Fourier Documentation

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Contents

CHAPTER 1

Overview

This document is the manual for the utility to perform the Fourier transformation of the correlation function in the site representation generated by mVMC or $\mathcal{H}\Phi$.

Prerequisite

The prerequisite of this utility is the same as that of mVMC or $\mathcal{H}\Phi$.

Supported quantities

This utility supports the Fourier transformation of the following quantities:

One-body correlations

$$\langle \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\rangle \equiv \frac{1}{N_{\mathrm{cell}}}\sum_{ij}^{N_{\mathrm{site}}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle \hat{c}^{\dagger}_{i\uparrow}\hat{c}_{j\uparrow}\rangle \tag{1.1}$$

$$\langle \hat{c}^{\dagger}_{\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\downarrow}\rangle \equiv \frac{1}{N_{\mathrm{cell}}}\sum_{ij}^{N_{\mathrm{site}}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle \hat{c}^{\dagger}_{i\downarrow}\hat{c}_{j\downarrow}\rangle \tag{1.2}$$

Density-density correlation

$$\langle \hat{\rho}_{\mathbf{k}}\hat{\rho}_{\mathbf{k}}\rangle \equiv \frac{1}{N^2_{\mathrm{cell}}}\sum_{ij}^{N_{\mathrm{site}}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle \hat{\rho}_i\hat{\rho}_j\rangle \tag{1.3}$$

Spin-Spin correlations

$$\langle \hat{S}^z_{\mathbf{k}}\hat{S}^z_{\mathbf{k}}\rangle \equiv \frac{1}{N^2_{\mathrm{cell}}}\sum_{ij}^{N_{\mathrm{site}}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle \hat{S}^z_i\hat{S}^z_j\rangle \tag{1.4}$$

$$\langle \hat{S}^+_{\mathbf{k}}\hat{S}^-_{\mathbf{k}}\rangle \equiv \frac{1}{N^2_{\mathrm{cell}}}\sum_{ij}^{N_{\mathrm{site}}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle \hat{S}^+_i\hat{S}^-_j\rangle \tag{1.5}$$

$$\langle \hat{\mathbf{S}}_{\mathbf{k}}\cdot\hat{\mathbf{S}}_{\mathbf{k}}\rangle \equiv \frac{1}{N^2_{\mathrm{cell}}}\sum_{ij}^{N_{\mathrm{site}}} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle \hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j\rangle \tag{1.6}$$

CHAPTER 2

Tutorial

This tutorial is done by using the input file in `sample/Standard/Spin/HeisenbergSquare/` (mVMC) or `sample/CG/Heisenberg/` (HPhi).

Run HPhi/vmc.out

- For $\mathcal{H}\Phi$

  Calculate the ground state and the correlation function at that state.

```
$ ../../../../src/HPhi -s stan.in
```

- For mVMC

  Optimize the trial wavefunction.

```
$ ../../../../src/vmc.out -s StdFace.def
```

  Add the following line in `StdFace.def` to compute the correlation function.

```
NVMCCalMode = 1
```

  Compute the correlation function.

```
$ ../../../../src/vmc.out -s StdFace.def output/zqp_opt.dat
```

Then the one- and two-body correlation function are written to files in the `output/` directory.

Related files

- StdFace.def (See the manuals for mVMC/$\mathcal{H}\Phi$)
- zqp_opt.dat (See the manual for mVMC)
- greenone.def (*Specify the index of correlation function to be computed*)
- greentwo.def (*Specify the index of correlation function to be computed*)

Fourier transformation of correlation functions

Perform the Fourier transformation of the correlation function by using the utility `fourier`.

```
$ ../../../../tool/fourier namelist.def geometry.dat
```

Then the Fourier-transformed correlation functions are written to a file in `output/`.

Related files

- output/zvo_cisajs_001.dat (*Results of correlation function in the site representation*)
- output/zvo_cisajs.dat (*Results of correlation function in the site representation*)
- output/zvo_cisajscktalt_001.dat (*Results of correlation function in the site representation*)
- output/zvo_cisajscktalt.dat (*Results of correlation function in the site representation*)
- geometry.dat (*Geometry*)
- output/zvo_corr.dat (*Correlation functions in the primitive Brillouin zone*)

Display correlation functions

Plot the correlation function in the k space by using the utility `corplot`.

```
$ ../../../../tool/corplot output/zvo_corr.dat
or
$ ../../../../tool/corplot output/zvo_corr_eigen0.dat
```

Then the following message appears in the terminal.

```
#####  Plot Start  #####

   Please specify target number from below (0 or Ctrl-C to exit):

   Real Part Without ErrorBar
     [ 1] Up-Up [ 2] Down-Down [ 3] Density-Density [ 4] SzSz [ 5] S+S- [ 6] S-S+
   Imaginary Part Without ErrorBar
     [11] Up-Up [12] Down-Down [13] Density-Density [14] SzSz [15] S+S- [16] S-S+
   Real Part With ErrorBar
     [21] Up-Up [22] Down-Down [23] Density-Density [24] SzSz [25] S+S- [26] S-S+
   Imaginary Part With ErrorBar
     [31] Up-Up [32] Down-Down [33] Density-Density [34] SzSz [35] S+S- [36] S-S+

   Target :
```

Type a number corresponding to the quantity to be plotted (for example `4`) and press `Enter`, then gnuplot is launched and the 3D figure is displayed (Fig. 2.1).

Related files

- kpoint.dat (*k-point file for corplot*)
- correlation.gp (*gnuplot script*)
- correlation.dat (*Correlation function at wide range of k*)

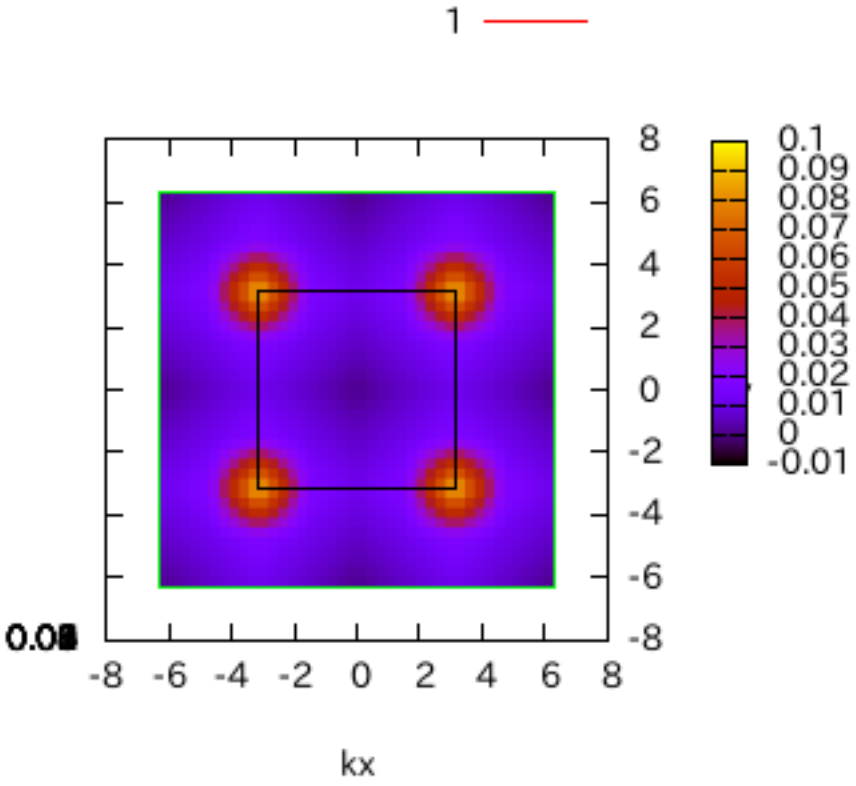

Fig. 2.1: The 3D picture when `Target : 4`. The solid black lines indicate the Brillouin zone.

CHAPTER 3

File format

Geometry

The file name in the *Tutorial* is `geometry.dat`. When we use Standard mode of mVMC/$\mathcal{H}\Phi$, this file is generated automatically. Therefore we do not have to care it.

```
1.000000     0.000000     0.000000  (1)
0.000000     1.000000     0.000000  (1)
0.000000     0.000000     1.000000  (1)
0.000000     0.000000     0.000000  (2)
4 0 0                                (3)
0 4 0                                (3)
0 0 1                                (3)
0.000000     0.000000     0.000000  (4)
1.000000     0.000000     0.000000  (4)
2.000000     0.000000     0.000000  (4)
3.000000     0.000000     0.000000  (4)
0.000000     1.000000     0.000000  (4)
1.000000     1.000000     0.000000  (4)
2.000000     1.000000     0.000000  (4)
3.000000     1.000000     0.000000  (4)
0.000000     2.000000     0.000000  (4)
1.000000     2.000000     0.000000  (4)
2.000000     2.000000     0.000000  (4)
3.000000     2.000000     0.000000  (4)
0.000000     3.000000     0.000000  (4)
1.000000     3.000000     0.000000  (4)
2.000000     3.000000     0.000000  (4)
3.000000     3.000000     0.000000  (4)
```

1. The unit lattice vectors. Arbitrary unit.
2. The phase for the one-body term across boundaries of the simulation cell (degree unit).
3. Three integer vector specifying the shape of the simulation cell. They are the same as the input parameters `a0W`, `a0L`, `a0H`, `a1W`... in Standard mode.
4. The position of each site. The fractional coordinate is used.

One- and Two-body correlation function in the site representation

Specify the index of correlation function to be computed

Specify the index of correlation functions computed with mVMC/$\mathcal{H}\Phi$. When we use the standard mode, this file is generated automatically. The general description is written in the manuals for mVMC/$\mathcal{H}\Phi$. The file names in the *Tutorial* are `greenone.def` (one body) and `greentwo.def` (two body).

For calculating correlation functions in *Supported quantities*, indices must be specified as follows:

- $\langle \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}\uparrow} \rangle$

  $\langle \hat{c}^\dagger_{i\uparrow} \hat{c}_{j\uparrow} \rangle$ with (i, j) ranging on the whole site.

- $\langle \hat{c}^\dagger_{\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\downarrow} \rangle$

  $\langle \hat{c}^\dagger_{i\downarrow} \hat{c}_{j\downarrow} \rangle$ with (i, j) ranging on the whole site.

- $\langle \hat{\rho}_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} \rangle$ and $\langle \hat{S}^z_{\mathbf{k}} \hat{S}^z_{\mathbf{k}} \rangle$

  $\langle \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma} \hat{c}^\dagger_{j\sigma'} \hat{c}_{j\sigma'} \rangle$ with (i, j) ranging on the whole site and (σ, σ') ranging from $\uparrow$ to $\downarrow$.

- $\langle \hat{S}^+_{\mathbf{k}} \hat{S}^-_{\mathbf{k}} \rangle$ and $\langle \hat{\mathbf{S}}_{\mathbf{k}} \cdot \hat{\mathbf{S}}_{\mathbf{k}} \rangle$

  For $\mathcal{H}\Phi$, $\langle \hat{c}^\dagger_{i\sigma} \hat{c}_{i-\sigma} \hat{c}^\dagger_{j-\sigma} \hat{c}_{j\sigma} \rangle$ with (i, j) ranging on the whole site and σ ranging from $\uparrow$ to $\downarrow$. For mVMC, $\langle \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \hat{c}^\dagger_{j-\sigma} \hat{c}_{i-\sigma} \rangle$ with (i, j) ranging on the whole site and σ ranging from $\uparrow$ to $\downarrow$. In the both cases, please care the order of operators.

In the default settings of Standard mode (`outputmode="corr"`), the above indices are specified automatically. Therefore we do not have to care it.

Results of correlation function in the site representation

The correlation functions having the indices specified in *Specify the index of correlation function to be computed* are computed by mVMC/$\mathcal{H}\Phi$, and written to files. The general description of this file is written in the manuals of mVMC/$\mathcal{H}\Phi$. File names in the *Tutorial* are `output/zvo_cisajs_001.dat` and `output/zvo_cisajscktalt_001.dat` (mVMC), or `output/zvo_cisajs.dat` and `output/zvo_cisajscktalt.dat` ($\mathcal{H}\Phi$).

The utility `fourier` reads these files before the calculation. If some of the correlation functions with indices written in *Specify the index of correlation function to be computed* are lacking (for example, because Standard mode was not used), this utility assume them as 0.

Correlation functions in the primitive Brillouin zone

This file contains the Fourier-transformed correlation function and generated by the utility `fourier`. The file name in the *Tutorial* is `output/zvo_corr.dat`.

```
#HPhi          16                                                  (1)
# kx[1] ky[2] kz[3](Cart.) UpUp[4,5] (Re. Im.) DownDown[6,7]    (2)
# Density[8,9] SzSz[10,11] S+S-[12,13] S-S+[14,15]              (2)
#k-offset      0.0000000      0.0000000      0.0000000          (3)
0.00000E+00    0.00000E+00    0.00000E+00    0.31250E-01  .... (4)
0.15708E+01    0.00000E+00    0.00000E+00    0.31250E-01  .... (4)
:                                                                :
```

1. `"#HPhi"` for the output of `HPhi`, `"#mVMC"` for the output of `vmc.out` The subsequent integer indicate the number of k points in the primitive Brillouine zone.
2. The description of the quantities in each column.
3. The k offset for the one-body correlation function. That is to say, the one-body correlation function in the 4-7 columns are those at the k point shifted from that point in the 1-3 column.
4. The k point (Cartesian) and correlation functions. The real- and the imaginary-part of each correlation function are written.

k-point file for corplot

This file is generated by `fourier` and read by `corplot` when the correlation function is plotted. The file name is `kpoint.dat`.

```
81           9                                          (1)
0.62832E+01    0.00000E+00    0.00000E+00               (2)
0.00000E+00    0.62832E+01    0.00000E+00               (2)
0.00000E+00    0.00000E+00    0.62832E+01               (2)
-0.62832E+01   -0.62832E+01    0.00000E+00      1        (3)
-0.47124E+01   -0.62832E+01    0.00000E+00      2        (3)
-0.31416E+01   -0.62832E+01    0.00000E+00      3
-0.15708E+01   -0.62832E+01    0.00000E+00      4
0.00000E+00   -0.62832E+01    0.00000E+00      1
0.15708E+01   -0.62832E+01    0.00000E+00      2
0.31416E+01   -0.62832E+01    0.00000E+00      3
0.47124E+01   -0.62832E+01    0.00000E+00      4
```

1. The total number of k points plotted by `corplot` and the number of columns for displaying by splot of gnuplot.
2. Reciprocal lattice vectors (Cartesian coordinate).
3. The k vector (Cartesian) and the index of the equivalent k point in the primitive Brillouin zone. This number is the same as that in *Correlation functions in the primitive Brillouin zone*

gnuplot script

This file is generated by `corplot`, and read from gnuplot launched automatically. We also can launch gnuplot independently and `load` this script. The file name is `correlation.gp`.

```
#set terminal pdf color enhanced \     (1)
#dashed dl 1.0 size 20.0cm, 20.0cm     (1)
#set output 'correlation.pdf'          (1)
#set view 60.0, 30.0                   (1)

set view equal xy
set ticslevel 0
set hidden3d
set xlabel 'kx'
set ylabel 'ky'
set zrange [    0.25000E-10:    0.18435E+00]

set pm3d
set pm3d interpolate 5, 5
set view 0.0, 0.0
```

```
#####  Set Brillouin-Zone Boundary  #####

set arrow from    -0.31416E+01,   -0.31416E+01,    ...
set arrow from    -0.31416E+01,    0.31416E+01,    ...
:
#####  End Set Brillouin-Zone Boundary  #####

splot \
'correlation.dat' u 1:2:3 w l tit '1' (2)
pause -1
```

1. When we want to write the figure to a file, this line is uncommented. For pasting this figure on the paper etc., we write the setting of font, line-color, and so on. For more details, please see the manual of gnuplot.
2. Plotting the file in *Correlation function at wide range of k*.

Correlation function at wide range of *k*

This file is generated by `corplot`, and read from gnuplot through *gnuplot script*. The file name is `correlation.dat`.

```
-0.62832E+01   -0.62832E+01    0.18435E+00    0.00000E+00
-0.47124E+01   -0.62832E+01    0.36159E-01    0.00000E+00
-0.31416E+01   -0.62832E+01    0.20921E-01    0.00000E+00
-0.15708E+01   -0.62832E+01    0.36159E-01    0.00000E+00
 0.00000E+00   -0.62832E+01    0.18435E+00    0.00000E+00
 0.15708E+01   -0.62832E+01    0.36159E-01    0.00000E+00
 0.31416E+01   -0.62832E+01    0.20921E-01    0.00000E+00
 0.47124E+01   -0.62832E+01    0.36159E-01    0.00000E+00
 0.62832E+01   -0.62832E+01    0.18435E+00    0.00000E+00

-0.62832E+01   -0.47124E+01    0.36159E-01    0.00000E+00
-0.47124E+01   -0.47124E+01    0.20921E-01    0.00000E+00
-0.31416E+01   -0.47124E+01    0.11372E-01    0.00000E+00
:
```

The 1st and the 2nd column contains the k vector (Cartesian). 3rd and the 4th column contains the correlation function and its standard error, respectively.

CHAPTER 4

Behavior of each utility

Utility `fourier`

This utility is used as follows:

```
$ ${PATH}/fourier ${NAMELIST} ${GEOMETRY}
```

where `${PATH}` is the path to the directory where the executable `fourier` exists, ${NAMELIST} is the NameList input-file name of $\mathcal{H}\Phi$/mVMC, and ${GEOMETRY} is the path to the *Geometry* file.

The behavior of this utility is slightly different between the correlation functions from each mode of $\mathcal{H}\Phi$ (Lanczos, TPQ, Full diagonalization, LOBCG) and mVMC. In the following cases, we assume that `CDataFileHead` in the ModPara input file is `"zvo"` (default).

HPhi-Lanczos

In this case, `HPhi` writes correlation functions to the files `zvo_cisajs.dat` (one body) and `zvo_cisajscktalt.dat` (two body) in `output/` directory. `fourier` utility reads this files, performs the Fourier transformation, and generate single file `zvo_corr.dat` in `output/` directory.

HPhi-TPQ

`HPhi` writes correlation functions to files `zvo_cisajs_run*step*.dat` (one body), `zvo_cisajscktalt_run*step*.dat` (two body) at each trial and TPQ step to the `output/` directory. `fourier` utility reads the one- and the two-body correlation function at each trial/TPQ-step, and performs Fourier transformation, and write to a file `zvo_corr_run*step*.dat` in `output/` directory.

HPhi-Full diagonalization and LOBCG

`HPhi` writes correlation functions to files `zvo_cisajs_eigen*.dat` (one body) and `zvo_cisajscktalt_eigen*.dat` (two body) for each wavefunction to the `output/` directory. `fourier` utility reads the one- and the two-body correlation function at each state and performs Fourier transformation, and write to a file `zvo_corr_eigen*.dat` in `output/`.

mVMC

`vmc.out` performs calculations according to the input parameters `NDataIdxStart` and `NDataQtySmp` in `ModPara` file, and it generates `zvo_cisajs_???.dat` (one body) and `zvo_cisajscktalt_???.dat` (two body) in `output/` directory. `fourier` utility reads all of these files, performs Fourier transformation, computes the average

$$\langle A \rangle = \frac{1}{N_{\mathrm{Try}}} \sum_{i=1}^{N_{\mathrm{Try}}} A_i \tag{4.1}$$

and the standard error

$$\delta A = \frac{1}{N_{\mathrm{Try}} - 1} \sqrt{\frac{1}{N_{\mathrm{Try}}} \sum_{i=1}^{N_{\mathrm{Try}}} (A_i - \langle A \rangle)^2} \tag{4.2}$$

of the real- and imaginary-part of each correlation function, and writes them to a file `zvo_corr_eigen*.dat` in `output/` directory.

Utility `corplot`

This utility is used as follows:

```
$ ${PATH}/corplot ${CORR1} ${CORR2} ${CORR3} ...
```

where `${PATH}` is the path to the directory which contains the executable `corplot`, ${CORR1}, ${CORR2}, ${CORR3}, ... are *Correlation functions in the primitive Brillouin zone* files generated by the utility `fourier`. Therefore, this utility can plot multiple files simultaneously (for example, to study the temperature dependence in the TPQ calculation).

CHAPTER 5

Contact

If you have any comments, questions, bug reports etc. about this utility, please contact to the main developer (Mitsuaki Kawamura) by sending the e-mail (the address is shown below).

```
mkawamura_at_issp.u-tokyo.ac.jp
```

Please change `_at_` into `@`, when you will send the e-mail.