QE-GIPAW User Manual

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QE-GIPAW is an improved version of the GIPAW code distributed in Quantum-Espresso. QE-GIPAW is distributed as a stand-alone package that must be compiled against Quantum-Espresso.

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- Norm-conserving and ultrasoft pseudopotentials
- Parallelization over k-points (pools) and g-vectors
- Automatic checkpoint and restart
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- NMR chemical shielding tensors
- Electric Field Gradients (EFG)
- EPR g-tensor
- Hyperfine couplings

Authors

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

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Build instructions

1. Configure and compile quantum-Espresso in the usual way. The supported version are 4.3, 4.3a, 4.3b and the current 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.tar.gz
   cd qe-gipaw-4.3
   From SVN:
   svn checkout svn://cvs.qe-forge.org/scmrepos/svn/qe-gipaw/trunk qe-gipaw
   cd qe-gipaw
3. Build QE-GIPAW:
   ./configure --with-qe-source=<quantum espresso folder containing make.sys>
   (for example: **./configure –with-qe-source=$HOME/Codes/espresso-4.3**)
   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.

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)

Input file description

The input file consists on only one namelist **&inputgipaw:**

Variable: **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 suscept. 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

Variable: **prefix** type: character default 'pwscf'
Description: prefix of files saved by program pw.x

Variable: **tmp_dir** type: character default: './scratch/'
Description: temporary directory where pw.x files resides

Variable: **max_seconds** type: real default: 10^7 units: s
Description: max wall time clock before writing the checkpoint and terminate

Variable: **conv_threshold** type: real default: 10^{-14} units: Rydberg^2
Description: convergence threshold for the diagonalization and for the Green's function solver

Variable: **isolve** type: integer default: 0
Description: diagonalization method (Davidson = 0, CG = 1)

Variable: **q_gipaw** type: real default: 0.01 units: $bohr^{-1}$
Description: the small wave-vector for linear response

Variable: **iverbosity** type: integer default: 0
Description: if iverbosity > 0 print debug information in output

Variable: **filcurr** character default: "
Description: file name for the induced current

Variable: **filfield** type: character default: "
Description: file name for the induced current

Variable: **use_nmr_macroscopic_shape** type: logical default: .false.
Description: correct the chemical shift by taking into account the macroscopic shape of the sample

Variable: **nmr_macroscopic_shape(3,3)** type: real default: 2/3
Description: shape tensor for the macroscopic shape correction

Variable: **spline_ps** type: logical default: .true.
Description: interpolate pseudopotentials with cubic splines

Variable: **q_efg(1..ntyp)** type: real default: 0.0 units: 10^{-30} m^2 = 0.01 barn
Description: for each atomic specie, the nuclear quadrupole

Variable: **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'

Variable: **hfi_nuclear_g_factor(1..ntyp)** type: real default: 0.0
Description: for each atomic specie, the nuclear g-factor

Obsolete/development variables (do not use):

- radial_integral_splines
- hfi_via_reconstruction_only
- hfi_extrapolation_npoints
- pawproj(1..ntyp)
- read_recon_in_paratec_fmt
- file_reconstruction(1..ntyp)

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.

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. 63, 245101 (2001)