

KGEC USER GUIDE

Kubo-Greenwood Electrical Conductivity Code

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I. Basics

- KGEC (Kubo-Greenwood Electrical Conductivity) is a post-processor module for use with Quantum Espresso. QE versions 5.1.2, 5.2.1, 5.4.0, 6.0, 6.1, 6.2.1, 6.3 and 6.4.1 are currently supported.

KGEC calculates the complex conductivity and dielectric tensors as well as the refraction, reflection, absorption coefficients and electron energy loss spectra.

QE 5.2.1 compiled for use in the Profess@QE suite [Comput. Phys. Commun. **185**, 3240 (2014)] also is supported. KGEC runs at both zero and non-zero temperature, with the temperature passed to KGEC via the occupation numbers (and associated Kohn-Sham orbitals and eigenvalues) from the QE calculation. Note that Profess@QE enables use of free-energy exchange-correlation functionals [e.g. Phys. Rev. Lett. **112**, 076403 (2014); Phys. Rev. E **93**, 063207 (2016); arXiv 1612.06266v2]. It also enables use of finite-temperature orbital-free DFT [Phys. Rev. B **88**, 161108(R) (2013)] for thermodynamic properties, including snapshot averages of electrical conductivity.

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- Licensure: GNU GPL.
- Main reference: “Kubo-Greenwood Electrical Conductivity Formulation and Implementation for Projector Augmented Wave Datasets”, L. Calderín, V.V. Karasiev, and S.B. Trickey (in preparation for submittal to Comput. Phys. Commun. as of this date).

II. Definitions, Abbreviations, and Notation

ω : frequency

$\sigma_1(\omega)$: real part of the complex conductivity $\sigma(\omega)$ tensor

$\sigma_2(\omega)$: imaginary part of the complex conductivity $\sigma(\omega)$ tensor

$\mathbf{k}; n, n'$: vector in the Brillouin zone; band indices

$\Omega; w_{\mathbf{k}}$: unit cell volume; reciprocal space integration weights

$\Delta\epsilon_{n\mathbf{k}, n'\mathbf{k}}$: difference in eigenvalues for bands n and n' at fixed \mathbf{k}

$\Delta f_{n\mathbf{k}, n'\mathbf{k}}$: difference in Fermi-Dirac occupation numbers for bands n and n' at fixed \mathbf{k}

$\delta(x)$: Dirac delta function

AC: Alternating Current (i.e. frequency dependent)

DC: Direct Current (i.e. frequency independent)

KS: Kohn-Sham

PAW: Projector Augmented Wave

QE: Quantum Espresso

A. Prerequisites and Assumptions

Prerequisites for the installation of KGEC are:

- Fortran 90 compiler (Makefiles for Intel or GNU Linux Fortran provided).
- QE 5.1.2, 5.2.1, 5.4.0, 6.0, 6.1, 6.3 and 6.4.1 installed for either serial or mpi-parallel execution (or QE 5.2.1 modified and installed using Intel for use with Profess@QE).
- MPI for parallel compilation.

KGEC operation assumes that an ordinary QE calculation has been done with QE options set to `wf_collect=.true.`, `smearing='fd'`, `nosym=.true.`, `noinv=.true.` and any of the options for KPOINTS except "KPOINTS gamma".

The QE calculation provides the KS orbitals, orbital energies, occupation numbers, and other relevant data via storage in the usual `outdir` directory. All of that data is made accessible to KGEC by the `QE_VAR` and `QE_P_PSI` modules. Note that KGEC uses the `make.sys` file generated for QE 5.x during QE installation or equivalently, the `make.inc` file for QE-6.x.

B. Installation and Trial Run Example

It is impossible to provide instructions for all operating systems and compilers. Here we provide instructions tested with Linux systems of the Red Hat family versions 6 and 7 (Red Hat, CentOS, Fedora 20-25) and SUSE Linux 11 (Cray) using Intel compilers and the Bourne-again shell (bash). These instructions should be relatively easy to adapt to other computational environments.

1. Installation

- Download the KGEC package from www.calderin.net (version 2.1 is at www.qtp.ufl.edu/ofdft).
- Unzip the package to the `kgec` root directory named `KGECDIR`, and change into that directory.
- Modify the appropriate Makefile in `KGECDIR` to get the variable `QE` to point to the path to the root directory of your QE installation. *Notice* that the last segment of the path must be of the form `$QEV-$TYPE`, where `$QEV` is the version of QE and `$TYPE` is either 'serial' or 'mpi'. For example, use `6.0-mpi` for QE version 6 compiled with MPI. To comply with this requirement, one may create a symbolic link with the required name to the actual QE installation. An alternative is to edit the variables `QE` and `SRCDIR` to fit your needs. Also note that for use with QE 5.2.1 modified and compiled for incorporation in Profess@QE, use `Makefile.for-qe-5.2.1m5` (tested only with Intel compilers).
- Run `make` on this directory to create `./for-qe-$QEV-$TYPE/kgec.x`

2. Trial Run

Input data and output for a trial example are provided. It is a nearly trivial case, namely fcc Aluminum with 4 atoms per unit cell at bulk density $\rho = 2.7 \text{ g/cm}^3$ and temperature $= 0.05 \text{ Ry} = 0.683 \text{ eV} = 7894.37 \text{ K}$. The PAW dataset provided was generated with the ATOMPAW code (see Al.UPF file for more details). Detailed descriptions of input and output are given below.

To run the trial example, proceed as follows:

- Change to the `./example/run` directory
- Execute QE for the input file provided (`Al-fcc-4.in`)
- Once QE has finished, run `kegc.x` in the same directory; see run command details below.
- Compare the resulting output files with those in `./example/reference` See detailed description of output below. Note that if you are using QE compiled for use with Profess@QE, you should compare with `./example/reference/for-qe-5.2.1m5-serial` or `./example/reference/for-qe-5.2.1m5-mpi` as appropriate.

For serial KGEC execution, use the command:

```
KGEC_DIR/kegc.x < INP_DIR/kegc.in > OUT_DIR/kegc.out
```

For parallel KGEC execution, use the `-n`, `-nk`, `-nb`, and `-np` parameters and the corresponding MPIEXEC command of your parallel environment as done for QE. For example, to run 8 processes with 2 each for k-points, bands, and plane waves, issue the command:

```
mpirun -n 8 KGEC_DIR/kegc.x -nk 2 -nb 2 -np 2 < INP_DIR/kegc.in  
> OUT_DIR/kegc.out
```

C. Input and Output

The input file contains a Fortran card image named `kegcpp`. All the possible variables are described in Table I. An input file example is

```
&kegcpp  
  outdir='./',  
  prefix='al'  
  calculation='tensor'  
  sigma1_exact=.true.  
  decomposition=.true.  
  calculate_sigma2=.true.  
/
```

Notice that at minimum the input file must contain the 'outdir' and 'prefix' variables.

Variable	Description
outdir	Output directory as specified in the QE calculation.
prefix	The prefix variable as specified for the QE calculation.
ac (=true.)	Calculate the frequency-dependent conductivity.
dc (=true.)	Calculate the DC conductivity.
calculation (=‘atrace’)	Use ‘tensor’ for the full tensor, ‘atrace’ for the average trace.
sigma1_exact (=true.)	Use exact or approximated formula.
sigma1_notintra (=false.)	Do not include intra-band for the exact formula (only valid with sigma1_exact=true.).
calculate_sigma2 (=false.)	Calculate the imaginary part of the conductivity.
sigma2_notintra (=false.)	Do not include intra-band and degenerate contributions (only valid with calculate_sigma2=true.).
calculate_epsilon1 (=false.)	Calculate the real part of the dielectric function.
calculate_epsilon2 (=false.)	Calculate the imaginary part of the dielectric function.
calculate_rrae (=false.)	Calculate the refraction indexes, reflection coef., absorption coef. and electron energy loss spectrum.
decomposition (=true.)	Separate contributions into intra-band, degenerate, and inter-band (only possible with sigma1_exact=true., sigma1_notintra=false. and sigma2_notintra=false.).
writegm (=false.)	Write gradient matrix elements to disk.
readgm (=false.)	Read gradient matrix elements from disk.
check_wfc (=false.)	Check the orthogonality of orbitals.
check_delta (=false.)	Compare the effect of Lorentzians and Gaussians as delta function representations.
deltarep (=‘2l’)	Representation for the Dirac delta function: use ‘l’ or ‘1l’ for a Lorentzian, ‘2l’ for two Lorentzians, ‘g’ or ‘1g’ for a Gaussian, ‘2g’ for two Gaussians (case insensitive).
deltawidth (=0.01)	Width of the Dirac delta function representation in eV.
wmin (=0.01)	Minimum frequency in eV.
wmax (=5.0)	Maximum frequency in eV (wmin fixed to zero in the code).
nw (=1000)	Number of frequency steps, less one, in the closed interval $[wmin, wmax]$
non_local (=false.)	Use a norm-conserving pseudo-pot even though non-local corrections to matrix elements are not implemented.
npwrecover (=false.)	Recover pw processes for band parallelization.
yessym (=false.)	Over-ride the non-use of symmetry
yesinv (=false.)	Over-ride the non-use of inversion symmetry

TABLE I: KGEC input variables. Default values given in parentheses.

During execution, KGEC writes information both to standard output and to specific files. A standard output example follows. Notice that it is fully commented and provides information about the files written to disk and their content.

III. Acknowledgments

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