

QE-GIPAW user's manual

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1 Introduction

QE-GIPAW is an improved version of the GIPAW once code distributed in Quantum-Espresso. Starting from QE 4.3, QE-GIPAW is distributed as a stand-alone package that to be compiled against Quantum-Espresso.

2 Features

- Periodic and isolated systems
- Norm-conserving and ultrasoft pseudopotentials
- Parallelization over k-points (pools) and g-vectors
- Automatic checkpoint and restart
- Magnetic susceptibility
- NMR chemical shielding tensors [[1](#), [2](#)]
- Electric Field Gradients (EFG)
- EPR g-tensor [[3](#)]
- Hyperfine couplings

3 Author contributions

- D. Ceresoli: bare susceptibility, hyperfine core polarization
- A. P. Seitsonen and U. Gerstmann: GIPAW reconstruction
- E. Kuçukbenli: ultrasoft and PAW pseudopotentials
- S. de Gironcoli: restart and bug fixes

For further information and to report bugs, please contact:

4 Quick build instructions

Thank to Layla Martin Samos, QE-GIPAW can be configured and compiled automatically once you download Quantum-Espresso version 4.3 and above.

1. Configure Quantum-Espresso (QE) version >4.3. If you have problems, read the QE user's guide at http://www.quantum-espresso.org/user_guide/user_guide.html
2. Type:

```
make gipaw
```

This will download from QE-forge the latest stable version of QE-GIPAW and it will compile it.

5 Build instructions

If you don't have a direct Internet connection on your machine, or if you want to build a different version of the code, or even the SVN version:

1. Configure and compile quantum-Espresso in the usual way. The supported version are >4.3 and the SVN version.
2. Download QE-GIPAW from tarball or from SVN. QE-GIPAW can be downloaded and built outside the Quantum-Espresso folder:
From tarball:

```
tar xzfv qe-gipaw-4.3.2.tar.gz  
cd qe-gipaw-4.3.2
```

From SVN:

```
svn checkout svn://cvs.qe-forge.org/scmrepos/svn/qe-gipaw/trunk qe-gipaw  
cd qe-gipaw
```

3. Configure and build QE-GIPAW:

```
./configure --with-qe-source=quantum espresso folder containing make.sys  
(for example: ./configure --with-qe-source=$HOME/Codes/espresso-4.3.2)  
make
```

QE-GIPAW will be built according to the options and libraries specified in `make.sys` and the `gipaw.x` executable will be placed in the `bin` folder.

6 Quick start

To calculate NMR/EPR parameters you need:

1. pseudopotentials containing the GIPAW reconstruction (look into folder `pseudo`)
2. run `pw.x` to perform the SCF calculation
3. run `gipaw.x` to calculate parameters (look into folder `examples` for NMR shielding, EFG, EPR g-tensor and hyperfine couplings)

7 Input file description

The input file consists on only one namelist `&inputgipaw` with the following keywords:

job (type: character, default: `'nmr'`)

Description: select calculation to perform. The possible values are:

<code>'f-sum'</code>	check the f-sum rule
<code>'nmr'</code>	compute the magnetic susceptibility and NMR chemical shifts
<code>'efg'</code>	compute the electric field gradients at the nuclei
<code>'g_tensor'</code>	compute the EPR g-tensor
<code>'hyperfine'</code>	compute the hyperfine couplings

prefix (type: character, default: `'pwscf'`)

Description: prefix of files saved by program `pw.x`

tmp_dir (type: character, default: `'./scratch/'`)

Description: temporary directory for `pw.x` restart files

max_seconds (type: real, default: 10^7)

Description: max wall time clock before writing the checkpoint and terminate

restart_mode (type: character, default: `'restart'`)

Description: if `'restart'` attempt to restart from a previous interrupted run. If `'from_scratch'`, discard any restart information

conv_threshold (type: real, default: 10^{-14} , units: Ry^2)

Description: convergence threshold for the diagonalization and for the Green's function solver

isolve (type: integer, default: 0)

Description: diagonalization method (Davidson = 0, CG = 1)

q_gipaw (type: real, default: 0.01, units: bohrradius^{-1})

Description: the small wave-vector for linear response

iverbosity (type: integer, default: 0)

Description: if `iverbosity > 0` print debug information in output

filcurr (type: character, default: `''`)

Description: write the induced current in this file

filfield (type: character, default: `''`)

Description: write the induced magnetic field in this file

use_nmr_macroscopic_shape (type: logical, default: `.false.`)

Description: correct the chemical shift by taking into account the macroscopic shape of the sample

nmr_macroscopic_shape(3,3) (type: real, default: $2/3$)

Description: shape tensor for the macroscopic shape correction

spline_ps (type: logical, default: `.true.`)

Description: interpolate pseudopotentials with cubic splines

q_efg(1..ntyp) (type: real, default: 0.0, units: $10^{-30} \text{ m}^2 = 0.01 \text{ barn}$)

Description: for each atomic specie, the nuclear quadrupole

hfi_output_unit (type: character, default: 'MHz')

Description: units for hyperfine couplings in output. The possible values are: 'MHz', 'mT', 'G', 'Gauss', '10e-4cm-1'

hfi_nuclear_g_factor(1..ntyp) (type: real, default: 0.0)

Description: for each atomic specie, the nuclear g-factor

core_relax_method (type: integer, default: 1)

Description: select the method to evaluate the core polarization contribution to the isotropic hyperfine (Fermi contact). The possible values are:

- 1 perturbative [4], exchange-only (Slater X- α)
- 2 perturbative [4], exchange-only
- 3 perturbative [4], exchange and correlation

There a number of obsolete or development variables that can be removed at any time from the code: **radial_integral_splines**, **hfi_via_reconstruction_only**, **hfi_extrapolation_npoints**, **pawproj(1..ntyp)**, **read_recon_in_paratec_fmt**, **file_reconstruction(1..ntyp)**.

8 Limitations

Symmetry operations that do not map cartesian axes are not allowed (i.e. 120° rotations). If you have a triclinic cell, remove all symmetries (**nosym** = **.true.**). In the special case of an hexagonal cell, you can use **ibrav** = 0 and orient the cell like in the quartz example. The keyword **CELL_PARAMETERS cubic** prevents PW to detect 120° rotations.

9 Resources

- Websites: <http://qe-forge.org/projects/qe-gipaw>, <http://www.gipaw.net/>
- NMR periodic table: <http://www.pascal-man.com/periodic-table/periodictable.html>
- Tutorials: http://www.gipaw.net/work_zurich09.html, <http://sites.google.com/site/cecamspectra2010/program> (day 2)

References

- [1] C. J. Pickard and F. Mauri, Phys. Rev. B **63**, 245101 (2001)
- [2] J. R. Yates, C. J. Pickard and F. Mauri, Phys. Rev. B **76**, 024401 (2007)
- [3] C. J. Pickard and F. Mauri, Phys. Rev. Lett. **88**, 086403 (2002)
- [4] M. S. Bahramy, M. H. F. Sluiter and Y. Kawazoe, Phys. Rev. B **76**, 035124 (2007)