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5th International ABINIT Developer Workshop

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Density-Functional Perturbation Theory and PAW :
miscellaneous features available now and soon in ABINIT

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Outline

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Introduction : historical reminder

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1995	DFPT available in ABINIT for Norm-Conserving PseudoPotentials
2004	PAW in ABINIT
2006-08	Writing of DFPT+PAW formalism
2009-10	DFPT+PAW in ABINIT for phonons, response to electric field
…	?

C. Audouze, F. Jollet, M. Torrent, X. Gonze, Phys. Rev. B ***73****, 235101* ***(2006)***

C. Audouze, F. Jollet, M. Torrent, X. Gonze, Phys. Rev. B ***78****, 035105* ***(2008)***

Introduction : historical reminder

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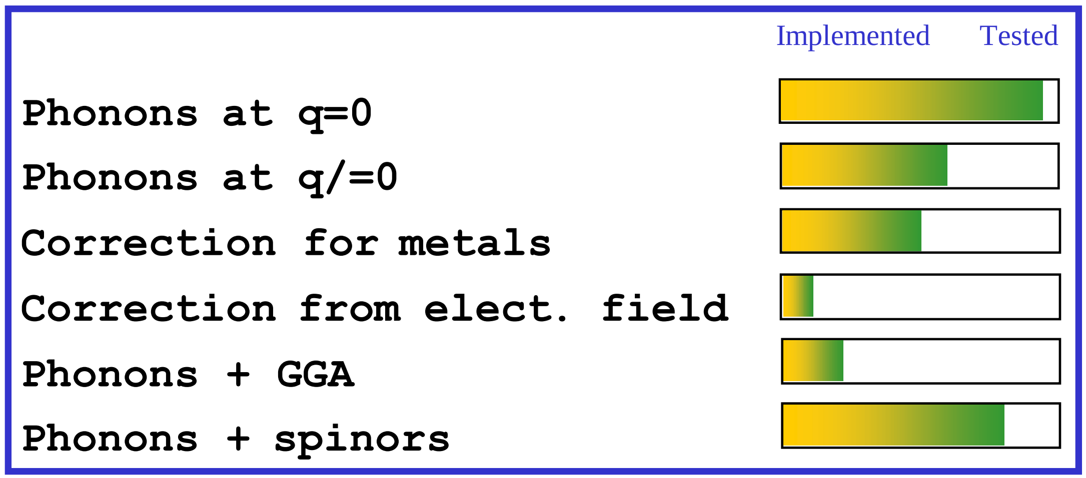
Presentation during the 4th ABINIT developer Workshop (Autrans, France, **2009**) :



DFPT+PAW : basics

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$$\left|\psi_n\right\rangle = \left|\tilde{\psi}_n\right\rangle + \sum_{R,i} \left\langle \tilde{p}_i^R \middle| \tilde{\psi}_n \right\rangle \cdot \left(\left|\phi_i\right\rangle - \left|\tilde{\phi}_i\right\rangle \right)$$

PAW linear transformation

Hamiltonian

$$\tilde{H} = -\frac{1}{2}\Delta + \tilde{v}_{eff} + \sum_{R,ij} \left|\tilde{p}_i^R\right\rangle D_{ij}^R \left\langle \tilde{p}_j^R\right|$$

Variable

Density

$$n(\mathrm{r}) = \sum_n f_n \left|\tilde{\Psi}_n(\mathrm{r})\right|^2 + \sum_{R,ij} \rho_{ij}^R \left(\phi_i(\mathrm{r})\phi_j(\mathrm{r}) - \tilde{\phi}_i(\mathrm{r})\tilde{\phi}_j(\mathrm{r})\right)$$

Occupations matrix

$$\rho_{ij}^R = \sum_n f_n \left\langle \tilde{\Psi}_n \middle| \tilde{p}_i^R \right\rangle \left\langle \tilde{p}_j^R \middle| \tilde{\Psi}_n \right\rangle$$

Pseudopotential strength

$$D_{ij}^R = D_{ij}^0 + \sum_{kl} \rho_{kl}^R E_{ijkl} + D_{ij}^{xc} + \sum_L \int_{R^3} \left[V_{Hxc} + V_{loc}\right](\mathbf{r}) \hat{Q}_{ij}^L(\mathbf{r}) d\mathbf{r}$$

Charge compensation

$$\hat{n}(\mathbf{r}) = \sum_{ij,L} \rho_{ij} \hat{Q}_{ij}^L(\mathbf{r})$$

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Density-functional Perturbation Theory

From a non-perturbed system ($E^{(0)}, \psi_m^{(0)}, n^{(0)}(r)$), we want to get the responses with respect to a perturbation λ…

Any physical quantity X is expanded as:

$$X[\lambda] = X^{(0)} + \lambda \cdot X^{(1)} + \lambda^2 \cdot X^{(2)} + \cdots \quad \text{with} \quad X^{(i)} = \frac{1}{i!}\left(\frac{d^i}{d\lambda^i} X\right)_{\lambda=0}$$

To be computed: $E^{(i)}, \psi_m^{(i)}, n^{(i)}(r), \quad \forall i \geq 1$

DFPT, 2n+1 theorem :

$E^{(2n)}$ obtained from $\Psi_m^{(n)}$,
solving a variational problem (Sternheimer equation)

$E^{(2n)}$ directly obtained from $\Psi_m^{(n)}$,
(non variational)

DFPT+PAW : basics

A typical DFPT calculation

Ground-State properties $\Psi_n^{(0)}, \varepsilon_n^{(0)}$

Frozen part of $\frac{\partial^2 E_{tot}}{\partial\lambda_{j1}\partial\lambda_{j2}}$

Depends on $\Psi_n^{(0)}, \varepsilon_n^{(0)}$

For each perturbation λ_{j1}

Minimize Stationnary expression of $\frac{\partial^2 E_{tot}}{\partial\lambda_{j1}^2}$

Solve Sternheimer equation

SCF cycle

1st-order properties $\Psi_n^{(j1)}, \varepsilon_n^{(j1)}$

For each perturbation λ_{j2}

Mix $\Psi_n^{(j1)}, \varepsilon_n^{(j1)}$ *with non self-consistent changes of* $\frac{\partial H}{\partial\lambda_{j2}}$ *and* $\frac{\partial\Psi_n}{\partial\lambda_{j2}}$

Using Non-stationnary expression of $\frac{\partial^2 E_{tot}}{\partial\lambda_{j1}\partial\lambda_{j2}}$

$$\frac{\partial^2 E_{tot}}{\partial\lambda_{j1}\partial\lambda_{j2}}$$

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Sternheimer equation:

$$P_c^*\left(\tilde{H}^{(0)}-\varepsilon_n^{(0)}S^{(0)}\right)P_c\left|\tilde{\Psi}_n^{(1)}\right\rangle=-P_c^*\left(\tilde{H}^{(1)}-\varepsilon_n^{(0)}S^{(1)}\right)\left|\tilde{\Psi}_n^{(0)}\right\rangle$$

$$P_c=I-\sum_{m=1}^{N}\left|\tilde{\Psi}_m^{(0)}\right\rangle\left\langle\tilde{\Psi}_m^{(0)}\right|S^{(0)} \qquad P_c^*=I-\sum_{m=1}^{N}S^{(0)}\left|\tilde{\Psi}_m^{(0)}\right\rangle\left\langle\tilde{\Psi}_m^{(0)}\right|$$

Parallel-transport gauge

$$\left\langle\tilde{\Psi}_i^{(1)}\middle|S^{(0)}\middle|\tilde{\Psi}_j^{(0)}\right\rangle=-\frac{1}{2}\left\langle\tilde{\Psi}_i^{(0)}\middle|S^{(1)}\middle|\tilde{\Psi}_j^{(0)}\right\rangle$$

DFPT+PAW : basics

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$$\tilde{H}^{(1)} = \left.\frac{\partial \tilde{H}}{\partial \lambda}\right|_{V_{Hxc}^{(0)}} + \tilde{V}_{Hxc}^{(1)}$$

$$\left.\frac{\partial \tilde{H}}{\partial \lambda}\right|_{V_{Hxc}^{(0)}} = V_H\left(\tilde{n}_{Zc}\right)^{(1)} + \sum_{R,ij} D_{ij}^{KV} \cdot \left(\left|\tilde{p}_i^R\right\rangle\left\langle\tilde{p}_j^R\right|\right)^{(1)}$$

$$+\sum_{R,ij}\left(\begin{array}{l}\left(\sum_L \int_{R^3} V_{Hxc}^{(0)}(\tilde{n}+\hat{n})\cdot \hat{Q}_{ij}^{L(1)}(\mathbf{r})\cdot d\mathbf{r}\right)\cdot\left(\left|\tilde{p}_i^R\right\rangle\left\langle\tilde{p}_j^R\right|\right) \\ +\left(\sum_L \int_{R^3} V_{Hxc}^{(0)}(\tilde{n}+\hat{n})\cdot \hat{Q}_{ij}^{L}(\mathbf{r})\cdot d\mathbf{r}\right)\cdot\left(\left|\tilde{p}_i^R\right\rangle\left\langle\tilde{p}_j^R\right|\right)^{(1)}\end{array}\right)$$

$$+\sum_{R,ij}\left(\begin{array}{l}\left\langle\phi_i\left|V_{Hxc}^{(0)}(n_1)\right|\phi_j\right\rangle_{\Omega_R} \\ -\left\langle\tilde{\phi}_i\left|V_{Hxc}^{(0)}(\tilde{n}_1+\hat{n}_1)\right|\tilde{\phi}_j\right\rangle_{\Omega_R} \\ -\sum_L \int_{\Omega_R} V_{Hxc}^{(0)}(\tilde{n}_1+\hat{n}_1)\cdot \hat{Q}_{ij}^{L}(\mathbf{r})d\mathbf{r}\end{array}\right)\cdot\left(\left|\tilde{p}_i^R\right\rangle\left\langle\tilde{p}_j^R\right|\right)^{(1)}$$

$$\tilde{V}_{Hxc}^{(1)} = V_{Hxc}\left(\tilde{n}+\hat{n}\right)^{(1)}$$

Compensation charge

$$+\sum_{R,ij}\left(\begin{array}{l}\sum_L \int_{R^3} V_{Hxc}^{(1)}(\tilde{n}+\hat{n})\cdot \hat{Q}_{ij}^{L}(\mathbf{r})\cdot d\mathbf{r} \\ \times\left(\left|\tilde{p}_i^R\right\rangle\left\langle\tilde{p}_j^R\right|\right)\end{array}\right)$$

$$+\sum_{R,ij}\left(\begin{array}{l}\left\langle\phi_i\left|V_{Hxc}^{(1)}(n_1)\right|\phi_j\right\rangle_{\Omega_R} \\ -\left\langle\tilde{\phi}_i\left|V_{Hxc}^{(1)}(\tilde{n}_1+\hat{n}_1)\right|\tilde{\phi}_j\right\rangle_{\Omega_R} \\ -\sum_L \int_{\Omega_R} V_{Hxc}^{(1)}(\tilde{n}_1+\hat{n}_1)\cdot \hat{Q}_{ij}^{L}(\mathbf{r})d\mathbf{r}\end{array}\right)\cdot\left(\left|\tilde{p}_i^R\right\rangle\left\langle\tilde{p}_j^R\right|\right)$$

On-site terms – **new in PAW**

Variational expression

$$E^{(2)} = E^{(2)}_{Frozen} + E^{(2)}_{WF} + E^{(2)}_{Hxc} + \dots$$

Frozen WF term

$$E^{(2)}_{Frozen} = \sum_n \left\langle \tilde{\Psi}^{(0)}_n \middle| \left.\frac{\partial^2 \tilde{H}}{\partial \lambda^2}\right|_{V^{(0)}_{Hxc}} - \varepsilon^{(0)}_n S^{(2)} \middle| \tilde{\Psi}^{(0)}_n \right\rangle$$

$$\left.\frac{\partial^2 \tilde{H}}{\partial \lambda^2}\right|_{V^{(0)}_{Hxc}} = V_H\left(\tilde{n}_{Zc}\right)^{(2)} + \sum_{R,ij} D^{KV}_{ij} \cdot \left(\left|\tilde{p}^R_i\right\rangle\left\langle\tilde{p}^R_j\right|\right)^{(2)} + \sum_{R,ij} \left(\begin{array}{l} \left(\sum_L \int_{R^3} V^{(0)}_{Hxc}\left(\tilde{n}+\hat{n}\right)\cdot \hat{Q}^{L(2)}_{ij}(\mathbf{r})\cdot d\mathbf{r}\right)\cdot\left(\left|\tilde{p}^R_i\right\rangle\left\langle\tilde{p}^R_j\right|\right) \\ + \left(\sum_L \int_{R^3} V^{(0)}_{Hxc}\left(\tilde{n}+\hat{n}\right)\cdot \hat{Q}^{L(1)}_{ij}(\mathbf{r})\cdot d\mathbf{r}\right)\cdot\left(\left|\tilde{p}^R_i\right\rangle\left\langle\tilde{p}^R_j\right|\right)^{(1)} \\ + \left(\sum_L \int_{R^3} V^{(0)}_{Hxc}\left(\tilde{n}+\hat{n}\right)\cdot \hat{Q}^{L}_{ij}(\mathbf{r})\cdot d\mathbf{r}\right)\cdot\left(\left|\tilde{p}^R_i\right\rangle\left\langle\tilde{p}^R_j\right|\right)^{(2)} \end{array} \right)$$

Compensation charge

$$+ \sum_{R,ij} \left(\left\langle \phi_i \middle| V^{(0)}_{Hxc}\left(n_1\right) \middle| \phi_j \right\rangle_{\Omega_R} - \left\langle \tilde{\phi}_i \middle| V^{(0)}_{Hxc}\left(\tilde{n}_1+\hat{n}_1\right) \middle| \tilde{\phi}_j \right\rangle_{\Omega_R} - \sum_L \int_{\Omega_R} V^{(0)}_{Hxc}\left(\tilde{n}_1+\hat{n}_1\right)\cdot \hat{Q}^L_{ij}(\mathbf{r}) d\mathbf{r} \right) \cdot \left(\left|\tilde{p}^R_i\right\rangle\left\langle\tilde{p}^R_j\right|\right)^{(2)}$$

On-site terms – **new in PAW**

DFPT+PAW : basics

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$$E^{(2)} = E^{(2)}_{Frozen} + E^{(2)}_{WF} + E^{(2)}_{Hxc} + \ldots$$

WF term

$$E^{(2)}_{WF} = \sum_n \left\{ \begin{array}{l} \left\langle \tilde{\Psi}^{(1)}_n \middle| \tilde{H}^{(0)} - \varepsilon^{(0)}_n S^{(0)} \middle| \tilde{\Psi}^{(1)}_n \right\rangle \\ + \left\langle \tilde{\Psi}^{(1)}_n \middle| \left. \frac{\partial \tilde{H}}{\partial \lambda} \right|_{V^{(0)}_{Hxc}} - \varepsilon^{(0)}_n S^{(1)} \middle| \tilde{\Psi}^{(0)}_n \right\rangle + c.c. \end{array} \right\}$$

V_{Hxc} term

$$E^{(2)}_{Hxc} = \frac{1}{2} \int_{R^3} V^{(1)}_{Hxc}(\tilde{n} + \hat{n})(\mathbf{r}') \cdot (\tilde{n} + \hat{n})^{(1)}(\mathbf{r})\, d\mathbf{r}' d\mathbf{r}$$

Compensation charge

$$+ \sum_R \left[\frac{1}{2} \int_{\Omega_R} V^{(1)}_{Hxc}(n_1)(\mathbf{r}') \cdot n_1^{(1)}(\mathbf{r})\, d\mathbf{r}' d\mathbf{r} - \frac{1}{2} \int_{\Omega_R} V^{(1)}_{Hxc}(\tilde{n}_1 + \hat{n}_1)(\mathbf{r}') \cdot (\tilde{n}_1 + \hat{n}_1)^{(1)}(\mathbf{r})\, d\mathbf{r}' d\mathbf{r} \right]$$

On-site terms – **new in PAW**

DFPT+PAW : difficulties (appeared during implementation)

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1. PAW non-local Hamiltonian depends on each atom (not only atom type)

2. PAW non-local Hamiltonian is self-consistent

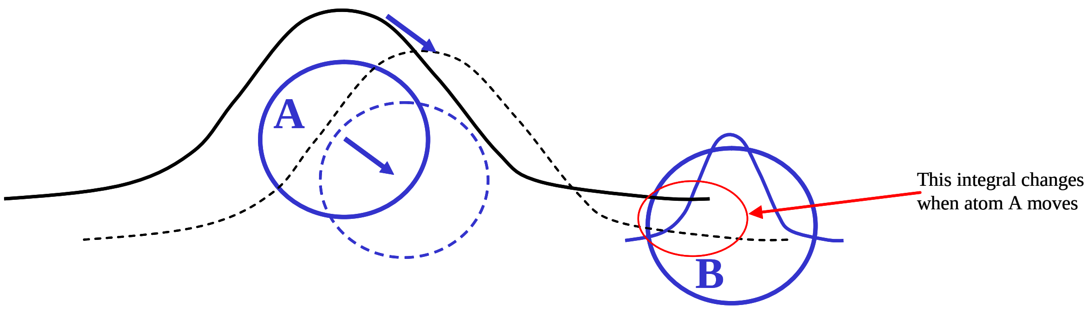
3. 2nd order « frozen » matrix is non-diagonal
   - because of long-range terms connecting 2 atomic sites
   - because of derivative of wave-function overlap

4. Non-stationnary expression of 2nd-order energy
   - is non-symetric
   - contains lot of additional terms (wr NC pseudopotentials)

DFPT+PAW : difficulties (appeared during implementation)

1. PAW non-local Hamiltonian depends on each atom (not only atom type)

$$\sum_{R,ij} \underbrace{\left(\sum_L \int_{R^3} V_{Hxc}^{(1)} \left(\tilde{n}+\hat{n}\right) \cdot \hat{Q}_{ij}^L(\mathbf{r}) \cdot d\mathbf{r} \right)}_{Part\,of\;\hat{D}_{ij}^{(1)}} \cdot \left(\left| \tilde{p}_i^R \right\rangle \left\langle \tilde{p}_j^R \right| \right)$$



DFPT+PAW : difficulties (appeared during implementation)

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2. PAW non-local Hamiltonian is self-consistent

$$+\sum_{R,ij}\left(D_{ij}^{(1)}\cdot\left(\left|\tilde{p}_i^R\right\rangle\left\langle\tilde{p}_j^R\right|\right)+D_{ij}\cdot\left(\left|\tilde{p}_i^R\right\rangle\left\langle\tilde{p}_j^R\right|\right)^{(1)}\right)$$

Depends on the density and the occupation matrix (and derivatives)

- Computation of H(1) had to be modularized
- Structure of ABINIT routines had to be strongly modified

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3. 2nd order « frozen » matrix is non-diagonal (wr to atoms)
> because of long-range terms connecting 2 atomic sites
> because of derivative of wave-function overlap

Change of wave-function overlap with respect to perturbation :

This term depends only on the change of the geometry…

$$\delta\tilde{\Psi}_n^{(1)} = \sum_{m=1}^{N} \left\langle \tilde{\Psi}_m^{(0)} \middle| S^{(1)} \middle| \tilde{\Psi}_n^{(0)} \right\rangle \cdot \tilde{\Psi}_m^{(0)}$$

Example of « frozen » term :

$$\left\langle \delta\tilde{\Psi}_n^{(\mathbf{j1})} \middle| \tilde{H}^{(\mathbf{j2})} - \varepsilon_n^{(0)} S^{(\mathbf{j2})} \middle| \tilde{\Psi}_n^{(0)} \right\rangle$$

j1, j2 are two different perturbations

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4. Non-stationnary expression of 2nd-order energy

> contains lot of additional terms *(wr to NC pseudopotentials)*

> is non-symetric

$\frac{\partial^2 E_{tot}}{\partial\lambda_1\partial\lambda_2}$ is obtained using a « non-stationnary » expression, variational with respect to one of the two perturbations

While in NC pseudopotential formalism, the non-stationnary expression is obtained by putting $\tilde{\Psi}_n^{(\mathbf{j2})} = 0$ in the stationnary expression,…

… within PAW it is obtained by putting $\tilde{\Psi}_n^{(\mathbf{j2})} = \delta\tilde{\Psi}_n^{(\mathbf{j2})}$ in the stationnary expression,…

Lot of new terms appear :

$$\left\langle \delta\tilde{\Psi}_n^{(\mathbf{j1})} \middle| \tilde{H}^{(\mathbf{j2})} - \varepsilon_n^{(0)} S^{(\mathbf{j2})} \middle| \tilde{\Psi}_n^{(0)} \right\rangle, \quad \left\langle \delta\tilde{\Psi}_n^{(\mathbf{j1})} \middle| \tilde{H}^{(0)} - \varepsilon_n^{(0)} S^{(0)} \middle| \tilde{\Psi}_n^{(\mathbf{j2})} \right\rangle \quad \ldots$$

DFPT+PAW : phonons

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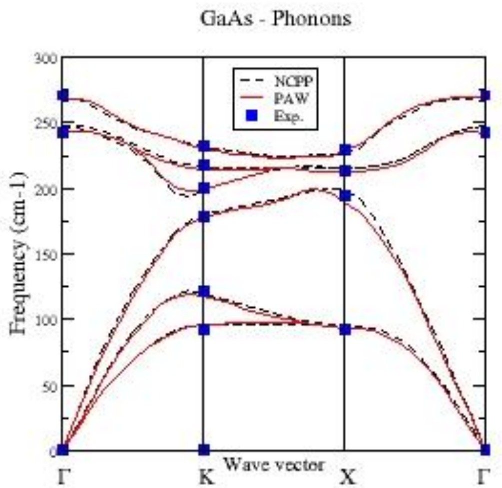
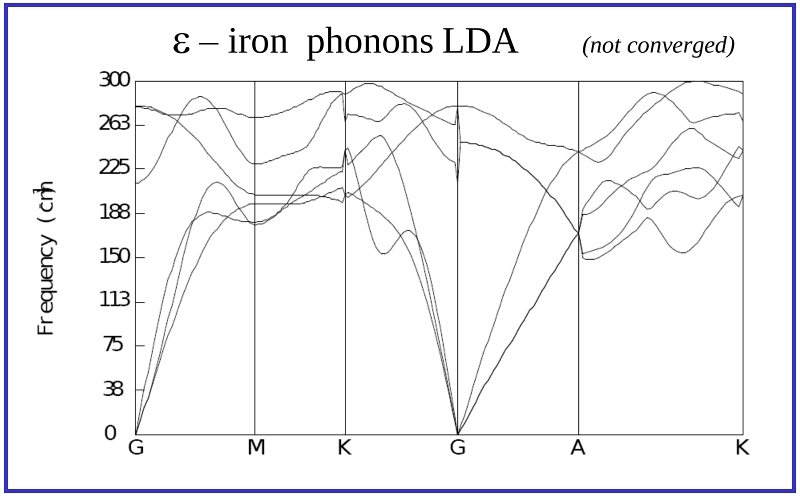
Implemented during the 2009-10 period :

- Phonons at non-zero q
- Completely rewritten non-stationnary expression of 2nd-order energy
- Several new terms not published in papers *(papers only valid for insulators at q=0)*
- Phonons for metals





DFPT+PAW : response to electric field

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Done in 2009

1- Implementation of 1st-order wave function
  $\rightarrow$ J. Zwanziger visit at CEA-Bruyères-le-Châtel *(May 09)*

2- Implementation of response to mixed perturbations
  (atomic position + electric field) $\rightarrow$ Born effective charges

New terms for Born Effective Charge:
  non-diagonal contribution to frozen terms

$$\widetilde{H}(\vec{\mathcal{E}}) = -\frac{1}{2}\Delta + \widetilde{v}_{eff} + \vec{\mathcal{E}}\cdot\vec{r} + \sum_{R,ij} \left|\widetilde{p}_i^R\right\rangle \left(D_{ij}^R(\vec{\mathcal{E}}) + S_{ij}^R\, \vec{\mathcal{E}}\cdot\vec{R}\right) \left\langle\widetilde{p}_j^R\right|$$

$$\frac{\partial^2 \widetilde{H}(\vec{\mathcal{E}})}{\partial R_\beta^a \partial \mathcal{E}_\alpha} = \sum_{ij,b}\left[\frac{\partial\left(\left|\widetilde{p}_i^R\right\rangle\left\langle\widetilde{p}_j^R\right|\right)}{\partial R_\beta^b}\left(X_{ij,\alpha}^R + S_{ij}^R R_\alpha^b\right)\right] + \delta_{a,b} G_{\alpha\beta}^{met} \sum_{ij}\left[\left|\widetilde{p}_i^R\right\rangle S_{ij}^R \left\langle\widetilde{p}_j^R\right|\right]$$

$$S_{ij}^R = \left\langle\phi_i^R\middle|\phi_j^R\right\rangle - \left\langle\widetilde{\phi}_i^R\middle|\widetilde{\phi}_j^R\right\rangle$$

$$X_{ij,\alpha}^R = \left\langle\phi_i^R\middle|r_\alpha - R_\alpha\middle|\phi_j^R\right\rangle - \left\langle\widetilde{\phi}_i^R\middle|r_\alpha - R_\alpha\middle|\widetilde{\phi}_j^R\right\rangle$$

```
 ==> Compute Derivative Database <==
..
 2nd-order matrix (non-cartesian coordinates, masses not included,
  asr not included )
    j1       j2             matrix element
 dir pert dir pert     real part     imaginary part
..
  1    1   1    1        5.1970177489        -0.0000000000
  1    1   2    1        2.8974276861        -0.2083331780
  1    1   3    1        2.2996058366        -0.2083335520
  1    1   1    2       -2.1529739716        -2.1529856454
  1    1   2    2       -2.2637511671        -0.0000123995
  1    1   3    2       -2.1529767949         0.1107713384
..
  2    1   1    1        2.8974270759         0.2083337358
  2    1   2    1        5.7948550464        -0.0000000000
  2    1   3    1        2.8974278341        -0.2083327220
  2    1   1    2       -2.0421972253        -0.0000125041
  2    1   2    2        0.0000005201        -0.0000252275
  2    1   3    2       -2.0422004924        -0.0000124574
..
```

DFPT+PAW : response to electric field

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GaAs

Electric tensor and
Born Effective Charges

```
 Dielectric tensor, in cartesian coordinates,
    j1       j2             matrix element
 dir pert dir pert     real part    imaginary part
..
   1    4   1    4         10.0184419580        -0.0000000000
   1    4   2    4         -0.0000000000        -0.0000000000
   1    4   3    4         -0.0000000000        -0.0000000000
..
   2    4   1    4         -0.0000000000        -0.0000000000
   2    4   2    4          9.9527284463        -0.0000000000
   2    4   3    4         -0.0000000000        -0.0000000000
..
   3    4   1    4         -0.0000000000        -0.0000000000
   3    4   2    4         -0.0000000000        -0.0000000000
   3    4   3    4          9.9439753269        -0.0000000000
..
 Effective charges, in cartesian coordinates,
 (from electric field response).
  if specified in the inputs, asr has been imposed
    j1       j2             matrix element
 dir pert dir pert     real part    imaginary part
..
   1    1   1    4          7.8973715868         0.0000000000
   2    1   1    4          0.0000000000         0.0000000000
   3    1   1    4          0.0000000000         0.0000000000
   1    2   1    4          0.4288167154         0.0000000000
   2    2   1    4          0.0000000000         0.0000000000
   3    2   1    4          0.0000000000         0.0000000000
..
   1    1   2    4          0.0000000000         0.0000000000
   2    1   2    4          7.8443360516         0.0000000000
   3    1   2    4          0.0000000000         0.0000000000
   1    2   2    4          0.0000000000         0.0000000000
   2    2   2    4          0.4284995080         0.0000000000
   3    2   2    4         -0.0000000000         0.0000000000
..
   1    1   3    4         -0.0000000000         0.0000000000
   2    1   3    4          0.0000000000         0.0000000000
   3    1   3    4          7.8585491314         0.0000000000
   1    2   3    4         -0.0000000000         0.0000000000
   2    2   3    4         -0.0000000000         0.0000000000
   3    2   3    4          0.4256180822         0.0000000000
```

DFPT+PAW : available functionnalities

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Available

Full usage of cut3d

- Spectra
- Phonon DOS
- LO-TO splitting

Electron-phonon coupling

Not available

- Spin-orbit coupling
- Elastic constants
- Non-linear response

Current status for phonons

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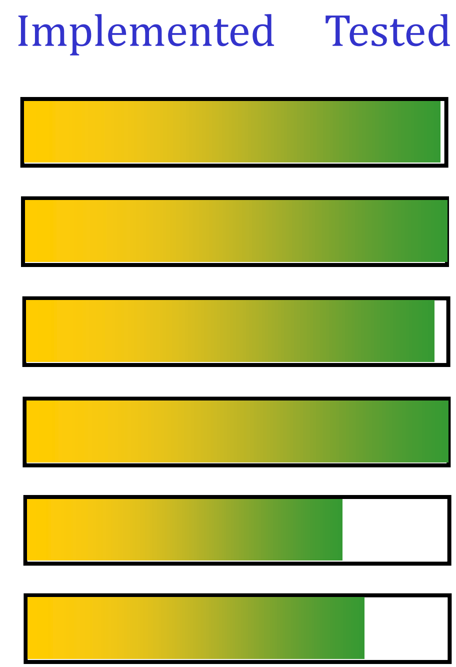
- Phonons at q=0
- Phonons at q/=0
- Correction for metals
- Correction from elect. field
- Phonons + GGA
- Phonons + spinors

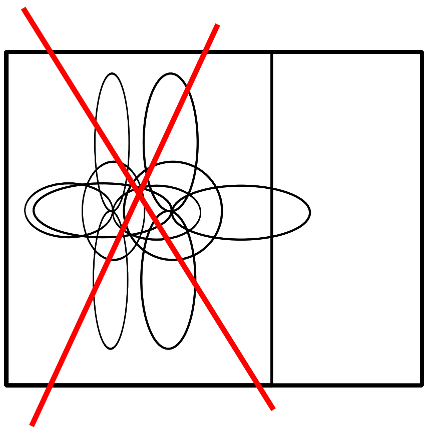


Project 1 : Elastic tensor

Formalism has to be derived :

No contribution from local basis change

- 2^{nd}-order Hamiltonan
- Non-stationnary expression of 2^{nd}-order energy



First-order Hamiltonian already implemented

(nonlocal Hamiltonian uses Ylm)

$$\tilde{H}^{(\alpha\beta)} = \left.\frac{\partial \tilde{H}}{\partial \varepsilon_{\alpha\beta}}\right|_{V_{Hxc}^{(0)}} + \tilde{V}_{Hxc}^{(\alpha\beta)}$$

$$\left.\frac{\partial \tilde{H}}{\partial \varepsilon_{\alpha\beta}}\right|_{V_{Hxc}^{(0)}} = V_H\left(\tilde{n}_{Zc}\right)^{(\alpha\beta)} + \sum_{R,ij} D_{ij}^{KV} \cdot \left(\left| \tilde{p}_i^R \right\rangle \left\langle \tilde{p}_j^R \right| \right)^{(\alpha\beta)}$$

$$+ \; on - site\,terms$$

$$\tilde{V}_{Hxc}^{(\alpha\beta)} = V_{Hxc}\left(\tilde{n} + \hat{n}\right)^{(\alpha\beta)}$$

$$+ \; on - site\,terms$$

Project 2 : non-linear response

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3rd derivative of total energy

- Formulae have been published in 2006 paper
- Only 1st-order wave-function(s) needed (already available within PAW)
- Complicated task : 3rd-order Hamiltonian $H^{(3)}$
- only q=0
- No change in *anaddb*

$$\frac{\partial^3 E_{tot}}{\partial \boldsymbol{\mathcal{E}}_k \, \partial \boldsymbol{\mathcal{E}}_j \, \partial \boldsymbol{\mathcal{E}}_i}$$

$$\frac{\partial^3 E_{tot}}{\partial \boldsymbol{\mathcal{E}}_k \, \partial \boldsymbol{\mathcal{E}}_j \, \partial R_i^B}$$

C. Audouze, F. Jollet, M. Torrent, X. Gonze, Phys. Rev. B ***73****, 235101* ***(2006)***

Conclusion

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- DFPT+PAW is an ongoing project…
- Phonons : done at 99%
  - Code structure has been revised in 2009-10
  - All capabilities of *cut3d* available
  - To be tested : spin-orbit
- (Mixed) response to electric field : OK
- Starting projects :
  - Elastic tensor
  - Non-linear response

WANTED

PhD
Post-docs

CEA & ENS Lyon

Contact :
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