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 and 6.1 currently are supported. 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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- Other code authors and testers, Valentin Karasiev (vkarasev@qtp.ufl.edu), Sam Trickey (trickey@qtp.ufl.edu).

- 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 Linux Fortran provided).
- QE 5.1.2, 5.2.1, 5.4.0, 6.0 or 6.1 installed for either serial or mpi-parallel execution (or QE 5.2.1 installed 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.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 $TYPE is either 'serial' or 'mpi'. For example, use 6.0-mpi for QE version 6 compiled with MPI. To comply with this requirement, one may create a symbolic link with the required name to the actual QE installation. An alternative is to edit the variables QE and SRCDIR to fit your needs. Also note that for use with QE 5.2.1 compiled for incorporation in Profess@QE, use Makefile.for-qe-5.2.1m5.
- Run `make` on this directory to create ./for-qe-$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 $\rho = 2.7$ g/cm^3 and temperature = 0.05 Ry = 0.683 eV= 7894.37 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:

```
KGECDIR/kegec.x < INPDIR/kegec.in > OUTDIR/kgec.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:

```
mpiexec -n 8 KGEC_DIR/kegec.x -nk 2 -nb 2 -np 2 < INP_DIR/kegec.in
> OUT_DIR/kgec.out
```

C. Input and Output

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

```
&kgecpp
  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.
notintra (.false.)	Do not include intra-band and degenerate contributions for the exact formula (only valid with sigma1_exact=.true.).
decomposition (=.true.)	Separate contributions into intra-band, degenerate, and inter-band (only possible with sigma1_exact=.true.).
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.
npwrecovery (=.false)	Recover pw processes for band parallelization.
calculate_sigma2 (=.false.)	Calculate the imaginary part of the conductivity.
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.

```
  Program KGEC v.6.0 (svn rev. 13079) starts on  9Nov2016 at 16:40:22

  This program is part of the open-source Quantum ESPRESSO suite
  for quantum simulation of materials; please cite
      "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
       URL http://www.quantum-espresso.org",
  in publications or presentations arising from this work. More details at
  http://www.quantum-espresso.org/quote

  Serial version

  Reading data from directory:
  ./al.save

Info: using nr1, nr2, nr3 values from input

Info: using nr1, nr2, nr3 values from input

  IMPORTANT: XC functional enforced from input :
  Exchange-correlation      = SLA PW NOGX NOGC ( 1  4  0  0 0 0)
  Any further DFT definition will be discarded
  Please, verify this is what you really want

           file Al.UPF: wavefunction(s)  Xn Xn Xn renormalized

  G-vector sticks info
  --------------------
  sticks:   dense  smooth     PW     G-vecs:    dense   smooth      PW
  Sum         373     373    129                 5449     5449    1045


  Check: negative/imaginary core charge=   -0.000005    0.000000

  negative rho (up, down):  8.965E-03 0.000E+00

  ------------------------------------------------------------
            Parameters from the QE calculation
  ------------------------------------------------------------
  System                    :  al
  Directory                 :  ./
  Number of electrons       :           12.000000
  Temperature (Ry)(degauss) :            0.050000
  Temperature (K) (degauss) :         7894.366199
  Temperature (eV)(degauss) :            0.680285
```

```
Number of bands           :                  10
Number of k-points        :                   8
Sum of k-weights          :            2.000000
Sum of band weights       :           12.000000
Fermi energy (eV)         :            3.814888
Volume (bohr^3)           :          700.632341
Wave function cutoff (ry) :           15.000000
Pseudo type               :                PAWs

---------------------------------------------------------------
            Parameters for the KG conductivity
---------------------------------------------------------------
Type of calculation       : tensor
Calculate                 : Sigma1 and Sigma2
Spherical Harmonics       : Real
Formulas                  : exact
   Decomposition          : yes
Delta function width (eV) :  0.010000  (Lorentzian)
Check the wave functions  : yes
Check delta function rep. : yes
DC components only        : no
Gradient matrix elements  : calculate
 Energies equal. tol. (eV):  1.000000000000000E-006
Recover plane waves procs.: no
Frequency grid:
   Frequency step (eV)    :  5.000000000000000E-003
   Frequency steps        :        1000
   Frequency range (eV)   :    0.0000 to     5.0000

---------------------------------------------------------------
                      Calculations
---------------------------------------------------------------

Calculating the re-normalization factors of | \Psi_{nk} > ...

Checking the duality of projectors and pseudo orbitals:
 Atom type:           1
 projector  l     pswfc     l      < proj | pswfc >
    1       0       1       0           0.999987
    1       0       2       0           0.000673
    1       0       3       1           0.0_DP    (orthogonal by angular momentum)
    1       0       4       1           0.0_DP    (orthogonal by angular momentum)
    2       0       1       0           0.000004
    2       0       2       0           0.999787
    2       0       3       1           0.0_DP    (orthogonal by angular momentum)
    2       0       4       1           0.0_DP    (orthogonal by angular momentum)
    3       1       1       0           0.0_DP    (orthogonal by angular momentum)
    3       1       2       0           0.0_DP    (orthogonal by angular momentum)
```

```
    3       1       3       1          0.999967
    3       1       4       1         -0.002609
    4       1       1       0          0.0_DP    (orthogonal by angular momentum)
    4       1       2       0          0.0_DP    (orthogonal by angular momentum)
    4       1       3       1         -0.000003
    4       1       4       1          0.999768

Checking orthogonality of the Wave Functions ... done

Calculating the gradient matrix elements over pseudo \Psi_{n,k} .. done.

Calculating the gradient matrix elements over atomic orbitals
and pseudo-orbitals and PAW correction ..  done.

Writing the gradient matrix elements ... done.

Calculating checks for delta function rep. ...  done.

Calculating sigma1 ... done.
Calculating sigma2 ... done.

Sum rule (exact)          :     1.218
Sum rule (int. over freq.):     1.200


-----------------------------------------------------------------
             SIGMA1 RELATED OUTPUT (ohm meter)^-1
-----------------------------------------------------------------
sigma1 DC tensor: all contributions
 9.5100501E+007      1.1626726E+005      9.6678146E+005
 1.1626726E+005      1.1911311E+007     -2.2290284E+004
 9.6678146E+005     -2.2290284E+004      7.5616526E+007
  DC ave. trace (all contributions)        :   60876112.3472120
sigma1 DC tensor: intra-bands contribution
 2.8089305E+000      1.9318712E-001      2.0842136E-001
 1.9318712E-001      1.4960353E-002      1.3331280E-002
 2.0842136E-001      1.3331280E-002      1.6582065E-002
  DC ave. trace (intra-bands contribution) :  0.946824310479595
sigma1 DC tensor: degeneracies contribution
 0.0000000E+000      0.0000000E+000      0.0000000E+000
 0.0000000E+000      0.0000000E+000      0.0000000E+000
 0.0000000E+000      0.0000000E+000      0.0000000E+000
  DC ave. trace (degeneracies contribution):  0.000000000000000E+000
sigma1 DC tensor: inter-bands contribution
 9.5100498E+007      1.1626707E+005      9.6678125E+005
 1.1626707E+005      1.1911311E+007     -2.2290297E+004
 9.6678125E+005     -2.2290297E+004      7.5616526E+007
  DC ave. trace (inter-bands contribution) :   60876111.4003877
```

```
     Real part of the conductivity tensor and/or average trace (in
     1/(ohm-meter)) vs frequencies (in eV) saved to sigma1*.dat file(s).

     ---------------------------------------------------------------
                 SIGMA2 RELATED OUTPUT (ohm meter)^-1
     ---------------------------------------------------------------
     sigma2 DC tensor: all contributions
      0.0000000E+000      0.0000000E+000      0.0000000E+000
      0.0000000E+000      0.0000000E+000      0.0000000E+000
      0.0000000E+000      0.0000000E+000      0.0000000E+000
       DC ave. trace (all contributions):  0.000000000000000E+000
        (sigma2 DC tensor must be zero)

     Imaginary part of the conductivity tensor and/or average trace (in
     1/(ohm-meter)) vs frequency (in eV) saved to sigma2*.dat file(s).

     ---------------------------------------------------------------
            Kubo Greenwood conductivity calculation finished
     ---------------------------------------------------------------

     KGEC         :     1.65s CPU         1.74s WALL


   This run was terminated on:  16:40:23   9Nov2016

=------------------------------------------------------------------------------=
   JOB DONE.
=------------------------------------------------------------------------------=
```

III. Acknowledgments

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