Orbital Magnetism

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Outline

Overview

Nuclear Magnetic Dipoles

Orbital Magnetization

Context

Orbital magnetism in insulators:

- Magnetic dipole moment density due to charge current (no spin)

$$\mathbf{M} \approx -\frac{1}{2} \sum_{n} \int_{\mathrm{BZ}} d\mathbf{k} \langle \psi_{n\mathbf{k}} | \mathbf{r} \times \mathbf{p} | \psi_{n\mathbf{k}} \rangle$$

- Induced by magnetic fields (external or nuclear dipoles)
- Observable: chemical shielding in NMR experiments
- Typical scale: $\alpha^2 \approx 5 \times 10^{-5}$

All-electron formulae

Chern number:

$$\begin{aligned} \mathbf{C} &= \frac{i}{2\pi}\sum_{n}\int_{\mathrm{BZ}} d\mathbf{k}\,\langle\partial_{\mathbf{k}}u_{n\mathbf{k}}|\times|\partial_{\mathbf{k}}u_{n\mathbf{k}}\rangle \\ &= \frac{i}{2\pi}\epsilon_{\alpha\beta\gamma}\hat{e}_{\alpha}\int_{\mathrm{BZ}} d\mathbf{k}\mathrm{Tr}\left[(\partial_{\beta}\rho_{\mathbf{k}})(1-\rho_{\mathbf{k}})(\partial_{\beta}\rho_{\mathbf{k}})\right] \end{aligned}$$

where $\rho_{\mathbf{k}}$ is the ground state density operator (valence bands).

- The Chern number is strictly zero in an insulator with TR symmetry
- Presence of magnetic field breaks TR symmetry
- Chern number measures presence of charge circulation.

See Ceresoli, Thonhauser, Vanderbilt, Resta, *PRB* **74**, 024408 (2006)

All-electron formulae

Magnetization

$$\mathbf{M} = \frac{i}{(2\pi)^3} \sum_n \int_{\mathrm{BZ}} d\mathbf{k} \left\langle \partial_{\mathbf{k}} u_{n\mathbf{k}} \right| \times \left(H_{\mathbf{k}} + E_{n\mathbf{k}} \right) \left| \partial_{\mathbf{k}} u_{n\mathbf{k}} \right\rangle$$

or more generally, energy due to external magnetic field:

$$E^{(n)} = \int_{\mathrm{BZ}} d\mathbf{k} \mathrm{Tr} \left[\left(\rho^{(n)}_{\mathbf{k}CC} + \rho^{(n)}_{\mathbf{k}VV} \right) H^{(0)}_{\mathrm{k}} \right],$$

where CC and VV refer to conduction and valence spaces, and $H^{(0)}$ is the field-free Hamiltonian.

Gonze and Zwanziger, *PRB* **84**, 064445 (2011)

Strategy for ABINIT

- Write PAW total energy in presence of external B field
- Compute first order change in energy due to external field (this is the magnetization through $E^{(1)} = \mathbf{M} \cdot \mathbf{B}$)
- The resulting **M** would be zero in an insulator due to TR symmetry so break this by *also* adding nuclear magnetic dipoles μ
- Result yields chemical shielding through converse method,

$$\sigma_{ij} = -\Omega \frac{\partial M_i}{\partial \mu_j}$$

Thonhauser, Ceresoli, Mostofi, Marzari, Resta, Vanderbilt, *J. Chem. Phys.* **131**, 101101 (2009)

Hamiltonian

A nuclear magnetic dipole moment $\mathbf{m}$ at site $\mathbf{R}$ generates a vector potential

$$\mathbf{A}_s = \frac{\mu_0}{4\pi} \frac{\mathbf{m} \times (\mathbf{r} - \mathbf{R})}{|\mathbf{r} - \mathbf{R}|^3}$$

and appears in the Hamiltonian as

$$H = \frac{1}{2m_e} (\mathbf{p} - q\mathbf{A}_s)^2 = \frac{p^2}{2m_e} - \frac{q}{m_e} \mathbf{A_s} \cdot \mathbf{p} + \ldots$$

to first order, in SI units. In this gauge, $\mathbf{A_s} \cdot \mathbf{p} = \mathbf{p} \cdot \mathbf{A_s}$.

Atomic units

In atomic units the first order nuclear dipole Hamiltonian is

$$\alpha^2 \frac{\mathbf{m} \times (\mathbf{r} - \mathbf{R}) \cdot \mathbf{p}}{|\mathbf{r} - \mathbf{R}|^3} \equiv \alpha^2 \frac{\mathbf{L_R} \cdot \mathbf{m}}{|\mathbf{r} - \mathbf{R}|^3}$$

where α is the fine structure constant, and the electron charge $q = -1$. $\mathbf{L_R} = (\mathbf{r} - \mathbf{R}) \times \mathbf{p}$. This term has lattice periodicity.

Application of the Hamiltonian

- PAW spheres: the Hamiltonian is applied as $H = \alpha^2 \frac{\mathbf{L_R} \cdot \mathbf{m}}{|\mathbf{r}-\mathbf{R}|^3}$.
- Planewaves: apply $\alpha^2 \mathbf{A_s} \cdot \mathbf{p}$
  - From $\mathbf{A_s}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{A_s}(\mathbf{G}) e^{-2\pi i \mathbf{G}.\mathbf{r}}$ we find

$$\mathbf{A_s}(\mathbf{G}) = \frac{-4\pi i}{2\pi\Omega} \frac{\mathbf{m} \times \mathbf{G}}{|\mathbf{G}|^2} e^{-2\pi i \mathbf{G}.\mathbf{R}}$$

  - Generate $\mathbf{A_s}(\mathbf{r})$ via FFT.
  - Apply $\mathbf{A_s}(\mathbf{r})$ to

$$\mathbf{p}|u_{n\mathbf{k}}\rangle = \sum_{\mathbf{G}} 2\pi(\mathbf{k}+\mathbf{G}) c_{\mathbf{k}}(\mathbf{G}) |\mathbf{G}\rangle$$

  by FFT, followed by multiplication, followed by FFT back to reciprocal space.

Total energy in external field

In SI units, the Hamiltonian and vector potential are

$$\begin{aligned} H &= \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A_0}\right)^2 + V, \\ \mathbf{A_0} &= \frac{1}{2}\mathbf{B} \times \mathbf{r}. \end{aligned}$$

The GIPAW transform operator is

$$T = 1 + \sum_{Ri} U \left[|\phi_{iR}\rangle - |\tilde{\phi}_{iR}\rangle \right] \langle \tilde{p}_{iR}| U^{\dagger}$$

where $U = \exp\left(-\frac{iq}{2\hbar}\mathbf{r} \cdot \mathbf{R} \times \mathbf{B}\right)$.

Pickard and Mauri, *PRB* **63**, 245101 (2001)

GIPAW Total Energy

Total energy consists of core terms, and $\tilde{E} + (E^1 - \tilde{E}^1)$ as usual. However, the following terms depend on $\mathbf{B}$:

- Kinetic energy includes $\mathbf{A_0}(\mathbf{r})$, and $\mathbf{A_0}(\mathbf{r} - \mathbf{R})$ on-site.
- $\rho_{ij} = \sum_{\text{occ}} \langle \psi_n | U | \tilde{p}_{iR} \rangle \langle \tilde{p}_{jR} | U^\dagger | \psi_n \rangle$
- $n^1(\mathbf{r}) = \sum_{ij} \rho_{ij} \langle \phi_i | \mathbf{r} \rangle \langle \mathbf{r} | \phi_j \rangle$
- $\tilde{n}^1(\mathbf{r}) = \sum_{ij} \rho_{ij} \langle \tilde{\phi}_i | \mathbf{r} \rangle \langle \mathbf{r} | \tilde{\phi}_j \rangle$
- $S = 1 + \sum_{Rij} U | \tilde{p}_{iR} \rangle \left[\langle \phi_{iR} | \phi_{jR} \rangle - \langle \tilde{\phi}_{iR} | \tilde{\phi}_{jR} \rangle \right] \langle \tilde{p}_{jR} | U^\dagger$

Still problematic due to $\mathbf{A_0}(\mathbf{r})$ and related terms.

Magnetic Translation Invariance

Key feature in the presence of an external magnetic field:

$$O(\mathbf{r_1}, \mathbf{r_2}) = \bar{O}(\mathbf{r_1}, \mathbf{r_2}) e^{-\frac{iq}{2\hbar}\mathbf{B}\cdot\mathbf{r_1}\times\mathbf{r_2}},$$

where $\bar{O}(\mathbf{r_1} + \mathbf{R}, \mathbf{r_2} + \mathbf{R}) = \bar{O}(\mathbf{r_1}, \mathbf{r_2})$.

Zak, *Phys. Rev.* **6**, 1602A (1964)

Hamiltonian and density operator

The energies are associated with a density operator and Hamiltonian via

$$E(\mathbf{B}) = \min_{\rho=\rho S\rho} \{\mathrm{Tr}[\rho H(\mathbf{B})]\} = \mathrm{Tr}[\bar{\rho}\bar{H}].$$

Both ρ and H have lattice periodic kernels, due to magnetic translation invariance. For the Hamiltonian this is just the zero-field Hamiltonian.

Density operator

The translationally invariant density operator kernel can be expressed through the idempotency condition, yielding to first order

$$\overline{\rho}_{\mathbf{k}} = \overline{\rho}_{\mathbf{k}}\overline{S}_{\mathbf{k}}\overline{\rho}_{\mathbf{k}} - \frac{i}{2}\epsilon_{\alpha\beta\gamma}B_{\alpha}\times$$
$$\left[(\partial_{\beta}\overline{\rho}_{\mathbf{k}})(\partial_{\gamma}\overline{S}_{\mathbf{k}})\overline{\rho}_{\mathbf{k}} + (\partial_{\beta}\overline{\rho}_{\mathbf{k}})\overline{S}_{\mathbf{k}}(\partial_{\gamma}\overline{\rho}_{\mathbf{k}}) + \overline{\rho}_{\mathbf{k}}(\partial_{\beta}\overline{S}_{\mathbf{k}})(\partial_{\gamma}\overline{\rho}_{\mathbf{k}})\right]$$

Now the B field dependency has been transferred off of H and onto ρ, in terms of lattice periodic $\overline{H}$ and $\overline{\rho}$.

Energy first order in B

The first order energy, arising from the planewave kinetic energy contribution $\mathbf{A_0}(\mathbf{r}) \cdot \mathbf{p}$ and ρ_{ij}, is obtained from the perturbed density operator as

$$\int d\mathbf{k} \ \mathrm{Tr}[\overline{\rho}^{(1)}_{\mathbf{k}} \ \overline{H}^{(0)}_{\mathbf{k}}]$$

Notice that with translational invariance restored, there is only $\overline{H}^{(0)}$, the zero-field Hamiltonian, all field-dependence is explicitly on $\overline{\rho}^{(1)}$. [N.B. there is also an explicit on-site term that is already translation invariant]

Perturbing the density operator

The idempotency condition $\rho = \rho S \rho$ yields in a perturbation expansion:

$$\begin{aligned}
\overline{\rho}^0_{\mathbf{k}} &= \overline{\rho}^0_{\mathbf{k}} \overline{S}^0_{\mathbf{k}} \overline{\rho}^0_{\mathbf{k}} \\
\overline{\rho}^1_{\mathbf{k}} &= \overline{\rho}^1_{\mathbf{k}} \overline{S}^0_{\mathbf{k}} \overline{\rho}^0_{\mathbf{k}} + \overline{\rho}^0_{\mathbf{k}} \overline{S}^1_{\mathbf{k}} \overline{\rho}^0_{\mathbf{k}} + \overline{\rho}^0_{\mathbf{k}} \overline{S}^0_{\mathbf{k}} \overline{\rho}^1_{\mathbf{k}} - \frac{i}{2} \epsilon_{\alpha\beta\gamma} B_\alpha \times \\
&\quad \left[(\partial_\beta \overline{\rho}^0_{\mathbf{k}})(\partial_\gamma \overline{S}^0_{\mathbf{k}}) \overline{\rho}^0_{\mathbf{k}} + (\partial_\beta \overline{\rho}^0_{\mathbf{k}}) \overline{S}^0_{\mathbf{k}} (\partial_\gamma \overline{\rho}^0_{\mathbf{k}}) + \overline{\rho}^0_{\mathbf{k}} (\partial_\beta \overline{S}^0_{\mathbf{k}})(\partial_\gamma \overline{\rho}^0_{\mathbf{k}}) \right]
\end{aligned}$$

Because the energy term depends only on $\mathrm{Tr}[\overline{\rho}^{(1)}_{\mathbf{k}} \, \overline{H}^{(0)}_{\mathbf{k}}]$, we need these expressions projected only in the unperturbed valence and conduction subspaces.

Subspace projections

Valence subspace:

$$(\overline{\rho}^0_{\mathbf{k}}\overline{S}^0_{\mathbf{k}})\overline{\rho}^1_{\mathbf{k}}(\overline{S}^0_{\mathbf{k}}\overline{\rho}^0_{\mathbf{k}}) = -\overline{\rho}^0_{\mathbf{k}}\overline{S}^1_{\mathbf{k}}\overline{\rho}^0_{\mathbf{k}} + \frac{i}{2}\epsilon_{\alpha\beta\gamma}B_\alpha(\overline{\rho}^0_{\mathbf{k}}\overline{S}^0_{\mathbf{k}})\,[\ldots]\,(\overline{S}^0_{\mathbf{k}}\overline{\rho}^0_{\mathbf{k}})$$

Conduction subspace:

$$\left(1-\overline{\rho}^0_{\mathbf{k}}\overline{S}^0_{\mathbf{k}}\right)\overline{\rho}^1_{\mathbf{k}}\left(1-\overline{S}^0_{\mathbf{k}}\overline{\rho}^0_{\mathbf{k}}\right) = - \frac{i}{2}\epsilon_{\alpha\beta\gamma}B_\alpha\left(1-\overline{\rho}^0_{\mathbf{k}}\overline{S}^0_{\mathbf{k}}\right)[\ldots]\left(1-\overline{S}^0_{\mathbf{k}}\overline{\rho}^0_{\mathbf{k}}\right)$$

where $[\ldots]$ are the three partial derivative terms.

Discretization

Derivatives with respect to k can be computed by a finite difference procedure:

$$\partial_\beta \rho_{\mathbf{k}} \approx \frac{\rho_{\mathbf{k}+\Delta_\beta} - \rho_{\mathbf{k}-\Delta_\beta}}{2\Delta_\beta}$$

$$\partial_\beta |\tilde{u}_{n\mathbf{k}}\rangle\langle\tilde{u}_{n\mathbf{k}}| \approx \frac{|\tilde{u}_{n\mathbf{k}+\Delta_\beta}\rangle\langle\tilde{u}_{n\mathbf{k}+\Delta_\beta}| - |\tilde{u}_{n\mathbf{k}-\Delta_\beta}\rangle\langle\tilde{u}_{n\mathbf{k}-\Delta_\beta}|}{2\Delta_\beta}$$

or more compactly, via $\sigma = \pm 1$:

$$\partial_\beta \rho = \frac{\partial}{\partial \mathbf{k}_\beta} \sum_n^{\text{occ}} |\tilde{u}_{n\mathbf{k}}\rangle\langle\tilde{u}_{n\mathbf{k}}| \approx \sum_n^{\text{occ}} \sum_{\sigma=\pm 1} \frac{\sigma |\tilde{u}_{n\mathbf{k}+\sigma\Delta_\beta}\rangle\langle\tilde{u}_{n\mathbf{k}+\sigma\Delta_\beta}|}{2\Delta_\beta}$$

k Derivatives (other tricks)

Differentiating the idempotency condition leads to

$$(\overline{\rho}^0_{\mathbf{k}}\overline{S}^0_{\mathbf{k}})\partial_{\mathbf{k}}\rho(\overline{S}^0_{\mathbf{k}}\overline{\rho}^0_{\mathbf{k}}) = -\rho(\partial_{\mathbf{k}}S)\rho \quad \text{valence}$$
$$(1-\overline{\rho}^0_{\mathbf{k}}\overline{S}^0_{\mathbf{k}})\partial_{\mathbf{k}}\rho(1-\overline{S}^0_{\mathbf{k}}\overline{\rho}^0_{\mathbf{k}}) = 0 \quad \text{conduction}$$

The valence-conduction cross terms are not zero.
The first order perturbation of S is

$$\overline{S}^1_{\mathbf{k}} = -\frac{i}{2}\epsilon_{\alpha\beta\gamma}\sum_{Rij}|\partial_\beta\tilde{p}_{Ri\mathbf{k}}\rangle\langle\partial_\gamma\tilde{p}_{Rj\mathbf{k}}|\left(\langle\phi_{Ri}|\phi_{Rj}\rangle - \langle\tilde{\phi}_{Ri}|\tilde{\phi}_{Rj}\rangle\right)$$

Typical term: CC

$$-\frac{i}{2}\epsilon_{\alpha\beta\gamma}\mathrm{Tr}[\bar{\rho}^{(1)}_{\mathbf{k}}\bar{H}^{(0)}_{\mathbf{k}}]_{\mathrm{CCI}} =$$

$$-\frac{i}{2}\epsilon_{\alpha\beta\gamma}\sum_{n}^{\mathrm{occ}}\langle\bar{u}^{(0)}_{n,\mathbf{k}}|\bar{S}^{(0)}_{\mathbf{k}}(\partial_\gamma\bar{\rho}^{(0)}_{\mathbf{k}})\bar{H}^{(0)}_{\mathbf{k}}(\partial_\beta\bar{\rho}^{(0)}_{\mathbf{k}})\bar{S}^{(0)}_{\mathbf{k}}|\bar{u}^{(0)}_{n,\mathbf{k}}\rangle.$$

The sum is evaluated using the discretized derivative as

$$\frac{1}{2\Delta_\beta 2\Delta_\gamma}\sum_{\sigma_\beta,\sigma_\gamma}\sigma_\beta\sigma_\gamma\sum_{n,n',n''}^{\mathrm{occ}}\langle\bar{u}^{(0)}_{n,\mathbf{k}}|\bar{S}^{(0)}_{\mathbf{k}}|\bar{u}^{(0)}_{n',\mathbf{k}+\sigma_\beta}\rangle$$

$$\langle\bar{u}^{(0)}_{n',\mathbf{k}+\sigma_\beta}|\bar{H}^{(0)}_{\mathbf{k}}|\bar{u}^{(0)}_{n'',\mathbf{k}+\sigma_\gamma}\rangle\langle\bar{u}^{(0)}_{n'',\mathbf{k}+\sigma_\gamma}|\bar{S}^{(0)}_{\mathbf{k}}|\bar{u}^{(0)}_{n,\mathbf{k}}\rangle.$$

Typical term: VV

$$+\frac{i}{2}\epsilon_{\alpha\beta\gamma}\mathrm{Tr}[\bar{\rho}^{(1)}_{\mathbf{k}}\bar{H}^{(0)}_{\mathbf{k}}]_{\mathrm{VVII}} =$$

$$+\frac{i}{2}\epsilon_{\alpha\beta\gamma}\sum_{n}^{\mathrm{occ}}\langle\bar{u}^{(0)}_{n,\mathbf{k}}|\bar{S}^{(0)}_{\mathbf{k}}(\partial_\beta\bar{\rho}^{(0)}_{\mathbf{k}})\bar{S}^{(0)}_{\mathbf{k}}(\partial_\gamma\bar{\rho}^{(0)}_{\mathbf{k}})$$

$$\bar{S}^{(0)}_{\mathbf{k}}\bar{\rho}^{(0)}_{\mathbf{k}}\bar{H}^{(0)}_{\mathbf{k}}\bar{\rho}^{(0)}_{\mathbf{k}}|\bar{u}^{(0)}_{n,\mathbf{k}}\rangle,$$

with the sum as

$$\frac{1}{2\Delta_\beta 2\Delta_\gamma}\sum_{\sigma_\beta,\sigma_\gamma}\sigma_\beta\sigma_\gamma\sum_{n,n',n''}^{\mathrm{occ}}\langle\bar{u}^{(0)}_{n,\mathbf{k}}|\bar{S}^{(0)}_{\mathbf{k}}|\bar{u}^{(0)}_{n',\mathbf{k}+\sigma_\beta}\rangle$$

$$\langle\bar{u}^{(0)}_{n',\mathbf{k}+\sigma_\beta}|\bar{S}^{(0)}_{\mathbf{k}}|\bar{u}^{(0)}_{n'',\mathbf{k}+\sigma_\gamma}\rangle\langle\bar{u}^{(0)}_{n'',\mathbf{k}+\sigma_\gamma}|\bar{S}^{(0)}_{\mathbf{k}}|\bar{u}^{(0)}_{n,\mathbf{k}}\rangle E_{n,\mathbf{k}}.$$

Objects needed

All expressions built from:

$\left\langle u_{n'\mathbf{k}+\Delta\mathbf{k}_\beta} \middle| \overline{S}^0_{\mathbf{k}} \middle| u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle$, as found in Berry phase polarization

Objects needed

All expressions built from:

$\left\langle u_{n'\mathbf{k}+\Delta\mathbf{k}_\beta} | \overline{S}^0_{\mathbf{k}} | u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle$, as found in Berry phase polarization

$\left\langle u_{n'\mathbf{k}} | \partial_\beta \overline{S}^0_{\mathbf{k}} | u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle$, analytical or finite difference

Objects needed

All expressions built from:

$$\left\langle u_{n'\mathbf{k}+\Delta\mathbf{k}_\beta} | \overline{S}^0_{\mathbf{k}} | u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle, \text{ as found in Berry phase polarization}$$

$$\left\langle u_{n'\mathbf{k}} | \partial_\beta \overline{S}^0_{\mathbf{k}} | u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle, \text{ analytical or finite difference}$$

$$\left\langle u_{n\mathbf{k}} | \overline{S}^1_{\mathbf{k}} | u_{n\mathbf{k}} \right\rangle, \text{ derivatives of } \texttt{cprj}$$

Objects needed

All expressions built from:

$\left\langle u_{n'\mathbf{k}+\Delta\mathbf{k}_\beta} | \overline{S}^0_{\mathbf{k}} | u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle$, as found in Berry phase polarization

$\left\langle u_{n'\mathbf{k}} | \partial_\beta \overline{S}^0_{\mathbf{k}} | u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle$, analytical or finite difference

$\left\langle u_{n\mathbf{k}} | \overline{S}^1_{\mathbf{k}} | u_{n\mathbf{k}} \right\rangle$, derivatives of `cprj`

$\left\langle u_{n\mathbf{k}} | \overline{H}^0_{\mathbf{k}} | u_{n\mathbf{k}} \right\rangle$, ground state energies

Objects needed

All expressions built from:

$\left\langle u_{n'\mathbf{k}+\Delta\mathbf{k}_\beta} | \overline{S}^0_{\mathbf{k}} | u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle$, as found in Berry phase polarization

$\left\langle u_{n'\mathbf{k}} | \partial_\beta \overline{S}^0_{\mathbf{k}} | u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle$, analytical or finite difference

$\left\langle u_{n\mathbf{k}} | \overline{S}^1_{\mathbf{k}} | u_{n\mathbf{k}} \right\rangle$, derivatives of `cprj`

$\left\langle u_{n\mathbf{k}} | \overline{H}^0_{\mathbf{k}} | u_{n\mathbf{k}} \right\rangle$, ground state energies

$\left\langle u_{n'\mathbf{k}+\Delta\mathbf{k}_\beta} | \overline{H}^0_{\mathbf{k}} | u_{n\mathbf{k}+\mathbf{\Delta}\mathbf{k}_\gamma} \right\rangle$, quite non-standard

Objects needed

All expressions built from:

$\left\langle u_{n'\mathbf{k}+\Delta\mathbf{k}_\beta} | \overline{S}^0_{\mathbf{k}} | u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle$, as found in Berry phase polarization

$\left\langle u_{n'\mathbf{k}} | \partial_\beta \overline{S}^0_{\mathbf{k}} | u_{n\mathbf{k}+\Delta\mathbf{k}_\gamma} \right\rangle$, analytical or finite difference

$\left\langle u_{n\mathbf{k}} | \overline{S}^1_{\mathbf{k}} | u_{n\mathbf{k}} \right\rangle$, derivatives of `cprj`

$\left\langle u_{n\mathbf{k}} | \overline{H}^0_{\mathbf{k}} | u_{n\mathbf{k}} \right\rangle$, ground state energies

$\left\langle u_{n'\mathbf{k}+\Delta\mathbf{k}_\beta} | \overline{H}^0_{\mathbf{k}} | u_{n\mathbf{k}+\mathbf{\Delta k}_\gamma} \right\rangle$, quite non-standard

$\left\langle \tilde{p}_{Ri\mathbf{k}+\Delta\mathbf{k}_\beta} | u_{n\mathbf{k}} \right\rangle$, computed from `mkffnl` and `getcprj`

Output

AlP, with dipole (1.0, 0.0, 0.0) on Al site.
ucvol = 273.25

```
 Chern number C from orbital magnetization
----C is a real vector, given along Cartesian directions----

 C(   1) : real, imag  -4.44485010E-08 -1.37238863E-16
 C(   2) : real, imag  -1.15269229E-11 -2.48938292E-16
 C(   3) : real, imag  -2.30421055E-12  3.75201531E-17

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```

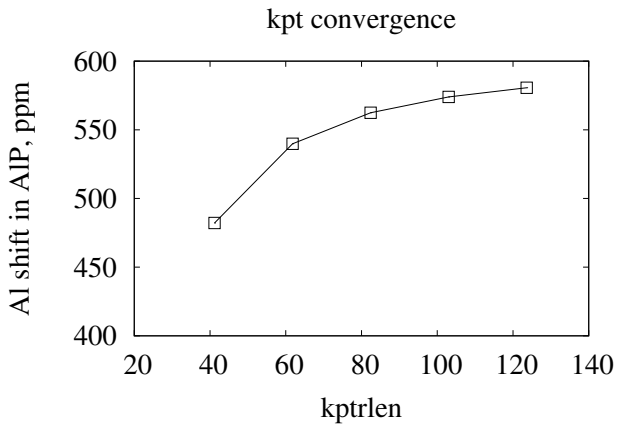


```
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 Orbital magnetization
----Orbital magnetization is a real vector, given along Cartesian directions----

 Orb Mag(   1) : real, imag  -2.05820419E-06  8.53048647E-15
 Orb Mag(   2) : real, imag  -2.21745487E-11  3.43814941E-14
 Orb Mag(   3) : real, imag  -5.59227864E-12 -4.18570117E-14

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```
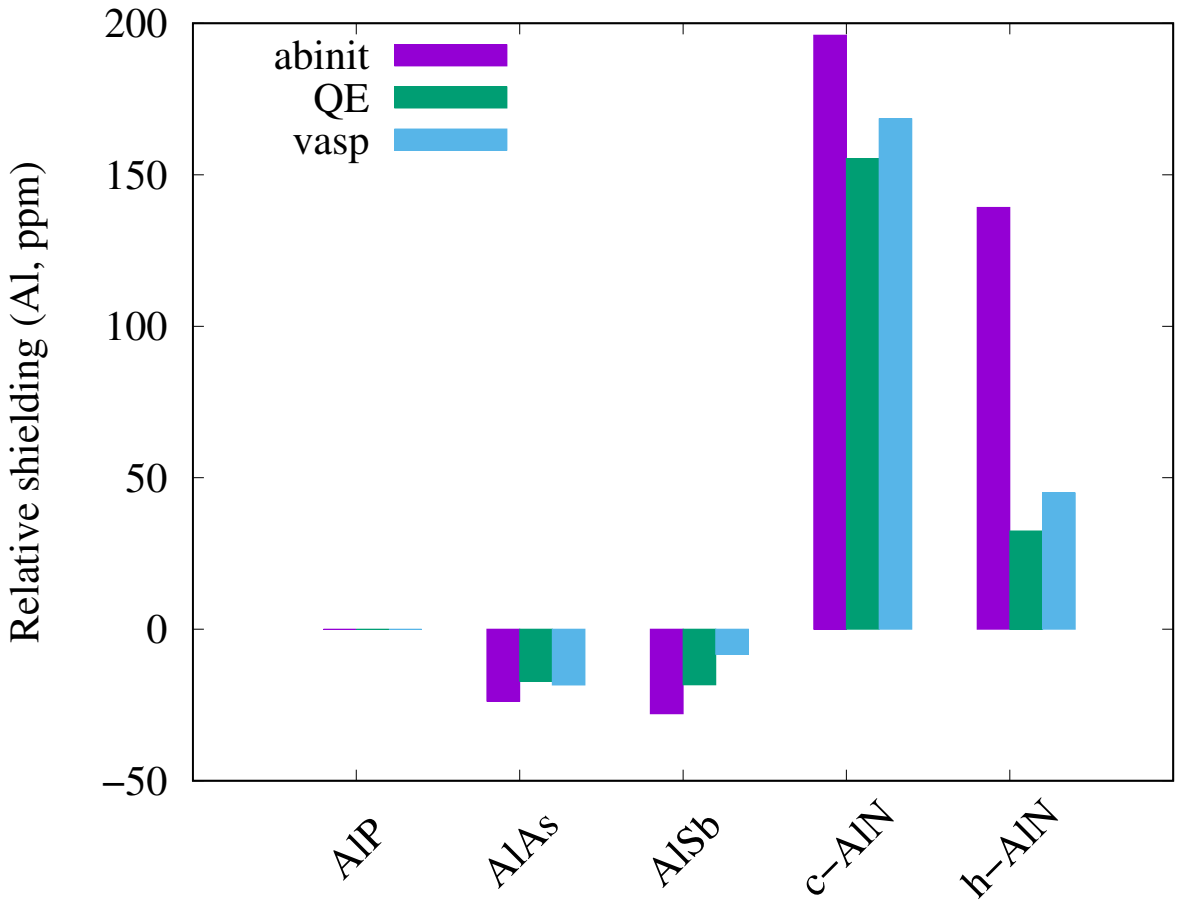

First results



Summary

- Orbital magnetism coded for insulators (see `m_orbmag.F90`), currently in extensive tests
- Requires PAW
- Parallelized over k pts
- So grateful to Xavier Gonze and Marc Torrent for much help and advice