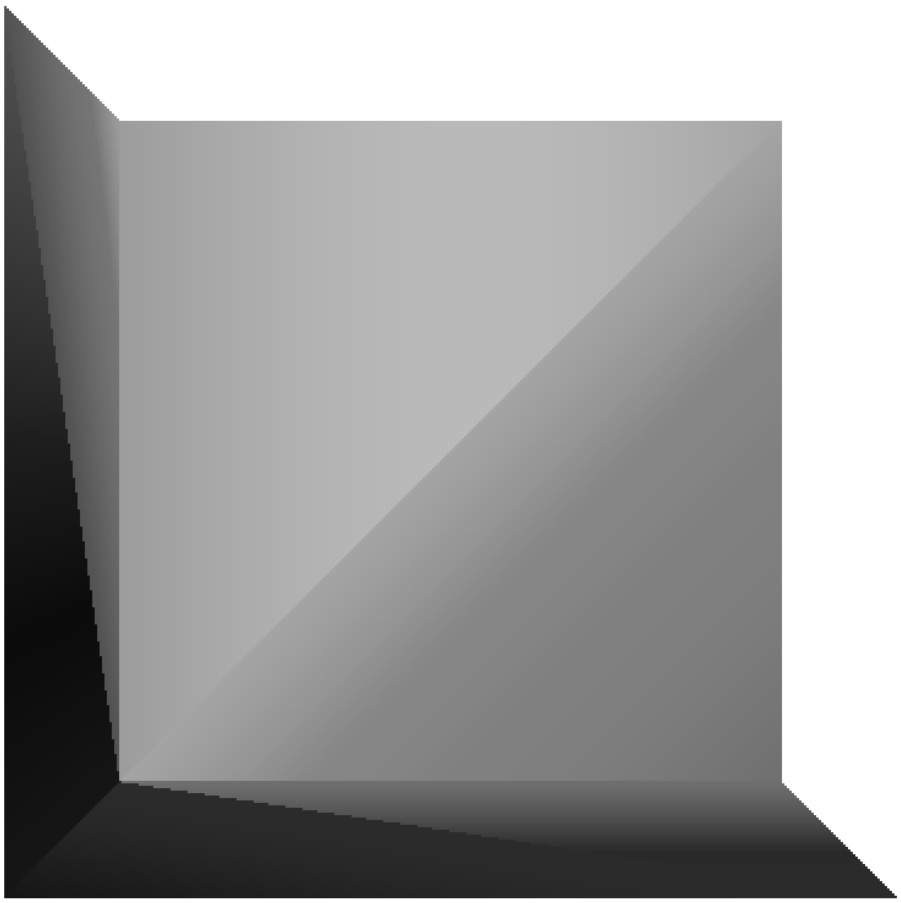

dHvA 3D Analysis Documentation

Release 1.1.0

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Content

Chapter 1 Introduction

This is a documentation for ***dHvA 3D Analysis***, a software for calculating and visualizing the first principle of quantum oscillations. ***dHvA 3D Analysis*** is based on the ***skeaf*** algorithm to calculate and visualize the fermi surface of the material, as well as visualize the polar orbital position, the polar orbital cross section, the polar selection process, etc. It also includes functions such as using different colors to distinguish different pockets, plotting group velocity, etc.

Chapter 2 Directtories And Important Files

- `mayavi_show.py`: algorithms for core functions of drawing fermi surface.
- `matplot_show.py`: algorithms for track section plotting and extremal section visualization plotting.
- `ds_files/`: pyqt interface function implementation files.
- `ui_py_files/`: pyqt interface files.
- `ui_py_files/ui_files/`: pyqt-related ui files.
- `share.py`: shared functions and parameter files.
- `comboCheckbox.py`: design file of multi-selectable combo box.
- `calc/`: calculate program and cache file.
- `main.py`: file to run program.

Chapter 3 Install

3.1 Installation in macOs

3.1.1. Testing environment

1. Python 3.8.13
2. PyQt5 5.15.4
3. traits 6.3.2
4. traitsui 7.3.1
5. pyface 7.4.1
6. mayavi 4.7.4
7. numpy 1.23.0
8. pandas 1.4.3
9. scipy 1.8.1
10. scikit-image 0.19.3
11. hdbscan 0.8.28
12. matplotlib 3.2.2

3.1.2. Install the required package

```
$ conda create -n dHvA python=3.8
$ conda activate dHvA
$ conda install mayavi
$ conda install pandas
$ conda install scikit-image
$ conda install hdbscan
$ conda install matplotlib
```

Chapter 4 Input File

4.1 input-file format

The input Fermi surface file format is ***BXSF*** file format, and the input ***results_long.out***, ***results_orbitoutlines_invau.out***, ***results_orbitoutlines_invAng.out*** files are the standard output files obtained from this program, which change some part of code from original ***skeaf*** algorithms.

Chapter 5 Control dHvA 3D Analysis

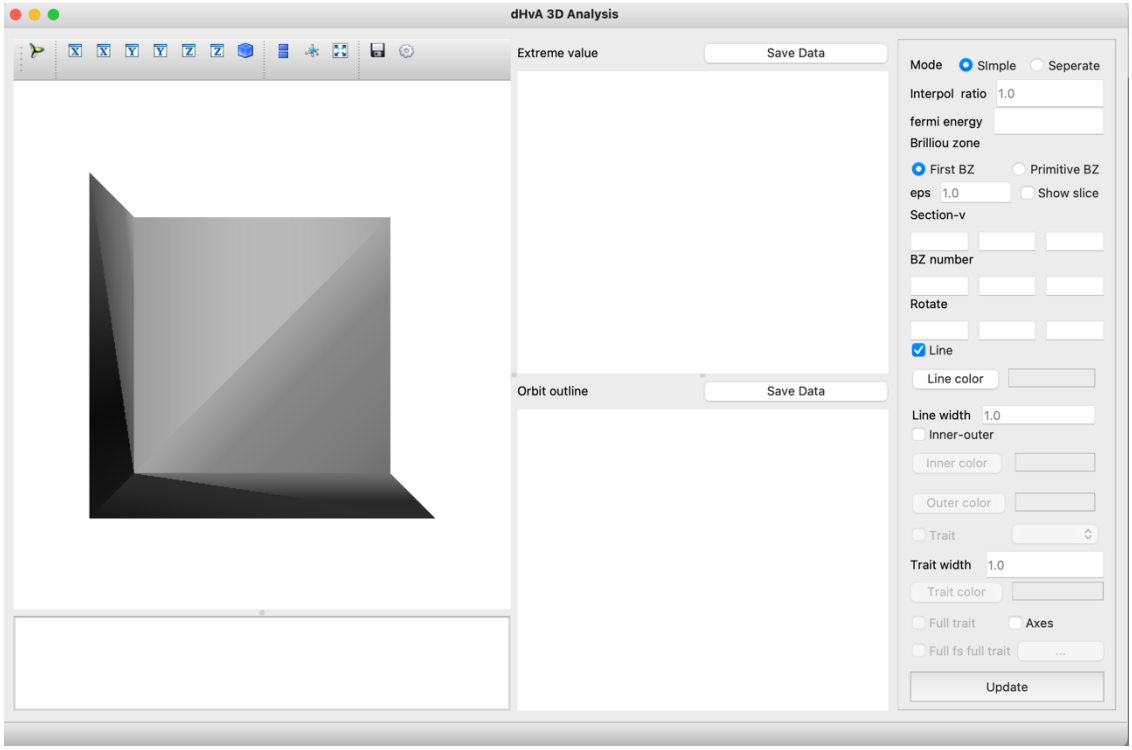
5.1 Launch

5.1.1 For Mac

You can launch generated executable as follows in terminal:

```
$ conda activate dHvA
$ cd <path_to_dHvA_3D_Analysis_directory>
$ python main.py
```

The following window will be obtained after successfully launched with the menu bar ***File***, ***Calc***, ***View*** and ***More***.



5.2 Input files

5.2.1 Input bxsf file

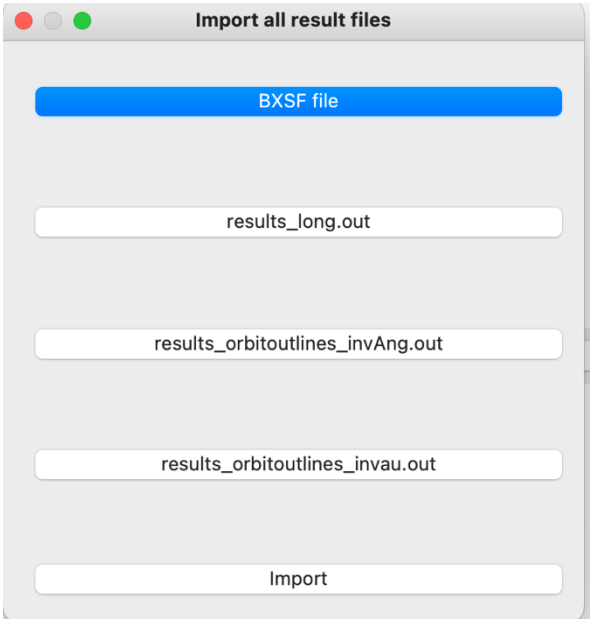
Click ***File*** -> ***Import bxsf file***, select the Fermi surface file you want to import and click ***Open***, there will be about 5-10s loading time after you click it, please don't close the program during that time.

5.2.2 Input result files

Click ***File*** -> ***Import skeaf file***, select the files ***results_long.out***, ***results_orbitoutlines_invau.out*** or ***results_orbitoutlines_invAng.out*** you want to import.
Note: The imported orbit file must match the long file, otherwise the program will report an error.

5.3.2 Import all files at once

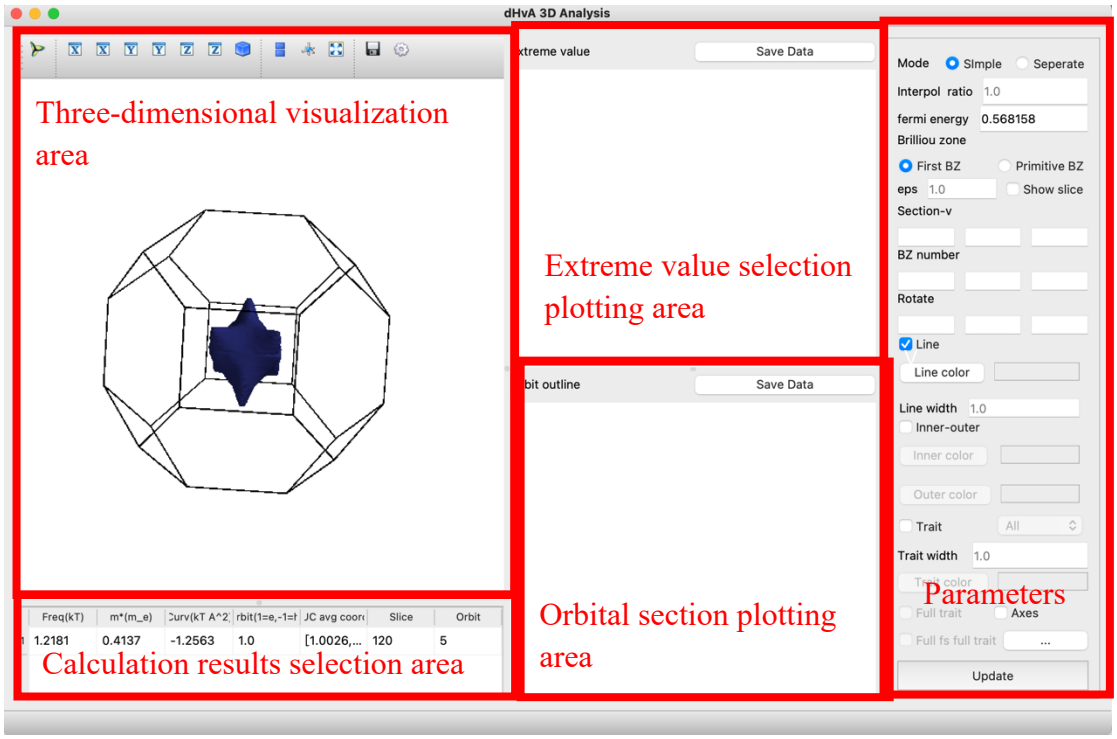
Click ***File*** -> ***Import skeaf file*** -> ***Import all results file***, the following screen appears:



Click any of the buttons to select the corresponding file for import, the absolute path of the file will be displayed at the bottom of the button for confirmation. When all files have been determined, click ***Import***, the program will load for a period of time based on the calculation results, please do not close the program during this period, and manually close the dialog box when the import is finished.

If you need to re-import the files, **it is recommended that you can re-open the program or re-import all the files**. Otherwise, the program will be updated according to the priority of the imported files, but there may be bugs.

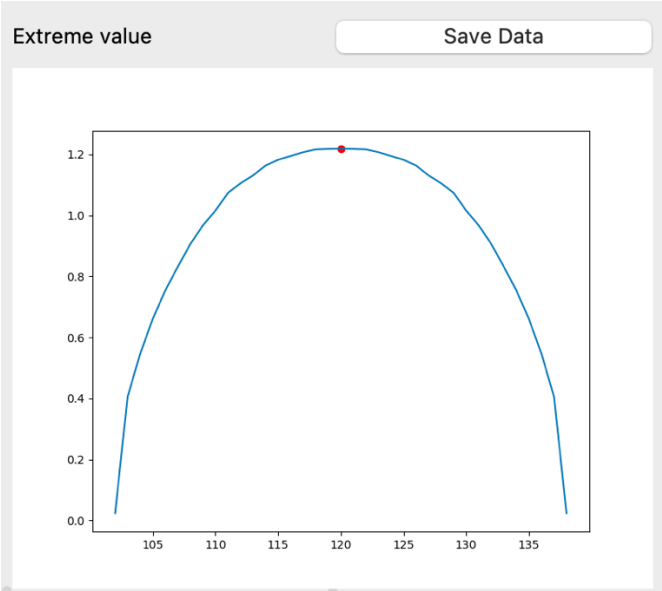
After a successful import you will get the following screen:



5.3 Visualization of extreme value selection

5.3.1 Visualization

If you import the standard output file ***result_long.out***, which is calculated by the software, and select the corresponding frequency in the area by clicking on the calculated result, the selection plotting will be displayed in the extreme value, i.e. the area change curve of the orbit along the magnetic field direction, as shown in the figure below.



The horizontal coordinate is the serial number of the slice and the vertical coordinate is the frequency in kT.

5.3.2 Save data format

Click ***Save Data*** to select the save file location and get the saved data file, which can be used for further plotting. The file is in csv format, named Ext_XXX.csv, where XXX is the frequency, and the contents of the file are shown below.

```
## Extreme value data file generated by Skeaf_demo
## Slice 120, orbit 5, freq1.2187
## slice,freq

1.020000000000000000e+02,2.350000000000000006e-02
1.030000000000000000e+02,4.057000000000000051e-01
1.040000000000000000e+02,5.463999999999999968e-01
...
1.360000000000000000e+02,5.463999999999999968e-01
1.370000000000000000e+02,4.057000000000000051e-01
1.380000000000000000e+02,2.350000000000000006e-02
```

The first column is the slice serial number and the second column is the frequency.

5.4 Visualization of extreme orbital sections

5.4.1 Visualization

If you import the standard output file ***results_orbitoutlines_invau.out*** or ***results_orbitoutlines_invAng.out*** calculated by the software, and click on the corresponding frequency in the ***Calculation results selection area***, the cross-section shape will be displayed in the ***Orbit outline***, the figure shows as follows:

5.4.2 Save data format

Click ***Save Data*** and select the save location to get the saved data file, which can be used for further plotting. The file is in csv format, named Orb_XXX.csv, where XXX is the frequency, and the contents of the file are shown below.

```
## Orbit data file generated by Skeaf_demo
## Freq 1.2181
## x,y

4.478030812557851070e-02,-1.977014914729296191e-01
4.601291321735462292e-02,-1.975747795017281372e-01
4.724302376840115725e-02,-1.974227912512758476e-01
...
4.231055732239641376e-02,-1.978827922299140618e-01
4.354607360540842936e-02,-1.978038915525861530e-01
4.478030812557849683e-02,-1.977014914729296469e-01
```

5.5 Mode

There are two modes, ***Simple*** and ***Separate***, and you can only choose one of them. ***Simple*** is a simple display mode, ***Separate*** is a mode based on ***dbscan*** algorithm to classify the closed area in Fermi surface, which can be used to display the pocket where the orbit of a specific frequency is located, with stronger visibility, generally applicable to the case where the Fermi surface contains multiple pockets.

5.6 Interpol ratio

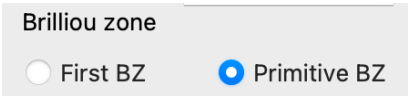
Interpolation accuracy function, the default is 1.0, it is recommended to input a number between 0.5 and 2.0 for adjustment, after inputting, press the keyboard ***Enter*** key, the Fermi surface will be recalculated and visualized, it will load for a period of time.

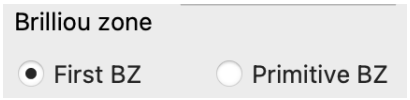
5.7 fermi energy

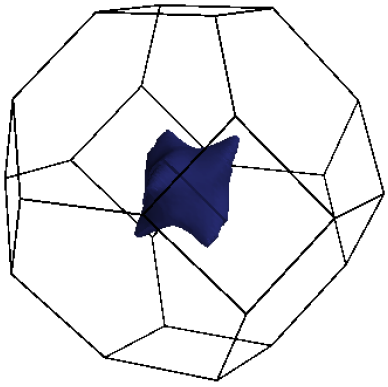
Fermi energy input, can be modified. After reading the ***bxsf*** file, it will automatically fill the ***fermi energy*** of the ***bxsf*** file,. and if you use the ***trait*** function, it will fill the fermi energy of the ***skeaf*** program calculation in priority. Please click **Update** to update after each modification.

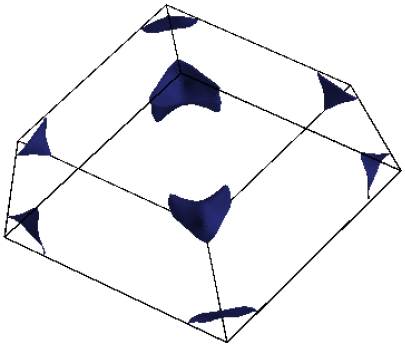
5.8 Brilliou Zone

Brillouin Zone mode is divided into ***First BZ*** (First Brillouin Zone) and ***Primitive BZ*** (Primary BZ) display mode, you can choose one of the two, as shown in the following figure.



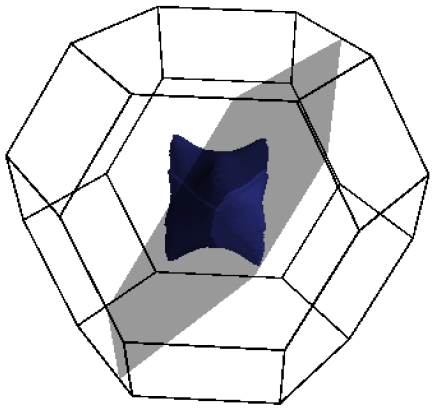






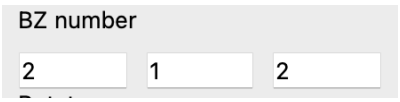
5.9 Show slice

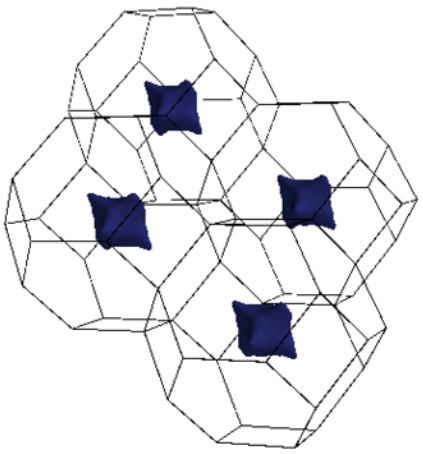
Turn on the ***Show Slice*** function, which is only useful when turning on ***trait*** function, opening the sync function of the ***Slice*** window or entering ***section-v***. The checkbox is pre-selected for the function and is implemented as shown in the following figure.



5.10 BZ number

Expand cell, you can enter the number of expanded cells in three directions and click ***Update*** for display, the loading time will become longer, as shown in the following figure.



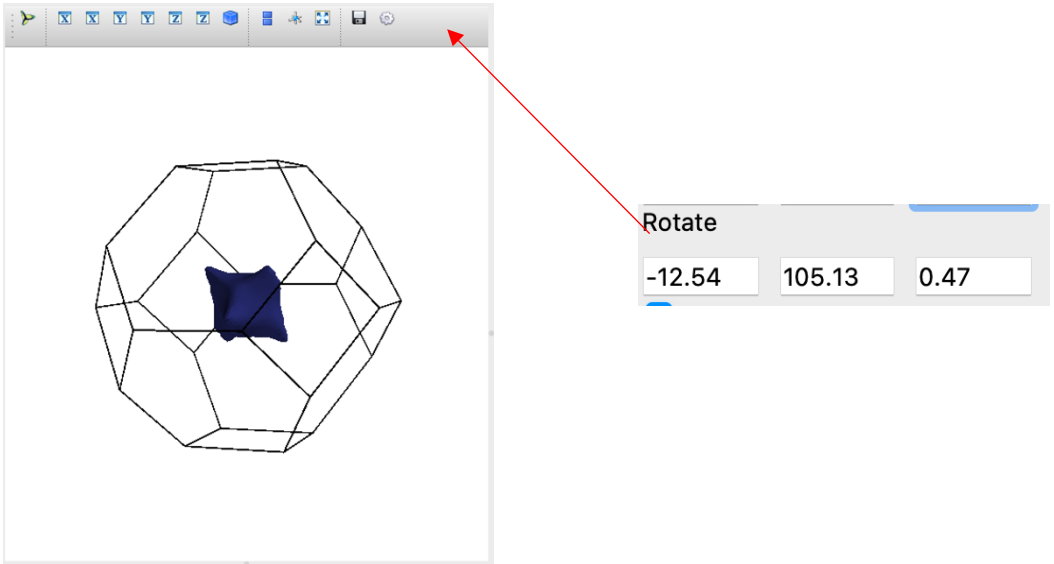


This function can be used with all other functions.

5.11 Rotate

5.11.1 Get current camera location

Display the current visualization camera location, which is convenient to unify the perspective and size of the picture. If you need to get the current camera location obtained after mouse dragging, you can click on the blank area of the visualization area toolbar (other blank areas are not available), and the three blank cells of Rotate will be filled with three numbers. The operation is shown in the figure.



5.11.2 Update camera location

Enter the camera location in ***Rotate***, the visualization area will be updated.

5.12 Line

Check whether to display the Fermi surface boundary line

5.13 Line color

Select the Fermi surface border line color, the default is black.

5.14 Line width

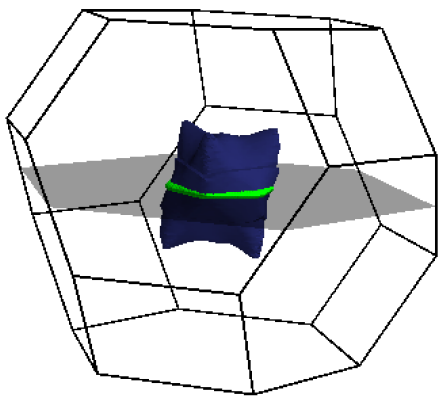
Select the Fermi surface boundary line thickness, the default is 1.0.

5.15 Inner-outer

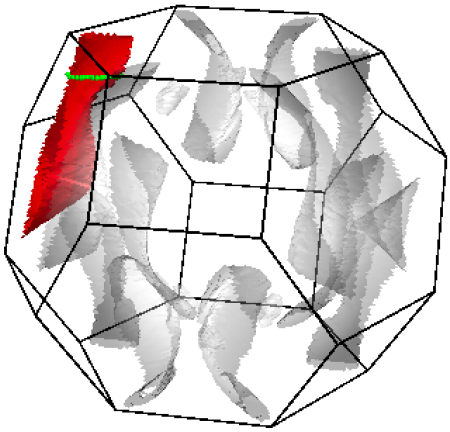
The function distinguishes between the inner and outer part of Fermi surface, which can be selected by ***Inner color*** and ***Outer color***. It is worth noting that the inner and outer surfaces are defined by Fermi energy and less than Fermi energy 0.0001 *Ryd*. Therefore, for the electron type Fermi surface, the outer surface is outer while for the hole type Fermi surface, the outer surface is inner.

5.16 Trait

If the standard output file ***results_orbitoutlines_invau.out*** or ***results_orbitoutlines_invAng.out*** file of ***skeaf*** calculation is imported, the ***Trait*** can be opened and displayed in the visualization area by clicking to select the frequency in the combo box. Adjust the thickness of the track display by ***Trait width***, color by ***Trait color***. And if ***Show slice*** is checked, it will display the cross section of the track in the visualization area, as shown below.



If the ***mode*** is ***Separate***, the corresponding pocket where the trait is located will be displayed, as shown below



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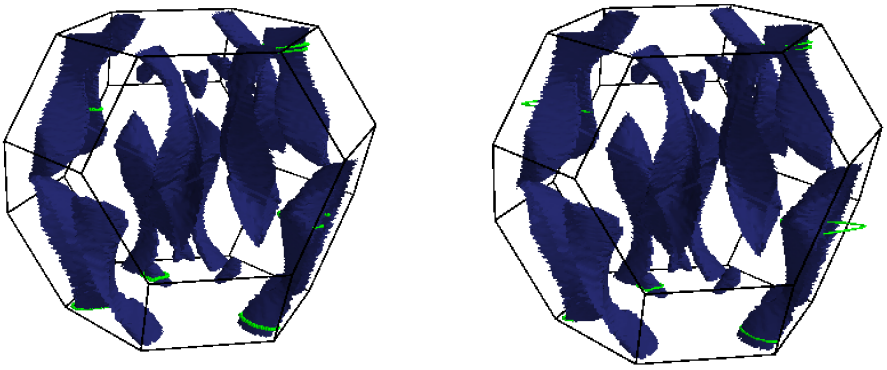
5.17 Full trait

Since not all Fermi surfaces form closed surfaces in the first Brillouin zone, i.e. the orbits are not all in the first Brillouin zone, checking ***Full trait*** will show the full shape of the orbits (including the cases that are not in the first Brillouin zone), as shown below (unchecked on the left, checked on the right).

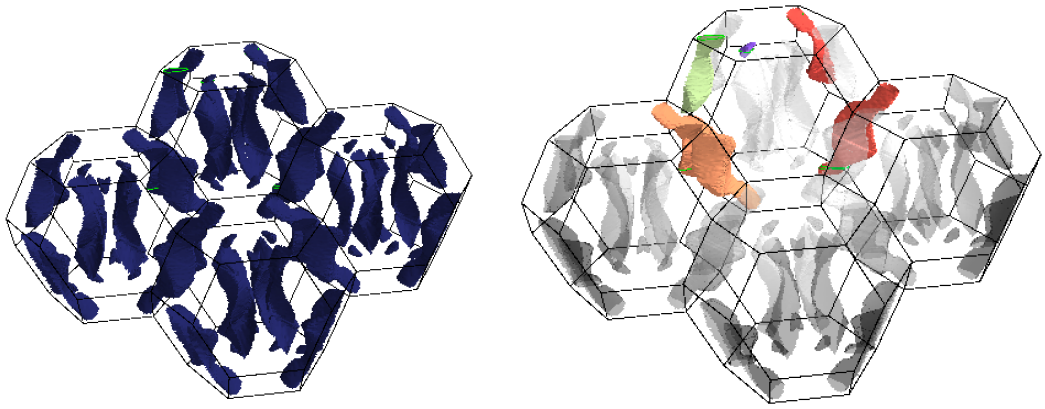


5.18 Axes

Show axis, default is not shown.

5.19 Full fs full trait

If you want to observe the complete shape of the orbit in the complete Fermi surface at once, you can check this option, which will be loaded for some time after checking, and eventually the program will automatically expand the cell to select the optimal display, as shown in the following figure.



5.20 More

Click **...** next to ***Full fs full trait*** to display more adjustment parameters, including:

5.20.1 FS Opacity

The opacity of the Fermi surface in Simple mode, which defaults to 1.0 (opaque), can be adjusted by adjusting the slider or by entering a decimal number from 0 to 1.

5.20.2 Line Opacity

The opacity of the borderline, also defaulted to 1.0, can be adjusted by adjusting the slider or by entering a decimal number from 0 to 1.

5.20.3 Trait Opacity

The opacity of the trait line, also defaulted to 1.0, can be adjusted by adjusting the slider or by entering a decimal number from 0 to 1.

5.20.4 Slice Opacity

The opacity of the slice, defaulted to 0.4, can be adjusted by adjusting the slider or by entering a decimal number from 0 to 1.

5.20.5 Background Color

Adjusts the background color of the visualization area.

5.20.6 Slice Color

Adjust the color of the slice.

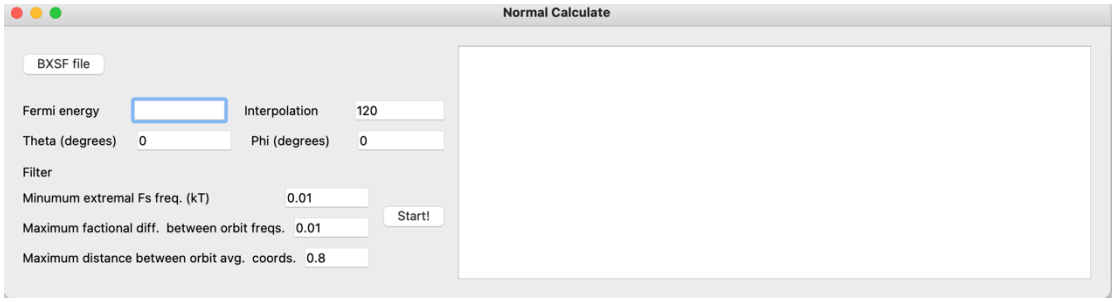
5.20.7 Magnetic Field

Display the direction of the magnetic field, which position is random, so it is only used for testing or verification purposes.

5.21 Calculation

5.21.1 Normal Calculation

Click ***Calc*** -> ***Normal Calculation*** -> ***Setting parameters*** in the menu bar, the following window will pop up:



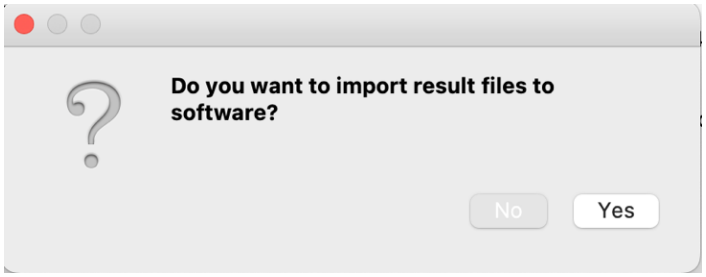
The left side is the parameter setting area, and the right side is the calculation process display. Steps:

1) Click the ***BXSF file*** and select the calculated Fermi surface file, noting that the length unit is *Bohr* and the energy unit is *Ryd*, and it contains only one energy band;
2) Confirm the ***Fermi energy***, generally the Fermi energy in the BXSF file will be filled automatically after importing the BXSF file, or you can modify it by yourself;
3) Enter ***Interpolation***, which defaults to 120 and does not exceed 150;
4) Enter ***Theta*** and ***Phi***, two parameters that can be determined through the ***B direction*** window, which defines the direction of the magnetic field;
5) Enter the first parameter in the ***Filter***, representing at most how much of the gap between the poles is considered to be the same polar orbit, with a default of 0.01kT.;
6) Enter the second parameter in ***Filter***, which represents the maximum difference in frequency between two orbits when they are considered to be the same orbit, default is 0.01 (percentage);
7) Enter the third parameter in the ***Filter***, which represents the most difference between the coordinates of two orbits between adjacent slices to be considered as the same orbit, the default is 0.8;
8) Click ***Start!*** button to start the calculation, it will load for a while.

It is worth noting that all error reports with wrong file formats are displayed in the right window, please check and modify the files/parameters according to the prompts in the right window.

5.21.2 Importing calculation results

When the calculation is finished successfully, the following dialog box will pop up:



Ask whether to import the calculation results, clicking ***Yes*** will import the results into the analysis software, ***No*** will not import, the import process will load for a period of time as well. It is best to observe in advance whether the calculation results are reasonable, the number of output orbits is reasonable, and then choose to import, otherwise the program will easily crash and exit.

5.21.3 Save calculation results

Click ***Calc*** -> ***Save results*** to save the latest result files, so please make sure to save the files first after each calculation.

5.22 Group velocity

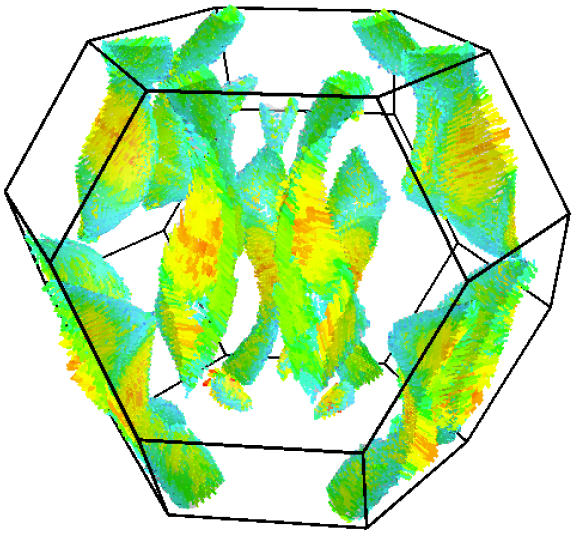
If the Fermi surface file has been imported, this function can be activated.

5.22.1 Calculate group velocity

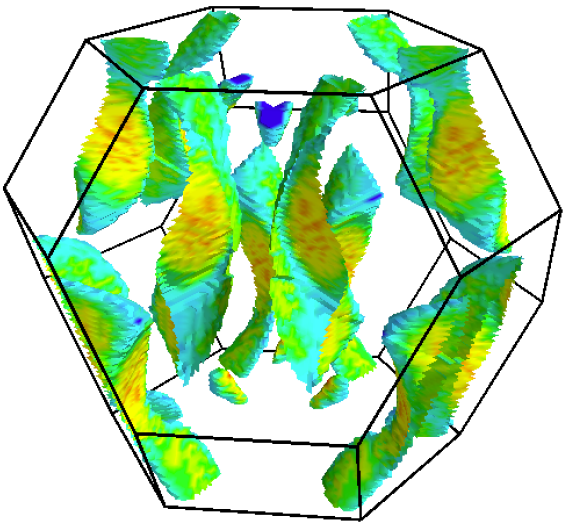
Click the menu bar ***View*** -> ***Group Velocity*** -> ***calculate*** and the software will calculate the group velocity of the current Fermi surface. Before displaying the group velocity, please make sure it has been calculate, if there are other bugs, you can reset the calculation by calculate again.

5.22.2 Display group velocity

Clicking ***View*** -> ***Group Velocity*** -> ***vector*** shows the vector pattern for the group velocity, as shown in the figure:

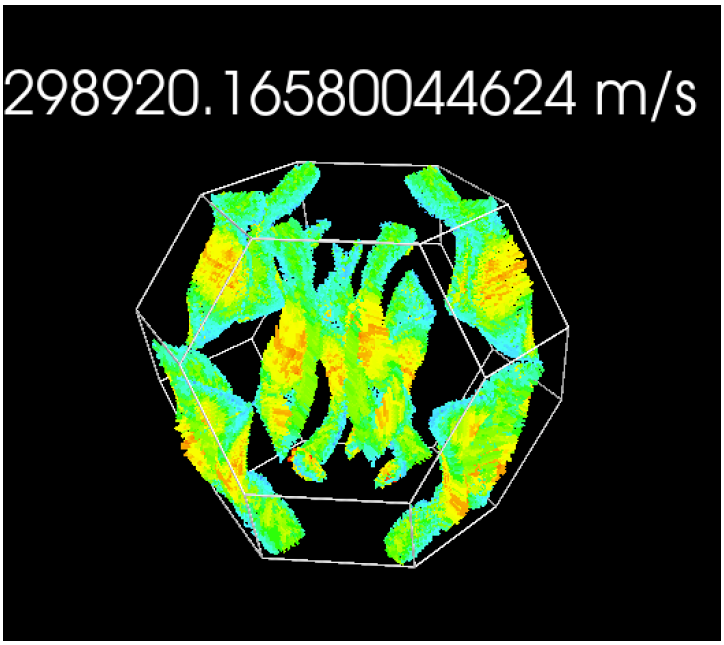


Clicking ***View*** -> ***Group Velocity*** -> ***mag*** shows the scalar mode for the group velocity, as shown in the figure:



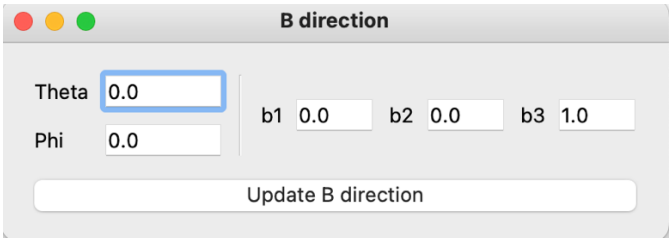
Both modes can be displayed simultaneously.

Click ***View*** -> ***Group Velocity*** -> ***avg***, it will show the average group velocity, but there is a problem with the calculation accuracy, the order of magnitude is basically accurate. The color is white, please set the background color to black for reading (it is also recommended to set it to black, because it is better to identify group velocity under black background), as shown in the following figure:

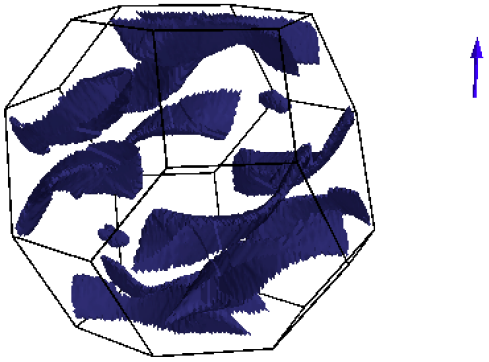


5.23 Magnetic field

Click on the menu bar ***View*** -> ***B direction***, the following screen will appear:



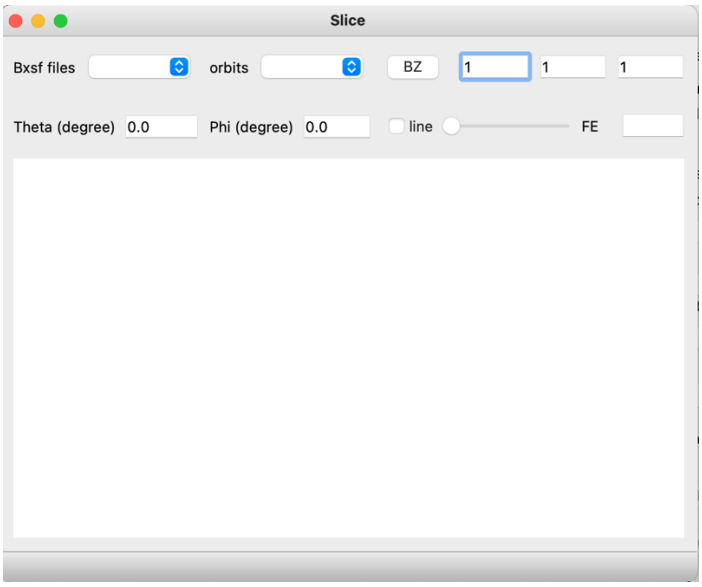
The magnetic field direction is determined by setting ***Theta*** (the angle between the projection of the magnetic field direction to the *xy* plane and the *x*-axis in degrees), ***Phi*** (the angle between the magnetic field direction and the *z*-axis in degrees), or the sum of the multiples of b1, b2 and b3 corresponding to the base vector. After setting, click ***Update B direction*** to see the blue arrow representing the set magnetic field direction in the visualization area, as shown in the figure:



The blue arrow will also disappear after closing the window.

5.24 Slice

Click the menu bar ***More*** -> ***Slice***, the following window will pop up:



This window is a separate window and can be used separately from the main window when running.

5.24.1 Import Fermi surface files

Click the menu bar ***files*** -> ***import bxsf files***, select the fermi surface to import, you can choose to import multiple fermi surface files multiple times.

5.24.2 Import orbit files

If you want to import the orbits calculated by XX Fermi surface after importing XX Fermi surface, you need to import the orbits file after performing 5.24.1, and then select another Fermi surface to import, so that the exact Fermi surface number corresponding to the track will appear in brackets in the orbits window.

5.24.3 Bxsf files

This is a multi-select combo box, pull down to select the Fermi surface to display.

5.24.4 orbits

This is a radio combo box that selects the case where the corresponding orbit is displayed in the slice.

5.24.5 BZ

Expand cell, please click ***BZ*** button to update after expanding cell, otherwise the expansion will not work.

5.24.6 Theta

Set the ***Theta*** of the magnetic field direction, which is automatically filled if the orbit file is entered. It can be modified later.

5.24.7 Phi

Set the ***Phi*** of the magnetic field direction, which is automatically filled if the orbit file is entered. It can be modified later.

5.24.8 line

Check to display the border.

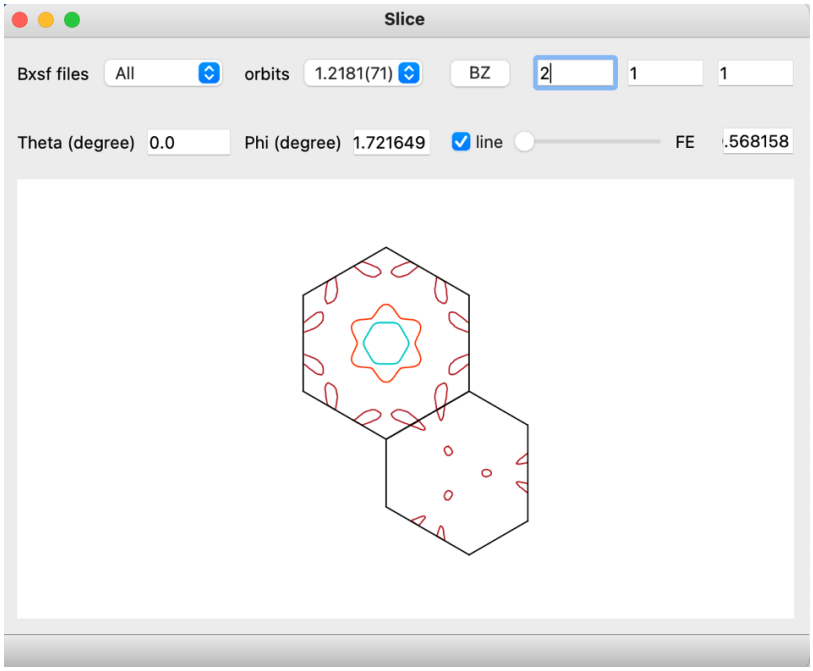
5.24.9 FE

Fermi energy, if you enter a Fermi surface file it will be filled automatically and can be modified later.

5.24.10 Slider

Slider can be used to display the cross section along the magnetic field direction from the bottom to the top (with orbits selection only one can be activated for use).

After the setup is completed the display will look like this:



5.24.11 Simultaneous display of section positions

Click the menu bar ***More*** -> ***sync***, it will show the specific location of the current section in 3D space. Before using this function, please make sure the Fermi surface of the main window and the slice window are the same (or at least one is the same), as shown in the figure.