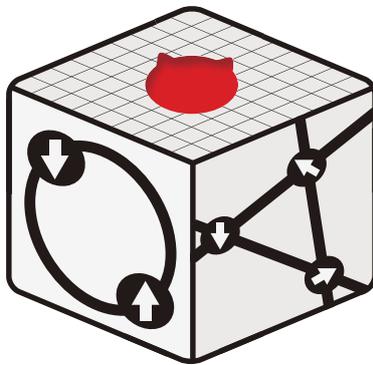


Manual for mVMC
ver. 1.0.2



mVMC

August 25, 2017

Contents

1	What is mVMC?	1
1.1	Overview of mVMC	1
1.2	License	2
1.3	Copyright	2
1.4	Contributors	2
1.5	Operating environment	3
2	How to use mVMC?	4
2.1	Prerequisite	4
2.2	Installation	4
2.2.1	Using <code>mVMCconfig.sh</code>	5
2.2.2	Using <code>cmake</code>	6
2.3	Directory structure	7
2.4	Basic usage	9
2.5	Printing version ID	10
3	Tutorial	11
3.1	List of sample files	11
3.2	Heisenberg model	11
3.3	Input files for Expert mode	16
3.4	Fourier transformation of correlation functions	17
4	File specification	18
4.1	Input files for Standard mode	18
4.1.1	Parameters about the kind of a calculation	19
4.1.2	Parameters for the lattice	19
4.1.3	Sublattice	23
4.1.4	Parameters for the Hamiltonian	23

4.1.5	Parameters for the numerical condition	27
4.2	Input files for Expert mode	31
4.2.1	List file for Input files (namelist.def)	34
4.2.2	ModPara file (modpara.def)	36
4.2.3	LocSpin file (locspn.def)	41
4.2.4	Trans file (trans.def)	43
4.2.5	InterAll file	45
4.2.6	CoulombIntra file (coulombintra.def)	47
4.2.7	CoulombInter file (coulombinter.def)	49
4.2.8	Hund file (hund.def)	51
4.2.9	PairHop file	53
4.2.10	Exchange file (exchange.def)	55
4.2.11	Gutzwiller file (gutzwiller.def)	57
4.2.12	Jastrow file (jastrow.def)	59
4.2.13	DH2 file	61
4.2.14	DH4 file	63
4.2.15	Orbital/OrbitalAntiParallel file (orbitalidx.def)	65
4.2.16	OrbitalParallel file	68
4.2.17	OrbitalGeneral file	71
4.2.18	TransSym file (qptransidx.def)	74
4.2.19	Files to set initial values of variational parameters	76
4.2.20	OneBodyG file (greenone.def)	78
4.2.21	TwoBodyG file (greentwo.def)	80
4.3	Output files	82
4.3.1	Output file for variational parameters (***_opt.dat)	82
4.3.2	Output files for variational parameters at each steps (xxx_var_yyy.dat)	82
4.3.3	Output file for gutzwiller factors (***_gutzwiller_opt.dat)	83
4.3.4	Output file for jastrow factors (***_jastrow_opt.dat)	83
4.3.5	Output file for doublonHolon 2-site factors (***_doublonHolon2site_opt.dat)	83
4.3.6	Output file for doublonHolon 4-site factors (***_doublonHolon4site_opt.dat)	83
4.3.7	Output file for pair orbitals	

	(***_orbital_opt.dat)	83
4.3.8	xxx_out_yyy.dat	83
4.3.9	xxx_CalcTimer.dat	84
4.3.10	xxx_time_zzz.dat	85
4.3.11	xxx_cisajs_yyy.dat	85
4.3.12	xxx_cisajscktalt_yyy.dat	86
4.3.13	xxx_ls_out_yyy.dat	87
4.3.14	xxx_ls_cisajs_yyy.dat	87
4.3.15	xxx_ls_cisajscktalt_yyy.dat	87
5	Algorithm	88
5.1	Variational Monte Carlo Method	88
5.2	Bogoliubov representation	88
5.3	Properties of the Pfaffian-Slater determinant	89
5.3.1	Relation between f_{ij} and $\Phi_{in\sigma}$ (the case of the anti-parallel pairing)	89
5.3.2	Relation between F_{IJ} and $\Phi_{In\sigma}$ (the case of the general pairing)	90
5.3.3	Singular value decomposition of f_{ij}	91
5.4	Power Lanczos method	91
5.4.1	Determination of α	91
5.4.2	Calculation of physical quantities	92
6	Acknowledgement	93
	A Program for the unrestricted Hartree-Fock approximation	94
A.1	Overview	94
A.1.1	Source code	94
A.1.2	How to compile	94
A.1.3	Input files	95
A.2	Usage	96

1

What is mVMC?

High-accuracy analyses of theoretical models for quantum many-body systems are expected to play important role for clarifying the nature of novel quantum phases such as high-temperature superconductivities and quantum spin liquids. Furthermore, recent theoretical progress enables us to obtain low-energy effective models for real materials with non-empirical way [1]. To clarify the electronic structures of real materials and control the physical properties, it is important to perform the high-accuracy analyses for the low-energy effective models. One of the most reliable theoretical tools for treating the strongly correlated electron systems is the exact diagonalization method. However, applicable range of system size is strongly limited in the exact diagonalization method. Variational Monte Carlo method [2] is one of promising way to perform the high-accuracy calculations for the larger system sizes beyond exact diagonalization method. Although the strong limitation of the variational wave function is the origin of the poor accuracy of the variational Monte Carlo method, recent development of the theoretical method and computers relaxes the limitation of the variational wave functions and enable us to perform the highly-accurate calculations [3–5].

mVMC (many-variable Variational Monte Carlo method) is a software for performing the highly-accurate variational Monte Carlo calculations with the simple and flexible user interface. mVMC also supports the large-scale parallelization. For the conventional models in strongly correlated electron systems such as the Hubbard model, the Heisenberg model, and the Kondo-lattice model, users can perform the calculation by preparing the one input files whose length is shorter than ten lines. By using the same input file, users can perform the exact diagonalization through HPhi. Thus, it is easy to examine the accuracy of the variational calculation for small system sizes and to perform the calculations for large system sizes that can not be treated by the exact diagonalization. A broad spectrum of users including experimental scientists is cordially welcome.

1.1 Overview of mVMC

By using mVMC, the following calculation can be done:

- The variational wave function which gives the minimum value of the expected value of energy in the range of the degree of freedoms of variational parameters is numerically generated. The calculation limited to the partial space divided by quantum numbers is also possible.

- The expected values of the physical quantities such as correlation functions can be calculated by using the generated variational wave functions.

The calculation flow in mVMC is shown as follows:

1. Read input files (*.def)
2. Optimize variational parameters α to minimize $\langle \mathcal{H} \rangle$
3. Calculate one body and two body Green functions
4. Output variational parameters and expected values

In calculation, the simple parallelization for the generation of the real space arrangement $|x\rangle$ and the collecting samples and the calculation result of expected energies is implemented. Following the procedure for each cluster computers, the parallelized calculation using MPI is automatically done by indicating the parallel number. However, mVMC cannot execute under the environment where the MPI job is forbidden such as the front-end of system B at ISSP. In mVMC, we use PFAPACK [6] to compute the Pfaffian matrix.

1.2 License

The distribution of the program package and the source codes for mVMC follows GNU General Public License version 3 (GPL v3).

We hope that you cite the following URL, <https://github.com/issp-center-dev/mVMC>, when you publish the results using mVMC (after writing the paper for mVMC, we will replace the URL to the paper's reference).

1.3 Copyright

©2016- The University of Tokyo. All rights reserved.

This software is developed under the support of “*Project for advancement of software usability in materials science*” by The Institute for Solid State Physics, The University of Tokyo.

1.4 Contributors

This software is developed by following contributors.

- ver.1.0.1 (released at 2017/6/8)
- ver.1.0.0 (released at 2017/5/23)
- ver.0.2.0 (released at 2017/3/16)

- ver.0.1.1 (released at 2016/12/16)
- ver.0.1.0 (released at 2016/10/26)
 - Developers
 - * Takahiro Misawa
(The Institute for Solid State Physics, The University of Tokyo)
 - * Satoshi Morita
(The Institute for Solid State Physics, The University of Tokyo)
 - * Takahiro Ogoe
(Department of Applied Physics, The University of Tokyo)
 - * Kota Ido
(Department of Applied Physics, The University of Tokyo)
 - * Masatoshi Imada
(Department of Applied Physics, The University of Tokyo)
 - * Yuichi Motoyama
(The Institute for Solid State Physics, The University of Tokyo)
 - * Mitsuaki Kawamura
(The Institute for Solid State Physics, The University of Tokyo)
 - * Kazusyohi Yoshimi
(The Institute for Solid State Physics, The University of Tokyo)
 - Project coordinator
 - * Takeo Kato
(The Institute for Solid State Physics, The University of Tokyo)

1.5 Operating environment

mVMC is tested in the following platform:

- The supercomputer system-B “sekirei”S in ISSP
- K computer
- OpenMPI + Intel Compiler + MKL
- MPICH + Intel Compiler + MKL
- MPICH + GNU Compiler + MKL

2

How to use mVMC?

2.1 Prerequisite

mVMC requires the following packages:

- C compiler (intel, Fujitsu, GNU, etc.)
- MPI library
- Option: ScaLAPACK library (intel MKL, Fujitsu, ATLAS, etc.)

Tips

E. g. / Settings of intel compiler

When you use the intel compiler, you can use easily scripts attached to the compiler. In the case of the bash in 64 bit OS, write the following in your `~/.bashrc`:

```
source /opt/intel/bin/compilervars.sh intel64
```

or

```
source /opt/intel/bin/iccvars.sh intel64
source /opt/intel/mkl/bin/mklvars.sh
```

Please read manuals of your compiler/library for more information.

2.2 Installation

You can download mVMC in the following place.
<https://github.com/issp-center-dev/mVMC/releases>

You can obtain the mVMC directory by typing

```
$ tar xzvf mVMC-xxx.tar.gz
```

There are two kind of procedures to install mVMC.

2.2.1 Using mVMCconfig.sh

Please run `mVMCconfig.sh` script in the `mVMC` directory as follow (for ISSP system-B "sekirei"):

```
$ bash mVMCconfig.sh sekirei
```

Then environmental configuration file `make.sys` is generated in `src/` directory. The command-line argument of `mVMCconfig.sh` is as follows:

- `sekirei` : ISSP system-B "sekirei"
- `kei` : K computer and ISSP system-C "maki"
- `intel-openmpi` : Intel compiler + OpenMPI
- `intel-mpich` : Intel compiler + MPICH2
- `intel-intelmpi` : Intel compiler + IntelMPI
- `gcc-openmpi` : GCC + OpenMPI
- `gcc-mpich-mkl` : GCC + MPICH + MKL

`make.sys` is as follows (for ISSP-system-B "sekirei"):

```
CC = mpicc
F90 = mpif90
CFLAGS = -O3 -no-prec-div -xHost -qopenmp -Wno-unknown-pragmas
FFLAGS = -O3 -implicitnone -xHost
LIBS = -L $(MKLR00T)/lib/intel64 -lmkl_scalapack_lp64 -lmkl_intel_lp64 \
      -lmkl_intel_thread -lmkl_core -lmkl_blacs_sgimpt_lp64 -lpthread -lm
SFMTFLAGS = -no-ansi-alias -DHAVE_SSE2
```

We explain macros of this file as:

- `CC` : C compiler (`mpicc`, `mpifccpx`)
- `F90` : fortran compiler (`ifort`, `frtpx`)
- `Libs` : Linker option
- `CFLAGS` : C compile option
- `FFLAGS` : fortran compile option

Then you are ready to compile `mVMC`. Please type

```
$ make mvmc
```

and obtain `vmc.out` and `vmcdry.out` in `src/` directory; you should add this directory to the `$PATH`.

Tips

You can make a `PATH` to mVMC as follows:

```
$ export PATH=${PATH}:mVMC_top_directory/src/
```

If you keep this `PATH`, you should write above in `~/.bashrc` (for `bash` as a login shell)

2.2.2 Using cmake

We can compile mVMC as

```
cd $HOME/build/mvmc
cmake -DCONFIG=gcc $PathTomvmc
make
```

Here, we set a path to mVMC as `$PathTomvmc` and to a build directory as `$HOME/build/mvmc`. After compilation, `src` folder is constructed below a `$HOME/build/mvmc` folder and we obtain an executable `vmc.out` in `src/` directory.

In the above example, we compile mVMC by using a `gcc` compiler. We can select a compiler by using the following options:

- `sekirei` : ISSP system-B “sekirei”
- `fujitsu` : Fujitsu compiler
- `intel` : Intel compiler + Linux PC
- `gcc` : GCC compiler + Linux PC.

An example of compiling mVMC by using the Intel compiler is shown as follows:

```
mkdir ./build
cd ./build
cmake -DCONFIG=intel ../
make
```

After compilation, `src` folder is created below the `build` folder and an execute `vmc.out` in the `\verbsrc—` folder. We can select ScaLAPACK instead of LAPACK for `vmc` calculation by adding the following as the `cmake` option

```
-DUSE_SCALAPACK=ON -DSCALAPACK_LIBRARIES="xxx".
```

Here, `xxx` is the libraries to use ScaLAPACK. Please note that we must delete the `build` folder and repeat the above operations when we change the compiler.

Tips

Before using cmake for sekirei, you must type

```
source /home/issp/materiapps/tool/env.sh
```

When we type the following in sekirei,

```
cmake -DCONFIG=sekirei ../ -DUSE_SCALAPACK=ON ,
```

-DSCALAPACK_LIBRARIES is automatically set as

```
-DSCALAPACK_LIBRARIES="\${MKLRROOT}/lib/intel64 -lmkl_scalapack_lp64
-lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core
-lmkl_blacs_sgimpt_lp64".
```

When the path to libraries for ScaLAPACK is different in your circumstance, please set -DSCALAPACK_LIBRARIES as the correct path.

2.3 Directory structure

When mVMC-xxx.tar.gz is unzipped, the following directory structure is composed.

```
COPYING
mVMCconfig.sh
doc/
  bib/
    elsart-num_mod.bst
    userguide.bib
  figs/
    *.pdf
    *.xbb
  fourier/
    en/
    figs/
    ja/
  jp/
    *.tex
  en/
    *.tex
sample/
  Standard/
    Hubbard/
    square/
    StdFace.def
```

```
reference/
    **.dat
triangular/
    ...
Kondo/
chain/
    ...
Spin/
    HeisenbergChain/
        ...
    HeisenbergSquare/
        ...
    Kagome/
        ...
src/
    mVMC/
        **.c
        include/
            **.h
    ComplexUHF/
        **.c
        include/
            **.h
    StdFace/
        **.c
        **.h
    pfapack/
        makefile_pfapack
        **.f
    sfmt/
        makefkie_sfmt
        **.c
        **.h
tool/
    **.f90
    makefile_tool
```

2.4 Basic usage

mVMC works as whether the following two modes:

- Expert mode

mVMC supports the arbitrary fermion-/spin-lattice system; we can specify the hopping, etc. at each site independently. Although this makes us able to specify flexibly the target this requires many input-files, and the setup of the calculation is complicated.

- Standard mode

For some typical models (such as the Heisenberg model on the square lattice), we can start calculation with a few parameters (for example, the size of the simulation cell, the common coupling parameter). In this case, the input-files for Expert mode are automatically generated. Although the number of available systems is smaller than that number of Expert mode, the setup of the calculation is easier than in Expert mode.

We can calculate by using these modes as follows:

1. Prepare a minimal input file

You can choose a model (the Heisenberg model, the Hubbard model, etc.) and a lattice (the square lattice, the triangular lattice, etc.) from ones provided; you can specify some parameters (such as the first/second nearest neighbor hopping integrals, the on-site Coulomb integral, etc.) for them. The input file format is described in the Sec. 4.1.

2. Run

Run a executable `vmc.out` in terminal by specifying the name of input file written in previous step (option `-s` is required).

```
$ mpiexec -np number_of_processes Path/vmc.out -s Input_file_name
```

When you use a queuing system in workstations or super computers, sometimes the number of processes is specified as an argument for the job-submitting command. If you need more information, please refer manuals for your system.

3. Watch calculation logs

Log files are outputted in the `output/` directory which is automatically made in the directory for a calculation scenario. The details of output files are shown in Sec. 4.3.

4. Results

If the calculation is finished normally, the result files are outputted in the `output/` directory. The details of output files are shown in Sec. 4.3.

5. Prepare and run Expert mode

In the above case, the calculation starts as soon as input files for Expert mode are generated. If we only generate files without starting the calculation, we can use a executable `vmcdry.out` as follows (MPI is not used in this step):

```
$ Path/vmcdry.out Input_file_name
```

Then, we can edit generated files by hand and run a executable `vmc.out` with `namelist.def` as an argument (option `-e` is required) as follows:

```
$ mpiexec -np number_of_processes Path/vmcdry.out -e namelist.def
```

Tips

The number of threads for OpenMP

If you specify the number of OpenMP threads for mVMC, you should set it as follows (in case of 16 threads) before the running:

```
export OMP_NUM_THREADS=16
```

2.5 Printing version ID

By using `-v` option as follows, you can check which version of mVMC you are using.

```
$ PATH/vmcdry.out -v
```

```
$ PATH/vmc.out -v
```

3

Tutorial

3.1 List of sample files

There are following tutorials in `samples/Standard/`.

- The Hubbard model on the two dimensional square lattice
(`samples/Standard/Hubbard/square/`)
- The Hubbard model on the two dimensional triangular lattice
(`samples/Standard/Hubbard/triangular/`)
- The one dimensional Kondo chain
(`samples/Standard/Kondo/chain/`)
- The one dimensional antiferromagnetic Heisenberg chain
(`samples/Standard/Spin/HeisenbergChain/HeisenbergChain/`)
- The antiferromagnetic Heisenberg model on the two dimensional square lattice
(`samples/Standard/Spin/HeisenbergSquare/`)
- The antiferromagnetic Heisenberg model on the two dimensional Kagome lattice
(`samples/Standard/Spin/Kagome/`)

We can perform these tutorials in the same way. In the following, the tutorial of the one dimensional antiferromagnetic Heisenberg chain is shown.

3.2 Heisenberg model

This tutorial should be performed in

`sample/Standard/Spin/HeisenbergChain/`.

This directory contains the following things:

The input file: `StdFace.def`

reference outputs: `reference/`

In this case, we treat the one dimensional antiferromagnetic Heisenberg chain which has a nearest neighbor spin coupling.

$$\hat{H} = J \sum_{i=1}^L \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1} \quad (3.1)$$

The input file is as follows:

```
L = 16
Lsub=4
model = "Spin"
lattice = "chain lattice"
J = 1.0
2Sz = 0
NMPtrans=1
```

In this tutorial, J and the number of sites are set to 1 (arbitrary unit) and 16 respectively.

Running

We execute the following command.

```
$ mpiexec -np number_of_processes Path/vmcdry.out -s StdFace.def
```

The MPI command depends on your system (such as `mpiexec`, `mpirun`, `mpijob`, `poe`, etc.). Then, the calculation starts and the following standard message is outputted in the terminal.

```
##### Standard Interface Mode STARTS #####

Open Standard-Mode Inputfile StdFace.def

KEYWORD : 1                | VALUE : 16
KEYWORD : lsub             | VALUE : 4
KEYWORD : model            | VALUE : spin
KEYWORD : lattice         | VALUE : chain
KEYWORD : j                | VALUE : 1.0
KEYWORD : nmptrans        | VALUE : 1

##### Parameter Summary #####

@ Lattice Size & Shape

      L = 16
    Lsub = 4
      L = 16
      W = 1
phase0 = 0.00000          ##### DEFAULT VALUE IS USED #####
```

@ Hamiltonian

```

      2S = 1          ##### DEFAULT VALUE IS USED #####
      h = 0.00000    ##### DEFAULT VALUE IS USED #####
    Gamma = 0.00000  ##### DEFAULT VALUE IS USED #####
      D = 0.00000    ##### DEFAULT VALUE IS USED #####
      JOx = 1.00000
      JOy = 1.00000
      JOz = 1.00000

```

@ Numerical conditions

```

      Lsub = 4
      Wsub = 1
    ioutputmode = 1      ##### DEFAULT VALUE IS USED #####

```

Print Expert input files

```

qptransidx.def is written.
  filehead = zvo      ##### DEFAULT VALUE IS USED #####
  filehead = zqp      ##### DEFAULT VALUE IS USED #####
  NVMCCalMode = 0     ##### DEFAULT VALUE IS USED #####
  NLanczosMode = 0   ##### DEFAULT VALUE IS USED #####
  NDataIdxStart = 1  ##### DEFAULT VALUE IS USED #####
  NDataQtySmp = 1    ##### DEFAULT VALUE IS USED #####
  NSPGaussLeg = 8    ##### DEFAULT VALUE IS USED #####
  NMPTrans = 1
  NSROptItrStep = 1000 ##### DEFAULT VALUE IS USED #####
  NSROptItrSmp = 100  ##### DEFAULT VALUE IS USED #####
  NVMCWarmUp = 10     ##### DEFAULT VALUE IS USED #####
  NVMCInterval = 1    ##### DEFAULT VALUE IS USED #####
  NVMCSample = 1000   ##### DEFAULT VALUE IS USED #####
  NExUpdatePath = 2
  RndSeed = 123456789 ##### DEFAULT VALUE IS USED #####
  NSplitSize = 1      ##### DEFAULT VALUE IS USED #####
  NStore = 0          ##### DEFAULT VALUE IS USED #####
  DSROptRedCut = 0.00100 ##### DEFAULT VALUE IS USED #####
  DSROptStaDel = 0.02000 ##### DEFAULT VALUE IS USED #####
  DSROptStepDt = 0.02000 ##### DEFAULT VALUE IS USED #####
  NSPStot = 0         ##### DEFAULT VALUE IS USED #####
  ComplexType = 0     ##### DEFAULT VALUE IS USED #####

```

locspn.def is written.

trans.def is written.

interall.def is written.

jastrowidx.def is written.

coulombintra.def is written.

coulombinter.def is written.

hund.def is written.

```

exchange.def is written.
orbitalidx.def is written.
gutzwilleridx.def is written.
namelist.def is written.
modpara.def is written.
greenone.def is written.
greentwo.def is written.

##### Input files are generated. #####
-----
Start: Read *def files.
  Read File namelist.def .
  Read File 'modpara.def' for ModPara.
  Read File 'locspn.def' for LocSpin.
  Read File 'trans.def' for Trans.
  Read File 'coulombintra.def' for CoulombIntra.
  Read File 'coulombinter.def' for CoulombInter.
  Read File 'hund.def' for Hund.
  Read File 'exchange.def' for Exchange.
  Read File 'gutzwilleridx.def' for Gutzwiller.
  Read File 'jastrowidx.def' for Jastrow.
  Read File 'orbitalidx.def' for Orbital.
  Read File 'qptransidx.def' for TransSym.
  Read File 'greenone.def' for OneBodyG.
  Read File 'greentwo.def' for TwoBodyG.
End : Read *def files.
Start: Read parameters from *def files.
End : Read parameters from *def files.
Start: Set memories.
End : Set memories.
Start: Initialize parameters.
End : Initialize parameters.
Start: Initialize variables for quantum projection.
End : Initialize variables for quantum projection.
Start: Optimize VMC parameters.
End : Optimize VMC parameters.
-----

```

In the beginning of this run, files describing the detail of considered Hamiltonian

- locspin.def
- trans.def
- coulombinter.def
- coulombintra.def
- exchange.def

- hund.def
- namelist.def
- modpara.def

and files for setting variational parameters

- gutzwilleridx.def
- jastrowidx.def
- orbitalidx.def
- qptransidx.def

and files specifying elements of correlation functions that will be calculated

- greenone.def
- greentwo.def

are generated. The details of these files are shown in Sec. 4.2.

During the calculation, the following files are outputted in `output` directory:

```
zvo_SRinfo.dat
zvo_out_001.dat
zvo_time_001.dat
zvo_var_001.dat
zvo_CalcTimer.dat
```

In `zvo_out_001.dat`, the following quantities are outputted at each bins

$$\langle H \rangle, \langle H^2 \rangle, \frac{\langle H^2 \rangle - \langle H \rangle^2}{\langle H \rangle^2}.$$

By seeing these informations, the conversion of the calculation can be judged. By using `gnuplot`, we can check the evolution of $\langle H \rangle$ as follows:

```
plot "zvo_out_001.dat" u 1
```

The details of these outputted files are shown in Sec. 4.3.

Output results

After finishing calculation normally, the files for the energy, the deviation, the optimized variational parameters and the time of execution for each calculation steps

are outputted in `output` directory. In the following, the outputted files are shown

```
gutzwiller_opt.dat
jastrow_opt.dat
orbital_opt.dat
zqp_opt.dat
ClacTimer.dat
```

The details of these outputted files are shown in Sec. 4.3.

Calculation of Green functions

After changing the value of `NVMCCalMode` from 0 to 1 in `modpara.def` file, we execute the following command. When we add "`zqp_opt.dat`" after "`namelist.dat`" as a command-line argument as follows, the calculation of Green functions is done by using the optimized variational parameters.

```
$ Path/vmc.out -e namelist.def output/zqp_opt.dat
```

After the calculation finishes, the following files are outputted in `output` directory.

```
zvo_cisajs_001.dat
zvo_cisajscktalt_001.dat
```

The details of these outputted files are shown in Sec. 4.3.

3.3 Input files for Expert mode

In mVMC, the calculation is done by reading input files categorized by the following six parts.

- (1) **List:** Specify the kinds and names of input files.
- (2) **Basic parameters:** Specify the basic parameters.
- (3) **Set Hamiltonian:** Specify the Hamiltonian.
- (4) **Set condition of variational parameters :** Specify the variational parameters to be optimized.
- (5) **Initial variational parameters:** Specify the initial values of the variational parameters.
- (6) **Output:** Specify the components of one-body and two-body Green's functions to be outputted.

The calculation for complex models can be done by directly making above input files. The details for each files are shown in Sec. 4.2.

3.4 Fourier transformation of correlation functions

This package has a utility which performs the Fourier transformation of the correlation function and plots that function. The manual of this utility is located in

```
doc/fourier/ja/_build/html/index.html  
doc/fourier/ja/_build/latex/fourier.pdf  
doc/fourier/en/_build/html/index.html  
doc/fourier/en/_build/latex/fourier.pdf
```

4

File specification

4.1 Input files for Standard mode

An example of input file for the standard mode is shown below:

```
W = 2
L = 4
model = "spin"

lattice = "triangular lattice"
//mu = 1.0
// t = -1.0
// t' = -0.5
// U = 8.0
//V = 4.0
//V'=2.0
J = -1.0
J'=-0.5
// nelec = 8
```

Basic rules for input files

- In each line, there is a set of a keyword (before an “=”) and a parameter(after an “=”); they are separated by “=”.
- You can describe keywords in a random order.
- Empty lines and lines beginning in a “//”(comment outs) are skipped.
- Upper- and lowercase are not distinguished. Double quotes and blanks are ignored.
- There are three kinds of parameters.
 1. Parameters that must be specified (if not, `vmcdry.out` will stop with error messages),
 2. Parameters that is not necessary be specified (if not, default values are used),
 3. Parameters that must not be specified (if specified, `vmcdry.out` will stop with error messages).An example of 3 is transfer t for the Heisenberg spin system. If you choose “model=spin”, you should not specify “ t ”.

We explain each keywords as follows:

4.1.1 Parameters about the kind of a calculation

- model

Type : String (Choose from "Fermion Hubbard", "Spin", "Kondo Lattice", "Fermion HubbardGC", "SpinGC", "Kondo LatticeGC") *1

Description : The target model is specified with this parameter; "Fermion Hubbard" denotes the canonical ensemble of the Fermion in the Hubbard model

$$H = -\mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - \sum_{i \neq j\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_{i \neq j} V_{ij} n_i n_j, \quad (4.1)$$

"Spin" denotes canonical ensemble in the Spin model ($\{\sigma_1, \sigma_2\} = x, y, z$)

$$H = -h \sum_i S_{iz} - \Gamma \sum_i S_{ix} + D \sum_i S_{iz} S_{iz} + \sum_{ij, \sigma_1} J_{ij\sigma_1} S_{i\sigma_1} S_{j\sigma_1} + \sum_{ij, \sigma_1 \neq \sigma_2} J_{ij\sigma_1\sigma_2} S_{i\sigma_1} S_{j\sigma_2}, \quad (4.2)$$

"Kondo Lattice" denotes canonical ensemble in the Kondo lattice model

$$H = -\mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \frac{J}{2} \sum_i \left\{ S_i^+ c_{i\downarrow}^\dagger c_{i\uparrow} + S_i^- c_{i\uparrow}^\dagger c_{i\downarrow} + S_{iz} (n_{i\uparrow} - n_{i\downarrow}) \right\}. \quad (4.3)$$

"Fermion HubbardGC", "SpinGC", and "Kondo LatticeGC" indicate the S_z -unconserved Fermion in the Hubbard model [Eqn. (4.1)], the S_z -unconserved Spin model [Eqn. (4.2)], and the S_z -unconserved Kondo lattice model [Eqn. (4.3)], respectively. Note: Although these flags has a word "GC" (=grandcanonical), the number of electrons are conserved in these system.

- lattice

Type : String (Choose from "Chain Lattice", "Square Lattice", "Triangular Lattice", "Honeycomb Lattice", "Kagome", "Ladder")

Description : The lattice shape is specified with this parameter; above words denote the one dimensional chain lattice (Fig. 4.1(a)), the two dimensional square lattice (Fig. 4.1(b)), the two dimensional triangular lattice (Fig. 4.1(c)), the two dimensional anisotropic honeycomb lattice (Fig. 4.2), the Kagome Lattice (Fig. 4.3), and the ladder lattice (Fig. 4.4), respectively.

4.1.2 Parameters for the lattice

Chain [Fig. 4.1(a)]

- L

Type : Integer

Description : The length of the chain is specified with this parameter.

*1GC=Grand Canonical

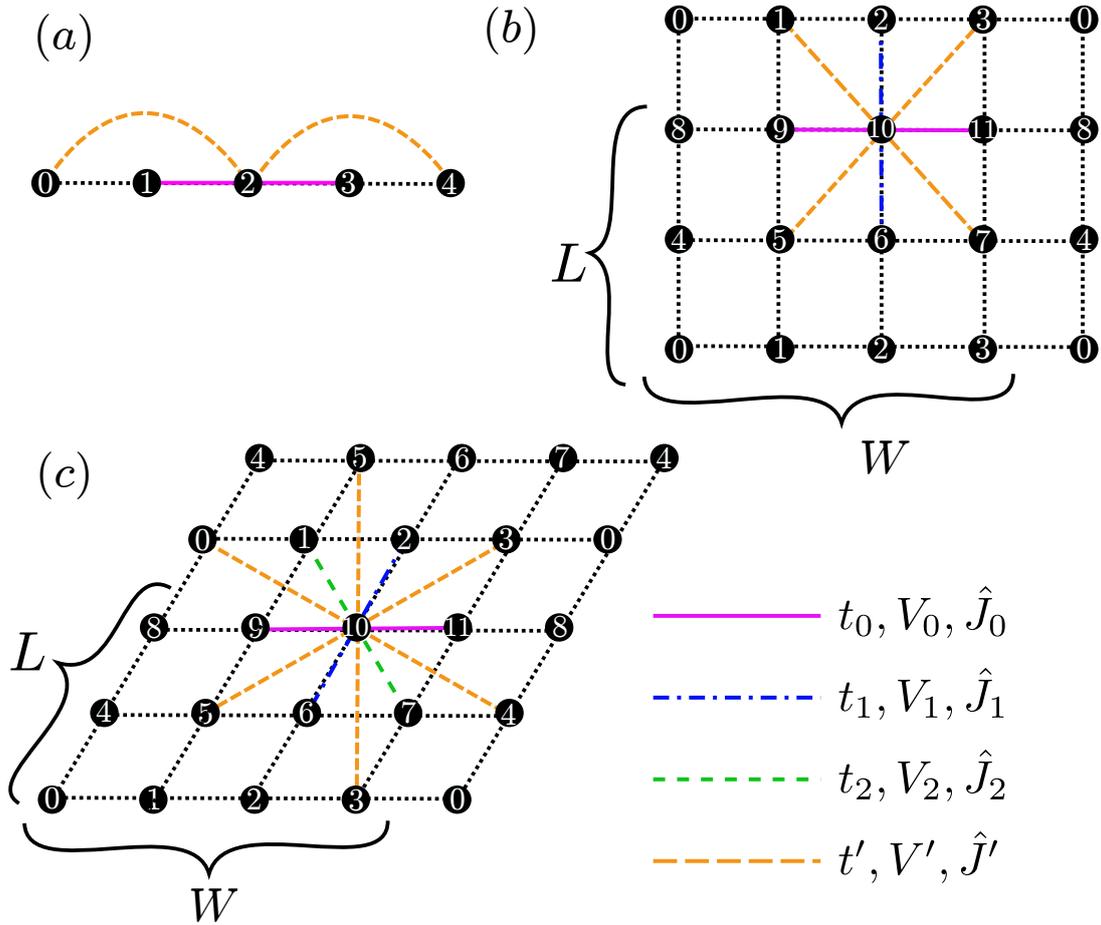


Figure 4.1: Schematic illustration of (a) one dimensional chain lattice, (b) two dimensional square lattice, and (c) two dimensional triangular lattice. They have t , V , and J as a nearest neighbor hopping, an onsite Coulomb integral, and a spin-coupling constant, respectively (magenta solid lines); They also have t' , V' , and J' as a next nearest neighbor hopping, onsite Coulomb integral, and spin-coupling constant, respectively (green dashed line).

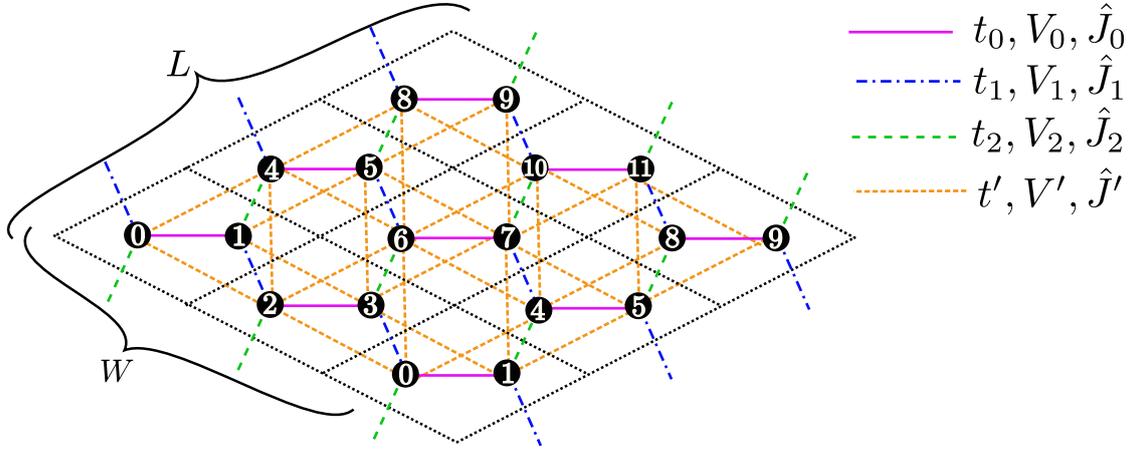


Figure 4.2: Schematic illustration of the anisotropic honeycomb lattice. The nearest neighbor hopping integral, spin coupling, offsite Coulomb integral depend on the bond direction. Those between second nearest neighbor sites are not supported.

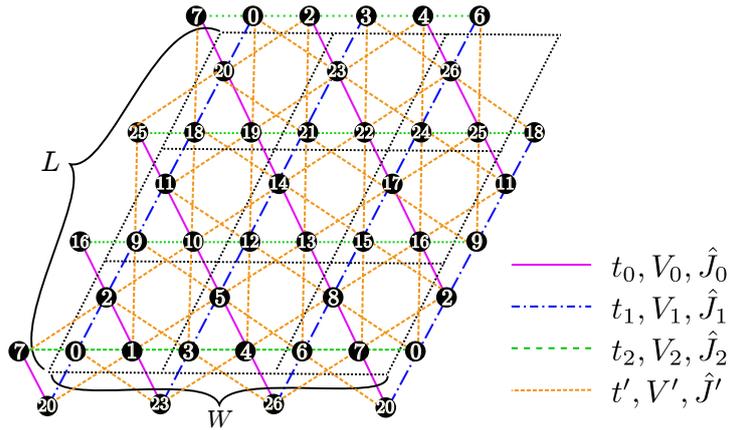


Figure 4.3: Schematic illustration of the Kagome lattice.

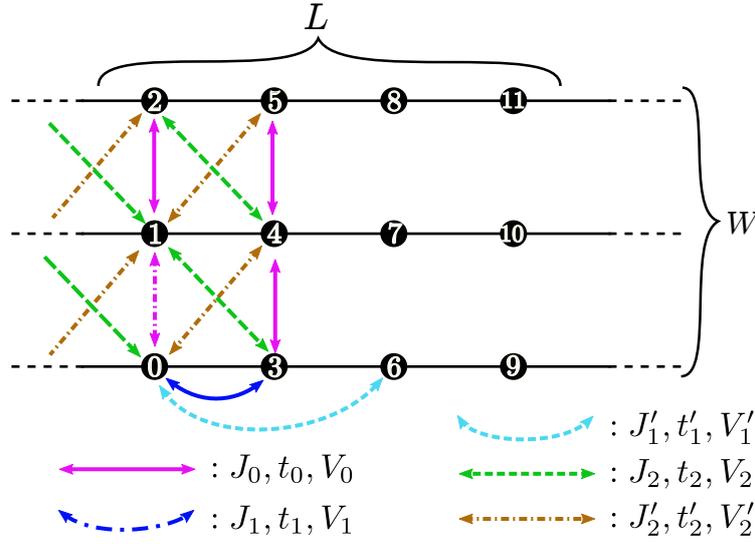


Figure 4.4: Schematic illustration of the ladder lattice.

Ladder (Fig. 4.4)

- L

Type : Integer

Description : The length of the ladder is specified with this parameter.

- W

Type : Integer

Description : The number of the ladder is specified with this parameter.

Square lattice [Fig. 4.1(b)], Triangular lattice[Fig. 4.1(c)], Honeycomb lattice(Fig. 4.2), Kagome lattice(Fig. 4.3)

In these lattices, we can specify the shape of the numerical cell by using the following two methods.

- W, L

Type : Integer

Description : The alignment of original unit cells (dashed black lines in Figs. 4.1 - 4.3) is specified with these parameter.

- a0W, a0L, a1W, a1L

Type : Integer

Description : We can specify two vectors ($\mathbf{a}_0, \mathbf{a}_1$) that surrounds the numerical cell (Fig. 4.5). These vectors should be specified in the Fractional coordinate.

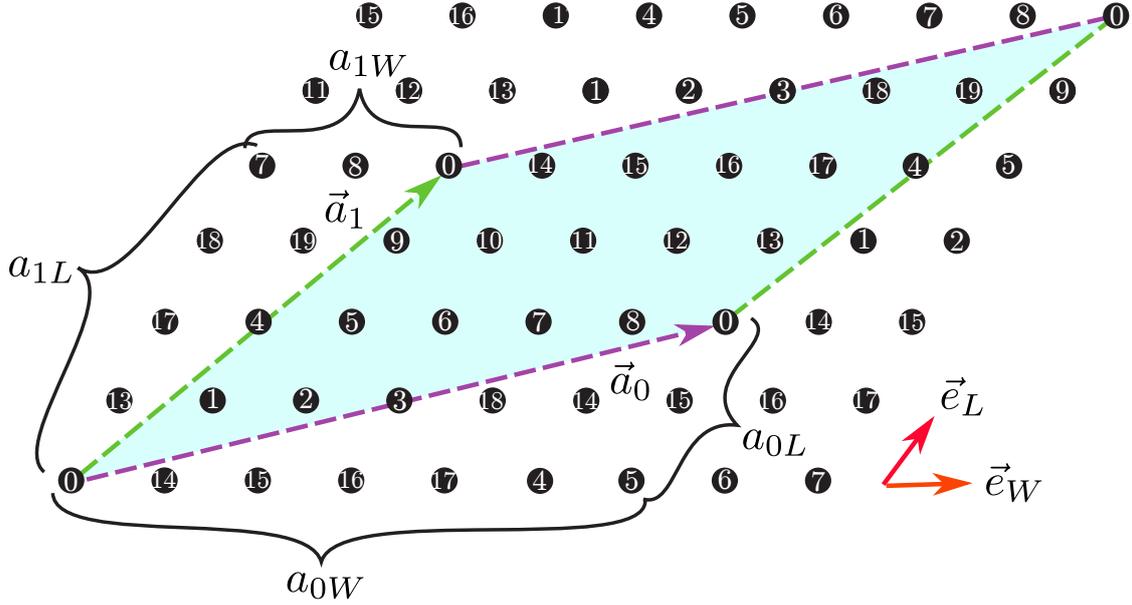


Figure 4.5: The shape of the numerical cell when $\mathbf{a}_0 = (6, 2)$, $\mathbf{a}_1 = (2, 4)$ in the triangular lattice. The region surrounded by \mathbf{a}_0 (Magenta dashed arrow) and \mathbf{a}_1 (Green dashed arrow) becomes the cell to be calculated (20 sites).

If we use both of these method, `vmcdry.out` stops.

We can check the shape of the numerical cell by using a file `lattice.gp` (only for square, triangular, honeycomb, and kagome lattice) which is written in the Standard mode. This file can be read by `gnuplot` as follows:

```
$ gnuplot lattice.gp
```

4.1.3 Sublattice

By using the following parameters, we can force the pair-orbital symmetrical to the translation of the sublattice.

- `a0Wsub`, `a0Lsub`, `a1Wsub`, `a1Lsub`, `Wsub`, `Lsub`

Type : Positive integer. In the default setting, `a0Wsub=a0W`, `a0Lsub=a0L`, `a1Wsub=a1W`, `a1Lsub=a1L`, `Wsub=W`, and `Lsub=L`. Namely, there is no sublattice.

Description : We can specify these parameter as we specify `a0W`, `a0L`, `a1W`, `a1L`, `W`, `L`. If the sublattice is incommensurate with the original lattice, `vmcdry.out` stops.

4.1.4 Parameters for the Hamiltonian

A default value is set as 0 unless a specific value is not defined in a description. Table 4.1 shows the parameters for each models. In the case of a complex type, a file format is “*a real part, an imaginary part*” while in the case of a real type, only “*a real part*”.

Local terms

- μ

Type : Real

Description : (Hubbard and Kondo lattice model) The chemical potential μ (including the site potential) is specified with this parameter.

- U

Type : Real

Description : (Hubbard and Kondo lattice model) The onsite Coulomb integral U is specified with this parameter.

- $J_x, J_y, J_z, J_{xy}, J_{yx}, J_{xz}, J_{zx}, J_{yz}, J_{zy}$

Type : Real

Description : (Kondo lattice model) The spin-coupling constant between the valence and the local electrons is specified with this parameter. If the exchange coupling J is specified in the input file, instead of J_x, J_y, J_z , the diagonal exchange couplings, J_x, J_y, J_z , are set as $J_x = J_y = J_z = J$. When both the set of exchange couplings (J_x, J_y, J_z) and the exchange coupling J are specified in the input file, `vmcdry.out` will stop.

- h, Gamma, D

Type : Real

Description : (Spin model) The longitudinal magnetic field, transverse magnetic field, and the single-site anisotropy parameter are specified with these parameters. The single-site anisotropy parameter is not available for `model=SpinGCBoost`.

The non-local terms described below should be specified in different ways depending on the lattice structure: For `lattice=Ladder`, the non-local terms are specified in the different way from `lattice=Chain Lattice, Square Lattice, Triangular Lattice, Honeycomb Lattice, Kagome`. Below, the available parameters for each lattice are shown in Table 4.1.

Interactions	1D chain	2D square	2D triangular	Honeycomb	Kagome	Ladder
J, t, V (simplified)	○	○	○	○	○	-
J', t', V'	○	○	○	○	○	-
J_0, t_0, V_0	○	○	○	○	○	○
J_1, t_1, V_1	-	○	○	○	○	○
J_2, t_2, V_2	-	-	○	○	○	○
J_1', t_1', V_1'	-	-	-	-	-	○
J_2', t_2', V_2'	-	-	-	-	-	○

Table 4.1: Interactions for each models defined in an input file. We can define spin couplings as matrix format.

Non-local terms[for Ladder (Fig. 4.4)]

- $t_0, t_1, t_1', t_2, t_2'$

Type : Complex

Description : (Hubbard and Kondo lattice model) Hopping integrals in the ladder lattice (See Fig. 4.4) is specified with this parameter.

- $V_0, V_1, V_1', V_2, V_2'$

Type : Real

Description : (Hubbard and Kondo lattice model) Offsite Coulomb integrals on the ladder lattice (Fig. 4.2) are specified with these parameters.

- $J_{0x}, J_{0y}, J_{0z}, J_{0xy}, J_{0yx}, J_{0xz}, J_{0zx}, J_{0yz}, J_{0zy}$
- $J_{1x}, J_{1y}, J_{1z}, J_{1xy}, J_{1yx}, J_{1xz}, J_{1zx}, J_{1yz}, J_{1zy}$
- $J_{1'x}, J_{1'y}, J_{1'z}, J_{1'xy}, J_{1'yx}, J_{1'xz}, J_{1'zx}, J_{1'yz}, J_{1'zy}$
- $J_{2x}, J_{2y}, J_{2z}, J_{2xy}, J_{2yx}, J_{2xz}, J_{2zx}, J_{2yz}, J_{2zy}$
- $J_{2'x}, J_{2'y}, J_{2'z}, J_{2'xy}, J_{2'yx}, J_{2'xz}, J_{2'zx}, J_{2'yz}, J_{2'zy}$

Type : Real

Description : (Spin model) Spin-coupling constants in the ladder lattice (See Fig. 4.4) are specified with these parameter. If the simplified parameter J_0 is specified in the input file instead of the diagonal couplings, J_{0x}, J_{0y}, J_{0z} , these diagonal couplings are set as $J_{0x} = J_{0y} = J_{0z} = J_0$. If both J_0 and the set of the couplings (J_{0x}, J_{0y}, J_{0z}) are specified, `vmcdry.out` will stop. The above rules are also valid for the simplified parameters, J_1, J_1', J_2 , and J_2' .

Non-local terms [other than Ladder (Figs. 4.1, 4.2, 4.3)]

- t_0, t_1, t_2

Type : Complex

Description : (Hubbard and Kondo lattice model) Nearest neighbor hoppings for each direction (See Figs. 4.1-4.3. These bonds are depicted with different line styles.) are specified with these parameter. If there is no bond dependence of the nearest-neighbor hoppings, the simplified parameter t is available to specify t_0, t_1 , and t_2 as $t_0 = t_1 = t_2 = t$. If both t and the set of the hoppings (t_0, t_1, t_2) are specified, `vmcdry.out` will stop.

- V_0, V_1, V_2

Type : Real

Description : (Hubbard and Kondo lattice model) Nearest-neighbor offsite Coulomb integrals V for each direction (See Figs. 4.1-4.3. These bonds are depicted with different line styles.) are specified with these parameters. If there is no bond dependence of the nearest-neighbor offsite Coulomb integrals, the simplified parameter V is available to specify V_0, V_1 , and V_2 as $V_0 = V_1 = V_2 = V$. If both V and the set of the Coulomb integrals (V_0, V_1, V_2) are specified, `vmcdry.out` will stop.

- $J_{0x}, J_{0y}, J_{0z}, J_{0xy}, J_{0yx}, J_{0xz}, J_{0zx}, J_{0yz}, J_{0zy}$
- $J_{1x}, J_{1y}, J_{1z}, J_{1xy}, J_{1yx}, J_{1xz}, J_{1zx}, J_{1yz}, J_{1zy}$
- $J_{2x}, J_{2y}, J_{2z}, J_{2xy}, J_{2yx}, J_{2xz}, J_{2zx}, J_{2yz}, J_{2zy}$

Type : Real

Description : (Spin model) Nearest-neighbor exchange couplings for each direction are specified with these parameters. If the simplified parameter J_0 is specified, instead of J_{0x}, J_{0y}, J_{0z} , the exchange couplings, J_{0x}, J_{0y}, J_{0z} , are set as $J_{0x} = J_{0y} = J_{0z} = J_0$. If both J_0 and the set of the exchange couplings (J_{0x}, J_{0y}, J_{0z}) are specified, `vmcdry.out` will stop. The above rules are valid for J_1 and J_2 .

If there is no bond dependence of the nearest-neighbor exchange couplings, the simplified parameters, $J_x, J_y, J_z, J_{xy}, J_{yx}, J_{xz}, J_{zx}, J_{yz}, J_{zy}$, are available to specify the exchange couplings for every bond as $J_{0x} = J_{1x} = J_{2x} = J_x$. If any simplified parameter ($J_{x\sim z}$) is specified in addition to its counter parts ($J_{0x\sim 2zy}$), `vmcdry.out` will stop. Below, examples of parameter sets for nearest-neighbor exchange couplings are shown.

- If there are no bond-dependent, no anisotropic and offdiagonal exchange couplings (such as J_{xy}), please specify J in the input file.
- If there are no bond-dependent and offdiagonal exchange couplings but are anisotropic couplings, please specify the non-zero couplings in the diagonal parameters, J_x, J_y, J_z .
- If there are no bond-dependent exchange couplings but are anisotropic and offdiagonal exchange couplings, please specify the non-zero couplings in the nine parameters, $J_x, J_y, J_z, J_{xy}, J_{yz}, J_{xz}, J_{yx}, J_{zy}, J_{zx}$.
- If there are no anisotropic and offdiagonal exchange couplings, but are bond-dependent couplings, please specify the non-zero couplings in the three parameters, J_0, J_1, J_2 .
- If there are no anisotropic exchange couplings, but are bond-dependent and offdiagonal couplings, please specify the non-zero couplings in the nine parameters, $J_{0x}, J_{0y}, J_{0z}, J_{1x}, J_{1y}, J_{1z}, J_{2x}, J_{2y}, J_{2z}$.
- If there are bond-dependent, anisotropic and offdiagonal exchange couplings, please specify the non-zero couplings in the twenty-seven parameters from J_{0x} to J_{2zy} .

- t'

Type : Complex

Description : (Hubbard and Kondo lattice model) Nearest neighbor hoppings for each direction (See Figs. 4.1-4.3) are specified with these parameter.

- V'

Type : Real

Description : (Hubbard and Kondo lattice model) Nearest neighbor-offsite Coulomb integrals V for each direction (See Figs. 4.1-4.3) are specified with these parameters.

- $J'x, J'y, J'z, J'xy, J'yx, J'xz, J'zx, J'yz, J'zy$

Type : Real

Description : (Spin model) Second nearest-neighbor exchange couplings are specified. However, for `lattice = Honeycomb Lattice` and `lattice = Kagome` with `model=SpinGBoost`, the second nearest-neighbor exchange couplings are not available in the *Standard* mode. If the simplified parameter J' is specified, instead of $J'x, J'y, J'z$, the exchange couplings are set as $J'x = J'y = J'z = J'$. If both J' and the set of the couplings ($J'x, J'y, J'z$), `vmcdry.out` will stop.

- `phase0, phase1`

Type : Double (0.0 as defaults)

Description : We can specify the phase for the hopping through the cell boundary with these parameter (unit: degree). These factor for the \mathbf{a}_0 direction and the \mathbf{a}_1 direction can be specified independently. For the one-dimensional system, only `phase0` can be used. For example, a hopping from i -th site to j -th site through the cell boundary with the positive direction becomes as

$$\exp(i \times \text{phase0} \times \pi/180) \times t \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma} + \exp(-i \times \text{phase0} \times \pi/180) \times t^* \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \quad (4.4)$$

4.1.5 Parameters for the numerical condition

- `nelec`

Type : int-type (must be specified)

Description : The number of itinerant electrons. It is the sum of the \uparrow and \downarrow electrons.

- `NVMCCalMode`

Type : int-type (default value: 0)

Description : [0] Optimization of variational parameters, [1] Calculation of one body and two body Green's functions.

- `NDataIdxStart`

Type : int-type (default value: 1)

Description : An integer for numbering of output files. For `NVMCCalMode=0`, `NDataIdxStart` is added at the end of the output files. For `NVMCCalMode=1`, the files are outputted with the number from `NDataIdxStart` to `NDataIdxStart+NDataQtySmp-1`.

- `NDataQtySmp`

Type : int-type (default value: 1)

Description : The set number for outputted files (only used for `NVMCCalMode=1`).

- `NSPGaussLeg`

Type : int-type (Positive integer, default value is 8 for `2Sz=0`)

Description : The mesh number for the Gauss-legendre quadrature about β integration (S_y rotation) for the spin quantum-number projection in actual numerical calculation.

- NSPStot

Type : int-type (greater equal 0, default value is 0 for 2Sz=0)

Description : The total spin quantum-number.

- 2Sz

Type : int-type (greater equal 0, default value is 0)

Description : The spin quantum-number S_z .

- NMPTrans

Type : int-type (Positive integer. Default 1)

Description : The number of the momentum and lattice translational quantum-number projection. In the case of not to apply the projection, this value must be set as 1.

- NSROptItrStep

Type : int-type (Positive integer, default value: 1000)

Description : The whole step number to optimize variational parameters by SR method. Only used for NVMCCalMode=0.

- NSROptItrSmp

Type : int-type (Positive integer, default value: NSROptItrStep/10)

Description : In the NSROptItrStep step, the average values of the each variational parameters at the NSROptItrStep step are adopted as the optimized values. Only used for NVMCCalMode=0.

- DSOptRedCut

Type : double-type (default value: 0.001)

Description : The stabilized factor for the SR method by truncation of redundant directions corresponding to ε_{wf} in the ref. [3].

- DSOptStaDel

Type : double-type (default value: 0.02)

Description : The stabilized factor for the SR method by modifying diagonal elements in the overwrap matrix corresponding to ε in the ref. [3].

- DSOptStepDt

Type : double-type (default value: 0.02)

Description : The time step using in the SR method.

- NVMCWarmUp

Type : int-type (Positive integer, default value: 10)

Description : Idling number for the Malkov chain Montecarlo Methods.

- **NVMCInterval**
Type : int-type (Positive integer, default value: 1)
Description : The interval step between samples. The local update will be performed $N_{\text{site}} \times \text{NVMCInterval}$ times.
- **NVMCSample**
Type : int-type (Positive integer, default value: 1000)
Description : The sample numbers to calculate the expected values.
- **NExUpdatePath**
Type : int-type (Positive integer)
Description : The option for local update about exchange terms. 0: not update, 1: update. The default value is set as 1 when the local spin exists, otherwise 0.
- **RndSeed**
Type : int-type (default value: 123456789)
Description : The initial seed of generating random number. For MPI parallelization, the initial seeds are given by $\text{RndSeed} + \text{my rank} + 1$ at each ranks.
- **NSplitSize**
Type : int-type (Positive integer, default value: 1)
Description : The number of processes of MPI parallelization.
- **NStore**
Type : int-type (0 or 1, default value: 1)
Description : The option of applying matrix-matrix product to calculate expected values $\langle O_k O_l \rangle$ (0: off, 1: on). This speeds up calculation but increases the amount of memory usage from $O(N_p^2)$ to $O(N_p^2) + O(N_p N_{\text{MCS}})$, where N_p is the number of the variational parameters and N_{MCS} is the number of Monte Carlo sampling.
- **NSRCG**
Type : int-type (0 or 1, default value: 0)
Description : The option of solving $Sx = g$ in the SR method without construting S matrix [7]. (0: off, 1: on). This reduces the amount of memory usage from $O(N_p^2) + O(N_p N_{\text{MCS}})$ to $O(N_p) + O(N_p N_{\text{MCS}})$ when $N_p > N_{\text{MCS}}$.
- **ComplexType**
Type : int-type (0 or 1. Default value is 0 for the S_z -conserved system and 1 for the S_z -unconserved system.)
Description : If it is 0, only the real part of the variational parameters are optimized. And the real and the imaginary part of them are optimized if this parameter is 1.

- **OutputMode**

Type : Choose from "none", "correlation", and "full" (correlation as a default)

Description : Indices of correlation functions are specified with this keyword. "none" indicates correlation functions will not be calculated. When `outputmode="correlation"`, the correlation function supported by the utility `fourier` is computed. For more details, see the document in `doc/fourier/`. If "full" is selected, $\langle c_{i\sigma}^\dagger c_{j\sigma'} \rangle$ is computed at all i, j, σ, σ' , and $\langle c_{i_1\sigma}^\dagger c_{i_2\sigma} c_{i_3\sigma'}^\dagger c_{i_4\sigma'} \rangle$ is computed at all $i_1, i_2, i_3, i_4, \sigma, \sigma'$.

In spin system, indices are specified as those on the Bogoliubov representation (See 5.2).

- **CDataFileHead**

Type : string-type (default : "zvo")

Description : A header for output files. For example, the output filename for one body Green's function becomes "`xxx_cisajs_yyy.dat`" (xxx are characters set by `CDataFileHead` and yyy are numbers given by numbers from `NDataIdxStart` to `NDataIdxStart + NDataQtySmp`).

- **CParaFileHead**

Type : string-type (default : "zqp")

Description : A header for output files of the optimized variational parameters. For example, the optimized variational parameters are outputted as `zzz_opt_yyy.dat` (zzz are characters set by `CParaFileHead` and yyy are numbers given by numbers from `NDataIdxStart` to `NDataIdxStart + NDataQtySmp-1`).

4.2 Input files for Expert mode

In this section, detailed input files (*.def) are explained. Input files are categorized by the following six parts. The files that are listed in parentheses correspond to the file made by vmcdry.out.

(1) List:

No keyword (namelist.def): This file is a list of input file names with keywords. Each keywords is fixed, but file names are free to be determined.

(2) Basic parameters:

ModPara (modpara.def): Set the parameters for basic parameters such as site number, electron number, Lanczos step *etc.*

LocSpin (locspn.def): Set the location of local spin.

(3) Hamiltonian:

Hamiltonian for mVMC is denoted by

$$\mathcal{H} = \mathcal{H}_T + \mathcal{H}_U + \mathcal{H}_V + \mathcal{H}_H + \mathcal{H}_E + \mathcal{H}_P + \mathcal{H}_I, \quad (4.5)$$

$$\mathcal{H}_T = - \sum_{i,j} \sum_{\sigma_1, \sigma_2} t_{ij\sigma_1\sigma_2} c_{i\sigma_1}^\dagger c_{j\sigma_2}, \quad (4.6)$$

$$\mathcal{H}_U = \sum_i U_i n_{i\uparrow} n_{i\downarrow}, \quad (4.7)$$

$$\mathcal{H}_V = \sum_{i,j} V_{ij} n_i n_j, \quad (4.8)$$

$$\mathcal{H}_H = - \sum_{i,j} J_{ij}^{\text{Hund}} (n_{i\uparrow} n_{j\uparrow} + n_{i\downarrow} n_{j\downarrow}), \quad (4.9)$$

$$\mathcal{H}_E = \sum_{i,j} J_{ij}^{\text{Ex}} (c_{i\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow}^\dagger c_{i\uparrow}), \quad (4.10)$$

$$\mathcal{H}_P = \sum_{i,j} J_{ij}^{\text{Pair}} c_{i\uparrow}^\dagger c_{j\uparrow} c_{i\downarrow}^\dagger c_{j\downarrow}, \quad (4.11)$$

$$\mathcal{H}_I = \sum_{i,j,k,l} \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} I_{ijkl\sigma_1\sigma_2\sigma_3\sigma_4} c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{l\sigma_4}, \quad (4.12)$$

as the format of interactions for electron system. Here, we define the charge density operator with spin σ at site i as $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ and the total charge density operator at site i as $n_i = n_{i\uparrow} + n_{i\downarrow}$. Each parameters are specified by the following files, respectively;

Trans (trans.def): $t_{ij\sigma_1\sigma_2}$ in \mathcal{H}_T ,

CoulombIntra (coulombintra.def): U_i in \mathcal{H}_U ,

CoulombInter (coulombinter.def): V_{ij} in \mathcal{H}_V ,

Hund (hund.def): J_{ij}^{Hund} in \mathcal{H}_H ,

Exchange (exchange.def): J_{ij}^{Ex} in \mathcal{H}_E ,

PairHop: J_{ij}^{Pair} in \mathcal{H}_P ,

InterAll: $I_{ijkl\sigma_1\sigma_2\sigma_3\sigma_4}$ in \mathcal{H}_I .

(4) Variational parameters to be optimized:

The variational parameters to be optimized are specified by using this categorized

files. In mVMC, the variational wave function is given as

$$|\psi\rangle = \mathcal{P}_G \mathcal{P}_J \mathcal{P}_{d-h}^{(2)} \mathcal{P}_{d-h}^{(4)} \mathcal{L}^S \mathcal{L}^K \mathcal{L}^P |\phi_{\text{pair}}\rangle, \quad (4.13)$$

$$\mathcal{P}_G = \exp \left[\sum_i g_i n_{i\uparrow} n_{i\downarrow} \right], \quad (4.14)$$

$$\mathcal{P}_J = \exp \left[\frac{1}{2} \sum_{i \neq j} v_{ij} (n_i - 1)(n_j - 1) \right], \quad (4.15)$$

$$\mathcal{P}_{d-h}^{(2)} = \exp \left[\sum_t \sum_{n=0}^2 (\alpha_{2nt}^d \sum_i \xi_{i2nt}^d + \alpha_{2nt}^h \sum_i \xi_{i2nt}^h) \right], \quad (4.16)$$

$$\mathcal{P}_{d-h}^{(4)} = \exp \left[\sum_t \sum_{n=0}^4 (\alpha_{4nt}^d \sum_i \xi_{i4nt}^d + \alpha_{4nt}^h \sum_i \xi_{i4nt}^h) \right], \quad (4.17)$$

$$\mathcal{L}_S = \frac{2S+1}{8\pi^2} \int d\Omega P_S(\cos \beta) \hat{R}(\Omega), \quad (4.18)$$

$$\mathcal{L}_K = \frac{1}{N_s} \sum_{\mathbf{R}} e^{i\mathbf{K} \cdot \mathbf{R}} \hat{T}_{\mathbf{R}}, \quad (4.19)$$

$$\mathcal{L}_P = \sum_{\alpha} p_{\alpha} \hat{G}_{\alpha}, \quad (4.20)$$

where $\Omega = (\alpha, \beta, \gamma)$ is the Euler angle, $\hat{R}(\Omega)$ is the rotational operator, $P_S(x)$ is the S -th polynomial, \mathbf{K} is the momentum operator of the whole system and $\hat{T}_{\mathbf{R}}$ is the translational operators corresponding to the translational vector \mathbf{R} , \hat{G}_{α} is the point group operator, and p_{α} is the parity operator, respectively. The details of $\mathcal{P}_{d-h}^{(2)}$ and $\mathcal{P}_{d-h}^{(4)}$ are shown in [3]. The one body part of the wavefunction is represented as the pair function of the real space:

$$|\phi_{\text{pair}}\rangle = \left[\sum_{i,j=1}^{N_s} \sum_{\sigma_1, \sigma_2} f_{i\sigma_1 j\sigma_2} c_{i\sigma_1}^{\dagger} c_{j\sigma_2}^{\dagger} \right]^{N/2} |0\rangle, \quad (4.21)$$

where N is the number of electrons and N_s is the number of sites. The setting for optimizing variational parameters or not is given by the following files (the parameters for \mathcal{L}_S are specified in the **ModPara** file).

Gutzwiller (gutzwilleridx.def): Set the target parameters g_i in \mathcal{P}_G to be optimized.

Jastrow (jastrowidx.def): Set the target parameters v_{ij} in \mathcal{P}_J to be optimized.

DH2: Set the target 2-site doublon-holon correlation factor $\alpha_{2nt}^{d(h)}$ in $\mathcal{P}_{d-h}^{(2)}$ to be optimized.

DH4: Set the target 4-site doublon-holon correlation factor $\alpha_{4nt}^{d(h)}$ in $\mathcal{P}_{d-h}^{(4)}$ to be optimized.

Orbital/OrbitalAntiParallel (orbitalidx.def): Set the pair orbital with anti-parallel spins $f_{i\uparrow j\downarrow}$ in $|\phi_{\text{pair}}\rangle$ to be optimized.

OrbitalParallel: Set the pair orbital with anti-parallel spins $f_{i\sigma j\sigma}$ in $|\phi_{\text{pair}}\rangle$ to be optimized.

OrbitalGeneral: Set the pair orbital with anti-parallel spins $f_{i\sigma j\sigma'}$ in $|\phi_{\text{pair}}\rangle$ to be

optimized.

TransSym (qptransidx.def): Set the the momentum projection operators \mathcal{L}_K and the lattice translational projection operators \mathcal{L}_P .

(5) Initial variational parameters:

Set the initial values of the variational parameters. When the keyword is not setting, the corresponding parameters are given by random values as default values.

InGutzwiller: Set the initial values of g_i in \mathcal{P}_G .

InJastrow: Set the initial values of v_{ij} in \mathcal{P}_J .

InDH2: Set the initial values of $\alpha_{2nt}^{d(h)}$ in $\mathcal{P}_{d-h}^{(2)}$.

InDH4: Set the initial values of $\alpha_{4nt}^{d(h)}$ in $\mathcal{P}_{d-h}^{(4)}$.

InOrbital /InOrbitalAntiParallel: Set the initial values of $f_{i\uparrow j\downarrow}$ in $|\phi_{\text{pair}}\rangle$.

InOrbitalParallel: Set the initial values of $f_{i\sigma j\sigma}$ in $|\phi_{\text{pair}}\rangle$.

InOrbitalGeneral: Set the initial values of $f_{i\sigma j\sigma'}$ in $|\phi_{\text{pair}}\rangle$.

(6) Output:

OneBodyG (greenone.def): Set the components of one-body green functions to output.

TwoBodyG (greentwo.def): Set the components of two-body green functions to output.

4.2.1 List file for Input files (namelist.def)

This file determines input filenames correlated with keywords. An example of the file format is shown as follows.

```
ModPara  modpara.def
LocSpin  zlocspn.def
Trans    ztransfer.def
InterAll zinterall.def
Orbital  orbitalidx.def
OneBodyG zcisajs.def
TwoBodyG zcisajscktaltdc.def
```

File format

[string01] [string02]

Parameters

- [string01]
Type : string-type
Description : Select a word from keywords.
- [string02]
Type : string-type
Description : An input filename which is correlated with keywords.

User rules

- After setting keywords at [string 01], half-width state is needed for writing a filename. You can set the filename freely.
- Keywords for input files are shown in Table 4.2.
- Essential keywords are “CalcMod”, “ModPara”, “LocSpin”, “Orbital” and “TransSym”.
- Keywords can be set in random order.
- If keywords or filenames are incorrect, the program is terminated.
- When the head of line is “#”, the line is skipped.

Keywords	Details for corresponding files
ModPara*	Parameters for calculation.
LocSpin*	Configurations of the local spins for Hamiltonian.
Trans	Transfer and chemical potential for Hamiltonian.
InterAll	Two-body interactions for Hamiltonian.
CoulombIntra	CoulombIntra interactions.
CoulombInter	CoulombInter interactions.
Hund	Hund couplings.
PairHop	Pair hopping couplings.
Exchange	Exchange couplings.
Gutzwiller	Gutzwiller factors.
Jastrow	Charge Jastrow factors.
DH2	2-site doublon-holon correlation factors.
DH4	4-site doublon-holon correlation factors.
Orbital*	Pair orbital factors with anti-parallel spins $f_{i\uparrow j\downarrow}$.
OrbitalAntiParallel	Pair orbital factors with anti-parallel spins $f_{i\uparrow j\downarrow}$.
OrbitalParallel	Pair orbital factors with parallel spins $f_{i\sigma j\sigma}$.
OrbitalGeneral	Pair orbital factors $f_{i\sigma_1 j\sigma_2}$.
TransSym*	Translational and lattice symmetry operation.
InGutzwiller	Initial values of Gutzwiller factors.
InJastrow	Initial values of charge Jastrow factors.
InDH2	Initial values of 2-site doublon-holon correlation factors.
InDH4	Initial values of 4-site doublon-holon correlation factors.
InOrbital	Initial values of pair orbital factors $f_{i\uparrow j\downarrow}$.
InOrbitalAntiParallel	Initial values of pair orbital factors $f_{i\uparrow j\downarrow}$.
InOrbitalParallel	Initial values of pair orbital factors $f_{i\sigma j\sigma}$.
InOrbitalGeneral	Initial values of pair orbital factors $f_{i\sigma_1 j\sigma_2}$.
OneBodyG	Output components for Green functions $\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle$
TwoBodyG	Output components for Correlation functions $\langle c_{i\sigma}^\dagger c_{j\sigma} c_{k\tau}^\dagger c_{l\tau} \rangle$

Table 4.2: List of the definition files. The files marked * are essential for executing.

4.2.2 ModPara file (modpara.def)

This file determines parameters for calculation. An example of the file format is shown as follows.

```

-----
Model_Parameters    0
-----
VMC_Cal_Parameters
-----
CDataFileHead    zvo
CParaFileHead    zqp
-----
NVMCCalMode      0
NLanczosMode     0
-----
NDataIdxStart    1
NDataQtySmp     1
-----
Nsite            16
Nelectron        8
NSPGaussLeg     1
NSPStot         0
NMPTrans        1
NSROptItrStep   1200
NSROptItrSmp    100
DSROptRedCut    0.001
DSROptStaDel    0.02
DSROptStepDt    0.02
NVMCWarmUp      10
NVMCInterval    1
NVMCSample      1000
NExUpdatePath   0
RndSeed         11272
NSplitSize      1
NStore          1

```

File format

- Lines 1 - 5: Header
- Line 6: [string01] [string02]
- Line 7: [string03] [string04]
- Line 8: Header
- Lines 9 - : [string05] [int01] (or [double01])

Parameters

- [string01]
Type : string-type (blank parameter not allowed)
Description : Set a keyword for header of output files.
- [string02]
Type : string-type (blank parameter not allowed)
Description : Set a header of output files. For example, the output file of one-body green's functions are named as **xxx_cisajs.dat**, where **xxx** is [string02].
- [string03]
Type : string-type (blank parameter not allowed)
Description : Set a keyword for header of output files for variational parameters.
- [string04]
Type : string-type (blank parameter not allowed)
Description : Set a header of output files for variational parameters. For example, the output file of optimized variational parameters are named as **xxx_opt.dat**, where **xxx** is [string04].
- [string05]
Type : string-type
Description : Select a word from keywords.
- [int01] ([double01])
Type : int (double)-type (blank parameter not allowed)
Description : A parameter which is correlated with a keyword.

User rules

- From Line 9: After setting keywords at [string 01], a half-width blank is needed for setting a parameter.
- From Line 9: When the first character of the line is “-”, the line is not read and skipped.

Keywords and parameters

- **NVMCCalMode**
Type : int-type (default value: 0)
Description : [0] Optimization of variational parameters, [1] Calculation of one body and two body Green's functions.

- **NLanczosMode**
Type : int-type (default value: 0)
Description : [0] Not using single Lanczos step, [1] Calculating energy by using Single Lanczos Step, [2] Calculating one body and two body Green's functions by using Single Lanczos Step (Condition: The options 1 and 2 can be selected when `NVMCCalMode = 1`).
- **NDataIdxStart**
Type : int-type (default value: 0)
Description : An integer for numbering of output files. For `NVMCCalMode= 0` , `NDataIdxStart` is added at the end of the output files. For `NVMCCalMode = 1`, the files are outputted with the number from `NDataIdxStart` to `NDataIdxStart+NDataQtySmp-1`.
- **NDataQtySmp**
Type : int-type (default value: 1)
Description : The set number for outputted files (only used for `NVMCCalMode = 1`).
- **Nsite**
Type : int-type (Positive integer)
Description : The number of sites.
- **Nelectron**
Type : int-type (Positive integer)
Description : The number of electron pairs (the electron number is given by `2 Nelectron`).
- **Ncond**
Type : int-type (greater than 0)
Description : The number of conduction electrons.
- **2Sz**
Type : int-type
Description : The value of $2S_z$. Since the electrons form pair, $2S_z$ must be even number.
- **NSPGaussLeg**
Type : int-type (Positive integer, default value: 8)
Description : The mesh number for the Gauss-legendre quadrature about β integration (S_y rotation) for the spin quantum-number projection in actual numerical calculation.
- **NSPStot**
Type : int-type (greater than 0, default value: 0)
Description : The spin quantum-number.

- **NMPTrans**

Type : int-type (default value: 1)

Description : The absolute value gives the number of the momentum and lattice translational quantum-number projection. When the value is negative, the mode of anti-periodic condition turns on. The quantum-number projection is used from the top to **NMPTrans** with the specified weight indicated in **TransSym** file. In the case of not applying the projection, this value must be equal to 1.

- **NSROptItrStep**

Type : int-type (Positive integer, default value: 1000)

Description : The whole step number to optimize variational parameters by SR method. Only used for **NVMCCalMode=0**.

- **NSROptItrSmp**

Type : int-type (Positive integer, default value: **NSROptItrStep/10**)

Description : In the **NSROptItrStep** step, the average values of the each variational parameters at the **NSROptItrStep** step are adopted as the optimized values. Only used for **NVMCCalMode=0**.

- **DSROptRedCut**

Type : double-type (default value: 0.001)

Description : The stabilized factor for the SR method by truncation of redundant directions corresponding to ε_{wf} in the ref. [3].

- **DSROptStaDel**

Type : double-type (default value: 0.02)

Description : The stabilized factor for the SR method by modifying diagonal elements in the overlap matrix corresponding to ε in the ref. [3].

- **DSROptStepDt**

Type : double-type

Description : The time step using in the SR method.

- **NSROptCGMaxIter**

Type : int-type (default value: 0)

Description : The maximum number of CG steps for the SR method. If this is zero or negative, CG steps will be run as many as the size of S matrix at maximum. Only used for **NSRCG!=0**.

- **DSROptCGTol**

Type : double-type (default value: 1.0e-10)

Description : The convergence condition of a CG step in the SR method. CG method runs until the root mean square of the residues becomes below this value. Only used for **NSRCG!=0**.

- **NVMCWarmUp**
Type : int-type (Positive integer, default value: 10)
Description : Idling number for the Malkov chain Montecarlo Methods.
- **NVMCInterval**
Type : int-type (Positive integer, default value: 1)
Description : The interval step between samples. The local update will be performed $N_{\text{site}} \times \text{NVMCInterval}$ times.
- **NVMCSample**
Type : int-type (Positive integer, default value: 1000)
Description : The sample numbers to calculate the expected values.
- **NExUpdatePath**
Type : int-type (Positive integer)
Description : The option for local update about exchange terms. 0: not update, 1: update for electron system. For Spin system, the value must be 2.
- **RndSeed**
Type : int-type
Description : The initial seed of generating random number. For MPI parallelization, the initial seeds are given by $\text{RndSeed} + \text{my rank} + 1$ at each ranks.
- **NSplitSize**
Type : int-type (Positive integer, default value: 1)
Description : The number of processes of MPI parallelization.
- **NStore**
Type : int-type (0 or 1, default value: 1)
Description : The option of applying matrix-matrix product to calculate expected values $\langle O_k O_l \rangle$ (0: off, 1: on). This speeds up calculation but increases the amount of memory usage from $O(N_p^2)$ to $O(N_p^2) + O(N_p N_{\text{MCS}})$, where N_p is the number of the variational parameters and N_{MCS} is the number of Monte Carlo sampling.
- **NSRCG**
Type : int-type (0 or 1, default value: 0)
Description : The option of solving $Sx = g$ in the SR method without construting S matrix [7]. (0: off, 1: on). This reduces the amount of memory usage from $O(N_p^2) + O(N_p N_{\text{MCS}})$ to $O(N_p) + O(N_p N_{\text{MCS}})$ when $N_p > N_{\text{MCS}}$.

4.2.3 LocSpin file (locspn.def)

This file determines sites with localized spins. An example of the file format is shown as follows.

```

=====
NlocalSpin      6
=====
=====i_0LocSpn_1IteElc =====
=====
  0      1
  1      0
  2      1
  3      0
  4      1
  5      0
  6      1
  7      0
  8      1
  9      0
 10     1
 11     0

```

File format

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3 - 5: Header
- Lines 6 -: [int02] [int03]

Parameters

Parameters

- [string01]

Type : string-type (blank parameter not allowed)

Description : A keyword for total number of localized spins. You can freely give a name of the keyword.
- [int01]

Type : int-type (blank parameter not allowed)

Description : An integer giving total number of localized spins.
- [int02]

Type : int-type (blank parameter not allowed)

Description : An integer giving a site index ($0 \leq [int02] < N_{site}$).

- [int03]

Type : int-type (blank parameter not allowed)

Description : An integer for selecting an electron state whether localized spin or itinerant electron states (0: Itinerant electron state, 1: localized spin state with $S = 1/2$).

Use rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of localized spins indicated by [int03].
- A program is terminated, when [int02] is different from the total number of sites.
- A program is terminated under the condition $[int02] < 0$ or $N_{site} \leq [int02]$.

4.2.4 Trans file (trans.def)

The Hamiltonian for general one-body interactions

$$\mathcal{H}_T = - \sum_{ij\sigma_1\sigma_2} t_{ij\sigma_1\sigma_2} c_{i\sigma_1}^\dagger c_{j\sigma_2}, \quad (4.22)$$

is added to the whole Hamiltonian by setting the parameters $t_{ij\sigma_1\sigma_2}$. An example of the file format is shown as follows.

```

=====
NTransfer      24
=====
=====i_j_s_tijs=====
=====
  0    0    2    0  1.000000  0.000000
  2    0    0    0  1.000000  0.000000
  0    1    2    1  1.000000  0.000000
  2    1    0    1  1.000000  0.000000
  2    0    4    0  1.000000  0.000000
  4    0    2    0  1.000000  0.000000
  2    1    4    1  1.000000  0.000000
  4    1    2    1  1.000000  0.000000
  4    0    6    0  1.000000  0.000000
  6    0    4    0  1.000000  0.000000
  4    1    6    1  1.000000  0.000000
  6    1    4    1  1.000000  0.000000
  6    0    8    0  1.000000  0.000000
  8    0    6    0  1.000000  0.000000
...

```

File format

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3-5: Header
- Lines 6-: [int02] [int03] [int04] [int05] [double01] [double02]

Parameters

- [string01]

Type : string-type (blank parameter not allowed)

Description : A keyword for total number of transfer integrals. You can freely give a name of the keyword.
- [int01]

Type : int-type (blank parameter not allowed)

Description : An integer giving total number of transfer integrals.

- [int02], [int04]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int02}], [\text{int04}] < \text{Nsite}$).
- [int03], [int05]
Type : int-type (blank parameter not allowed)
Description : An integer giving a spin index,
0: up-spin,
1: down-spin.
- [double01]
Type : double-type (blank parameter not allowed)
Description : A value for a real part of $t_{ij\sigma_1\sigma_2}$.
- [double02]
Type : double-type (blank parameter not allowed)
Description : A value for an imaginary part of $t_{ij\sigma_1\sigma_2}$.

Use rules

- Headers cannot be omitted.
- Blank line is not allowed.
- A program is terminated, when [int01] is different from the total number of transfer integrals defined in this file.
- A program is terminated, when [int02]-[int05] are out of range from the defined values.
- Since Hamiltonian must be Hermitian, the following relation must be satisfied,

$$t_{ij\sigma_1\sigma_2} = t_{ji\sigma_2\sigma_1}^\dagger.$$

4.2.5 InterAll file

The Hamiltonian for general two-body interactions

$$\mathcal{H}_I = \sum_{i,j,k,l} \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} I_{ijkl\sigma_1\sigma_2\sigma_3\sigma_4} c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{l\sigma_4}. \quad (4.23)$$

is added to the whole Hamiltonian by setting the parameters $I_{ijkl\sigma_1\sigma_2\sigma_3\sigma_4}$. An example of file format is shown as follows.

```

=====
NInterAll      36
=====
=====zInterAll=====
=====
0   0   0   1   1   1   1   0   0.50  0.0
0   1   0   0   1   0   1   1   0.50  0.0
0   0   0   0   1   0   1   0   0.25  0.0
0   0   0   0   1   1   1   1  -0.25  0.0
0   1   0   1   1   0   1   0  -0.25  0.0
0   1   0   1   1   1   1   1   0.25  0.0
2   0   2   1   3   1   3   0   0.50  0.0
2   1   2   0   3   0   3   1   0.50  0.0
2   0   2   0   3   0   3   0   0.25  0.0
2   0   2   0   3   1   3   1  -0.25  0.0
2   1   2   1   3   0   3   0  -0.25  0.0
2   1   2   1   3   1   3   1   0.25  0.0
4   0   4   1   5   1   5   0   0.50  0.0
4   1   4   0   5   0   5   1   0.50  0.0
4   0   4   0   5   0   5   0   0.25  0.0
4   0   4   0   5   1   5   1  -0.25  0.0
4   1   4   1   5   0   5   0  -0.25  0.0
4   1   4   1   5   1   5   1   0.25  0.0
...

```

File format

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3 - 5: Header
- Lines 6 -: [int02] [int03] [int04] [int05] [int06] [int07] [int08] [int09] [double01] [double02]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)

Description : A keyword for total number of generalized two body interactions. You can freely give a name of the keyword.

- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of generalized two body interactions.
- [int02], [int04], [int06], [int08]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int02}], [\text{int04}], [\text{int06}], [\text{int08}] < N_{\text{site}}$).
- [int03], [int05], [int07], [int09]
Type : int-type (blank parameter not allowed)
Description : An integer giving a spin index,
 0: up-spin,
 1: down-spin.
- [double01]
Type : double-type (blank parameter not allowed)
Description : A value for a real part of $I_{ijkl\sigma_1\sigma_2\sigma_3\sigma_4}$.
- [double02]
Type : double-type (blank parameter not allowed)
Description : A value for an imaginary part of $I_{ijkl\sigma_1\sigma_2\sigma_3\sigma_4}$.

Use rules

- Headers cannot be omitted.
- Since Hamiltonian must be Hermitian, the following relation must be satisfied,

$$I_{ijkl\sigma_1\sigma_2\sigma_3\sigma_4} = I_{lkji\sigma_4\sigma_3\sigma_2\sigma_1}^\dagger.$$
- A program is terminated, when [int01] is different from the total number of generalized two body interactions defined in this file.
- A program is terminated, when [int02]-[int09] are out of range from the defined values.

4.2.6 CoulombIntra file (coulombintra.def)

The Hamiltonian for the coulombintra interactions

$$\mathcal{H}_U = \sum_i U_i n_{i\uparrow} n_{i\downarrow} \quad (4.24)$$

is added to the whole Hamiltonian by setting U_i . An example of the file format is shown as follows.

```

=====
NCoulombIntra 6
=====
=====i_0LocSpn_1IteElc =====
=====
 0  4.000000
 1  4.000000
 2  4.000000
 3  4.000000
 4  4.000000
 5  4.000000

```

File format

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3 - 5: Header
- Lines 6 -: [int02] [double01]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)
Description : A keyword for total number of on-site interactions. You can freely give a name of the keyword.
- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of on-site interactions.
- [int02]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int02}] < \text{Nsite}$).
- [double01]
Type : double-type (blank parameter not allowed)
Description : A value for U_i .

Use rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of on-site interactions defined in this file.
- A program is terminated, when [int02] is out of range from the defined values.

4.2.7 CoulombInter file (coulombinter.def)

The Hamiltonian for the coulombinter interactions

$$\mathcal{H}_V = \sum_{i,j} V_{ij} n_i n_j \quad (4.25)$$

is added to the whole Hamiltonian by setting V_{ij} . An example of the file format is shown as follows.

```

=====
NCoulombInter 6
=====
=====CoulombInter =====
=====
  0    1  1.0000
  1    2  1.0000
  2    3  1.0000
  3    4  1.0000
  4    5  1.0000
  5    0  1.0000

```

File format

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3 - 5: Header
- Lines 6 -: [int02] [int03] [double01]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)
Description : A keyword for total number of off-site interactions. You can freely give a name of the keyword.
- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of off-site interactions.
- [int02], [int03]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int02}], [\text{int03}] < N_{\text{site}}$).
- [double01]
Type : double-type (blank parameter not allowed)
Description : A value for V_{ij} .

Use rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of off-site interactions defined in this file.
- A program is terminated, when either [int02] or [int03] are out of range from the defined values.

4.2.8 Hund file (hund.def)

The Hamiltonian for Hund couplings

$$\mathcal{H}_H = - \sum_{i,j} J_{ij}^{\text{Hund}} (n_{i\uparrow} n_{j\uparrow} + n_{i\downarrow} n_{j\downarrow}) \quad (4.26)$$

is added to the whole Hamiltonian by setting the parameters J_{ij}^{Hund} . An example of the file format is shown as follows.

```

=====
NHund 6
=====
=====Hund =====
=====
  0      1 -0.250000
  1      2 -0.250000
  2      3 -0.250000
  3      4 -0.250000
  4      5 -0.250000
  5      0 -0.250000

```

File format

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3 - 5: Header
- Lines 6 -: [int02] [int03] [double01]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)
Description : A keyword for total number of Hund couplings. You can freely give a name of the keyword.
- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of Hund couplings.
- [int02], [int03]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int02}], [\text{int03}] < N_{\text{site}}$).
- [double01]
Type : double-type (blank parameter not allowed)
Description : A value for J_{ij}^{Hund} .

Use rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of Hund couplings defined in this file.
- A program is terminated, when either [int02] or [int03] are out of range from the defined values.

4.2.9 PairHop file

The Hamiltonian for PairHop couplings

$$\mathcal{H}_P = \sum_{i,j} J_{ij}^{\text{Pair}} (c_{i\uparrow}^\dagger c_{j\uparrow} c_{i\downarrow}^\dagger c_{j\downarrow} + c_{j\downarrow}^\dagger c_{i\downarrow} c_{j\uparrow}^\dagger c_{i\uparrow}) \quad (4.27)$$

is added to the whole Hamiltonian by setting the parameters J_{ij}^{Pair} . An example of the file format is shown as follows.

```

=====
NPairhop 6
=====
=====Pairhop =====
=====
    0      1  0.50000
    1      2  0.50000
    2      3  0.50000
    3      4  0.50000
    4      5  0.50000
    5      0  0.50000

```

File format

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3 - 5: Header
- Lines 6 -: [int02] [int03] [double01]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)
Description : A keyword for total number of PairHop couplings. You can freely give a name of the keyword.
- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of PairHop couplings.
- [int02], [int03]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int02}], [\text{int03}] < \text{Nsite}$).
- [double01]
Type : double-type (blank parameter not allowed)
Description : A value for J_{ij}^{Pair} .

Use rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of PairHop couplings defined in this file.
- A program is terminated, when either [int02] or [int03] are out of range from the defined values.

4.2.10 Exchange file (exchange.def)

The Hamiltonian for exchange couplings

$$\mathcal{H}_E = \sum_{i,j} J_{ij}^{\text{Ex}} (c_{i\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow}^\dagger c_{i\uparrow}) \quad (4.28)$$

is added to the whole Hamiltonian by setting J_{ij}^{Ex} . An example of the file format is shown as follows.

```

=====
NExchange 6
=====
=====Exchange =====
=====
  0      1  0.50000
  1      2  0.50000
  2      3  0.50000
  3      4  0.50000
  4      5  0.50000
  5      0  0.50000

```

File format

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3-5: Header
- Lines 6-: [int02] [int03] [double01]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)
Description : A keyword for total number of Exchange couplings. You can freely give a name of the keyword.
- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of Exchange couplings.
- [int02], [int03]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int02}], [\text{int03}] < N_{\text{site}}$).
- [double01]
Type : double-type (blank parameter not allowed)
Description : A value for J_{ij}^{Ex} .

Use rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of Exchange couplings defined in this file.
- A program is terminated, when either [int02] or [int03] are out of range from the defined values.

4.2.11 Gutzwiller file (gutzwiller.def)

This file sets the calculation conditions of Gutzwiller factors

$$\mathcal{P}_G = \exp \left[\sum_i g_i n_{i\uparrow} n_{i\downarrow} \right]. \quad (4.29)$$

A site number i and the variational parameters g_i are specified. An example of the file format is shown as follows.

```

=====
NGutzwillerIdx 2
ComplexType 0
=====
=====
    0    0
    1    0
    2    0
    3    1
(continue...)
   12    1
   13    0
   14    0
   15    0
    0    1
    1    0

```

File format

In the following, we define the whole number of sites as N_s and variational parameters as N_g , respectively.

- Line 1: Header
- Line 2: [string01] [int01]
- Line 3: [string02] [int02]
- Lines 4 - 5: Header
- Lines 6 - (5+ N_s): [int03] [int04]
- Lines (6+ N_s) - (5+ N_s + N_g): [int05] [int06]

Parameters

- [string01]

Type : string-type (blank parameter not allowed)

Description : A keyword for total number of variational parameters g_i . You can freely give a name of the keyword.

- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of variational parameters g_i .
- [string02]
Type : string-type (blank parameter not allowed)
Description : A keyword for indicating the double or complex type of variational parameters g_i . You can freely give a name of the keyword.
- [int02]
Type : int-type (blank parameter not allowed)
Description : An integer indicates the double or complex type of variational parameters g_i (0: double, 1: complex).
- [int03]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int03}] < \text{Nsite}$).
- [int04]
Type : int-type (blank parameter not allowed)
Description : An integer setting kinds of variational parameters g_i ($0 \leq [\text{int04}] < [\text{int01}]$).
- [int05]
Type : int-type (blank parameter not allowed)
Description : An integer giving kinds of variational parameters ($0 \leq [\text{int05}] < [\text{int01}]$).
- [int06]
Type : int-type (blank parameter not allowed)
Description : An integer to select the target of variational parameters indicated at [int05] to be optimized or not (0: not optimize, 1: optimize).

User rules

- Headers cannot be omitted.
- A program is terminated, when components of variational parameters are double counted.
- A program is terminated, when [int01] is different from the total number of variational parameters defined in this file.
- A program is terminated, when [int02] - [int06] are out of range from the defined values.

4.2.12 Jastrow file (jastrow.def)

This file sets the calculation conditions of Jastrow factors

$$\mathcal{P}_J = \exp \left[\frac{1}{2} \sum_{i \neq j} v_{ij} (n_i - 1)(n_j - 1) \right] \quad (4.30)$$

Site numbers i , j , and the variational parameters v_{ij} are specified. An example of the file format is shown as follows.

```

=====
NJastrowIdx 5
ComplexType 0
=====
=====
  0    1    0
  0    2    1
  0    3    0
(continue...)
  0    1
  1    1
  2    1
  3    1
  4    1

```

File format

In the following, we define the total number of sites as N_s and variational parameters as N_j , respectively.

- Line 1: Header
- Line 2: [string01] [int01]
- Line 3: [string02] [int02]
- Lines 4 - 5: Header
- Lines 6 - (5+ $N_s \times (N_s - 1)$): [int03] [int04] [int05]
- Lines (6+ $N_s \times (N_s - 1)$) - (5+ $N_s \times (N_s - 1)$ + N_j): [int06] [int07]

Parameters

- [string01]

Type : string-type (blank parameter not allowed)

Description : A keyword for total number of variational parameters v_{ij} . You can freely give a name of the keyword.

- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of variational parameters v_{ij} .
- [string02]
Type : string-type (blank parameter not allowed)
Description : A keyword for indicating the double or complex type of variational parameters v_{ij} . You can freely give a name of the keyword.
- [int02]
Type : int-type (blank parameter not allowed)
Description : An integer indicates the double or complex type of variational parameters v_{ij} (0: double, 1: complex).
- [int03], [int04]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int03}], [\text{int04}] < N_{\text{site}}$).
- [int05]
Type : int-type (blank parameter not allowed)
Description : An integer setting kinds of variational parameters v_{ij} ($0 \leq [\text{int05}] < [\text{int01}]$).
- [int06]
Type : int-type (blank parameter not allowed)
Description : An integer giving kinds of variational parameters ($0 \leq [\text{int06}] < [\text{int01}]$).
- [int07]
Type : int-type (blank parameter not allowed)
Description : An integer to select the target of variational parameters indicated at [int06] to be optimized or not (0: not optimize, 1: optimize).

User rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of variational parameters defined in this file.
- A program is terminated, when [int02] - [int07] are out of range from the defined values.

4.2.13 DH2 file

This file sets the calculation conditions of 2-site doublon-holon correlation factors

$$\mathcal{P}_{d-h}^{(2)} = \exp \left[\sum_t \sum_{n=0}^2 (\alpha_{2nt}^d \sum_i \xi_{i2nt}^d + \alpha_{2nt}^h \sum_i \xi_{i2nt}^h) \right]. \quad (4.31)$$

A site number i , the two sites around i site and the variational parameters $\alpha_{2nt}^{d(h)}$ which have t kinds at each sites are specified. The details of the parameters $\alpha_{2nt}^{d(h)}$ and the operator $\xi_{i2nt}^{d(h)}$ are shown in ref. [3]. An example of the file format is shown as follows.

```

=====
NDoublonHolon2siteIdx 2
ComplexType 0
=====
=====
    0    5   15    0
    0   13    7    1
  (continue...)
   15    8    2    1
    0    1
  (continue...)
   11    1
=====

```

File format

In the following, we define the total number of sites as N_s and variational parameters as N_{dh2} , respectively.

- Line 1: Header
- Line 2: [string01] [int01]
- Line 3: [string02] [int02]
- Lines 4 - 5: Header
- Lines 6 - $(5+N_s \times N_{dh2})$: [int03] [int04] [int05] [int06]
- Lines $(6+N_s \times N_{dh2}) - (5+(N_s + 6) \times N_{dh2})$: [int07] [int08]

Parameters

- [string01]
 - Type :** string-type (blank parameter not allowed)
 - Description :** A keyword for total number of variational parameters. You can freely give a name of the keyword.
- [int01]
 - Type :** int-type (blank parameter not allowed)
 - Description :** An integer giving total number of variational parameters.

- [string02]
Type : string-type (blank parameter not allowed)
Description : A keyword for indicating the double or complex type of variational parameters. You can freely give a name of the keyword.
- [int02]
Type : int-type (blank parameter not allowed)
Description : An integer indicates the double or complex type of variational parameters (0: double, 1: complex).
- [int03], [int04], [int05]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [int03], [int04], [int05] < N_{site}$).
- [int06]
Type : int-type (blank parameter not allowed)
Description : An integer setting kinds of variational parameters ($0 \leq [int06] < [int01]$).
- [int07]
Type : int-type (blank parameter not allowed)
Description : An integer giving kinds of variational parameters. The value is $(2n + s) \times [int01] + t$, where n , s and t are given by the following relation:
 - n : The number of doublon (holon) around the center site (0, 1, 2),
 - s : When the center is doublon (holon), $s=0$ (1),
 - t : The kind of variational parameters (0, \dots $[int01]-1$).
- [int08]
Type : int-type (blank parameter not allowed)
Description : An integer to select the target of variational parameters indicated at [int07] to be optimized or not (0: not optimize, 1: optimize).

User rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of variational parameters defined in this file.
- A program is terminated, when [int02] - [int08] are out of range from the defined values.

4.2.14 DH4 file

This file sets the calculation conditions of 4-site doublon-holon correlation factors

$$\mathcal{P}_{d-h}^{(4)} = \exp \left[\sum_t \sum_{n=0}^4 (\alpha_{4nt}^d \sum_i \xi_{i4nt}^d + \alpha_{4nt}^h \sum_i \xi_{i4nt}^h) \right] \quad (4.32)$$

A site number i , the four sites around i site and the variational parameters $\alpha_{4nt}^{d(h)}$ which have t kinds at each sites are specified. The details of the parameters $\alpha_{4nt}^{d(h)}$ and the operator $\xi_{i4nt}^{d(h)}$ are shown in ref. [3]. An example of the file format is shown as follows.

```

=====
NDoublonHolon4siteIdx 1
ComplexType 0
=====
=====
  0   1   3   4  12   0
  1   2   0   5  13   0
(continue...)
 15  12  14   3  11   0
  0   1
(continue...)
  9   1

```

File format

In the following, we define the total number of sites as N_s and variational parameters as N_{dh4} , respectively.

- Line 1: Header
- Line 2: [string01] [int01]
- Line 3: [string02] [int02]
- Lines 4 - 5: Header
- Lines 6 - $(5+N_s \times N_{dh4})$: [int03] [int04] [int05] [int06] [int07] [int08]
- Lines $(6+N_s \times N_{dh4})$ - $(5+(N_s + 10) \times N_{dh4})$: [int09] [int10]

Parameters

- [string01]

Type : string-type (blank parameter not allowed)

Description : A keyword for total number of variational parameters. You can freely give a name of the keyword.
- [int01]

Type : int-type (blank parameter not allowed)

Description : An integer giving total number of variational parameters.

- [string02]
Type : string-type (blank parameter not allowed)
Description : A keyword for indicating the double or complex type of variational parameters. You can freely give a name of the keyword.
- [int02]
Type : int-type (blank parameter not allowed)
Description : An integer indicates the double or complex type of variational parameters (0: double, 1: complex).
- [int03], [int04], [int05], [int06], [int07]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int03}], \dots, [\text{int07}] < N_{\text{site}}$).
- [int08]
Type : int-type (blank parameter not allowed)
Description : An integer setting kinds of variational parameters ($0 \leq [\text{int08}] < [\text{int01}]$).
- [int09]
Type : int-type (blank parameter not allowed)
Description : An integer giving kinds of variational parameters. The value is $(2n + s) \times [\text{int01}] + t$, where n , s and t are given by the following relation:
 - n : The number of doublon (holon) around the center site (0, 1, 2, 3, 4),
 - s : When the center is doublon (holon), $s=0$ (1),
 - t : The kind of variational parameters (0, \dots $[\text{int01}]-1$).
- [int10]
Type : int-type (blank parameter not allowed)
Description : An integer to select the target of variational parameters indicated at [int09] to be optimized or not (0: not optimize, 1: optimize).

User rules

- Headers cannot be omitted.
- A program is terminated, when components of variational parameters are double counted.
- A program is terminated, when [int01] is different from the total number of variational parameters defined in this file.
- A program is terminated, when [int02] - [int10] are out of range from the defined values.

4.2.15 Orbital/OrbitalAntiParallel file (orbitalidx.def)

This file sets the calculation conditions of pair orbitals

$$|\phi_{\text{pair}}\rangle = \left[\sum_{i,j=1}^{N_s} f_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \right]^{N/2} |0\rangle. \quad (4.33)$$

Site numbers i, j and the variational parameters f_{ij} are indicated. An example of the file format is shown as follows.

```

=====
NOrbitalIdx 64
ComplexType 0
=====
=====
    0    0    0
    0    1    1
    0    2    2
    0    3    3
  (continue...)
   15    9   62
   15   10   63
    0    1
    1    1
  (continue...)
   62    1
   63    1

```

File format

In the following, we define the total number of sites as N_s and variational parameters as N_o , respectively.

- Line 1: Header
- Line 2: [string01] [int01]
- Line 3: [string02] [int02]
- Lines 4 - 5: Header
- Lines 6 - $(5+N_s^2)$: [int03] [int04] [int05] [int06]
- Lines $(6+N_s^2)$ - $(5+N_s^2 + N_o)$: [int06] [int07]

Parameters

- [string01]

Type : string-type (blank parameter not allowed)

Description : A keyword for total number of variational parameters. You can freely give a name of the keyword.

- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of variational parameters.
- [string02]
Type : string-type (blank parameter not allowed)
Description : A keyword for indicating the double or complex type of variational parameters. You can freely give a name of the keyword.
- [int02]
Type : int-type (blank parameter not allowed)
Description : An integer indicates the double or complex type of variational parameters (0: double, 1: complex).
- [int03], [int04]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int03}], [\text{int04}] < N_{\text{site}}$).
- [int05]
Type : int-type (blank parameter not allowed)
Description : An integer setting kinds of variational parameters ($0 \leq [\text{int05}] < [\text{int01}]$).
- [int06]
Type : int-type
Description : When the mode of the anti-periodic condition turns on (the mode turns on when the value of `NMPTrans` in `ModPara` file is negative), the sign of f_{ij} is specified by setting $[\text{int06}] = \pm 1$. This term can be omitted when the mode of the anti-periodic condition is off.
- [int07]
Type : int-type (blank parameter not allowed)
Description : An integer giving kinds of variational parameters ($0 \leq [\text{int07}] < [\text{int01}]$).
- [int08]
Type : int-type (blank parameter not allowed)
Description : An integer to select the target of variational parameters indicated at [int06] to be optimized or not (0: not optimize, 1: optimize).

User rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of variational parameters defined in this file.

- A program is terminated, when [int02] - [int09] are out of range from the defined values.

4.2.16 OrbitalParallel file

This file sets the calculation conditions of pair orbitals

$$|\phi_{\text{pair}}\rangle = \left[\sum_{i,j=1}^{N_s} \sum_{\sigma} f_{i\sigma j\sigma} c_{i\sigma}^{\dagger} c_{j\sigma}^{\dagger} \right]^{N/2} |0\rangle. \quad (4.34)$$

Site numbers i, j , the spin index σ and the variational parameters $f_{i\sigma j\sigma}$ are indicated. The indexes of $f_{i\sigma j\sigma}$ must satisfy the condition $i < j$, where $\sigma = 0$ or 1 and process will terminate when the condition is broken. An example of the file format is shown as follows.

```

=====
NOrbitalIdx 120
ComplexType 0
=====
=====
  0    1    0
  0    2    1
  0    3    2
(continue...)
 15   13   118
 15   14   119
  0    1
  1    1
(continue...)
 118    1
 119    1

```

File format

In the following, we define the total number of sites as N_s and variational parameters as N_o , respectively.

- Line 1: Header
- Line 2: [string01] [int01]
- Line 3: [string02] [int02]
- Lines 4 - 5: Header
- Lines 6 - $(5+N_s * (N_s - 1)/2)$: [int03] [int04] [int05] [int06]
- Lines $(6+N_s * (N_s - 1)/2)$ - $(5+N_s * (N_s - 1)/2 + N_o)$: [int06] [int07]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)
Description : A keyword for total number of variational parameters. You can freely give a name of the keyword.

- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of variational parameters.
- [string02]
Type : string-type (blank parameter not allowed)
Description : A keyword for indicating the double or complex type of variational parameters. You can freely give a name of the keyword.
- [int02]
Type : int-type (blank parameter not allowed)
Description : An integer indicates the double or complex type of variational parameters (0: double, 1: complex).
- [int03], [int04]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int03}], [\text{int04}] < N_{\text{site}}$).
- [int05]
Type : int-type (blank parameter not allowed)
Description : An integer setting kinds of variational parameters ($0 \leq [\text{int05}] < [\text{int01}]$).
- [int06]
Type : int-type
Description : When the mode of the anti-periodic condition turns on (the mode turns on when the value of `NMPTrans` in `ModPara` file is negative), the sign of f_{ij} is specified by setting $[\text{int06}] = \pm 1$. This term can be omitted when the mode of the anti-periodic condition is off.
- [int07]
Type : int-type (blank parameter not allowed)
Description : An integer giving kinds of variational parameters ($0 \leq [\text{int07}] < [\text{int01}]$).
- [int08]
Type : int-type (blank parameter not allowed)
Description : An integer to select the target of variational parameters indicated at [int06] to be optimized or not (0: not optimize, 1: optimize).

User rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of variational parameters defined in this file.

- A program is terminated, when [int02] - [int09] are out of range from the defined values.

4.2.17 OrbitalGeneral file

This file sets the calculation conditions of pair orbitals

$$|\phi_{\text{pair}}\rangle = \left[\sum_{i,j=1}^{N_s} \sum_{\sigma_1, \sigma_2} f_{i\sigma_1 j\sigma_2} c_{i\sigma_1}^\dagger c_{j\sigma_2}^\dagger \right]^{N/2} |0\rangle. \quad (4.35)$$

Site numbers i, j , spin indexes σ_1, σ_2 and the variational parameters $f_{i\sigma_1 j\sigma_2}$ are indicated. The indexes of $f_{i\sigma_1 j\sigma_2}$ must satisfy the condition $i + \sigma_1 N_s < j + \sigma_2 N_s$, where $\sigma_i = 0$ or 1 and process will terminate when the condition is broken. An example of the file format is shown as follows.

```

=====
NOrbitalIdx 255
ComplexType 0
=====
=====
    0  0  0  1  0
    0  0  1  1  1
  (continue...)
   14  0  15  1  253
   15  0  15  1  254
    0   1
    1   1
  (continue...)
   253  1
   254  1

```

File format

In the following, we define the total number of sites as N_s and variational parameters as N_o , respectively. A total number of variational parameters N_p is given by N_s^2 , $2N_s^2 - N_s$ in S_z conserved and S_z unconserved system, respectively.

- Line 1: Header
- Line 2: [string01] [int01]
- Line 3: [string02] [int02]
- Lines 4 - 5: Header
- Lines 6 - (5+ N_p): [int03] [int04] [int05] [int06] [int07] [int08]
- Lines (6+ N_p) - (5+ N_p + N_o): [int09] [int10]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)

Description : A keyword for total number of variational parameters. You can freely give a name of the keyword.

- [int01]

Type : int-type (blank parameter not allowed)

Description : An integer giving total number of variational parameters.

- [string02]

Type : string-type (blank parameter not allowed)

Description : A keyword for indicating the double or complex type of variational parameters. You can freely give a name of the keyword.

- [int02]

Type : int-type (blank parameter not allowed)

Description : An integer indicates the double or complex type of variational parameters (0: double, 1: complex).

- [int03], [int05]

Type : int-type (blank parameter not allowed)

Description : An integer giving a site index ($0 \leq [\text{int03}], [\text{int04}] < N_{\text{site}}$).

- [int04], [int06]

Type : int-type (blank parameter not allowed)

Description : An integer giving a spin index (0 : \uparrow spin, 1 : \downarrow spin).

- [int07]

Type : int-type (blank parameter not allowed)

Description : An integer setting kinds of variational parameters ($0 \leq [\text{int07}] < [\text{int01}]$).

- [int08]

Type : int-type

Description : When the mode of the anti-periodic condition turns on (the mode turns on when the value of `NMPTrans` in `ModPara` file is negative), the sign of $f_{i\sigma_1 j\sigma_2}$ is specified by setting $[\text{int08}] = \pm 1$. This term can be omitted when the mode of the anti-periodic condition is off.

- [int09]

Type : int-type (blank parameter not allowed)

Description : An integer giving kinds of variational parameters ($0 \leq [\text{int09}] < [\text{int01}]$).

- [int10]

Type : int-type (blank parameter not allowed)

Description : An integer to select the target of variational parameters indicated at `[int09]` to be optimized or not (0: not optimize, 1: optimize).

User rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of variational parameters defined in this file.
- A program is terminated, when [int02] - [int10] are out of range from the defined values.

4.2.18 TransSym file (qptransidx.def)

This file sets the weight and corresponding site numbers of momentum projection $\mathcal{L}_K = \frac{1}{N_s} \sum_{\mathbf{R}} e^{i\mathbf{K} \cdot \mathbf{R}} \hat{T}_{\mathbf{R}}$ and lattice translational projection $\mathcal{L}_P = \sum_{\alpha} p_{\alpha} \hat{G}_{\alpha}$. The patterns of projection are indicated by (α, \mathbf{R}) . We note that the weight must be equal to 1.0 when the projection is not done. An example of the file format is shown as follows.

```

=====
NQPTrans 4
=====
== TrIdx_TrWeight_and_TrIdx_i_xi ==
=====
  0  1.000000
  1  1.000000
  2  1.000000
  3  1.000000
  0   0   0
(continue...)
  3  12   1
  3  13   2

```

File format

In the following, we define the total number of sites as N_s and projection patterns as N_{TS} , respectively.

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3 - 5: Header
- Lines 6 - (5+ N_{TS}): [int02] [double01]
- Lines (6+ N_{TS}) - (5+($N_s + 1$) \times N_{TS}): [int03] [int04] [int05] [int06]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)
Description : A keyword for total number of projection patterns. You can freely give a name of the keyword.
- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of projection patterns.
- [int02]
Type : int-type (blank parameter not allowed)
Description : An integer giving the projection pattern (α, \mathbf{R}) ($0 \leq [\text{int02}] < [\text{int01}]$).

- [double01]
Type : double-type (blank parameter not allowed)
Description : The weight $p_\alpha \cos(\mathbf{K} \cdot \mathbf{R})$ of the projection pattern (α, \mathbf{R}) .
- [int03]
Type : int-type (blank parameter not allowed)
Description : An integer giving kinds of the projection pattern (α, \mathbf{R}) ($0 \leq [\text{int03}] < [\text{int01}]$).
- [int04], [int05]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [\text{int04}], [\text{int05}] < \text{Nsite}$). The site number [int05] is given by applying the translation and point group transformation indicated by [int03] to the site [int04].
- [int06]
Type : int-type
Description : When the mode of the anti-periodic condition turns on (the mode turns on when the value of NMPTrans in ModPara file is negative), the sign of the translational operator is specified by setting [int06] = ± 1 . This term can be omitted when the mode of the anti-periodic condition is off.

User rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of projection patterns defined in this file.
- A program is terminated, when [int02] - [int06] are out of range from the defined values.

4.2.19 Files to set initial values of variational parameters

This file sets the initial values of variational parameters. The kinds of variational parameters are specified by setting the following keywords in `List` file (`namelist.def`): `InGutzwiller`, `InJastrow`, `InDH2`, `InDH4`, `InOrbital`, `InOrbitalAntiParallel`, `InOrbitalParallel`, `InOrbitalGeneral`.

The file format is common and an example of the `InJastrow` file is shown as follows.

```

=====
NJastrowIdx  28
=====
== i_j_JastrowIdx  ===
=====
0 -8.909963465082626488e-02  0.000000000000000000e+00
1  5.521681211878626955e-02  0.000000000000000000e+00
(continue...)
27 -9.017586139930480749e-02  0.000000000000000000e+00

```

File format

In the following, we define the total number of variational parameters as N_v .

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3 - 5: Header
- Lines 6 - (5+ N_v): [int03] [double01] [double02]

Parameters

- [string01]

Type : string-type (blank parameter not allowed)

Description : A keyword for total number of variational parameters. You can freely give a name of the keyword.
- [int01]

Type : int-type (blank parameter not allowed)

Description : An integer giving total number of variational parameters.
- [int02]

Type : int-type (blank parameter not allowed)

Description : An integer setting kinds of variational parameters ($0 \leq [\text{int02}] < [\text{int01}]$).
- [double01]

Type : double-type (blank parameter not allowed)

Description : The real part of the variational parameter indicated by [int01].

- [double02]

Type : double-type

Description : The imaginary part of the variational parameter indicated by [int01].

User rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of variational parameters defined in this file.

4.2.20 OneBodyG file (greenone.def)

This file determines the target components to calculate and output one-body Green's function $\langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle$. An example of file format is shown as follows.

```

=====
NCisAjs          24
=====
===== Green functions =====
=====
  0    0    0    0
  0    1    0    1
  1    0    1    0
  1    1    1    1
  2    0    2    0
  2    1    2    1
  3    0    3    0
  3    1    3    1
  4    0    4    0
  4    1    4    1
  5    0    5    0
  5    1    5    1
  6    0    6    0
  6    1    6    1
  7    0    7    0
  7    1    7    1
  8    0    8    0
  8    1    8    1
  9    0    9    0
  9    1    9    1
 10    0   10    0
 10    1   10    1
 11    0   11    0
 11    1   11    1

```

File format

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3 - 5: Header
- Lines 6 -: [int02] [int03] [int04] [int05]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)

Description : A keyword for total number of one-body Green's functions. You can freely give a name of the keyword.

- [int01]

Type : int-type (blank parameter not allowed)

Description : An integer giving total number of one-body Green's functions.

- [int02], [int04]

Type : int-type (blank parameter not allowed)

Description : An integer giving a site index ($0 \leq [int02], [int04] < N_{site}$).

- [int03], [int05]

Type : int-type (blank parameter not allowed)

Description : An integer giving a spin index,
0: up-spin,
1: down-spin.

Use rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of one-body Green's functions defined in this file.
- A program is terminated, when [int02]-[int05] are out of range from the defined values.

4.2.21 TwoBodyG file (greentwo.def)

This file determines the target components to calculate and output two-body Green's function $\langle c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{l\sigma_4} \rangle$. For Spin, the condition $i = j$ and $k = l$ must be satisfied. An example of file format is shown as follows.

```

=====
NCisAjsCktAltDC          576
=====
===== Green functions for Sq AND Nq =====
=====
  0   0   0   0   0   0   0   0
  0   0   0   0   0   1   0   1
  0   0   0   0   1   0   1   0
  0   0   0   0   1   1   1   1
  0   0   0   0   2   0   2   0
  0   0   0   0   2   1   2   1
  0   0   0   0   3   0   3   0
  0   0   0   0   3   1   3   1
  0   0   0   0   4   0   4   0
  0   0   0   0   4   1   4   1
  0   0   0   0   5   0   5   0
  0   0   0   0   5   1   5   1
  0   0   0   0   6   0   6   0
  0   0   0   0   6   1   6   1
  0   0   0   0   7   0   7   0
  0   0   0   0   7   1   7   1
  0   0   0   0   8   0   8   0
  0   0   0   0   8   1   8   1
  0   0   0   0   9   0   9   0
  0   0   0   0   9   1   9   1
  0   0   0   0  10   0  10   0
  0   0   0   0  10   1  10   1
  0   0   0   0  11   0  11   0
  0   0   0   0  11   1  11   1
  0   1   0   1   0   0   0   0
  ...

```

File format

- Line 1: Header
- Line 2: [string01] [int01]
- Lines 3 - 5: Header
- Lines 6 -: [int02] [int03] [int04] [int05] [int06] [int07] [int08] [int09]

Parameters

- [string01]
Type : string-type (blank parameter not allowed)
Description : A keyword for total number of two-body Green's functions. You can freely give a name of the keyword.
- [int01]
Type : int-type (blank parameter not allowed)
Description : An integer giving total number of two-body Green's functions.
- [int02], [int04],[int06], [int08]
Type : int-type (blank parameter not allowed)
Description : An integer giving a site index ($0 \leq [int02], [int04], [int06], [int08] < N_{site}$).
- [int03], [int05],[int07], [int09]
Type : int-type (blank parameter not allowed)
Description : An integer giving a spin index,
0: up-spin,
1: down-spin.

Use rules

- Headers cannot be omitted.
- A program is terminated, when [int01] is different from the total number of two-body Green's functions defined in this file.
- A program is terminated, when [int02]-[int09] are out of range from the defined values.

4.3 Output files

The list of output files are shown in Table 4.3, where `***` and `xxx` are the header indicated by `CParaFileHead`, `CDataFileHead` in `ModPara` file, respectively. `yyy` is a number given by `NDataIdxStart...NDataIdxStart+NDataQtySmp`, where both `NDataIdxStart` and `NDataQtySmp` are defined in `ModPara` file and `zzz` is a number given by `NDataIdxStart` in `ModPara`.

Name	Details for corresponding files
<code>***_opt.dat</code>	All optimized parameters.
<code>***_gutzwiller_opt.dat</code>	Optimized gutzwiller factors.
<code>***_jastrow_opt.dat</code>	Optimized jastrow factors.
<code>***_doublonHolon2site_opt.dat</code>	Optimized 2-site doublon-holon correlation factors.
<code>***_doublonHolon4site_opt.dat</code>	Optimized 4-site doublon-holon correlation factors.
<code>***_orbital_opt.dat</code>	Optimized pair orbital factors.
<code>xxx_out_yyy.dat</code>	Energy and deviation.
<code>xxx_var_yyy.dat</code>	Progress information for optimizing variational parameters.
<code>xxx_CalcTimer.dat</code>	Computation time for each processes.
<code>xxx_time_zzz.dat</code>	Progress information for MonteCalro samplings.
<code>xxx_cisaajs_yyy.dat</code>	One body Green's functions.
<code>xxx_cisajscktalt_yyy.dat</code>	Correlation functions.

Table 4.3: List of the output files.

4.3.1 Output file for variational parameters (`***_opt.dat`)

The average and deviation values of variational parameters and the energy optimized by the SR method are outputted in the following order:

$$\langle H \rangle, \langle H^2 \rangle, g_i, v_{ij}, \alpha_{2nt}^{d(h)}, \alpha_{4nt}^{d(h)}, f_{ij}.$$

The type of average values is a complex number, while that of the deviation is a real number. Since the initial values of all variational parameters are specified at the beginning of the calculation, the calculation of physical quantities is done by using this file file. Here, `***` is the header indicated by `CParaFileHead` in `ModPara` file.

4.3.2 Output files for variational parameters at each steps (`xxx_var_yyy.dat`)

The average and deviation values of variational parameters and the energy optimized by the SR method are postscripted by the order same as `$$$_opt.dat` file (the deviation is always outputted as 0). Here, `xxx` is the header indicated by `CDataFileHead` in `ModPara` file and `yyy` is a number given by `NDataIdxStart...NDataIdxStart+NDataQtySmp`, where both `NDataIdxStart` and `NDataQtySmp` are defined in `ModPara` file.

4.3.3 Output file for gutzwiller factors (*****_gutzwiller_opt.dat**)

The optimized Gutzwiller factors by SR method are outputted. The file format is same as the `InGutzwiller` file defined in Sec. 4.2.19.

4.3.4 Output file for jastrow factors (*****_jastrow_opt.dat**)

The optimized Jastrow factors by SR method are outputted. The file format is same as the `InJastrow` file defined in Sec. 4.2.19.

4.3.5 Output file for doublonHolon 2-site factors (*****_doublonHolon2site_opt.dat**)

The optimized 2-site doublon-holon correlation factors by SR method are outputted. The file format is same as the `InDH2` file defined in Sec. 4.2.19.

4.3.6 Output file for doublonHolon 4-site factors (*****_doublonHolon4site_opt.dat**)

The optimized 4-site doublon-holon correlation factors by SR method are outputted. The file format is same as the `InDH4` file defined in Sec. 4.2.19.

4.3.7 Output file for pair orbitals (*****_orbital_opt.dat**)

The optimized pair orbitals by SR method are outputted. The file format is same as the `InOrbital` file defined in Sec. 4.2.19.

4.3.8 **xxx_out_yyy.dat**

The calculation information at each bins are outputted in the order:

$$\langle H \rangle, \langle H^2 \rangle, \frac{\langle H^2 \rangle - \langle H \rangle^2}{\langle H \rangle^2}, \langle S^z \rangle, \langle (S^z)^2 \rangle.$$

The type of $\langle H \rangle$ is a complex number, and that of the others is a real number. Here, `xxx` is the header indicated by `CDataFileHead` in `ModPara` file and `yyy` is a number given by `NDataIdxStart...NDataIdxStart+NDataQtySmp`, where both `NDataIdxStart` and `NDataQtySmp` are defined in `ModPara` file. An example of outputted file is shown as follows.

```

1.151983765704212992e+01  8.124622418360909482e-01  \
1.619082955438887268e+02  2.019905203939084959e-01
1.288482613817423150e+01  5.006903733262847433e-01  \
1.972000325276957824e+02  1.824505193695792893e-01
1.308897206011880421e+01  5.701244886956570168e-01  \
2.072610167083121837e+02  2.029162857569105916e-01
...

```

4.3.9 xxx_CalcTimer.dat

After finishing calculation, the processing time is outputted in the order of the name, the number assigned by the process and the seconds at each processes. An example of outputted file is shown as follows.

```

All [0] 15.90724
Initialization [1] 0.04357
  read options [10] 0.00012
  ReadDefFile [11] 0.00082
  SetMemory [12] 0.00002
  InitParameter [13] 0.03026
VMCParaOpt [2] 15.86367
  VMCMakeSample [3] 12.85650
...

```

4.3.10 xxx_time_zzz.dat

The calculation information at each bins are outputted in the order of the sampling number, the acceptance ratio for hopping and exchange term (acc_hopp, acc_ex), trial numbers to update for hopping and exchange term (n_hopp, n_ex) and the time stamp. Here, xxx is the header indicated by CDataFileHead in ModPara file and zzz is a number given by NDataIdxStart in ModPara. An example of outputted file is shown as follows.

```
00000  acc_hop acc_ex  n_hop    n_ex      : Mon Jul 25 14:03:29 2016
00001  0.59688 0.00000 320      0         : Mon Jul 25 14:03:30 2016
00002  0.47727 0.00000 176      0         : Mon Jul 25 14:03:30 2016
00003  0.50000 0.00000 176      0         : Mon Jul 25 14:03:30 2016
00004  0.49432 0.00000 176      0         : Mon Jul 25 14:03:30 2016
00005  0.57386 0.00000 176      0         : Mon Jul 25 14:03:30 2016
00006  0.55114 0.00000 176      0         : Mon Jul 25 14:03:30 2016
...
```

4.3.11 xxx_cisajs_yyy.dat

This file is the outputted files for one-body Green's function $\langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle$. The target components are set in the input file with the keyword "OneBodyG". Here, xxx is the header indicated by CDataFileHead in ModPara file and yyy is a number given by NDataIdxStart...NDataIdxStart+NDataQtySmp, where both NDataIdxStart and NDataQtySmp are defined in ModPara file.

An example of the file format is as follows.

```
0 0 0 0 0.4452776740 0.0000000000
0 1 0 1 0.4452776740 0.0000000000
1 0 1 0 0.5000000000 0.0000000000
1 1 1 1 0.5000000000 0.0000000000
2 0 2 0 0.4452776740 0.0000000000
2 1 2 1 0.4452776740 0.0000000000
3 0 3 0 0.5000000000 0.0000000000
3 1 3 1 0.5000000000 0.0000000000
...
```

File format

- [int01] [int02] [int03] [int04] [double01] [double02]

Parameters

- [int01], [int03]

Type : Int

Description : The integer of the site number. [int01] and [int03] show the i and j site numbers, respectively.

- [int02], [int04]

Type : Int

Description : The integer of the spin index:

0: Up-spin

1: Down-spin.

[int02] and [int04] show σ_1 and σ_2 , respectively.

- [double01], [double02]

Type : Double

Description : The value of $\langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle$.

[double01] and [double02] show the real and imaginary part of $\langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle$, respectively.

4.3.12 xxx_cisajsckalt_yyy.dat

This file is the outputted files for the two-body Green's function $\langle c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{l\sigma_4} \rangle$. The target components are set in the input file with the keyword "TwoBodyG". Here, xxx is the header indicated by CDataFileHead in ModPara file and yyy is a number given by NDataIdxStart...NDataIdxStart+NDataQtySmp, where both NDataIdxStart and NDataQtySmp are defined in ModPara file. An example of the file format is as follows.

```

0 0 0 0 0 0 0 0 0.4452776740 0.0000000000
0 0 0 0 0 1 0 1 0.1843355815 0.0000000000
0 0 0 0 1 0 1 0 0.1812412105 0.0000000000
0 0 0 0 1 1 1 1 0.2640364635 0.0000000000
0 0 0 0 2 0 2 0 0.0279690007 0.0000000000
0 0 0 0 2 1 2 1 0.2009271524 0.0000000000
0 0 0 0 3 0 3 0 0.2512810778 0.0000000000
0 0 0 0 3 1 3 1 0.1939965962 0.0000000000
...
```

File format

- [int01] [int02] [int03] [int04] [int05] [int06] [int07] [int08] [double01] [double02].

Parameters

- [int01], [int03],[int05], [int07]

Type : Int

Description : The integer of the site number. [int01], [int03], [int05], and [int07] show the i , j , k , and l site numbers, respectively.

- [int02], [int04],[int06], [int08]

Type : Int

Description : The integer of the spin index:

0: Up-spin

1: Down-spin.

[int02], [int04], [int06], and [int08] show σ_1 , σ_2 , σ_3 , and σ_4 , respectively.

- [double01], [double02]

Type : Double

Description : The value of $\langle c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{l\sigma_4} \rangle$.

[double01] and [double02] show the real and imaginary part of $\langle c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{l\sigma_4} \rangle$, respectively.

4.3.13 xxx_ls_out_yyy.dat

This file is the outputted files for $\langle H \rangle$, $\langle H^2 \rangle$, and the optimized parameter α obtained by Power Lanczos method. This file is outputted when `NVMCCalMode = 1`, `NLanczosmode = 1` or `2` are set in `ModPara` file. Here, `xxx` is the header indicated by `CDataFileHead` in `ModPara` file and `yyy` is a number given by `NDataIdxStart...NDataIdxStart+NDataQtySmp`, where both `NDataIdxStart` and `NDataQtySmp` are defined in `ModPara` file.

4.3.14 xxx_ls_cisajs_yyy.dat

This file is the outputted files for one-body Green's function $\langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle$ obtained by Power Lanczos method. The file format is same as the `xxx_cisajs_yyy.dat` file. This file is outputted when `NVMCCalMode = 1`, `NLanczosmode = 2` are set in `ModPara` file.

4.3.15 xxx_ls_cisajscktalt_yyy.dat

This file is the outputted files for the two-body Green's function $\langle c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{l\sigma_4} \rangle$ obtained by Power Lanczos method. The file format is same as the `xxx_cisajscktalt_yyy.dat` file. This file is outputted when `NVMCCalMode = 1`, `NLanczosmode = 2` are set in `ModPara` file.

5

Algorithm

5.1 Variational Monte Carlo Method

The variational Monte Carlo (VMC) method is a method for calculating approximate wave functions of a ground state and low-lying excited states by optimizing variational parameters included in a trial wave function. In calculating expectation values of physical quantities for the trial wave functions, the Markov chain Monte Carlo method is applied for efficient important sampling.

In the mVMC package, we choose a spatial configuration for electrons as a complete set of bases in sampling:

$$|x\rangle = \prod_{n=1}^{N/2} c_{r_{n\uparrow}}^\dagger \prod_{n=1}^{N/2} c_{r_{n\downarrow}}^\dagger |0\rangle, \quad (5.1)$$

where $r_{n\sigma}$ is a position of n -th electron with σ ($=\uparrow$ or \downarrow) spin, and $c_{r_{n\sigma}}^\dagger$ is a creation operator of electrons. By using this basis set, the expectation value of an operator A is expressed as

$$\langle A \rangle = \frac{\langle \psi | A | \psi \rangle}{\langle \psi | \psi \rangle} = \sum_x \frac{\langle \psi | A | x \rangle \langle x | \psi \rangle}{\langle \psi | \psi \rangle}. \quad (5.2)$$

If we define a weight of the Markov chain Monte Carlo method as

$$\rho(x) = \frac{|\langle x | \psi \rangle|^2}{\langle \psi | \psi \rangle} \geq 0, \quad \sum_x \rho(x) = 1, \quad (5.3)$$

we can rewrite $\langle A \rangle$ in the following form:

$$\langle A \rangle = \sum_x \rho(x) \frac{\langle \psi | A | x \rangle}{\langle \psi | x \rangle}. \quad (5.4)$$

By using this form, the Markov chain Monte Carlo method is performed for sampling with respect to x . The local Green's function $G_{ij\sigma\sigma'}(x)$, which is defined as

$$G_{ij\sigma\sigma'}(x) = \frac{\langle \psi | c_{i\sigma}^\dagger c_{j\sigma'} | \psi \rangle}{\langle \psi | x \rangle}, \quad (5.5)$$

is also evaluated by the same sampling method by taking $A = c_{i\sigma}^\dagger c_{j\sigma'}$. We adopt the Mersenne twister method as a random number generator for sampling [8].

5.2 Bogoliubov representation

In the VMC calculation for spin systems, we use the Bogoliubov representation. In the input files defining the one-body term (`transfer`) and the two-body term (`InterAll`), and

the output files for correlation functions, the indices must be assigned by the Bogoliubov representation, in which the spin operators are generally expressed by creation/annihilation operators of fermions as

$$S_{iz} = \sum_{\sigma=-S}^S \sigma c_{i\sigma}^\dagger c_{i\sigma}, \quad (5.6)$$

$$S_i^+ = \sum_{\sigma=-S}^{S-1} \sqrt{S(S+1) - \sigma(\sigma+1)} c_{i\sigma+1}^\dagger c_{i\sigma}, \quad (5.7)$$

$$S_i^- = \sum_{\sigma=-S}^{S-1} \sqrt{S(S+1) - \sigma(\sigma+1)} c_{i\sigma}^\dagger c_{i\sigma+1}. \quad (5.8)$$

Since the present package support only $S = 1/2$ spin systems, the Bogoliubov representation obtained by substituting $S = 1/2$ into the above equations is used.

5.3 Properties of the Pfaffian-Slater determinant

In this section, we explain some properties of the Pfaffian-Slater determinant. We derive the general relation between a Pfaffian-Slater determinant and a single Slater determinant in Sec. 5.3.1 and 5.3.2. We also discuss meaning of the singular value decomposition of coefficients f_{ij} in Sec. 5.3.3.

5.3.1 Relation between f_{ij} and $\Phi_{in\sigma}$ (the case of the anti-parallel pairing)

In the many-variable variational Monte Carlo (mVMC) method, the one-body part of the trial wave function is expressed by the Pfaffian Slater determinant defined as

$$|\phi_{\text{Pf}}\rangle = \left(\sum_{i,j=1}^{N_s} f_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \right)^{N_e/2} |0\rangle, \quad (5.9)$$

where N_s is number of sites, N_e is number of total particles, and f_{ij} are variational parameters. For simplicity, we assume that f_{ij} are a real number. The single Slater determinant is defined as

$$|\phi_{\text{SL}}\rangle = \left(\prod_{n=1}^{N_e/2} \psi_{n\uparrow}^\dagger \right) \left(\prod_{m=1}^{N_e/2} \psi_{m\downarrow}^\dagger \right) |0\rangle, \quad (5.10)$$

$$\psi_{n\sigma}^\dagger = \sum_{i=1}^{N_s} \Phi_{in\sigma} c_{i\sigma}^\dagger, \quad (5.11)$$

Here, $\Phi_{in\sigma}$ is an orthonormal basis, i.e., satisfies

$$\sum_{i=1}^{N_s} \Phi_{in\sigma} \Phi_{im\sigma} = \delta_{nm}, \quad (5.12)$$

where δ_{nm} is the Kronecker's delta. From this orthogonality, we can prove the relation

$$[\psi_{n\sigma}^\dagger, \psi_{m\sigma}]_+ = \delta_{nm}, \quad (5.13)$$

$$G_{ij\sigma} = \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle = \frac{\langle \phi_{\text{SL}} | c_{i\sigma}^\dagger c_{j\sigma} | \phi_{\text{SL}} \rangle}{\langle \phi_{\text{SL}} | \phi_{\text{SL}} \rangle} \quad (5.14)$$

$$= \sum_n \Phi_{in\sigma} \Phi_{jn\sigma}. \quad (5.15)$$

Next, let us prove the relation between f_{ij} and $\Phi_{in\sigma}$ by modifying $|\phi_{\text{SL}}\rangle$. By the commutation relation for $\psi_{n\sigma}^\dagger$, $|\phi_{\text{SL}}\rangle$ is rewritten as

$$|\phi_{\text{SL}}\rangle \propto \prod_{n=1}^{N_e/2} \left(\psi_{n\uparrow}^\dagger \psi_{\mu(n)\downarrow}^\dagger \right) |0\rangle, \quad (5.16)$$

where $\mu(n)$ represents permutation of a sequence of natural numbers, $n = 1, 2, \dots, N_e/2$. For simplicity, let us take identity permutation ($\mu(n) = n$). By defining $K_n^\dagger = \psi_{n\uparrow}^\dagger \psi_{n\downarrow}^\dagger$, and by using the relation $K_n^\dagger K_m^\dagger = K_m^\dagger K_n^\dagger$, we can derive the relation

$$|\phi_{\text{SL}}\rangle \propto \prod_{n=1}^{N_e/2} \left(\psi_{n\uparrow}^\dagger \psi_{n\downarrow}^\dagger \right) |0\rangle = \prod_{n=1}^{N_e/2} K_n^\dagger |0\rangle \quad (5.17)$$

$$\propto \left(\sum_{n=1}^{N_e/2} K_n^\dagger \right)^{N_e/2} |0\rangle = \left(\sum_{i,j=1}^{N_s} \left[\sum_{n=1}^{N_e/2} \Phi_{in\uparrow} \Phi_{jn\downarrow} \right] c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \right) |0\rangle. \quad (5.18)$$

This result indicates that f_{ij} is expressed by the coefficients of the single Slater determinant as

$$f_{ij} = \sum_{n=1}^{N_e/2} \Phi_{in\uparrow} \Phi_{jn\downarrow}. \quad (5.19)$$

We note that this is one of a number of possible expressions of f_{ij} derived from one single Slater determinant. Since f_{ij} depends not only on the choice of the pairing degrees of freedom (i.e., the choice of $\mu(n)$) but also on the choice of the gauge degrees of freedom (i.e., the sign of $\Phi_{in\sigma}$), the parameter f_{ij} has huge redundancy.

5.3.2 Relation between F_{IJ} and $\Phi_{In\sigma}$ (the case of the general pairing)

We extend the relation between the Pfaffian-Slater wave function and the single Slater wave function into the general pairing case including the spin-parallel pairing. We define the Pfaffian-Slater wave function and the single Slater wave function as

$$|\phi_{\text{Pf}}\rangle = \left(\sum_{I,J=1}^{2N_s} F_{IJ} c_I^\dagger c_J^\dagger \right)^{N_e/2} |0\rangle, \quad (5.20)$$

$$|\phi_{\text{SL}}\rangle = \left(\prod_{n=1}^{N_e} \psi_n^\dagger \right) |0\rangle, \quad \psi_n^\dagger = \sum_{I=1}^{2N_s} \Phi_{In} c_I^\dagger, \quad (5.21)$$

respectively, where I, J denote the site index including the spin degrees of freedom. By the similar argument as the anti-parallel pairing case, we can derive the following relation:

$$F_{IJ} = \sum_{n=1}^{\frac{N_e}{2}} \left(\Phi_{In} \Phi_{Jn+1} - \Phi_{Jn} \Phi_{In+1} \right). \quad (5.22)$$

Because this relation hold for the case of anti-parallel pairing, we employ this relation in mVMC ver 1.0 and later.

5.3.3 Singular value decomposition of f_{ij}

We define matrices F , Φ_{\uparrow} , Φ_{\downarrow} , and Σ as

$$(F)_{ij} = f_{ij}, \quad (\Phi_{\uparrow})_{in} = \Phi_{in\uparrow}, \quad (\Phi_{\downarrow})_{in} = \Phi_{in\downarrow}, \quad (5.23)$$

$$\Sigma = \text{diag}[\underbrace{1, \dots, 1}_{N_e/2}, 0, 0, 0]. \quad (5.24)$$

When f_{ij} (i.e., the matrix F) is related with a single Slater determinant of the wave function, we can show that the singular value decomposition of F becomes

$$F = \Phi_{\uparrow} \Sigma \Phi_{\downarrow}^t. \quad (5.25)$$

This result indicates that when the number of nonzero singular values is $N_e/2$, and when all the nonzero singular values of F are one in the singular value decomposition of F , the Pfaffian-Slater wave function parametrized by f_{ij} coincides with a single Slater determinant (i.e. a solution of the mean-field approximation). In other words, the numbers of the nonzero singular values and their difference from one offer a quantitative criterion how the Pfaffian-Slater determinant deviates from the single Slater determinant.

5.4 Power Lanczos method

In this section, we show how to determine α in the power-Lanczos method. We also explain the calculation of physical quantities after the single-step Lanczos method.

5.4.1 Determination of α

First, we briefly explain the sampling procedure of the variational Monte Carlo (VMC) method. Physical properties \hat{A} are calculated as follows:

$$\langle \hat{A} \rangle = \frac{\langle \phi | \hat{A} | \phi \rangle}{\langle \phi | \phi \rangle} = \sum_x \rho(x) F(x, \hat{A}), \quad (5.26)$$

$$\rho(x) = \frac{|\langle \phi | x \rangle|^2}{\langle \phi | \phi \rangle}, \quad F(x, \hat{A}) = \frac{\langle x | \hat{A} | \phi \rangle}{\langle x | \phi \rangle}. \quad (5.27)$$

There are two ways to calculate the product of the operators $\hat{A}\hat{B}$.

$$\langle \hat{A}\hat{B} \rangle = \sum_x \rho(x) F(x, \hat{A}\hat{B}), \quad (5.28)$$

$$\langle \hat{A}\hat{B} \rangle = \sum_x \rho(x) F^\dagger(x, \hat{A}) F(x, \hat{B}). \quad (5.29)$$

As we explain later, in general, the latter way is numerical stable one. For example, we consider the expectation value of the variance, which is defined as $\sigma^2 = \langle (\hat{H} - \langle \hat{H} \rangle)^2 \rangle$. There are two ways to calculate the variance.

$$\sigma^2 = \sum_x \rho(x) F(x, (\hat{H} - \langle \hat{H} \rangle)^2) = \sum_x \rho(x) F(x, \hat{H}^2) - \left[\sum_x \rho(x) F(x, \hat{H}) \right]^2, \quad (5.30)$$

$$\begin{aligned} \sigma^2 &= \sum_x \rho(x) F^\dagger(x, \hat{H} - \langle \hat{H} \rangle) F(x, \hat{H} - \langle \hat{H} \rangle) \\ &= \sum_x \rho(x) F^\dagger(x, \hat{H}) F(x, \hat{H}) - \left[\sum_x \rho(x) F(x, \hat{H}) \right]^2 \end{aligned} \quad (5.31)$$

From its definition, the latter way gives the positive definitive variance even for the finite sampling while the former way does not guarantee the positive definitiveness of the variance. Here, we consider the expectation values of energy and variance for the (single-step) power Lanczos wave function $|\phi\rangle = (1 + \alpha\hat{H})|\psi\rangle$. The energy is calculated as

$$E_{LS}(\alpha) = \frac{\langle \phi | \hat{H} | \phi \rangle}{\langle \phi | \phi \rangle} = \frac{h_1 + \alpha(h_{2(20)} + h_{2(11)}) + \alpha^2 h_{3(12)}}{1 + 2\alpha h_1 + \alpha^2 h_{2(11)}}, \quad (5.32)$$

where we define h_1 , $h_{2(11)}$, $h_{2(20)}$, and $h_{3(12)}$ as

$$h_1 = \sum_x \rho(x) F^\dagger(x, \hat{H}), \quad (5.33)$$

$$h_{2(11)} = \sum_x \rho(x) F^\dagger(x, \hat{H}) F(x, \hat{H}), \quad (5.34)$$

$$h_{2(20)} = \sum_x \rho(x) F^\dagger(x, \hat{H}^2), \quad (5.35)$$

$$h_{3(12)} = \sum_x \rho(x) F^\dagger(x, \hat{H}) F(x, \hat{H}^2). \quad (5.36)$$

From the condition $\frac{\partial E_{LS}(\alpha)}{\partial \alpha} = 0$, i.e., by solving the quadratic equations, we can determine the α . The variance is calculate in the similar way.

5.4.2 Calculation of physical quantities

By using the optimized parameter α , we can calculate the expected value of the operator \hat{A} as

$$A_{LS}(\alpha) = \frac{\langle \phi | \hat{A} | \phi \rangle}{\langle \phi | \phi \rangle} = \frac{A_0 + \alpha(A_{1(10)} + A_{1(01)}) + \alpha^2 A_{2(11)}}{1 + 2\alpha h_1 + \alpha^2 h_{2(11)}}, \quad (5.37)$$

where we define A_0 , $A_{1(10)}$, $A_{1(01)}$, and $A_{2(11)}$ as

$$A_0 = \sum_x \rho(x) F(x, \hat{A}), \quad (5.38)$$

$$A_{1(10)} = \sum_x \rho(x) F^\dagger(x, \hat{H}) F(x, \hat{A}), \quad (5.39)$$

$$A_{1(01)} = \sum_x \rho(x) F(x, \hat{A} \hat{H}), \quad (5.40)$$

$$A_{2(11)} = \sum_x \rho(x) F^\dagger(x, \hat{H}) F(x, \hat{A} \hat{H}). \quad (5.41)$$

6

Acknowledgement

We would like to express our sincere gratitude to Mr. Daisuke Tahara for providing us his code of variational Monte Carlo method. A part of mVMC is based on his original code. We also acknowledge Dr. Hiroshi Shinaoka, Dr. Youhei Yamaji, Dr. Moyuru Kurita, and Dr. Ryui Kaneko for their cooperation on developing mVMC. We would also like to thank the support from “ Project for advancement of software usability in materials science ” by The Institute for Solid State Physics, The University of Tokyo, for development of mVMC ver.0.1, ver. 0.2, and ver. 1.0.

A

Program for the unrestricted Hartree-Fock approximation

In mVMC package, there is a program to calculate the initial values of the pair orbital parameters f_{ij} by using the unrestricted Hartree-Fock (UHF) approximation (relation between Pfaffian Slater determinant and single Slater determinant is explained in sec. 5.3). It is noted that the target system of this program is the itinerant electron system.

A.1 Overview

In UHF approximation, two-body interaction terms are approximated as one-body interaction terms by taking into account of the fluctuation, $\delta A \equiv A - \langle A \rangle$, up to the first order. As an example, we consider the inter-site coulomb interactions

$$\mathcal{H}_V = \sum_{i,j} V_{ij} n_i n_j, \quad (\text{A.1})$$

where we define $i \equiv (i, \sigma)$, $j \equiv (j, \sigma')$ for simplicity. Then, the interaction terms can be approximated as

$$\begin{aligned} n_i n_j &= (\langle n_i \rangle + \delta n_i)(\langle n_j \rangle + \delta n_j) - \left[\langle c_i^\dagger c_j \rangle + \delta(c_i^\dagger c_j) \right] \left[\langle c_j^\dagger c_i \rangle + \delta(c_j^\dagger c_i) \right] \\ &\sim \langle n_i \rangle n_j + \langle n_j \rangle n_i - \langle c_i^\dagger c_j \rangle c_j^\dagger c_i - \langle c_j^\dagger c_i \rangle c_i^\dagger c_j - \langle n_i \rangle \langle n_j \rangle + \langle c_j^\dagger c_i \rangle \langle c_i^\dagger c_j \rangle. \end{aligned} \quad (\text{A.2})$$

Also for other types of interaction, the problem can be attributed to a one-body problem by using a similar approximation. Actual calculation is performed iteratively until that self-consistent solution for the mean values of the above observables are obtained.

A.1.1 Source code

A set of source codes are included in the directory `src/ComplexUHF/src`.

A.1.2 How to compile

To compile source codes, move to the directory just below the main directory of mVMC, and execute

```
$ make mvmc
```

in a similar way as the compile of mVMC. After compiling, an executable file `UHF` is generated in `src/ComplexUHF/src`.

A.1.3 Input files

A file for assigning input files (`namelist.def`)

The following files are needed to use the program of UHF. The format of `namelist.def` is the same as defined in 4.2.1.

- `ModPara`
- `LocSpin`
- `Trans`
- `CoulombIntra`
- `CoulombInter`
- `Hund`
- `PairHop`
- `Exchange`
- `Orbital/OrbitalAntiParallel`
- `OrbitalParallel`
- `OrbitalGeneral`
- `Initial`

Although the format of these files are the same as those for mVMC basically, the following items are different:

- Parameters assigned in `ModPara` file.
- Addition of `Initial` file.

We explain details of the format of these files as follows.

Parameters assigned in `ModPara` file

The parameters needed in the program of UHF are as follows:

- `Nsite`
- `Ne`
- `Mix`
- `EPS`
- `IterationMax`

The parameters, `Nsite` and `Ne`, are common as mVMC. The other three parameters are specific to UHF:

- **Mix**
Linear mixing is assigned by double-type. When `mix=1`, a new Green's function is fully updated without using a old one.
- **EPS**
A condition for convergence is assigned by int-type. When a residual error between a new Green's function and a previous one is less than $10^{-\text{eps}}$, the iteration of calculation is stopped.
- **IterationMax**
A maximum number of the loop is assigned by int-type.

If there are the other parameters for mVMC in this file , warning is output to the standard output (the calculation is not stopped).

Initial file

Initial values of Green's function $G_{ij\sigma_1\sigma_2} \equiv \langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle$ are given. The format is the same as `Trans` file, and instead of $t_{ij\sigma_1\sigma_2}$, values of $G_{ij\sigma_1\sigma_2}$ are described. Green's function is set as zero if values are not given.

A.2 Usage

Calculation of UHF is performed by the same way as mVMC, i.e., by executing the command

```
$ UHF namelist.def
```

The routine of the calculation is as follows.

1. Reading files
2. Construction of a Hamiltonian
3. Self-consistent calculation of Green's function
4. Output of f_{ij} and other files

Examples of output after calculation are as follows.

- `zvo_result.dat`: The energy and the particle number are output.

```
energy -15.2265348135
num    36.0000000000
```

- `zvo_check.dat`: The step number of the iteration, the mean of the absolute value of the residual error in Green's function, the energy in convergence process, and the particle number are output in order.

```
0  0.004925645652 -544.963484605164 36.000000
1  0.002481594941 -278.304285708488 36.000000
2  0.001274395448 -147.247026925130 36.000000
3  0.000681060599 -82.973664527606 36.000000
...
```

- `zvo_UHF_cisajs.dat`: Convergent one-body Green's function $G_{ij\sigma_1\sigma_2} \equiv \langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle$ is output.

For all the components, $i, \sigma_1, j, \sigma_2, \text{Re}[G_{ij\sigma_1\sigma_2}], \text{Im}[G_{ij\sigma_1\sigma_2}]$ are output in order.

```

0  0  0  0  0.5037555283  0.0000000000
0  0  0  1  0.4610257618  0.0003115503
0  1  0  0  0.4610257618 -0.0003115503
0  1  0  1  0.4962444717  0.0000000000
...
```

- `zvo_eigen.dat`: Convergent eigenvalues of the Hamiltonian are output in ascending order.

```

1  -2.9425069199
2  -2.9425069198
3  -1.5005359205
...
```

- `zvo_gap.dat`: For the total electron number N_{tot} , the energy difference $\Delta E = E(N_{\text{tot}} + 1) - E(N_{\text{tot}})$ is output.

```

5.2208232631
```

- `zvo_orbital_opt.dat`: f_{ij} generated from the Slater determinant. The file with the same format as `InOrbital`, `InOrbitalAntiParallel`, `InOrbitalParallel`, `InOrbitalAntiGeneral` file is output. By referring `Orbital`, `OrbitalAntiParallel`, `OrbitalParallel`, `OrbitalAntiGeneral` file, f_{ij} is calculated (for the same type of parameters, the averaged value is calculated).

References

- [1] M. Imada, T. Miyake, J. Phys. Soc. Jpn. **79**, 112001 (2010).
- [2] C. Gros, Ann. Phys. **189**, 53–88 (1989).
- [3] D. Tahara, M. Imada, Journal of the Physical Society of Japan **77**, 114701 (2008).
- [4] T. Misawa, M. Imada, Phys. Rev. B **90**, 115137 (2014).
- [5] S. Morita, R. Kaneko, M. Imada, J. Phys. Soc. Jpn. **84**, 024720 (2015).
- [6] M. Wimmer: ACM Trans. Math. Software 38 30 (2012).
- [7] E. Neuscamman, C. J. Umrigar, G. K.-L. Chan, Phys. Rev. B **85**, 045103 (2012).
- [8] <http://www.math.sci.hiroshima-u.ac.jp/m-mat/MT/SFMT>.