This document is out of date. Need fixing

Spectrum function of G.

How to calculate $\langle {\bf q} n|\Sigma(\omega)|{\bf q} n\rangle$

We have an example at {\tt ecalj/MATERIALS/SiSigma/}, where
you can just type {\tt job}. It calls a shell script {\tt gwsigma}, which is
just a modification of {\tt gwsc} for spectrum function plotting.
If you have {\tt sigm.*}, it will automatically read it as in the case
of {\tt gwsc}.

By the script {\tt gwsigma}, we calculate the diagonal elements
$\langle \psi({\bf q},n)|\sigma_{\rm c}(\omega) |\psi({\bf q},n)\rangle$.
Thus we need to set $\bf q$ and band index n for which we calcualte.
In addition, we need to set resolution of ω.

~~Set <QPNT> section~~(-->probably QforGW instead). This section is to set the q point, and band index for which we calculate the self energy. In addition, energy mesh for plotting is set.

(A) ~~Set q point set~~ --> We now use QforGW probably
(--- following is not correct. ---)
If you set

```
  *** all q -->1, otherwise 0;  up only -->1, otherwise 0
         1          0
  ----------
  You will have self-energy for all irreducible k points. This may be
needed for A(omega).
  or
  You have to set all q points as
  ----------
  *** q-points, which shoud be in qbz.,See KPNTin1BZ.
         3           <--- number of readin q point
  1     0.0000000000000000     0.0000000000000000     0.0000000000000000
<--1st number is irrelevant
  2    -0.5000000000000000     0.5000000000000000     0.5000000000000000
  3     0.0000000000000000     0.0000000000000000     1.0000000000000000
```

To know allowed q points on regular mesh point, run the command "mkGWIN_lmf2", then supply n1,n2,n3. The templete of GWinput.tmp contains all possible q points. Edit it.

~~NOTE:Anyq option can allow you to specify any q points by shifted mesh technique.~~
~~(if necessary, but only for some special purpose).~~

(B)
~~Band index set~~ --> instead, We now use EMAXforGW probably

It is specified by the section

```
*** no. states and band index for calculation.
2
4  5
----------
means the self-energy for band index 4 and 5. Just two bands.
If you like to plot self energy from 1 through 8, use
*** no. states and band index for calculation.
8
1 2 3 4 5 6 7 8
```

If you need 17 bands for example, it should be 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
in addition to 17 (number of bands at the first line).

(C) ~~energy mesh set ~~ We now use Histbin

```
  At the bottom of <QPNT> section, we have
  ----------------
  *****
   0.01 2.0
  ----------------
   Two real number should be supplied.
   These are dwplot and omegamaxin, read in hsfp0.m.F by a line
     read (ifqpnt,*,err=2038,end=2038) dwplot,omegamaxin
   dwplot (=0.01 Ry) is mesh for self energy.
   omegamaxin=(2.0 Ry) means the range "-2 Ry to 2 Ry" for self-energy
plot.

   Note that imaginary part of Sigma is given as the comvolution of
ImW(omega) and the pole of Green's function
   (esmr in GWinput gives energy smearing of the pole). Resolution for
Im W (near omega=0) is by dw in GWinput.)
   I think that the reolution of self-energy is ~ 0.05 eV in the default
setting.
   This is because {\tt dw} \sim {\tt esmr} \sim 0.05 eV.


  Run gwsigma. This will run
    echo 4| mpirun -np 24 hsfp0,
  after dielectric funcition is calculated.
  Then we have SEComg.UP (DN) files, Look for file handle, ifoutsec,
  for the file in fpgw/main/hsfp0.m.F to see format for the file.
  (not hsfp0.sc.m.F but hsfp0.m.F). Search a line
       open(ifoutsec,file='SEComg'//sss) (around hsfp0.m.F L1052)
   You can find that we use folloing lines to plot SEComg.*.
    ----------------
          write(ifoutsec,"(4i5,3f10.6,3x,f10.6,2x,f16.8,x,3f16.8)")
     &          iw,itq(i),ip,is, q(1:3,ip),  eqx(i,ip,is),
```

```
     &          (omega(i,iw)-ef)*rydberg(),  hartree*zsec(iw,i,ip)
!,sumimg                                                  -------------
---
     This means we use energy in eV.
     iw:      omega index
     itq(iq): band index specified by <QPNT>
     ip:      k point index specified by <QPNT>
     is:      spin index
     q:       q vector (cartesian in 2pi/alat)
     eqx:     eigenvalue in eV. (I think relative to the Fermi energy)
     (omega(i,iw)-ef)*rydberg():  omega relative to the Fermi energy
     hartree*zsec(iw,i,ip):       Self energy. real and imaginary part.
(complex, two values)

   You can only repeat echo 4| mpirun -np 24 hsfp0
   when you change setting in <QPNT> section.

* Example.  There is an example MATERIALS/SiSigma/
  plot 'SEComg.UP' u ($9):($10) w l,'' u ($9):($11) w l
  can give a plot for Re (Sigma_c(omega)) and Im(Sigma_c).

  9th:  energy in eV   (omega(i,iw)-ef)*rydberg()
  10th: real part      Re hartree*zsec(iw,i,ip)
  11th: imag part      Im hartree*zsec(iw,i,ip)

## 4
 To get integrated spectrum function (DOS), we need to superpose all the
spectrum function
 (All q points and all band index). Be careful about the degeneracy
(multiplicity) for each q points.
  You have to build it from SEComg file.
  To know the multiplicity, search following lines ofkeyword {\tt
Multiplicity} in the console output of qg4gw (lqg4gw).

  Anyway, consider about ``is it worth to do?''
  To confirm your result, use sum rule (sum of spectrum weight). And pay
attention to the relation
  between real and imag parts (Hilbert transformation).
```