The AbinitioDΓA Project v1.0: Non-local correlations beyond and susceptibilities within dynamical mean-field theory: README (December 2017)

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1 Introduction

Diagrammatic extensions of dynamical mean field theory (DMFT) such as the dynamical vertex approximation (DΓA) allow us to include non-local correlations beyond DMFT on all length scales and proved their worth for model calculations. Here, we detail the implementation of an AbinitioDΓA approach. We go through each major step in the workflow and discuss the input and output data files (including their structure).

2 DMFT data

Starting point of any calculation is a converged DFT+DMFT solution, which we obtain, e.g. from the package `w2dynamics`. The latter writes all output data into an HDF5 file, from which we extract the datasets `siw`, `dc`, `mu`, `beta`, `giw` (self-energy, double counting correction, chemical potential, inverse temperature, Green's function) and—depending on the run options—also `hk` (Hamiltonian). The data structure of the `w2dynamics` output is shown in Listing 1. In order to keep these instructions as concise as possible, only the parts relevant for AbinitioDGA are shown. (Information about the full contents and structure of an HDF5 file can usually be retrieved via `h5ls -lr`. For a basic HDF5 introduction please visit `/documentation/hdf5_intro.pdf`) In order to use input from another (DMFT) program, it is necessary to convert it into the group structure shown in Listings 1 and 2. Examplary HDF5 templates with the existing structures can be found in `/documentation/hdf5_templates/`.

Listing 1: HDF5-structure of the DMFT output

```
/.axes/                                  Group
/.axes/iw                                Dataset {2*NIW}
/.config                                 Group
/dmft-001/                               Group
/dmft-001/ineq-001/                      Group
/dmft-001/ineq-001/siw                   Group
/dmft-001/ineq-001/siw/value             Dataset {NBANDS, NSPINS, 2*NIW}
/dmft-001/ineq-001/giw                   Group
/dmft-001/ineq-001/giw/value             Dataset {NBANDS, NSPINS, 2*NIW}
/dmft-001/ineq-001/dc                    Group
/dmft-001/ineq-001/dc/value              Dataset {NBANDS, NSPINS}
/dmft-001/mu                             Group
/dmft-001/mu/value                       Dataset {SCALAR}
...
```

Please note that instead of actual numbers, we use upper-case variables here in order to keep the description general. `NIW` is the number of positive fermionic frequencies of the one-particle quantities, `NBANDS` is the number of correlated orbitals of the inequivalent atom `ineq-001`, and `NSPINS` is equal to 2.
On top of this DMFT solution, the impurity two-particle Green's function ("vertex") is computed, e.g. within `w2dynamics`, which has the following structure: (again, groups not necessary for AbinitioDΓA are omitted here.)

Listing 2: HDF5-structure of the worm-sampled vertex

```
/.axes/                                  Group
/.axes/iwb-g4                            Dataset {2*N4IWB+1}
/.axes/iwf-g4                            Dataset {2*N4IWF}
/worm-001/                               Group
/worm-001/ineq-001/                      Group
/worm-001/ineq-001/g4iw-worm/            Group
/worm-001/ineq-001/g4iw-worm/00001/      Group
/worm-001/ineq-001/g4iw-worm/00001/value Dataset {2*N4IWF, 2*N4IWF, 2*N4IWB+1}
/worm-001/ineq-001/g4iw-worm/00001/error Dataset {2*N4IWF, 2*N4IWF, 2*N4IWB+1}
...
/worm-001/ineq-001/g4iw-worm/NGRPS/      Group
/worm-001/ineq-001/g4iw-worm/NGRPS/value Dataset {2*N4IWF, 2*N4IWF, 2*N4IWB+1}
/worm-001/ineq-001/g4iw-worm/NGRPS/error Dataset {2*N4IWF, 2*N4IWF, 2*N4IWB+1}
...
```

`N4IWF` and `N4IWB` are the number of positive fermionic and bosonic Matsubara frequencies of the two-particle Green's function, respectively. `NGRPS` is the maximal number of band-spin combinations, $(2n_{dim})^4$. The group names in front of the `value` and `error` groups are integers from from 1 to NGRPS and represent a one-to-one mapping from a *band-spin combination* to an integer, e.g. 00001 $\rightarrow (1\uparrow, 1\uparrow, 1\uparrow, 1\uparrow)$. In general, the transformation of band-spin combination to an index ($b_i \in [1, n_{ndim}]$, $s_i \in [1, 2] = [\uparrow, \downarrow]$)

$$b_1 s_1, b_2 s_2, b_3 s_3, b_4 s_4 \rightarrow \text{index},$$

is achieved via

$$\text{index} = 2^3 n_{dim}^3 (2b_1 + s_1 - 3) + 2^2 n_{dim}^2 (2b_2 + s_2 - 3) + 2n_{dim}(2b_3 + s_3 - 3) + 2b_1 + s_4 - 2$$

where n_{dim} represents the number of correlated bands whithin the atom under consideration. The number of existing groups can be calculated via

$$\text{density} - \text{density interactions}: \; N = n_{dim}^2 \times 6$$
$$\text{Kanamori parametrization}: \; N = \left[3n_{dim}^2 - 2n_{ndim}\right] \times 6,$$

where the factor 6 comes from all the possible SU(2) combinations allowed for a given band combination.

3 Fully nonlocal V(q) data

The $V(\mathbf{q})$ file creation is currently completely independent of the AbinitioDΓA package but it must respect a certain HDF5 structure, which will be explained by considering an example of a three-band system (a template can be found in /documentation/hdf5_templates/):

Listing 3: $V(q)$ file structure

```
/                          Group
/.axes                     Group
/.axes/Q-points            Dataset {8000, 3}
/00001                     Dataset {8000}
/00005                     Dataset {8000}
...
/00077                     Dataset {8000}
/00081                     Dataset {8000}
```

The `Q-points` dataset contains all $\mathbf{q}$-point vectors starting from $(0,0,0)$ and going through all other points in the following manner (e.g., for a 20x20x20 q-mesh of the Brillouin zone):

$$\begin{aligned}
i = 0 \quad & q = (0,0,0) \\
i = 1 \quad & q = (0,0,0.05) \\
& \vdots \\
i = 19 \quad & q = (0,0,0.95) \\
i = 20 \quad & q = (0,0.05,0) \\
i = 21 \quad & q = (0,0.05,0.05) \\
& \vdots \\
i = 399 \quad & q = (0,0.95,0.95) \\
i = 400 \quad & q = (0.05,0,0) \\
i = 401 \quad & q = (0.05,0,0.05) \\
& \vdots \\
i = 7999 \quad & q = (0.95,0.95,0.95)
\end{aligned}$$

in units of 2π/lattice constant. The other groups then contain the $V(\mathbf{q})$ information along this list of points for the specific band combinations. The transformation of band combination to an index

$$i_1, i_2, i_3, i_4 \rightarrow \text{index},$$

is achieved via

$$\text{index} = n_{dim}^3(i_1 - 1) + n_{dim}^2(i_2 - 1) + n_{dim}(i_3 - 1) + i_4,$$

where n_{dim} represents the number of correlated bands.

4 `setupvertex` - symmetrizing the vertex

In order to use the vertex it must first be symmetrized and transformed into the density and magnetic channels according to

$$G_d = \frac{1}{2}\left[G_{\uparrow\uparrow\uparrow\uparrow} + G_{\downarrow\downarrow\downarrow\downarrow} + G_{\uparrow\uparrow\downarrow\downarrow} + G_{\downarrow\downarrow\uparrow\uparrow}\right]$$

$$G_m = \frac{1}{2}\left[G_{\uparrow\downarrow\downarrow\uparrow} + G_{\downarrow\uparrow\uparrow\downarrow}\right],$$

where we additionally used the SU(2) symmetry. This symmetrization can be done with the `setupvertex` program. One simply has to execute this program, with `$ADGA_DIR` as your `ADGA` parent directory, and follow the instructions given (colored text represents user input).

Listing 4: exemplary setupvertex execution

```
$ $ADGA_DIR/bin/setupvertex
Number of inequivalent atoms: 1
Vertex file : srvo3-2pg-repo.hdf5
Number of correlated bands for inequivalent atom 1: 3
Outputfile for symmetrized Vertex: srvo3-2pg-symmetrized.hdf5

SU2 symmetry only (s) or SU2 AND orbital symmetry (o)?: o
```

This produces an HDF5 file of the following structure:

Listing 5: symmetrized vertex structure

```
/                                       Group
/ineq-001                               Group
/ineq-001/dens                          Group
/ineq-001/dens/00000                    Group
/ineq-001/dens/00000/00001              Group
/ineq-001/dens/00000/00001/value        Dataset {2*N4IWF}
...
/ineq-001/magn                          Group
/ineq-001/magn/00000                    Group
/ineq-001/magn/00000/00001              Group
/ineq-001/magn/00000/00001/value        Dataset {2*N4IWF}
...
```

which is the centerpiece of the `ADGA` input. The group names in front of the `value` groups again represent a one-to-one mapping from a *band combination* to an integer. (00001 $\rightarrow$ (1, 1, 1, 1)). The group before that represents a bosonic frequency which is shifted so we start at 0 (00000) and go to 2*`N4IWB`.

5 abinitiodga - main program

The last preparational step is the configuring of ADGA. The main program's input options are contained in a config file (of arbitrary name). This config file is segmented into groups marked by squared braces. Subgroups are marked by double squared braces. In the [General] group we define what we want to calculate and how large our calculation should be (i.e. frequency box, momentum-space grid). In the [Atoms] group we define our local interactions and give information about the number of bands. In the [One-Particle] and [Two-Particle] group we define our files and in the [Output] group we define additional output parameters. One important thing to mention is that this config file is read by routines written in Fortran. Any kind of typos will not produce errors unless a check is imposed on that variable (Checks are mainly done for the existance of files and crucial run options).

At the moment there are four (4) different run options:

- calc-eom = T, calc-sus = T, QDataFile empty → calculation on q-grid
- calc-eom = T, calc-sus = F, QDataFile empty → calculation on q-grid
- calc-eom = F, calc-sus = T, QDataFile empty → calculation on q-grid
- calc-eom = F, calc-sus = T, QDataFile **exists** → calculation along these q-points.

Listings 7 and 8 contain example config files with the first first and the fourth run option respectively. For a complete overview over all input options please check out /documentation/configspec where all options are described in detail.

Once the config file is prepared, we can run the program with the following commands, depending on whether the compilation was performed with or without MPI (colored text as user input).

Listing 6: abinitiodga run commands

```
with MPI:
$ mpirun -np 3 $ADGA_DIR/bin/abinitiodga config_file
without MPI:
$ $ADGA_DIR/bin/abinitiodga config_file
```

A recommendation for real (large) calculations: First start a full calculation on a single core in order to check whether the config file is complete and to get an estimation of the full run time. After one loop the out file (see Listing 9) prints the necessary time per loop together with the number of necessary loops. This gives an estimation of the full run time and the amount of parallelization necessary.

Listing 7: config file for q-grid calculation

```
[General]
# calculate the momentum-dependent susceptibilities
calc-susc = T
# calculate the dga-selfenergy via the equation of motion
calc-eom  = T

NAt = 1 # Number of atoms

# number of positive f/b frequencies used from the vertex
N4iwf = -1 # full box
N4iwb = -1 # full box

HkFile = srvo3_k20.hk # Wannier Hamiltonian

k-grid = 20 20 20 # Wannier Hamiltonian and eom grid - must be fixed at all times
q-grid = 20 20 20 # Grid we run our calculation on and susc grid

[Atoms] # fully local interaction parameters
[[1]]
Interaction = Kanamori
Nd = 3 # number of d-bands
Np = 0 # number of p-bands
Udd = 5.0
Vdd = 3.5
Jdd = 0.75

[One-Particle]
1PFile = srvo3-1pg.hdf5 # DMFT 1PG
orb-sym = T

[Two-Particle]
2PFile = srvo3-2pg-symmetrized.hdf5 # symmetrized vertex
vertex-type = 0 # 0: 2PGF, 1: chi_con, 2: chi

[Output]
text-output = T # additionally output the data in form of text-files
```

Listing 8: config file for q-path calculation

```
[General]
# calculate the momentum-dependent susceptibilities
calc-susc = T
calc-eom  = F # must be turned off for q-path calculation

NAt = 1 # Number of atoms

# number of positive f/b frequencies used from the vertex
N4iwf = -1 # full fermionic box
N4iwb = 0  # only at w=0

HkFile = srvo3_k20.hk # Wannier Hamiltonian

k-grid = 20 20 20 # Wannier Hamiltonian and eom grid - must be fixed all times
# q-grid = 20 20 20 -- this gets ignored if we run with QDataFile

QDataFile = qpath_template
# this file can be found in /documentation/examples/qpath_template

Output = output-qpath

[Atoms] # fully local interaction parameters
[[1]]
Interaction = Kanamori
Nd = 3 # number of d-bands
Np = 0 # number of p-bands
Udd = 5.0
Vdd = 3.5
Jdd = 0.75

[One-Particle]
1PFile = srvo3-1pg.hdf5 # DMFT 1PG
orb-sym = T

[Two-Particle]
2PFile = srvo3-2pg-symmetrized.hdf5 # symmetrized vertex
vertex-type = 0 # 0: 2PGF, 1: chi_con, 2: chi

[Output]
text-output = T # additionally output the data in form of text-files
```

6 abinitiodga - output

The first thing created by abinitiodga is a log file called out in the output directory. This text file represents a basic log file, contains most of the run options and shows the progress of the calculation.

Listing 9: ADGA log file

```
/------------------------------------------------------------------\
|  Ab initio dynamical vertex approximation program (abinitiodga)  |
|  Running on           2 core(s) with     20    20    20 k-points |
|     time              date            host                       |
| 114824.952        20171220          l32                        |
\------------------------------------------------------------------/

one particle quantities in
srvo3-1pg.hdf5

two particle quantities in
srvo3-2pg-symmetrized.hdf5

Calculating with maximum number of fermionic frequencies =      30
orb_symmetry =  T
beta=    10.0000000000000
mu=    1.73411511496015
dc= (0.000000000000000E+000,0.000000000000000E+000)
(0.000000000000000E+000,0.000000000000000E+000)
(0.000000000000000E+000,0.000000000000000E+000)
(0.000000000000000E+000,0.000000000000000E+000)
(0.000000000000000E+000,0.000000000000000E+000)
(0.000000000000000E+000,0.000000000000000E+000)
Reading giw from file. (The QMC green's function)
Creating U matrix from input parameters.

Running the calculation without V(q)

Frequency information:
iwmax=         2000
 (number of fermionic matsubara frequencies of one-particle quantities)
iwfmax=           30 iwfmax_small=           30
 (number of fermionic matsubara frequencies of two-particle quantities)
iwbmax=           30 iwbmax_small=            0
 (number of bosonic matsubara frequencies of two-particle quantities)
k-point information:
        8000 k-points in the mesh
          41 q-points in the q-path

mpi_distribute: average number of iqw points per rank (floored):       20
Constructing the local (frequency summed) susceptibilities from chi^{qvv'}_loc.
Writing hdf5 output to
output-qpath/adga-20171220-114824.952-output.hdf5


Starting the main loop:
To supress the progress indicator, use the verbose keyword Noprogress.
--------------------------------------------------------------------------------
Core:   0  Completed qw-point:    1 (from     1 to    20)  Time per point:    0.7421
...
...
Core:   0  Completed qw-point:    9 (from     1 to    20)  Time per point:    0.5335
--------------------------------------------------------------------------------

End of Program
```

Unless otherwise specified by `text-output = T` in the `[Output]` group the data produced by `abinitiodga` is put into a partially compressed HDF5 file (for a basic HDF5 introdution please visit `/documentation/hdf5_intro.pdf`) . This data file contains, depending on the run options `calc-eom` and `calc-susc`, the following datasets:

Listing 10: ADGA HDF5 output format for a q-grid

```
/input                                  Group
/input/beta                             Dataset {SCALAR}
/input/dc                               Dataset {NBANDS, NSPINS}
/input/giw                              Dataset {NBANDS, 2*NIW}
/input/hk                               Dataset {NBANDS, NBANDS, NKX, NKY, NKZ}
/input/iwbmax                           Dataset {SCALAR}
/input/iwbmax_small                     Dataset {SCALAR}
/input/iwfmax                           Dataset {SCALAR}
/input/iwfmax_small                     Dataset {SCALAR}
/input/iwmax                            Dataset {SCALAR}
/input/mu                               Dataset {SCALAR}
/input/n_dmft                           Dataset {NBANDS}
/input/n_dmft_k                         Dataset {NBANDS, NBANDS, NKX, NKY, NKZ}
/input/nkp                              Dataset {SCALAR}
/input/nkpxyz                           Dataset {NBANDS}
/input/nqp                              Dataset {SCALAR}
/input/nqpxyz                           Dataset {NBANDS}
/input/siw                              Dataset {NBANDS, 2*NIW}
/occupation                             Group
/occupation/n_dga                       Dataset {NBANDS}
/occupation/n_dga_k                     Dataset {NBANDS, NBANDS, NKX, NKY, NKZ}
/selfenergy                             Group
/selfenergy/loc                         Group
/selfenergy/loc/dga_ksum                Dataset {NBANDS, NBANDS, 2*N4IWF}
/selfenergy/loc/dmft                    Dataset {NBANDS, NBANDS, 2*N4IWF}
/selfenergy/nonloc                      Group
/selfenergy/nonloc/dga                  Dataset {NBANDS, NBANDS, NKX, NKY, NKZ, 2*N4IWF}
/selfenergy/nonloc/hartree_fock         Dataset {NBANDS, NBANDS, NKX, NKY, NKZ, 2*N4IWF}
/susceptibility                         Group
/susceptibility/loc                     Group
/susceptibility/loc/bubble_loc          Dataset {NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/loc/dens                Dataset {NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/loc/magn                Dataset {NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/nonloc                  Group
/susceptibility/nonloc/bubble_nl        Dataset {NBANDS, NBANDS, NQX, NQY, NQZ, 2*N4IWB+1}
/susceptibility/nonloc/dens             Dataset {NBANDS, NBANDS, NQX, NQY, NQZ, 2*N4IWB+1}
/susceptibility/nonloc/magn             Dataset {NBANDS, NBANDS, NQX, NQY, NQZ, 2*N4IWB+1}
```

Since full generalized susceptibilities have four orbital indices, they consume a massive amount of storage space. However, the physical spin and charge susceptibilities consist only of terms which have two pairs of equal indices, (i, i, j, j), which reduces the number of components from n_{dim}^4 to n_{dim}^2. If nevertheless the output of all components is required, one has to set `susc-full-output = T` in the config group `[Output]`. If susceptibilities are calculated only for certain q-points, as specified in `QDataFile`, the q-points are written explicitly to `/input/qpath` and the susceptibility datasets have only one q-dimension.
The susceptibility output formats are shown in the following Listing:

Listing 11: susceptibility output comparison

```
Q-Path calculation - reduced (QDataFile = qpath)

/input/qpath                        Dataset {NQP}
/susceptibility                     Group
/susceptibility/loc                 Group
/susceptibility/loc/bubble_loc      Dataset {NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/loc/dens            Dataset {NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/loc/magn            Dataset {NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/nonloc              Group
/susceptibility/nonloc/bubble_nl    Dataset {NBANDS, NBANDS, NQP, 2*N4IWB+1}
/susceptibility/nonloc/dens         Dataset {NBANDS, NBANDS, NQP, 2*N4IWB+1}
/susceptibility/nonloc/magn         Dataset {NBANDS, NBANDS, NQP, 2*N4IWB+1}


Q-Path calculation - full (QDataFile = qpath)

/input/qpath                        Dataset {NQP}
/susceptibility                     Group
/susceptibility/loc                 Group
/susceptibility/loc/bubble_loc      Dataset {NBANDS, NBANDS, NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/loc/dens            Dataset {NBANDS, NBANDS, NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/loc/magn            Dataset {NBANDS, NBANDS, NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/nonloc              Group
/susceptibility/nonloc/bubble_nl    Dataset {NBANDS, NBANDS, NBANDS, NBANDS, NQP, 2*N4IWB+1}
/susceptibility/nonloc/dens         Dataset {NBANDS, NBANDS, NBANDS, NBANDS, NQP, 2*N4IWB+1}
/susceptibility/nonloc/magn         Dataset {NBANDS, NBANDS, NBANDS, NBANDS, NQP, 2*N4IWB+1}


Q-Grid calculation - reduced (q-grid = nqx, nqy, nqz)

/susceptibility                     Group
/susceptibility/loc                 Group
/susceptibility/loc/bubble_loc      Dataset {NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/loc/dens            Dataset {NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/loc/magn            Dataset {NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/nonloc              Group
/susceptibility/nonloc/bubble_nl    Dataset {NBANDS, NBANDS, NQX, NQY, NQZ, 2*N4IWB+1}
/susceptibility/nonloc/dens         Dataset {NBANDS, NBANDS, NQX, NQY, NQZ, 2*N4IWB+1}
/susceptibility/nonloc/magn         Dataset {NBANDS, NBANDS, NQX, NQY, NQZ, 2*N4IWB+1}

Q-Grid calculation - full (q-grid = nqx, nqy, nqz)

/susceptibility                     Group
/susceptibility/loc                 Group
/susceptibility/loc/bubble_loc      Dataset {NBANDS, NBANDS, NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/loc/dens            Dataset {NBANDS, NBANDS, NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/loc/magn            Dataset {NBANDS, NBANDS, NBANDS, NBANDS, 2*N4IWB+1}
/susceptibility/nonloc              Group
/susceptibility/nonloc/bubble_nl    Dataset {NBANDS, NBANDS, NBANDS, NBANDS, NQX, NQY, NQZ, 2*N4IWB+1}
/susceptibility/nonloc/dens         Dataset {NBANDS, NBANDS, NBANDS, NBANDS, NQX, NQY, NQZ, 2*N4IWB+1}
/susceptibility/nonloc/magn         Dataset {NBANDS, NBANDS, NBANDS, NBANDS, NQX, NQY, NQZ, 2*N4IWB+1}
```

7 abinitiodga - srvo3 test results

Finally, we present the results for the test data from the repository (`/srvo3-testdata/`). Using the config files in Listings 7 and 8, as well as the plot scripts found in `/documentation/scripts/`, we obtain the following results:

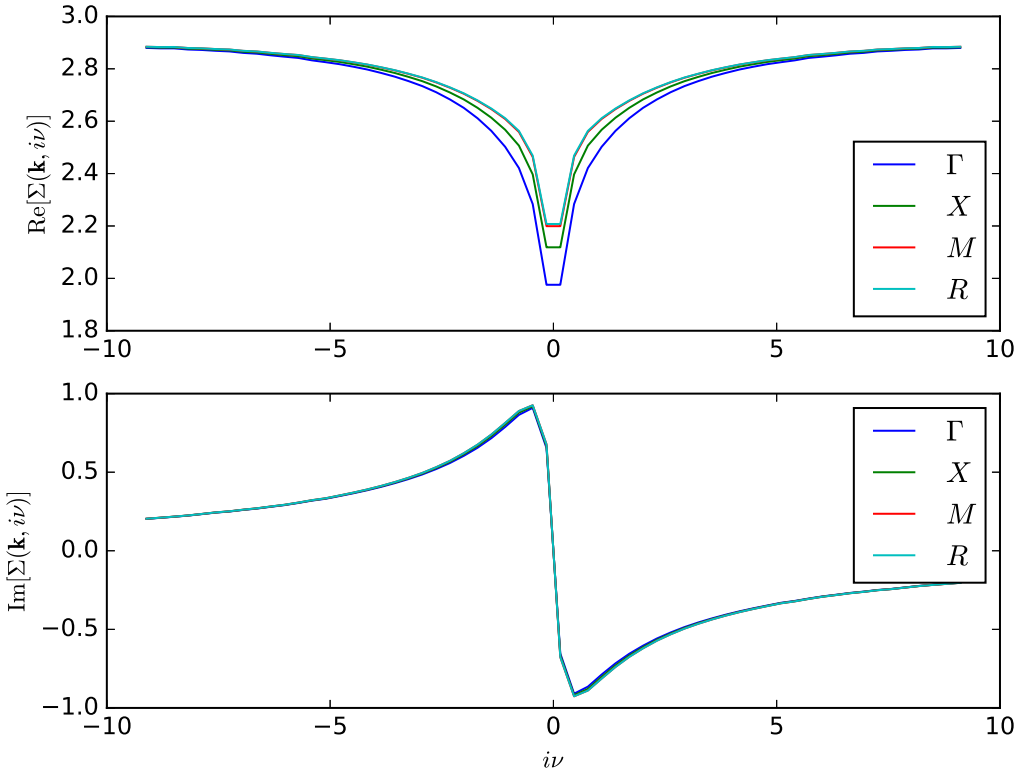

Figure 7.1: Selfenergy results for a Q-qrid calculation at high symmetry points. The plot script can be found in `/documentation/scripts/1D_plot_selfenergy.py`

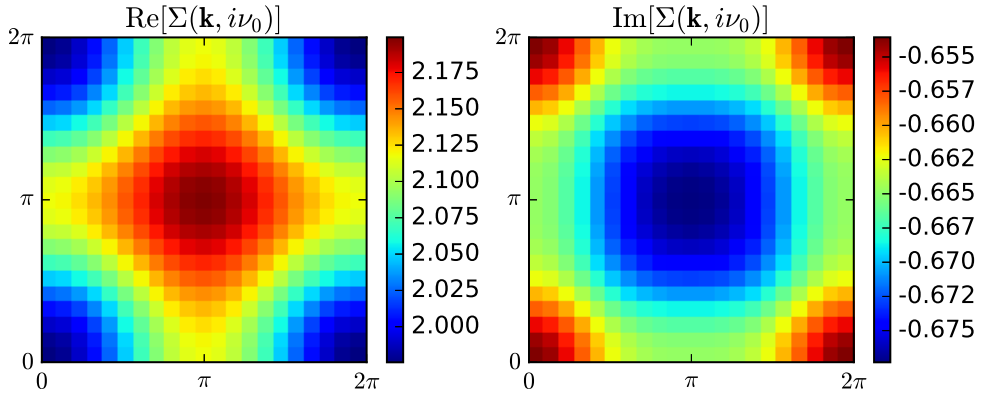

Figure 7.2: Selfenergy results for a Q-qrid calculation in the $k_z = 0$ plane. Please note that the Γ point is located at the bottom left corner. The plot script can be found in `/documentation/scripts/2D_plot_selfenergy_plane.py`

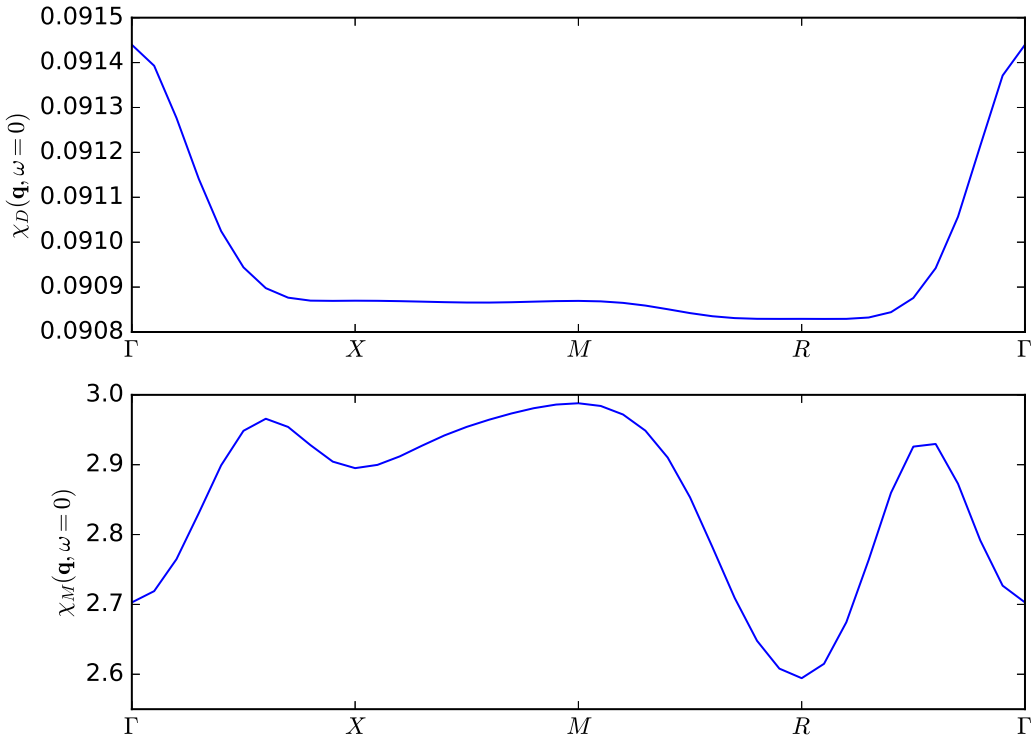

Figure 7.3: Susceptibility results for a Q-path calculation. Please note that a prefactor of 2 is necessary to get the actual magnetic susceptibility. The plot script can be found in `/documentation/scripts/1D_plot_qpath.py`

Please note that these results are not the same as in arXiv:1710.06651, where we used much larger box sizes in combination with asymptotic vertex behaviour.