QE-CONVERSE user's manual

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Last revision: June 7, 2024

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

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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: Ry^2)
Description: Convergence threshold (ethr) for iterative diagonalization.

conv_threshold (type: real, default: 10^{-8}, units: Ry^2)
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.

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]