QE-GIPAW user's manual

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Last revision: December 9, 2011

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
- Electric Field Gradients (EFG)
- EPR g-tensor
- 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 zxfv 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:

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

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: $10^{-30}\ \text{m}^2 = 0.01$ 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

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 triclinc 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

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