

QE-CONVERSE user's manual

Simone Fioccola, sfioccola@laas.fr

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1 Introduction

The QE-CONVERSE implement a non-perturbative approach (converse) to compute the orbital magnetization in isolated and periodic systems. The calculation of orbital magnetization allows ab-initio computation of macroscopic properties like the Nuclear Magnetic Resonance (NMR) chemical shifts and the Electronic Paramagnetic Resonance (EPR) g tensor.

2 Features

- Periodic and isolated systems
- Norm-conserving pseudopotentials
- Parallelization over bands and g-vectors
- NMR shielding tensors
- EPR g-tensor
- LDA and GGA functionals

3 Author contributions

S. Fioccola, L. Giacomazzi, D. Ceresoli, N. Richard, A. Hemeryck, L. Martin-Samos

4 Build instructions

This current version of the code is compatible with the version 7.2 of Quantum-Espresso package.

1. A Quantum-Espresso package version 7.2 must be previously installed (<https://gitlab.com/QEF/q-e/-/releases/qe-7.2>). To take advantage of the enhancements in linear algebra operations, the configuration with scaLAPACK package or ELPA library is suggested. QE user's guide at http://www.quantum-espresso.org/user_guide/user_guide.html
2. Type:

```
git clone https://github.com/mammasmias/QE-CONVERSE
```

This will download from github the latest stable version of QE-CONVERSE.

3. Type:

```
cd QE-CONVERSE
```

4. Copy the source files and the Makefile from `/src/` dictory into `/PP/` directory of Quantum-Espresso.

5. In the main directory of QE-7.2 type `make pp`. You should find the binary file `qe-converse.x` in the `/bin/` directory of Quantum-Espresso.

5 Quick start

To calculate NMR/EPR parameters you need:

1. pseudopotentials containing the GIPAW reconstruction (<https://sites.google.com/site/dceresoli/pseudopotentials>)
2. run `pw.x` to perform the SCF calculation
3. run `qe-converse.x` to calculate parameters (look into folder `examples` for NMR shielding, EPR g-tensor.)

6 Input file description

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

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

Description: prefix of files saved by program `pw.x`. The value of this keyword must be the same used in the SCF calculation.

outdir (type: character, default: `'./'`)

Description: temporary directory for `pw.x` restart files. The value of this keyword must be the same used in the SCF calculation.

diagonalization (type: string, default: `'david'`)

Description: diagonalization method (only allowed values: `'david'`)

verbosity (type: string default: `'high'`)

Description: verbosity level (allowed values: `'low'`, `'medium'`, `'high'`)

q_gipaw (type: real, default: 0.01, units: bohrradius⁻¹)

Description: the small wave-vector for the covariant finite difference formula.

dudk_method (type: string, default: `'covariant'`)

Description: k-point derivative method (only allowed values: `'covariant'`)

diag_thr_init (type: real, default: 10⁻⁷, units: Ry²)

Description: Convergence threshold (ethr) for iterative diagonalization.

conv_threshold (type: real, default: 10⁻⁸, units: Ry²)

Description: convergence threshold for the diagonalization in the SCF step.

mixing_beta (type: real, default: 0.5)

Description: mixing factor for self-consistency.

lambda_so(1,...,3) (type: real, default: 0.0, units: Bohr magneton)

Description: Cartesian components of electron spin. The value (1,...,3) denotes the spin-orbit coupling direction.

m_0(1,...,3) (type: real, default: 0.0, units: nuclear magneton)

Description: Cartesian components of nuclear dipole. The value (1,...,3) denotes the nuclear dipole moment direction.

m_0_atom (type: integer, default: 0)

Description: Atom index carrying the nuclear magnetic dipole.

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

Description: If `.true.`, temporary du/dk files (wavefunction k-derivatives) are deleted after the orbital magnetization calculation.

7 Limitations

Parallelization on k-point (pool) is not allowed.

K_POINTS GAMMA are not supported. For Gamma-point calculations use: K_POINTS automatic and '1 1 1 0 0 0'

8 Resources

- NMR periodic table: <http://www.pascal-man.com/periodic-table/periodictable.html>

References

[1]