/\partial\tau_y$	0	7.25 (*8.49*)	0	$\partial/\partial\tau_y$	0	24.63 (*22.57*)	0
		$\partial/\partial\tau_z$	0	0	-0.91 (*-0.67*)	$\partial/\partial\tau_z$	0	0	-15.01 (*-15.34*)
O_{api}	1b	$\partial/\partial\tau_x$	2.80 (*1.74*)	0	0	$\partial/\partial\tau_x$	-6.12 (*-5.52*)	0	0
		$\partial/\partial\tau_y$	0	2.80 (*1.74*)	0	$\partial/\partial\tau_y$	0	-6.12 (*-5.52*)	0
		$\partial/\partial\tau_z$	0	0	0.11 (*0.10*)	$\partial/\partial\tau_z$	0	0	-0.57 (*-1.83*)

New properties

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Visualisation of DMCs: