Optical conductivity using abinit with norm-conserving pseudopotentials

V. Recoules

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1 Kubo-Greewood formula implementation

The real part of the optical conductivity versus frequency ω is computed using the Kubo-Greenwood formulation [1, 2] and can be expressed as :

$$\sigma(\omega) = \frac{2\pi}{3}\frac{1}{\Omega}\sum_{\boldsymbol{k}} W(\boldsymbol{k})\sum_{n,m}(f_n^{\boldsymbol{k}} - f_m^{\boldsymbol{k}})$$

$$\frac{1}{(2\pi)^2} \times \left|\left\langle \psi_n^{\boldsymbol{k}} \left| \frac{\partial \hat{H}}{\partial \boldsymbol{k}} \right| \psi_m^{\boldsymbol{k}} \right\rangle\right|^2 \delta(E_m^{\boldsymbol{k}} - E_n^{\boldsymbol{k}} - \omega) \tag{1}$$

where

- Ω is the volume of the unit cell,

- $W(\boldsymbol{k})$ is the $\boldsymbol{k}$-point weight in the Monkhorst-Pack scheme,

- $f_n^{\boldsymbol{k}}$ is the Fermi-Dirac occupations for the band n and the k-point $\boldsymbol{k}$,

- the matrix element $\left\langle \psi_n^{\boldsymbol{k}} \left| \frac{\partial \hat{H}}{\partial \boldsymbol{k}} \right| \psi_m^{\boldsymbol{k}} \right\rangle$ are computed using a response function calculation. Technical details on the computation of matrix elements can be found in Refs. [3, 4].

- The δ function can be resolved by averaging over a finite frequency interval $\Delta\omega$ [5]:
$$\sigma(\omega_l) = \frac{1}{\Delta\omega} \int_{\omega_l - \frac{\Delta\omega}{2}}^{\omega_l + \frac{\Delta\omega}{2}} \sigma(\omega)d\omega \tag{2}$$

This was done until version 4.0.2, and now, a Gaussian is used to represent the delta function:

$$G(\omega) = \frac{1}{\sqrt{\pi}\Delta} exp\left[-((E_m^{\boldsymbol{k}} - E_n^{\boldsymbol{k}} - \hbar\omega)/\Delta)^2\right] \tag{3}$$

2 Abinit computation

An example of input file for abinit is given in Test_v3/t78.in. Five linked calculations have to be run to obtained all the needed quantities to evaluate the optical conductivity.

- First calculation is a scf evaluation of the electronic density, with iscf=3 and prtden=1. The Fermi-Dirac occupations is obtained at this step.

- Second calculation is a non-scf calculation (iscf=-2) starting from the previous electronic density and wave functions. It gives the Khon-Sham eigenvalues needed.

- The three last calculations are calculations of response function (iscf=-3) and gives the derivative of the Hamiltonian with respect to the wave vector for the three directions. There is one calculation for each direction. They start from the wave functions of the previous non-scf calculation (getwfk=2).

3 conducti module

An example of input file for conducti is given in Test_v3/t79.in.

```
1                    ! 1 for norm-conserving calculations
t78o_DS3_1WF4
t78o_DS4_1WF5
t78o_DS5_1WF6
t78o_DS2_WFK
9.5E-04
1.00000
0.00735 2.0
```

- the three first lines are the name of the xxx_1WFxx function for the three directions,

- then there is the name of the wave function file obtained with the non-scf calculation.

- The temperature is given in a.u.

- The weight of the k-vector is given exactly with the same format as the output file.

- The first number is the value of Δ in a.u., the conductivity is computed up to the second number.

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When conducti runs, you will have to answer with the name of the input file containing all the above informations and the name of the output file.

4 Output content

First, you get some information (as rprimd, the number of bands, of k-points, etc..) to be sure that the reading is okay.

The sum rule is computed [1]:

$$S = \frac{2m_e\Omega}{\pi e^2 n_e} \int_0^\infty \sigma(\omega)d\omega \tag{4}$$

where m_e is the electron mass and n_e the electronic density. S must be equal to 1 (or as close as possible). To obtain a well converged sum rule, more unoccupied electronic states is needed than for the determination of the DC electrical conductivity $\sigma(\omega \to 0)$.

At last, since a finite number of excited states is included in the calculation, $\sigma(\omega)$ is computed correctly for $\hbar\omega < |E_{\max} - E_{\mathrm{f}}|$ where E_{f} is the Fermi level and $E_{\max}$ is the energy of the highest level computed. This value is computed.

The output file contain the energy value in Ha and eV and the optical conductivity in a.u and $(\mathrm{ohm.cm})^{-1}$.

The DC electrical conductivity σ_{DC} computation is made by extrapolating optical conductivity to $\omega = 0$. An example of application is given in [6].

Conducti produces different files, with the following brief description : (1) the zero limit of *.STP is the thermopower ; (2) *.SIG is the real part of the optical conductivity, the zero limit gives the electrical conductivity ; (3) the zero limit of *.KTH gives the thermal conductivity ; (4) *.TENS is the electrical tensor including the non-diegonal terms.

References

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