



Fermisurfer Documentation

Release 2.4.0

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**CHAPTER
ONE**

INTRODUCTION

This document is a manual for the Fermi surface drawing program “FermiSurfer”. FermiSurfer has been developed since 2012 by Mitsuaki Kawamura (ISSP, The University of Tokyo); it is opened on web at November, 2014. It draws Fermi surfaces, and plot k -depend matrix elements such as the superconducting gap and orbital character with colors.

**CHAPTER
TWO**

DIRECTORIES AND IMPORTANT FILES

- **doc/** [Directory for manuals]
 - doc/index.html : Index page
- **examples/** : Directory for samples
- **src/** : Directory for source code
- **configure** : Configuration script for build

INSTALL

3.1 Installation in Linux and macOS

1. Install the required package

- For Debian/Ubuntu

```
$ sudo aptitude install libwxgtk3.0-dev
```

- For Red Hat Enterprise Linux/CentOS

```
$ sudo yum install wxGTK3-devel.x86_64
```

- macOS (Homebrew)

```
$ brew install wxmac
```

- macOS (Mac Ports)

```
$ port install wxWidgets-3.0
```

2. Install

```
$ ./configure  
$ make  
$ sudo make install
```

Then a binary file `src/fermisurfer` is generated and copied into `/usr/local/bin/`.

3.2 Installation in Windows

Download the binary file.

Alternatively, we can build FermiSurfer by ourselves after we install wxWidgets library. We can use `fermisurfer.vcxproj` together with VisualStudio.

CHAPTER
FOUR

INPUT FILE

4.1 input-file format

You have to prepare following data:

- The number of k grid (three direction)
- Reciprocal lattice vectors
- The number of bands
- The orbital energy at each band and k (We call it “energy”).
- Variables that you want to plot with color (We call it “matrix elements”).

The input file is as follows (`mgb2_vfz.fs`):

```
40          40          36          (1)
0                      (2)
3                      (3)
1.0000000      0.57735026      -0.0000000 (4)
0.0000000      1.1547005       0.0000000 (5)
0.0000000      -0.0000000      0.87206507 (6)
2.91340202E-02                          (7)
2.93242838E-02
2.98905596E-02
3.08193434E-02
:
:
0.14393796
0.12800488
0.0000000          (8)
0.36269817
0.71675694
1.0535113
1.3644149
:
:
-26.409407
-19.318560
-10.315671
```

1. The number of k in each direction

2. Switch to specify type of k grid (Choose from 0, 1, 2)

k grid is represented as follows:

$$\mathbf{k}_{i,j,k} = x_i \mathbf{b}_1 + y_j \mathbf{b}_2 + z_k \mathbf{b}_3, \quad (4.1)$$

where $i, j, k = 1 \dots N_1, 1 \dots N_2, 1 \dots N_3$, and N_1, N_2, N_3 are the number of k in each direction.

x_i, y_j, z_k can be chosen from below:

- 0 (Monkhorst-Pack grid) : $x_i = \frac{2i-1-N_1}{2N_1}$
- 1 : $x_i = \frac{i-1}{N_1}$
- 2 : $x_i = \frac{2i-1}{2N_1}$

3. The number of bands

4. Reciprocal lattice vector 1 (arbitrary unit)

5. Reciprocal lattice vector 2

6. Reciprocal lattice vector 3

7. Energy (The order of component is written in [How to produce the input file in C and fortran programs](#))

`fermisurfer` assume that the Fermi energy is 0.0 in the default. You can shift the Fermi energy by using Shift Fermi Energy menu described at the section 6.5.

8. Matrix elements (The order of component is written in [How to produce the input file in C and fortran programs](#))

Same as the energy, but in this case we can write 0 to 3 blocks for this quantity, i.e. we can omit to write this.

4.2 BXSF format

The BXSF format also can be treated by FermiSurfer. In this case this program behaves as “Matrix elements” are omitted.

4.3 How to produce the input file in C and fortran programs

fortran

```
real(4) :: bvec1(3), bvec2(3), bvec3(3) ! Reciplocal lattice vector
integer :: nk1, nk2, nk3 ! k-grid of each direction
integer :: ishift ! 1 for shifted grid, 0 for unshifted grid.
integer :: nbnd ! The number of bands
real(4) :: eig(nk3,nk2,nk1,nbnd) ! energy
real(4) :: x(nk3,nk2,nk1,nbnd) ! matrix element

integer :: ik1, ik2, ik3, ibnd, fo

open(fo, file = "sample.fs")
write(fo,*) nk1, nk2, nk3
write(fo,*) ishift
write(fo,*) nbnd
```

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```

write(fo,*)
real(bvec1(1:3))
real(bvec2(1:3))
real(bvec3(1:3))
do ibnd = 1, nbnd
  do ik1 = 1, nk1
    do ik2 = 1, nk2
      do ik3 = 1, nk3
        write(fo,*) real(eig(ik3,ik2,ik1,ibnd))
      end do
    end do
  end do
end do
do ibnd = 1, nbnd
  do ik1 = 1, nk1
    do ik2 = 1, nk2
      do ik3 = 1, nk3
        write(fo,*) real(x(ik3,ik2,ik1,ibnd))
      end do
    end do
  end do
end do
close(fo)

```

C

```

float bvec1[3], bvec2[3], bvec3[3]; /*Resiplocal lattice vector*/
int nk1, nk2, nk3; /*k-grid of each direction*/
int ishift; /*1 for shifted grid, 0 for unshifted grid.*/
int nbnd; /*The number of bands*/
float eig[nbnd][nk1][nk2][nk3]; /*Energy*/
float x[nbnd][nk1][nk2][nk3]; /*Matrix element*/

FILE* fo;
int ibnd, ik1, ik2, ik3;

fo = fopen("sample.frmsf", "w");
ierr = fprintf(fo, "%d %d %d\n", nk1, nk2, nk3);
ierr = fprintf(fo, "%d\n", iswitch);
ierr = fprintf(fo, "%d\n", nbnd);
ierr = fprintf(fo, "%e %e %e\n", bvec1[0], bvec1[1], bvec1[2]);
ierr = fprintf(fo, "%e %e %e\n", bvec2[0], bvec2[1], bvec2[2]);
ierr = fprintf(fo, "%e %e %e\n", bvec3[0], bvec3[1], bvec3[2]);
for (ibnd = 0; ibnd < nbnd; ++ibnd) {
  for (ik1 = 0; ik1 < nk1; ++ik1) {
    for (ik2 = 0; ik2 < nk2; ++ik2) {
      for (ik3 = 0; ik3 < nk3; ++ik3) {
        ierr = fprintf(fo, "%e\n", eig[ibnd][ik1][ik2][ik3]);
      }
    }
  }
}
for (ibnd = 0; ibnd < nbnd; ++ibnd) {

```

(continues on next page)

(continued from previous page)

```

for (ik1 = 0; ik1 < nk1; ++ik1) {
    for (ik2 = 0; ik2 < nk2; ++ik2) {
        for (ik3 = 0; ik3 < nk3; ++ik3) {
            ierr = fprintf(fo, "%e\n", x[ibnd][ik1][ik2][ik3]);
        }
    }
}
fclose(fo);

```

4.4 For the 2D color plot (See `srvo3_t2g.frmsf` in examples)

fortran

```

real(4) :: bvec1(3), bvec2(3), bvec3(3) !Reciprocal lattice vector
INTEGER :: nk1, nk2, nk3 !k-grid of each direction
integer :: ishift !1 for shifted grid, 0 for unshifted grid.
integer :: nbnd !The number of bands
real(4) :: eig(nk3,nk2,nk1,nbnd) !energy
real(4) :: x(nk3,nk2,nk1,nbnd,2) !matrix element (2D or complex)

integer :: ik1, ik2, ik3, ibnd, fo, ii

open(fo, file = "sample.frmsf")
write(fo,*) nk1, nk2, nk3
write(fo,*) ishift
write(fo,*) nbnd
write(fo,*) real(bvec1(1:3))
write(fo,*) real(bvec2(1:3))
write(fo,*) real(bvec3(1:3))
do ibnd = 1, nbnd
    do ik1 = 1, nk1
        do ik2 = 1, nk2
            do ik3 = 1, nk3
                write(fo,*) real(eig(ik3,ik2,ik1,ibnd))
            end do
        end do
    end do
end do
do ii = 1, 2
    do ibnd = 1, nbnd
        do ik1 = 1, nk1
            do ik2 = 1, nk2
                do ik3 = 1, nk3
                    write(fo,*) real(x(ik3,ik2,ik1,ibnd,ii))
                end do
            end do
        end do
    end do
close(fo)

```

4.5 Omit the quantity for the color plot

fortran

```
real(4) :: bvec1(3), bvec2(3), bvec3(3) ! Resiplocal lattice vector
INTEGER :: nk1, nk2, nk3 ! k-grid of each direction
integer :: ishift ! 1 for shifted grid, 0 for unshifted grid.
integer :: nbnd ! The number of bands
real(4) :: eig(nk3,nk2,nk1,nbnd) ! energy

integer :: ik1, ik2, ik3, ibnd, fo, ii

open(fo, file = "sample.frmsf")
write(fo,*) nk1, nk2, nk3
write(fo,*) ishift
write(fo,*) nbnd
write(fo,*) real(bvec1(1:3))
write(fo,*) real(bvec2(1:3))
write(fo,*) real(bvec3(1:3))
do ibnd = 1, nbnd
    do ik1 = 1, nk1
        do ik2 = 1, nk2
            do ik3 = 1, nk3
                write(fo,*) real(eig(ik3,ik2,ik1,ibnd))
            end do
        end do
    end do
end do
end do
```

CONTROL FERMISURFER

5.1 Launch

5.1.1 For Linux, Unix, Mac

You can launch generated executable as follows:

```
$ fermisurfer mgb2_vfz.fs
```

You need a space between the command and input-file name. (The sample input file `mgb2_vfz.fs` contains z element of the Fermi velocity in MgB₂.)

5.1.2 For Windows

Click mouse right button on the input file. Choose “Open With ...” menu, then choose `fermisurfer.exe`.

Then, Operations are printed, and Fermi surfaces are drawn (Fig. 1).

The following operations are available:

- Rotation of objects with mouse drag
- Expand and shrink with mouse wheel
- Window re-sizing
- Moving objects with cursor keys (wasd for Windows). Also we can shift objects with double click.
- Operate by using the panel

Here, we can see all menus.

Note: Some operations are not applied immediately, and after the “Update” button is pushed they are applied. Such operations are referred as “Update required”.

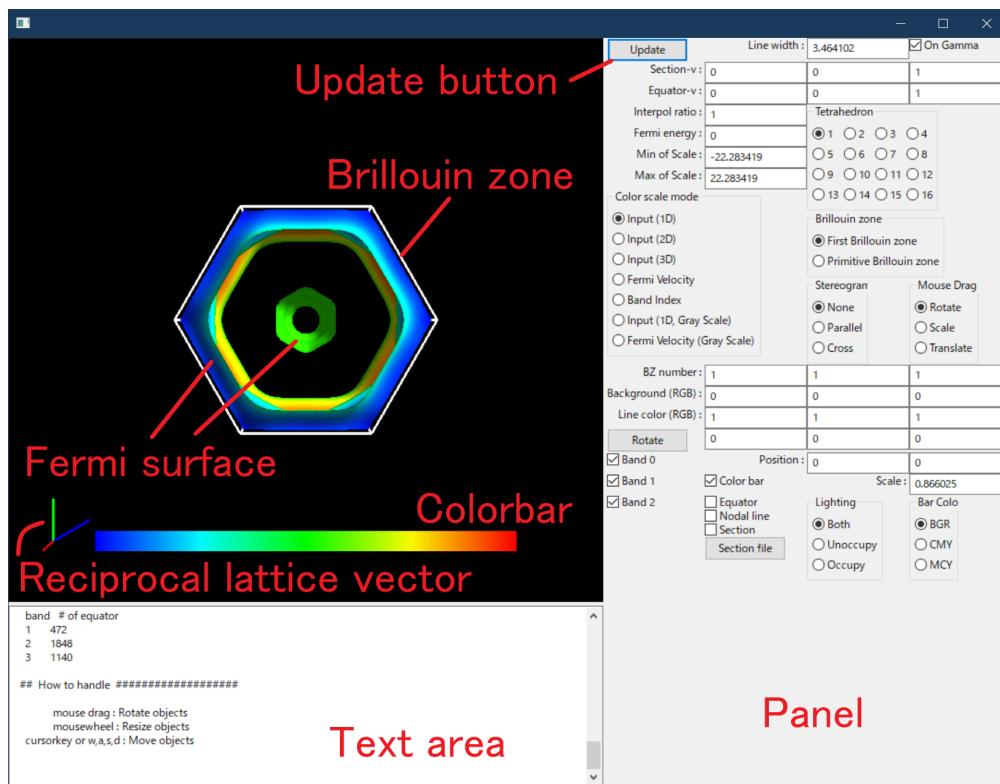


Fig. 1: Main view.

5.2 Background color

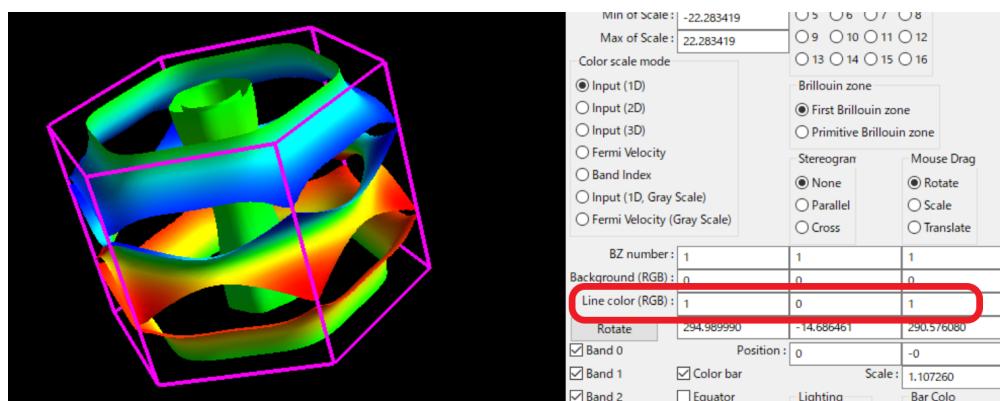
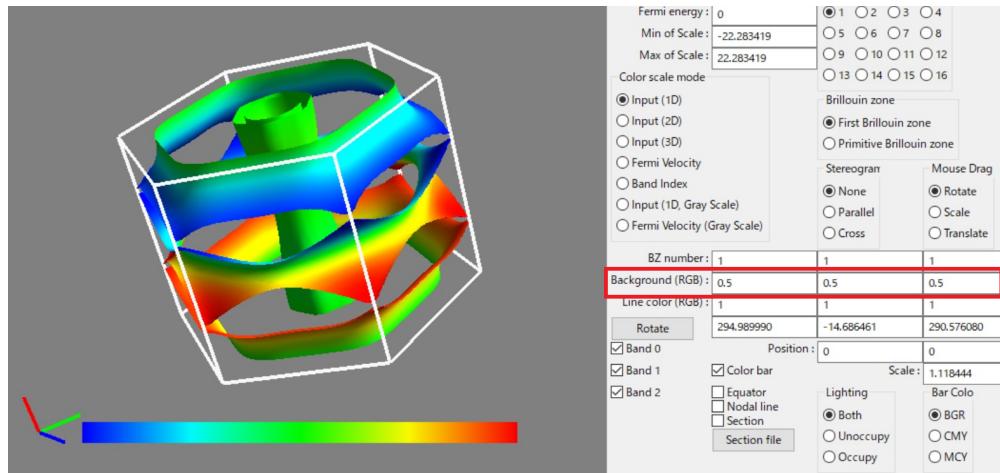
Background (RGB) : The background color is specified as RGB.

5.3 Line width

Line width : Modify the width of the Brillouin-zone boundary, the nodal line, etc.

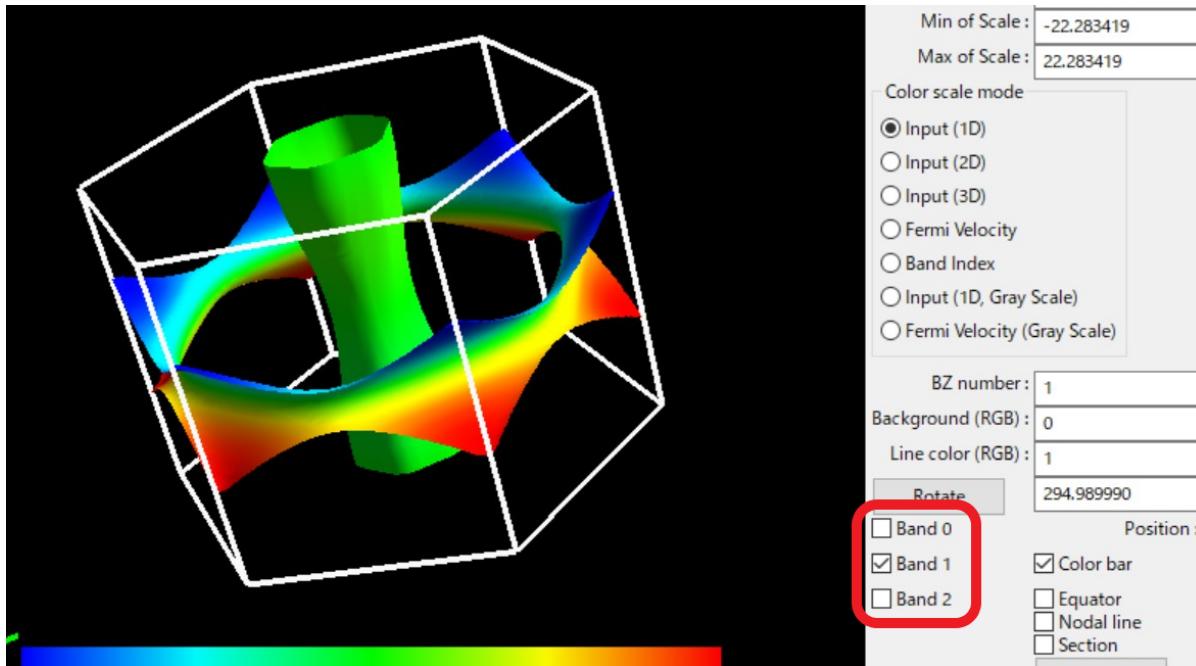
5.4 Line color

Line color (RGB) : The line color is specified with RGB.



5.5 Band

Band 0, RGB, Band 1, RGB ... : It makes each band enable/disable (Fig. ??).



5.6 Brillouin zone (Update required)

Brillouin zone : We choose Brillouin-zone type as follows (Fig. 2):

First Brillouin Zone The region surrounded by Bragg's planes the nearest to Γ point.

Primitive Brillouin Zone A hexahedron whose corner is the reciprocal lattice point.

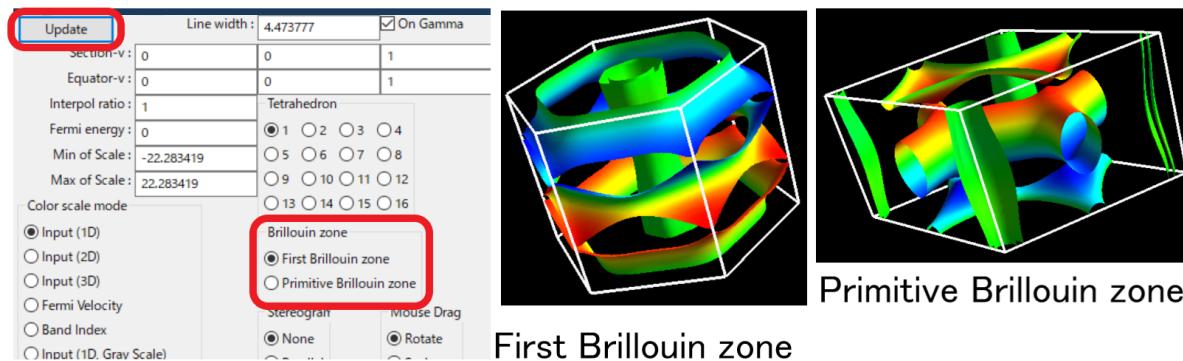
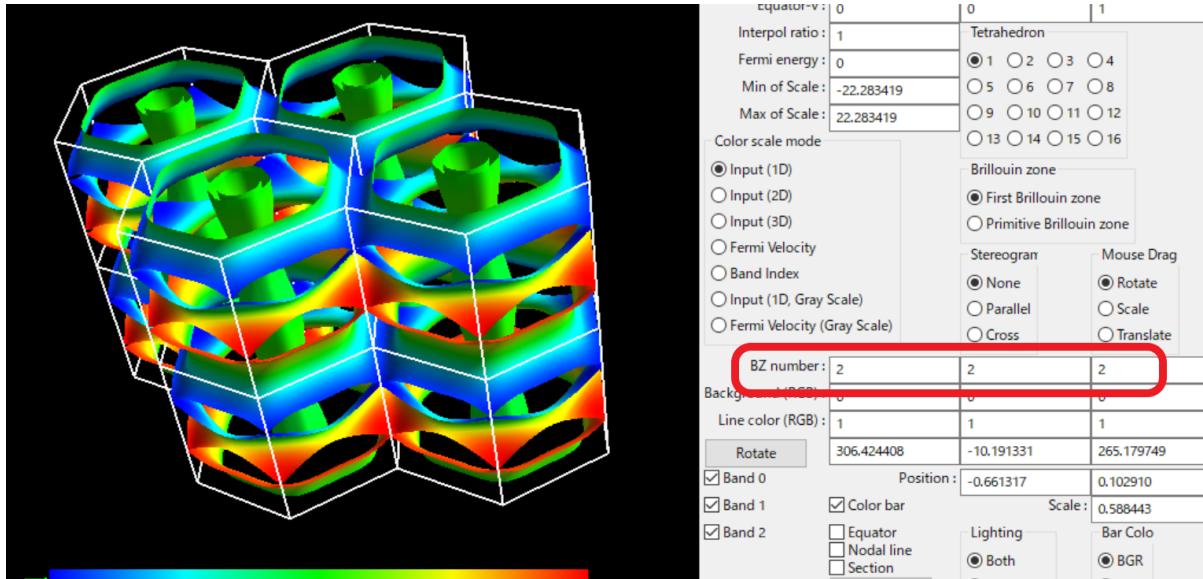


Fig. 2: You can change the type of the Brillouin zone with “Brillouin zone” menu.

5.7 Number of Brillouin zone (Update required)

BZ number : We can specify how many zones are displayed along each reciprocal lattice vector.



5.8 Color bar

Color bar : The color bar becomes enable/disable (Fig. 3).

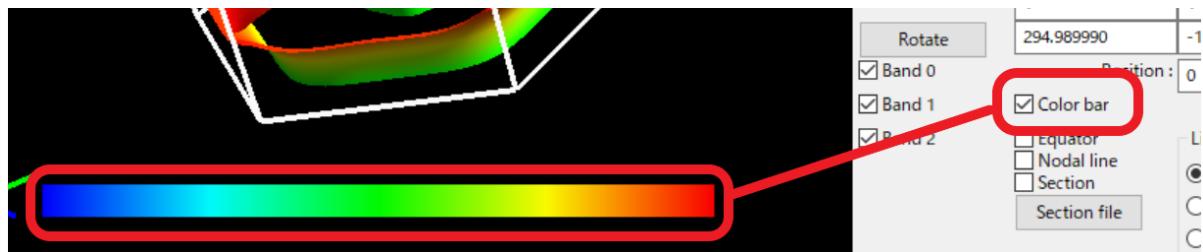


Fig. 3: Toggling the color bar with “Color bar On/Off” menu.

5.9 Color scale mode (Update required)

Color scale mode : It turns color pattern on Fermi surfaces (Fig. 4).

Input (1D) (default for the single input quantity) : It makes blue as the minimum on Fermi surfaces and red as the maximum on them.

Input (2D) (default for the double input quantity) : The color plot is shown with the color circle (see the figure).

Input (3D) (default for the triple input quantity) : The input value is shown as arrows (thin triangles) on the Fermi surfaces. The color of the Fermi surfaces are the same as “Band Index” case.

Fermi velocity (default for no input quantity) Compute the Fermi velocity $\mathbf{v}_F = \nabla_k \epsilon_k$ with the numerical differentiation of the energy, and plot the absolute value of that.

Band Index : Fermi surfaces of each band are depicted with uni-color without relation to the matrix element.

Input (1D, Gray), Fermi Velocity (Gray) : Plot with gray scale.

Min of Scale, Max of Scale : We can change the range of the color plot by inputting into the text boxes. For 3D arrow plot the length of arrows can be changed by **Max of Scale**.

3D arrow step : Change the interval to display arrows at “Input (3D)” mode. Larger number indicates fewer arrows.

Arrow width : Change the thickness of arrow (triangle) at “Input (3D)” mode.

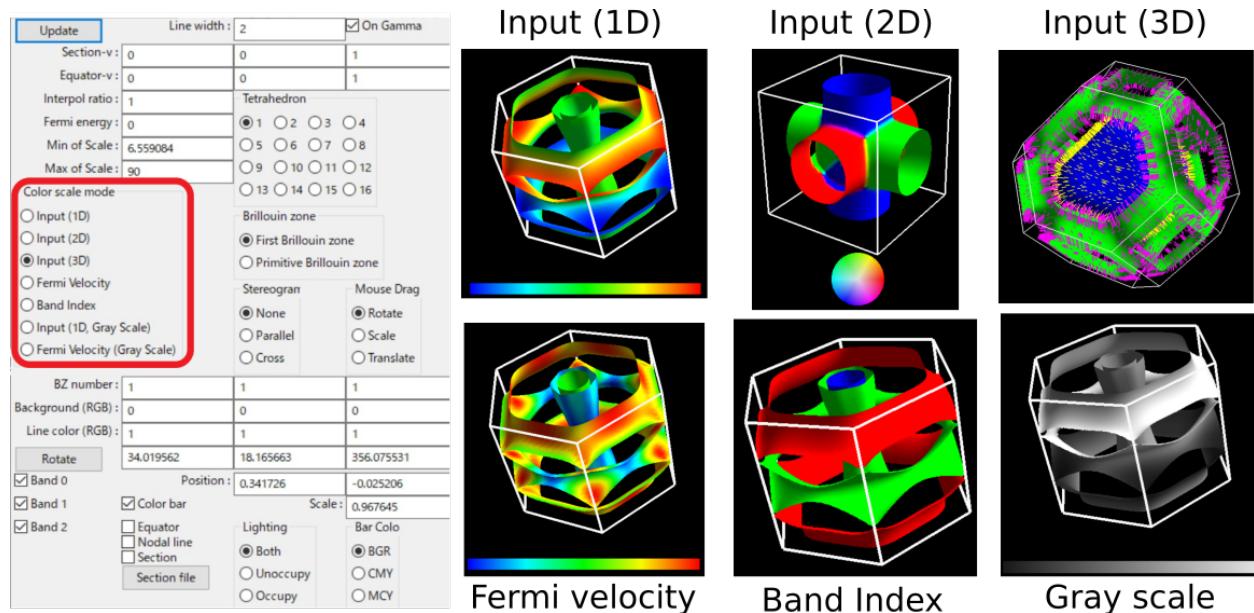


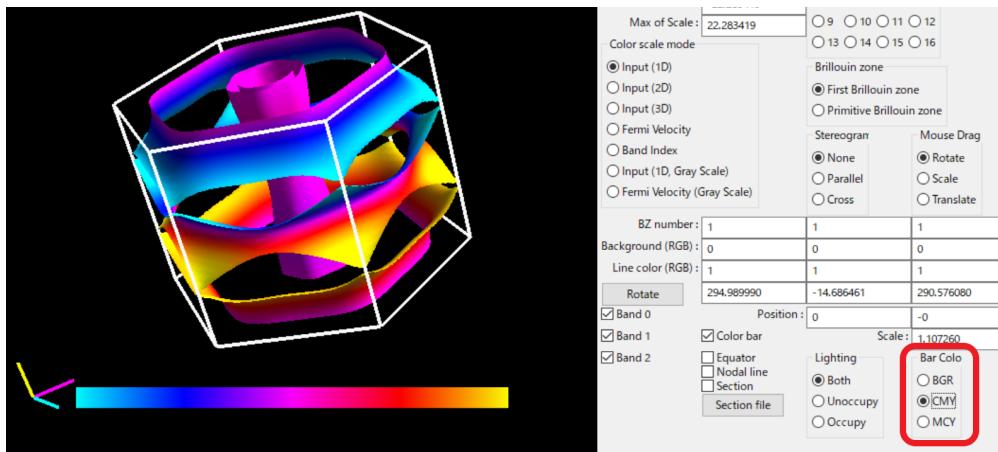
Fig. 4: “Color scale mode” menu.

5.10 Perspective

Perspective : Turn on/off the perspective view.

5.11 Color sequence for plot

Bar Color : We can specify the sequence of color plot. “BGR” is Blue-Cyan-Green-Yellow-Red, “CMY” is Cyan-Blue-Magenta-Red-Yellow, “MCY” is Magenta-Blue-Cyan-Green-Yellow.



5.12 Equator (Update required)

We can draw the line where $\mathbf{v}_F \cdot \mathbf{k} = 0$ for a vector \mathbf{k} . See fig. 5. When it was created, Kawamura misunderstood that this coincides with the extremal orbit in dHvA (it is not true!). Maybe it is related to the ultrasonic attenuation.

Equator : We can toggle equator. This operation does not require the update.

Equator-v : Modify the direction of the tangent vector \mathbf{k} (**fractional coordinate**). We need to push Update to reflect the change.

5.13 Interpolation (Update required)

Interpol ratio : Smooth the Fermi surface with the interpolation (Fig. 6). The time for the plot increases with the interpolation ratio.

5.14 Which (or both) side of Fermi surface is illuminated

Lighting : We can choose the illuminated side of the Fermi surface (Fig. 7).

Both : Light both sides.

Unoccupy : Light unoccupied side.

Occupy : Light the occupied side.

5.15 Mouse Drag

Mouse Drag : It turns the event of the mouse-left-drag.

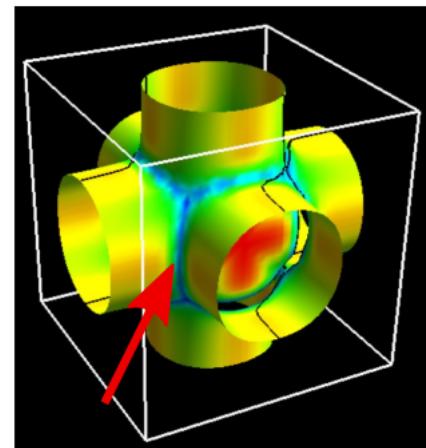
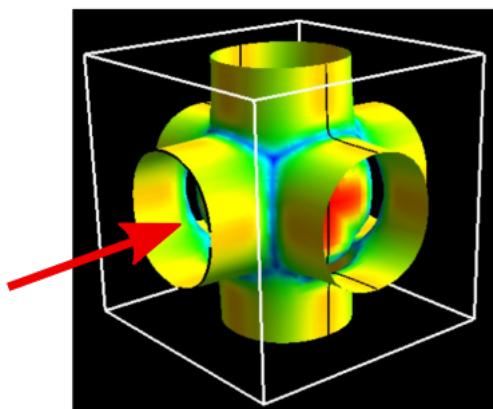
Rotate(default) Rotate the figure along the mouse drag.

Scale Expand/shrink the figure in upward/downward drag.

Translate Translate the figure along the mouse drag.

Update	Line width :	3.141042	<input checked="" type="checkbox"/> On Gamma
Section-v :	1	1	1
Equator-v :	1	1	0
Interpol ratio :	1	Tetrahedron	
Fermi energy :	0	<input checked="" type="radio"/> 1	<input type="radio"/> 2
Min of Scale :	0.163095	<input type="radio"/> 3	<input type="radio"/> 4
Max of Scale :	0.256061	<input type="radio"/> 5	<input type="radio"/> 6
Color scale mode		<input type="radio"/> 7	<input type="radio"/> 8
<input type="radio"/> Input (1D)		<input type="radio"/> 9	<input type="radio"/> 10
<input type="radio"/> Input (2D)		<input type="radio"/> 11	<input type="radio"/> 12
<input type="radio"/> Input (3D)		<input type="radio"/> 13	<input type="radio"/> 14
<input checked="" type="radio"/> Fermi Velocity		<input type="radio"/> 15	<input type="radio"/> 16
<input type="radio"/> Band Index			
<input type="radio"/> Input (1D, Gray Scale)			
<input type="radio"/> Fermi Velocity (Gray Scale)			
Rotate	299.183624	1.229718	28.416000
<input checked="" type="checkbox"/> Band 0	Position :	-0.059396	0.142908
<input checked="" type="checkbox"/> Band 1		Scale :	1.398358
<input checked="" type="checkbox"/> Band 2	<input checked="" type="checkbox"/> Equator		
	<input type="checkbox"/> Nodal line		
	<input type="checkbox"/> Section		
Lighting		Background colc	
<input checked="" type="radio"/> Both		<input checked="" type="radio"/> Black	
<input type="radio"/> Unoccupy		<input type="radio"/> White	
<input type="radio"/> Occupy			

Equator-v:1 0 0

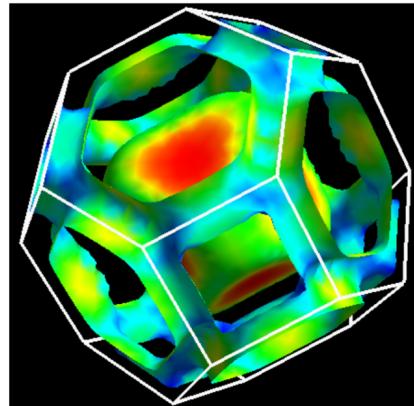


Equator-v:1 1 0

Fig. 5: Display the equator with the “Equator” menu.

Update	Line width :	4	<input checked="" type="checkbox"/> On Gamma
Section-v :	0	0	1
Equator-v :	0	0	1
Interpol ratio :	4	Tetrahedron	
Fermi energy :	0	<input checked="" type="radio"/> 1	<input type="radio"/> 2
Min of Scale :	6.921616	<input type="radio"/> 3	<input type="radio"/> 4
Max of Scale :	16.480536	<input type="radio"/> 5	<input type="radio"/> 6
Color scale mode		<input type="radio"/> 7	<input type="radio"/> 8
<input type="radio"/> Input (1D)		<input type="radio"/> 9	<input type="radio"/> 10
<input type="radio"/> Input (2D)		<input type="radio"/> 11	<input type="radio"/> 12
<input type="radio"/> Input (3D)		<input type="radio"/> 13	<input type="radio"/> 14
<input checked="" type="radio"/> Fermi Velocity		<input type="radio"/> 15	<input type="radio"/> 16
<input type="radio"/> Band Index			
<input type="radio"/> Input (1D, Gray Scale)			
<input type="radio"/> Fermi Velocity (Gray Scale)			
Rotate	309.276184	-70.846390	291.730133
<input checked="" type="checkbox"/> Band 0	Position :	0	0
<input checked="" type="checkbox"/> Band 1	<input checked="" type="checkbox"/> Color bar	Scale :	0.849414
<input checked="" type="checkbox"/> Band 2	<input type="checkbox"/> Equator		
	<input type="checkbox"/> Nodal line		
	<input type="checkbox"/> Section		
Lighting		Background colc	
<input checked="" type="radio"/> Both		<input checked="" type="radio"/> Black	
<input type="radio"/> Unoccupy		<input type="radio"/> White	
<input type="radio"/> Occupy			

Interpol ratio : 1



Interpol ratio : 4

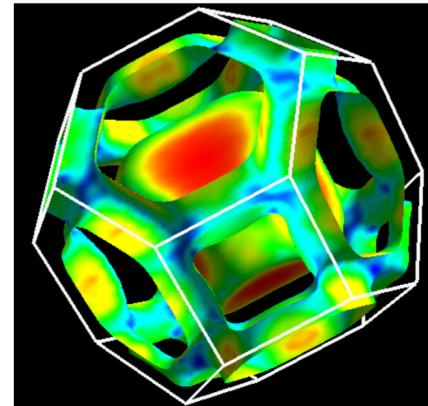


Fig. 6: Modify the number of interpolation points from 1 to 4 with “Interpolate” menu.

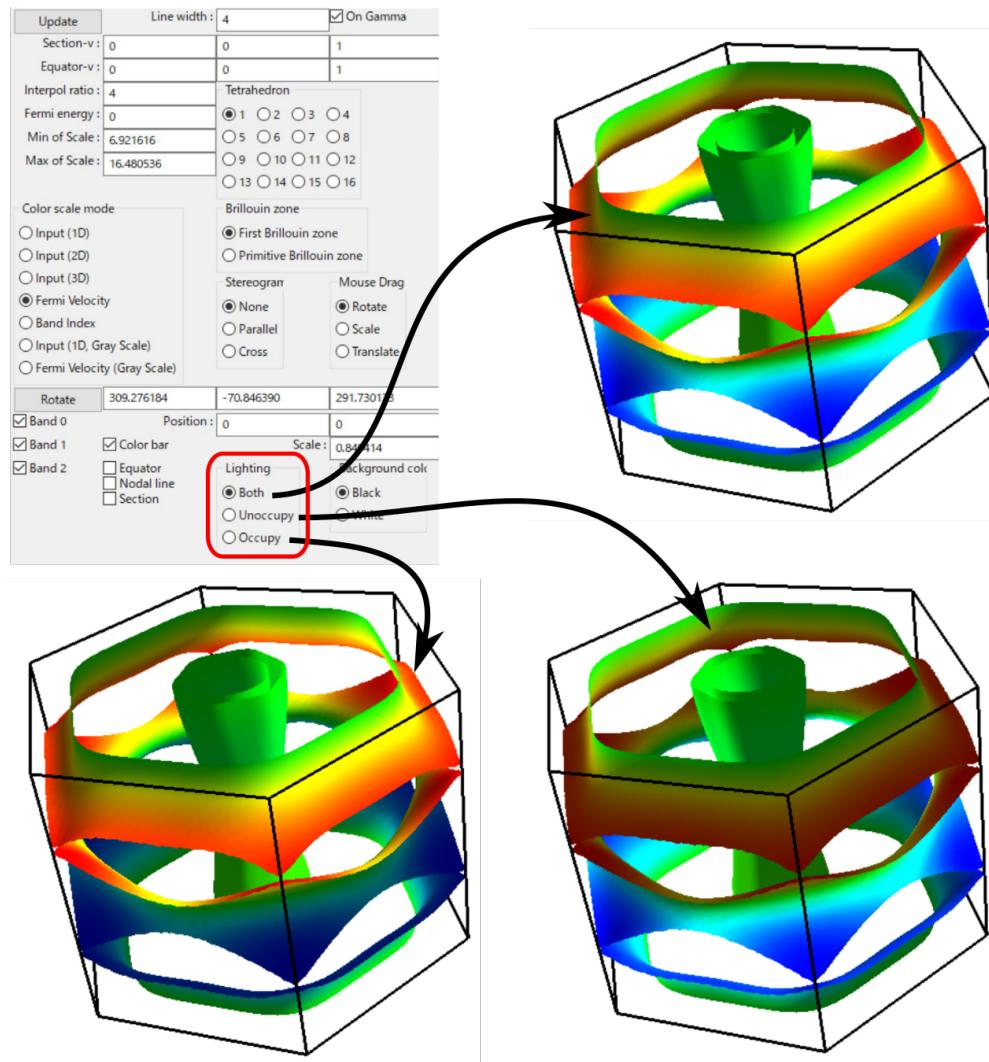
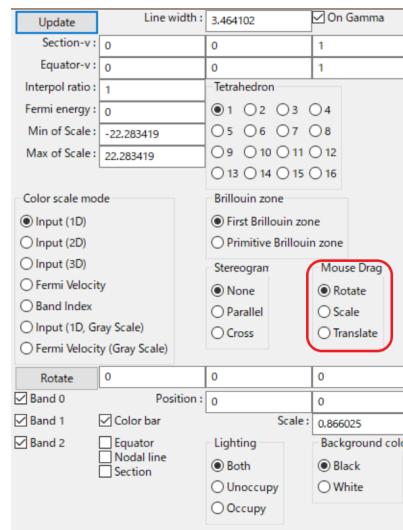


Fig. 7: Change the lighted side by using the “Lighting” menu.



5.16 Nodal line

Nodal Line : The line on which the matrix element becomes 0 (we call it nodal line) becomes enable/disable (Fig. 8).

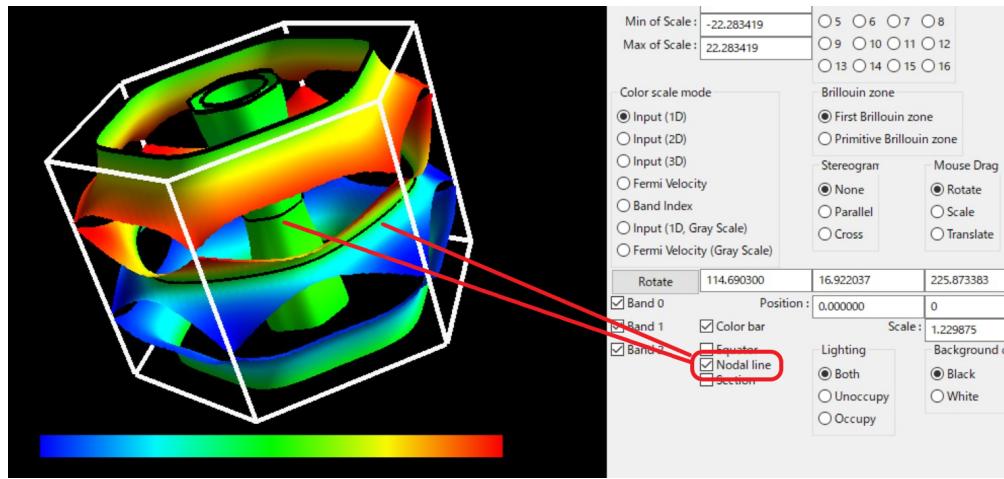


Fig. 8: Toggling the node line with “Nodal line” menu.

5.17 Section of the Brillouine zone (Update required)

Display a 2D plot of the Fermi surface (line) on an arbitrary section of the Brillouin zone (Fig. 9).

Section : We can toggle it with the checkbox (this operation does not require update).

Section-v : We can change the normal vector with the textbox (**fractional coordinate**).

On Gamma If the it is turned on, the section crosses Γ point.

Section (RGB) : Change the color of plane representing the section in BZ.

5.18 Output section of the Brillouine zone

Section file : Above section of the Brillouin zone and Fermi surfaces are outputted into files “fermi_line.dat” and “bz_line.dat” by pushing this button.

These files are plotted in gnuplot as follows:

```
plot "fermi_line.dat" w 1, "bz_line.dat" w 1
```

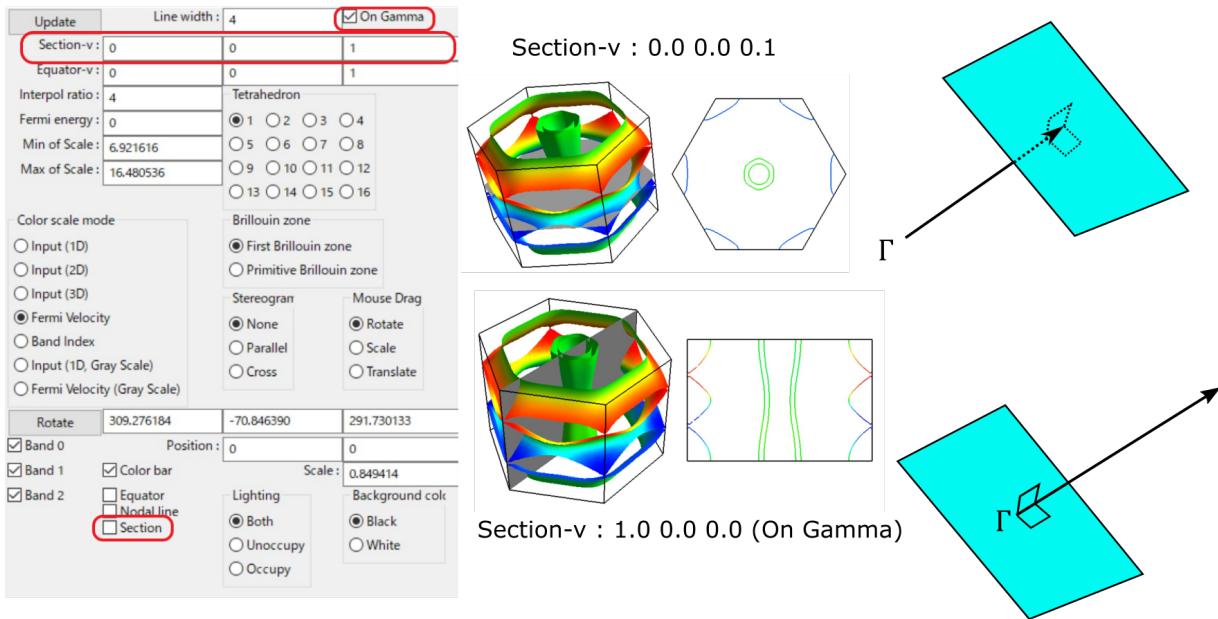
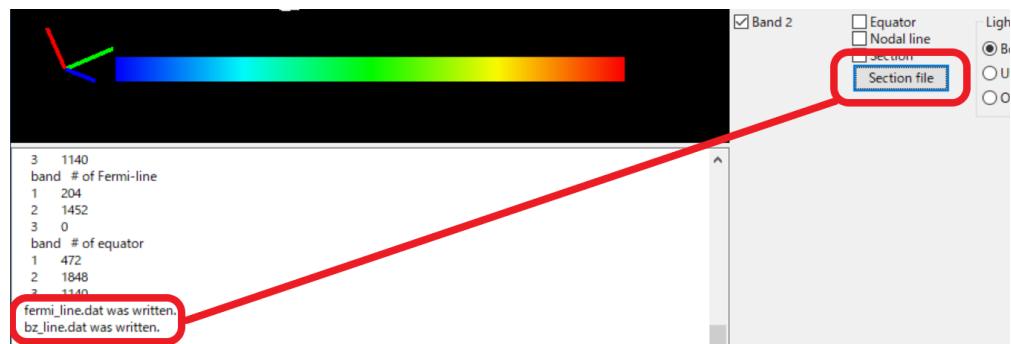


Fig. 9: Display 2D plot of the Fermi surface (line) with “Section” menu.



5.19 Shift Fermi energy (Update required)

Fermi energy : It shifts the Fermi energy (= 0 in default) to arbitrary value (Fig. 10).

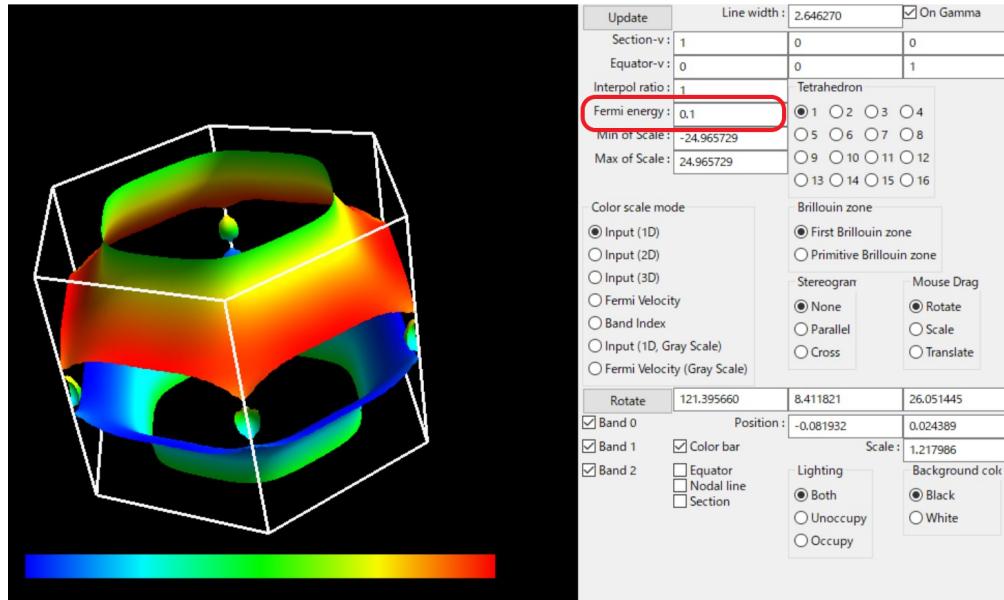


Fig. 10: The Fermi energy is set from 0 Ry to 0.1 Ry with “Shift Fermi energy” menu

5.20 Stereogram

Stereogram : The stereogram (parallel eyes and cross eyes) becomes enabled/disabled (Fig. 11).

None (Default)

Parallel Parallel-eyes stereogram

Cross Cross-eyes stereogram

5.21 Tetrahedron (Update required)

Tetraghedron : You change the scheme to divide into tetrahedra (`tetra # 1` as default). It is experimental.

5.22 View point

Changing the view point.

Scale : Change the size of the figure.

Position : Change the xy position of the figure.

Rotate : Change angles at x-, y-, z- axis. Rotations are performed as z-y-x axis if the “Roate” buttone is pushed.

In each menu, first the current value is printed. then a prompt to input the new value appears (Fig. 12).

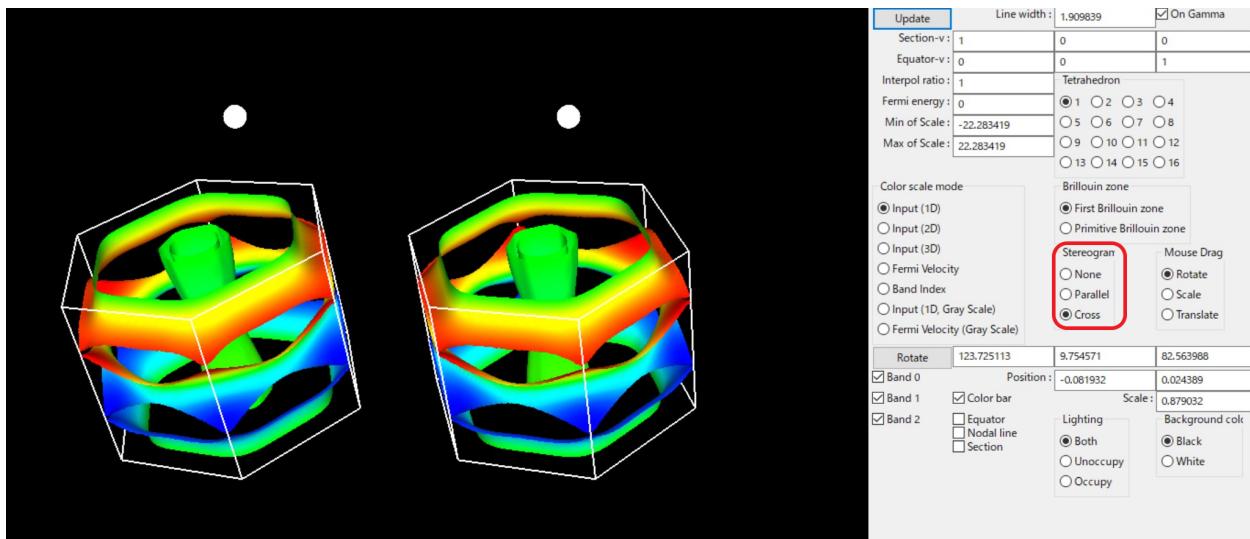
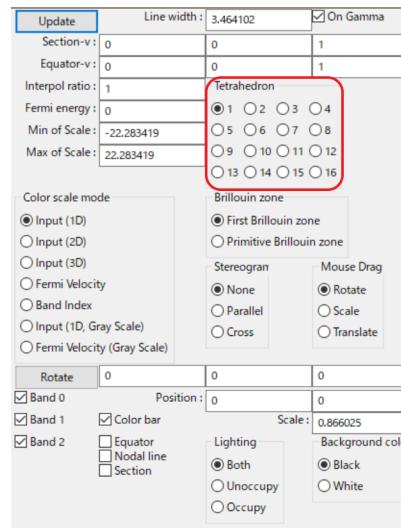


Fig. 11: The stereogram becomes enabled/disabled with “Stereogram” menu.



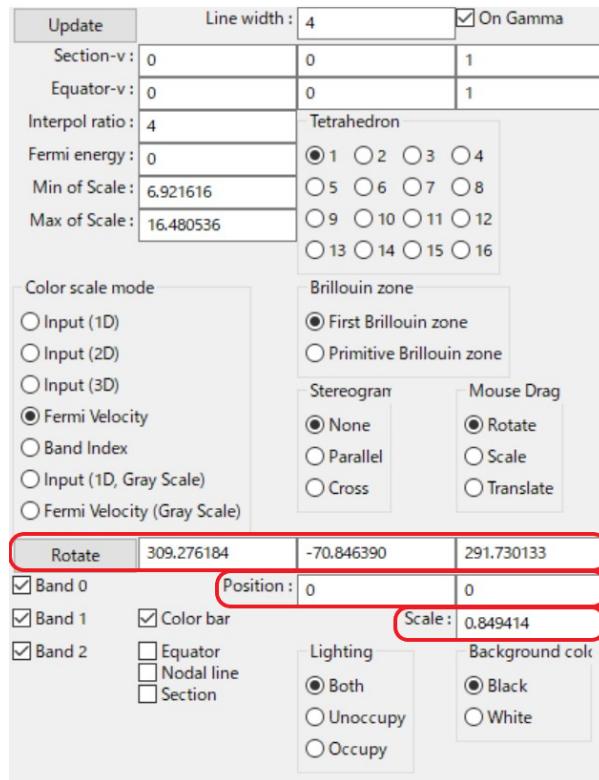


Fig. 12: Modify the view point by using “View point” menu

5.23 Arrow

Show an arrow (thin triangle) at arbitrary place. The following are specified in the fractional coordinate.

Arrow (Start) : Starting point

Arrow (End) : End point

Arrow (Diff) : Difference of above. **Arrow (End)** and **Arrow (Diff)** affects each other.

Arrow width : Modify the thickness of arrow (triangle).

5.24 Wireframe sphere

Show a wireframe sphere at arbitrary place. This is utilized together with HiLAPW. The following are specified in the Cartesian coordinate.

Sphere center : Center of sphere.

Sphere radius : Radius of sphere.

5.25 Nesting function

The following two kinds of nesting function are computed and written into a file readable by FermiSurfer.

delta*delta : File name is “doubledelta.frmsf”

$$\sum_{nn'k} \delta(\varepsilon_{nk} - \varepsilon_F) \delta(\varepsilon_{n'k+q} - \varepsilon_F)$$

Lindhard : File name is “lindhard.frmsf”

$$-\sum_{nn'k} \frac{\theta(\varepsilon_F - \varepsilon_{n'k+q}) - \theta(\varepsilon_F - \varepsilon_{nk})}{\varepsilon_{n'k+q} - \varepsilon_{nk}}$$

5.26 Saving images

`fermisurfer` does not have any functions to save images to a file. Please use the screenshot on your PC.

CHAPTER
SIX

BATCH MODE

By using “Batch mode”, we can generate an image (PNG) file drawn by FermiSurfer only with the command-line operation. By using this batch mode, we can easily make [this kind of many figures](#).

For example, in `example/` directory, when we execute

```
$ fermisurfer mgb2_vfz.frmsf frmsf.in 500 500
```

we will obtain an image file `frmsf.in.png`. The last two numbers are the width and the height of the window. `frmsf.in` is a configuration file for the batch mode; its contents are as follows:

```
backgroundcolor 1 1 0
linecolor 0 0 1
band 0 0 1
#brillouinzone primitive
  colorbar 1
  colorscale fermivelocity
    minmax -22 22
#   equator 1.0 0.0 0.0
  interpol 4
  linewidth 3.0
  lighting both
  nodalline 0
#   section 1.0 0.0 0.0
acrossgamma 1
  position 0.0 0.0 0.0
  scale 1.0
  rotation 120.0 40.0 0.0
fermienergy 0.0
stereogram none
tetrahedron 1
```

They are corresponding to the operations in the panel written in the previous section, and the available keywords are as follows (for the ignored keyword, each default value is used) :

Key-word	Available parameter	Default value	Description
background	float float float	0 0 0	Background color
band	1 or 0 for each band	1 1 1 1 ...	Show(1) or hide(0) each band
brillouin-zone	first, primitive	first	Kind of the Brillouin zone
colorbar	0, 1	1	Show(1) or hide (0) the color bar
colorscale	input1d, input2d, input3d, fermivelocity, bandindex, inputgray, fermivelocitygray	input1d	Kind of the color plot
minmax	float float	The min. and max. through Fermi surfaces	the range of the color scale
equator	float float float	If it is not specified, equator is not shown	Tangent vector for equator (fractional coordinate)
interpol	int	1	Degree of the interpolation
linewidth	float	3.0	Line width
lighting	both, unoccupied, occupied	both	Which side is illuminated
nodalline	0, 1	0	Show(1) or hide(0) the nodal line
section	float float float	Section is not shown	Normal vector for the section (fractional coordinate)
across-gamma	0, 1	1	Whether math: <i>rm Gamma</i> is included (1) or not (0) in the section.
position	float float	0.0, 0.0	The position of the figure
scale	float	1.0	The scale of the figure
rotation	float float float	0.0, 0.0, 0.0	Rotation arround x-, y-, and z-axis
fermienergy	float	0.0	Fermi energy
stereogram	none, parallel, cross	none	Stereogram
tetrahedron	int from 0 to 15	0	Direction to cut tetrahedra

Note: This function uses “import” command to get the screen-shot in ImageMagic. Therefore ImageMagic have to be installed to use this function.

TUTORIAL WITH QUANTUM ESPRESSO

Since the version 6.2, Quantum ESPRESSO can generate data-files for FermiSurfer. The following quantities can be displayed through FermiSurfer.

- The absolute value of the Fermi velocity $|v_F|$ (`fermi_velocity.x`).
- The projection onto each atomic orbital $|\langle \phi_{nlm} | \psi_{nk} \rangle|^2$ (`fermi_proj.x`)

7.1 Building PostProcess tool

For displaying the above quantities with FermiSurfer, we have to build PostProcess tools (tools for plotting the band structure, the charge density, etc.) in QuantumESPRESSO as follows:

```
$ make pp
```

7.2 SCF calculation

Now we will move on the tutorial. First, we perform the electronic-structure calculation with `pw.x`. We will treat MgB₂ in this tutorial. The input file is as follows.

`scf.in`

```
&CONTROL
  calculation = 'scf',
  pseudo_dir = './',
  prefix = 'mgb2' ,
  outdir = './'
/
&SYSTEM
  ibrav = 4,
  celldm(1) = 5.808563789,
  celldm(3) = 1.145173082,
  nat = 3,
  ntyp = 2,
  ecutwfc = 50.0 ,
  ecutrho = 500.0 ,
  occupations = 'tetrahedra_opt',
/
&ELECTRONS
```

(continues on next page)

(continued from previous page)

```

/
ATOMIC_SPECIES
Mg    24.3050  Mg.pbe-n-kjpaw_psl.0.3.0.upf
B     10.811   B.pbe-n-kjpaw_psl.0.1.upf
ATOMIC_POSITIONS crystal
Mg    0.000000000  0.000000000  0.000000000
B     0.333333333  0.666666667  0.500000000
B     0.666666667  0.333333333  0.500000000
K_POINTS automatic
16 16 12 0 0 0

```

Pseudopotentials used in this example are included in PS Library, and they can be downloaded from the following address:

- http://theosrv1.epfl.ch/uploads/Main/NoBackup/Mg.pbe-n-kjpaw_psl.0.3.0.upf
- http://theosrv1.epfl.ch/uploads/Main/NoBackup/B.pbe-n-kjpaw_psl.0.1.upf

We put the input file and the pseudopotential in the same directory, and run `pw.x` at that directory.

```
$ mpiexec -np 4 pw.x -npool 4 -in scf.in
```

the number of processes and the number of blocks for k -paralleliztion (`npool`) can be arbitrary numbers. We also can perform additional non-scf calcultion with a different k -grid.

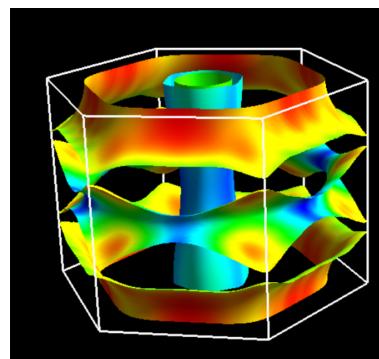
7.3 Compute and display Fermi velocity

We run `fermi_velocity.x` program with the same input file as `pw.x`.

```
$ mpiexec -np 1 fermi_velocity.x -npool 1 -in scf.in
```

For this calculation, the number of blocks for k -paralleliztion (`npool`) should be 1 (or not specified). Then, the file for the Fermi velocity, `vfermi.frmsf`, is generated; this file can be read from FermiSurfer as

```
$ fermisurfer vfermi.frmsf
```



For the case of the collinear spin calculation, two files, `vfermi1.frmsf` and `vfermi2.frmsf` associated to each spin are generated.

7.4 Compute and display projection onto the atomic orbital

Then we will compute the projection onto the atomic orbital. First we run `projwfc.x` with the following input file: `proj.in`

```
&PROJWFC
 outdir = './'
  prefix='mgb2'
  Emin=-0.3422,
  Emax=10.0578,
  DeltaE=0.1
/
2
6 10
```

The input dates after the end of the name-list PROJWFC (/) is not used by `projwfc.x`. The number of processes and the number of blocks for the k -parallelization (`npool`) must to be the same as those for the execution of `pw.x`.

```
$ mpixexec -np 4 projwfc.x -npool 4 -in proj.in
```

excepting `wf_collect=.true.` in the input of `pw.x`.

the following description can be found in the beginning of the standard output of `projwfc.x`.

```
Atomic states used for projection
(read from pseudopotential files):
```

```
state # 1: atom 1 (Mg ), wfc 1 (l=0 m= 1)
state # 2: atom 1 (Mg ), wfc 2 (l=1 m= 1)
state # 3: atom 1 (Mg ), wfc 2 (l=1 m= 2)
state # 4: atom 1 (Mg ), wfc 2 (l=1 m= 3)
state # 5: atom 2 (B ), wfc 1 (l=0 m= 1)
state # 6: atom 2 (B ), wfc 2 (l=1 m= 1)
state # 7: atom 2 (B ), wfc 2 (l=1 m= 2)
state # 8: atom 2 (B ), wfc 2 (l=1 m= 3)
state # 9: atom 3 (B ), wfc 1 (l=0 m= 1)
state # 10: atom 3 (B ), wfc 2 (l=1 m= 1)
state # 11: atom 3 (B ), wfc 2 (l=1 m= 2)
state # 12: atom 3 (B ), wfc 2 (l=1 m= 3)
```

This indicates the relationship between the index of the atomic orbital (`state #`) and its character (for more details, please see `INPUT_PROJWFC.html` in QE). When we choose the projection onto the atomic orbital plotted on the Fermi surface, we use this index. For example, we run `fermi_proj.x` with above `proj.in` as an input file,

```
$ mpixexec -np 1 fermi_proj.x -npool 1 -in proj.in
```

and we obtain the data-file for FermiSurfer, `proj.frmsf`. In this case, after / in `proj.in`

```
2
6 10
```

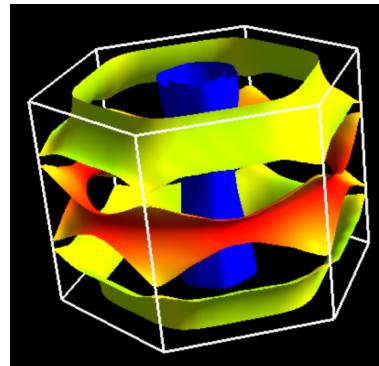
we specify the total number of the displayed projection onto the atomic orbital as the first value (2) and projections to be summed as following indices. In this input, the sum of the 2pz of the first B atom (6) and the 2pz of the first B atom

(10),

$$|\langle \phi_{B_1 2p_z} | \psi_{nk} \rangle|^2 + |\langle \phi_{B_2 2p_z} | \psi_{nk} \rangle|^2$$

is specified. We can display the Fermi surface as

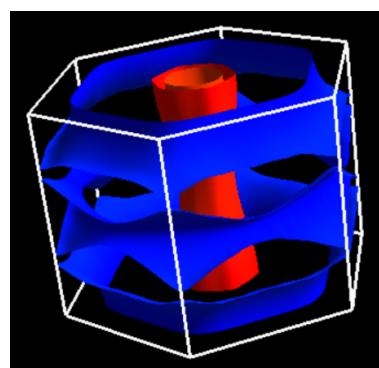
```
$ fermisurfer proj.frmsf
```



If we want to plot the projections onto 2px and 2py orbitals of all B atoms, the input file for `fermi_proj.x` becomes

```
&PROJWFC
outdir = './'
prefix='mgb2'
Emin=-0.3422,
Emax=10.0578,
DeltaE=0.1
/
4
7 8 11 12
```

We do not have to run `projwfc.x` again.



FERMISURFER ON WEB

We can use FermiSurfer on Web at the following URL: <http://163.220.177.91/fsonweb/index.php>

8.1 Control FermiSurfer on Web

Although we are planning to port all functions of *the app version of Fermisurfer*, part of them have not been supported yet.

8.2 How to input file

Fermi surfaces are displayed by choosing a local FRMSF file (BXSF is not supported yet) through the file-explore at left top of the window. Several time-lag may be expected.

8.3 Open online file

We can open an input file placed online by just clicking the link by a URL with an argument:

<http://163.220.177.91/fsonweb/index.php?frmsf=http://163.220.177.91/fsonweb/Pb.js>

We add the URL where the input file locates after `http://163.220.177.91/fsonweb/index.php?frmsf=`. This function can be used in research-introduction pages.

The input file `Pb.js` is as follows:

```
frmsf="16 16 16 1 2 -0.67303315756516724 0.67303315756516724 ... ";
```

This is a javascript source in which a single-lined string generated by replacing new-line letters in *FRMSF-formatted file* with spaces is inputted into a variable `frmsf`. BXSF format has not been supported.

We can convert a FRMSF-formatted file into the above format as

```
sed -e '1i frmsf="" -e '$a ";" ANY.frmsf | perl -pe 's/\n/ /g' | sed -E -e 's/ +/ /g' -e 's/" "/g' -e 's/ \"/g' > ANY.js
```

The following bash script file also do this conversion

<http://163.220.177.91/fsonweb/frmsf2js.sh>

Usage:

```
$ bash frmsf2js.sh ANY.frmsf
```

where ANY is an arbitrary string. Then a file ANY.js which should be uploaded onto an Web server is generated.

**CHAPTER
NINE**

ACKNOWLEDGMENT

I thank Dr. Yusuke Konishi in ISSP; he performed a test in Mac OSX, and proposed Makefiles and a patch.

RE-DISTRIBUTION OF THIS PROGRAM

10.1 Contain Fermisurfer in your program

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**CHAPTER
ELEVEN**

CONTACT

Please post bag reports and questions to the forum

<https://github.com/mitsuaki1987/fermisurfer/issues>

When you want to join us, please contact me as follows.

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