

dHvA

Klaus Koepernik

July 4, 2022

We will walk you through a basic setup of a dHvA calculation. The module is discussed in depth in a section of FPL022.00-62/DOC/MANUAL/doc.pdf.

The solutions are to be found in the `solution` directory and you will work in `task`.

dHvA has two stages. The first calculates the Fermi surface and the second calculates the dHvA spectrum. The first stage saves the data in the file `+isoergcache`. This cache file is designed for re-use. If you want to increase the accuracy of the Fermi surface you can change the settings accordingly and simply re-run `fplo`. It will read the cache data and only calculates data, which are not yet present in the file. Consequently, a fresh calculation would require to delete this file. Consult `doc.pdf` for more details as mentioned above.

- Go into the directory `task`.
- Let's start by setting up stage one: the creation of the Fermi surface. Open `fedit` and go to the `dHvA` submenu (hotkeys `space d`). Switch on `Iso Surface Run`, set `initial subdivision` to `6,,` and leave `bisections` at zero. Leave the submenu and `Quit/Save` `fedit`.
- Run

```
fplo22.00-62-x86_64 | tee out
```

- Have a look at the relevant output

```
grep ISO: out|less
```

In contrast to other modules this module determines the Fermi surface in a adaptive way. It will find a minimal reciprocal cell which is printed after

```
ISO: Reciprocal iso cell vectors/(2*pi):
```

subdivide it according to `subdivision` in the `fedit` submenu and prints a suggestion, which subdivision ratios are optimal in the line

```
ISO: Most homogenous initial subdivision would be: 6 6 5 or multiples of these.
```

On this initial grid all cells containing the Fermi surface will be determined. This means that very tiny parts might be missed if the `subdivision` is too course. (If in doubt use `xfpo` to get an idea which sheets must exist.)

After this initial step the resulting non-empty cells will be subdivided into 8 equal parts of which again the cells which contain the Fermi surface will be registered. These subdivision steps are repeated up to `bisection` times (zero means no bisection at all — just the original mesh is used). At the end we have a set of cells, which finely wraps around the Fermi surfaces. The resulting Fermi surfaces are extracted sheet-wise (sheet = band number) and part-wise (disconnected sheets) and written to files called e.g. `+iso_b00011_p0001_spin1` (b=band number, p=part number).

- Check the files

```
ls -l +iso_*
```

You will find one part of band number 11 and 6 parts of band number 12. (That there are 6 parts is an artifact of the low resolution, which results in disconnected parts).

- Let's visualize the result

```
xfplo -raw +iso_* # the underscore matters!
```

Use **Ctrl-R** **r** to re-scale the scene and **left click + mouse move** to rotated the picture.

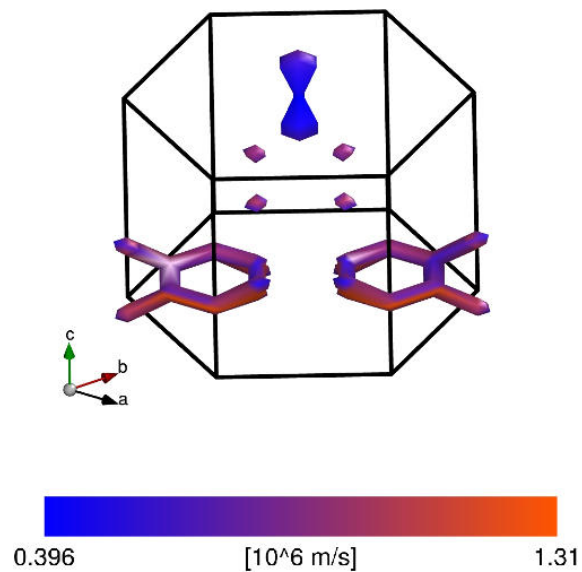


Figure 1: The first approximation of the Fermi surfaces.

Later you will find that the little blobs in Fig. 1 belong to the two ring-like sheets.

- Note, the size of +isoergcache

```
ls -lh +isoergcache
```

It has 328KB.

- Open fedit and in the **dHvA** submenu increase the **bisection** to 2 and **quit/save** fedit.
- Re-run fplo

```
fplo22.00-62-x86_64 | tee out
```

- and visualize

```
xfplo -raw +iso_* # the underscore matters!
```

to get Fig. 2

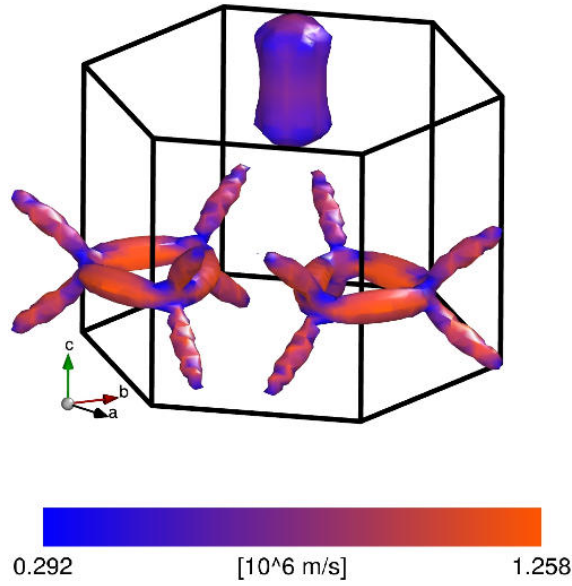


Figure 2: The two-bisections approximation of the Fermi surfaces.

We still have 6 parts of sheet 12. If you type

```
ls -lh +iso* # no underscore
```

you will find out that `+isoergcache` now has 7MB and that all but part 1 and 2 are very smaller. Let's load an isolated part

```
xfplo -raw +iso_b00012_p0003_spin1
```

You will not see much: this tiny part is a little spec at the end of the arms of the ring like sheets, which got separated due to the finite resolution. It is basically un-important.

Our approximation is still not very good, but for teaching purpose let's continue to the second stage: the dHvA spectrum.

- Open `fedit` and in the `dHvA` submenu put the `Number of fields` to 4. Edit the fields to look like this

No.	Label	field
(1)	: [0001]	: 0 0 1
(2)	: [10-10]	: 1 0 0
(3)	: [11-20]	: 0.866025403784 0.5 0
(4)	: [001]	: 0. 0. 1.

Set `Parts` (hotkey `t`) to 1. This will ignore all but the first part of each sheet. This makes sense since band 12 has two symmetry related parts and sheet 11 has only one part. Note, that the number and the numbering of parts can change depending in the value for `bisections`. Hence, it is always a good idea to check the `+iso_*` files.

- Now, run

```
fdhva22.00-62-x86_64
```

When done, have a look at the files created:

```
ls -ltr
```

We have a `dHvAdata` directory, `+area` and `+mass` files for parts 1 of both sheets and an xfbp script `area_vs_angle.cmd` which we will use now

```
xfbfp area_vs_angle.cmd
```

Open the `Edit > World > properties` dialog and set `Y-max` to 1000.

You see Fig. 3. It is quite a mess.

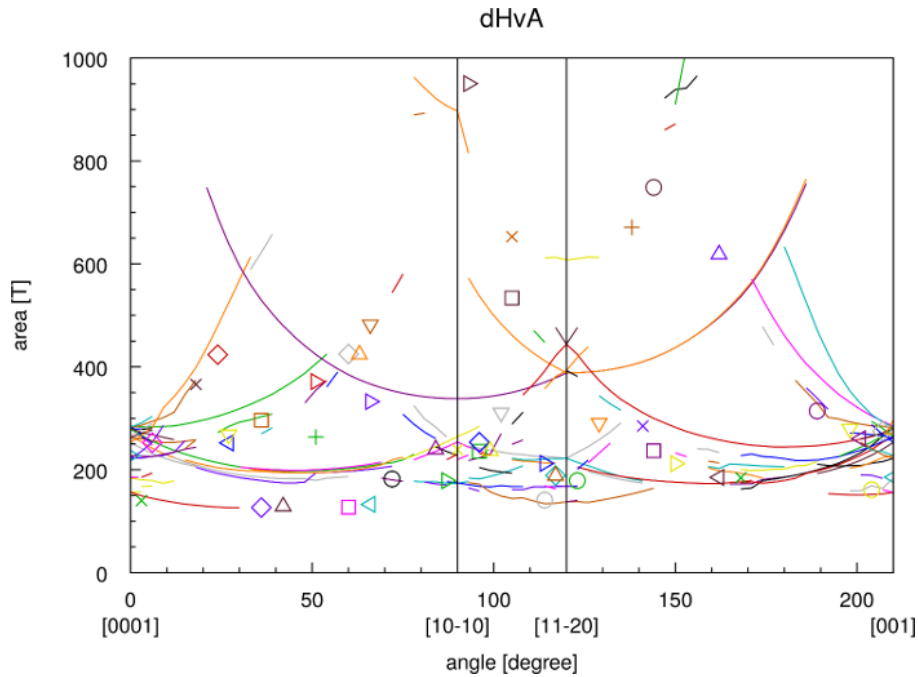


Figure 3: Our first dHvA spectrum.

We will not explain the details of the algorithm here. For this we strongly encourage to read the dHvA section in `doc.pdf`. We will however increase the accuracy.

- In the `dHvA` submenu of `fedit` change the `angle subdiv` to 60 and the `No of planes` to 200.
- Re-run

```
fdhva22.00-62-x86_64
```

Have a look at the result

```
xfbfp area_vs_angle.cmd
```

It is a bit better in that there are more lines and less isolated symbols. However, there seem to be doublings of lines.

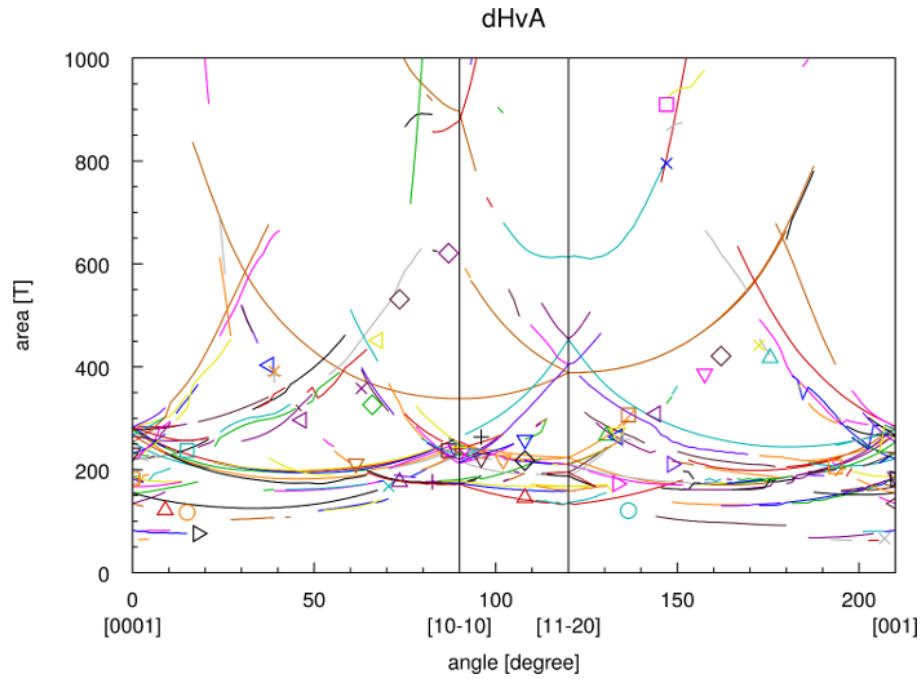


Figure 4: A better dHvA spectrum.

We cannot do much better here, since most of the trouble comes from the crude Fermi surface Fig. 2.

- Open fedit and in the dHvA submenu increase the bisection to 4 and quit/save fedit.
- Re-run fplo

```
fplo22.00-62-x86_64 | tee out
```

After some time (1min) we can visualize the Fermi surfaces

```
xfplo -raw +iso_*
```

Now that is much better

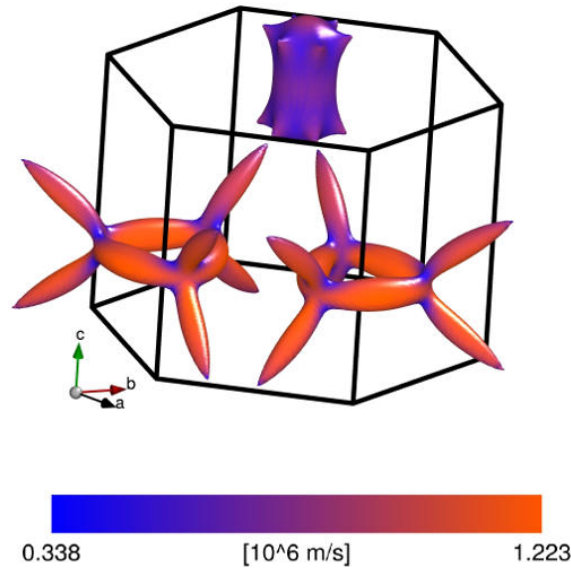


Figure 5: Bisection 4.

- To convince yourself that the cache-file works re-run

```
fplo22.00-62-x86_64 | tee out
```

It basically does not take any time.

- Let's check the files:

```
ls -lh +iso* # no underscore
```

We now have only 3 `+iso_` files: band 11 part 1 and parts 1 and 2 of sheet 12. You will notice that the older `+iso_` files have vanished. This was triggered by the `delete old files` option in the `fedit` submenu. It is for your convenience in order to avoid outdated files from previous runs.

Furthermore, you will notice that the cache has 111MB. The size of the Fermi surface data is growing exponentially with the number of bisections. (Well, who would have thought that 2^n is an exponential. But seriously, keep this in mind. At any state, the next higher bisection could flood all your RAM and make the system swap.)

We approximate from our three calculations that the size grows as $\text{mem} = 0.3 \cdot 4.8^n$, which gives 760 MB for bisection 5. Indeed we get 440MB, so the estimate is rough. Moreover, the cache data is not all. The RAM actually used for bisection 5 was 700MB. So, be cautious.

The intel MKL library has a bug on some machines, which makes the memory grow. If you see such behaviour compile without it.

- Let's proceed to the dHvA spectrum. Re-run

```
fdhva22.00-62-x86_64
```

When done have a look at the result

```
xfbp area_vs_angle.cmd
```

This is the best we can show in such a tutorial. We could increase the bisections to 6 to obtain the results shown in `doc.pdf`.

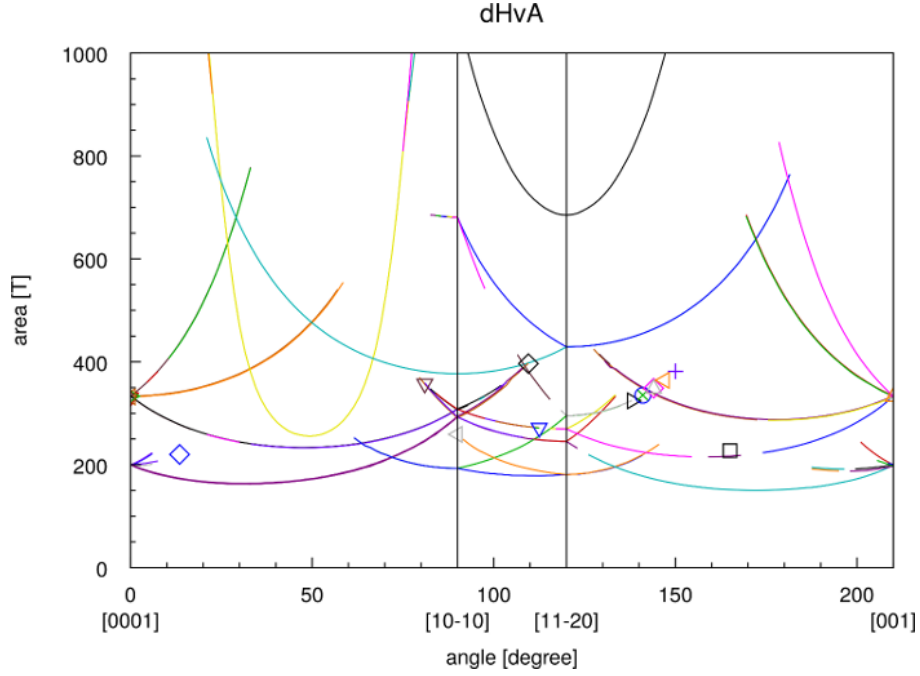
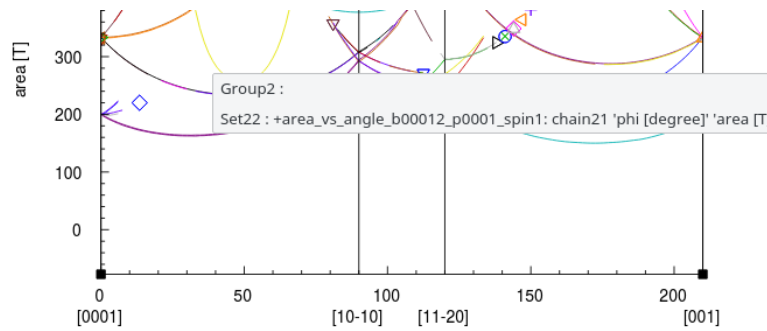


Figure 6: Our final result for this tutorial.

- Finally, we will display the extremal orbits. Execute

```
xfbp area_vs_angle.cmd
```

- Set the **world ymax** to 1000. In the viewport **right click** close to the yellow parabolic curve (bottom 250T, angle at minimum 50) to get this



It tells you that this curve belongs to sheet 12 part 1 chain21.

We use this information to load the extremal orbits belonging to this curve.

- Execute the following command. Hint: use tab-completion to avoid typing.

```
xfplo -raw +iso_b00012_p0001_spin1 dHvAdata/b00012_p0001_spin1/extrorbit_chain00021_*
```

We changed the color of the sheet to get this picture

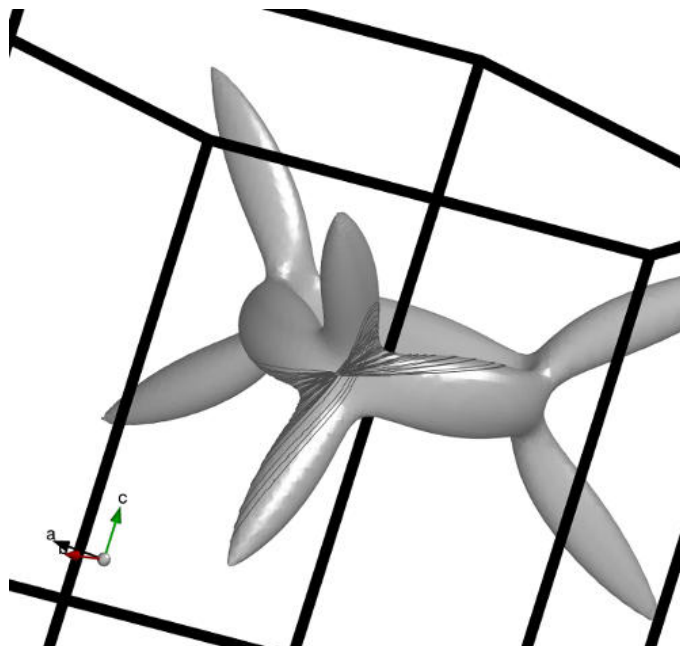


Figure 7: Extremal orbits of chain 21

Of course there are more files like this. In a real application you might be interested to check them out.

- As a final exercise we load

```
xfplo +iso_* # without the raw option
```

which loads the sheets and backfolds them into the boundary. We changed the boundary a bit to obtain this final picture.

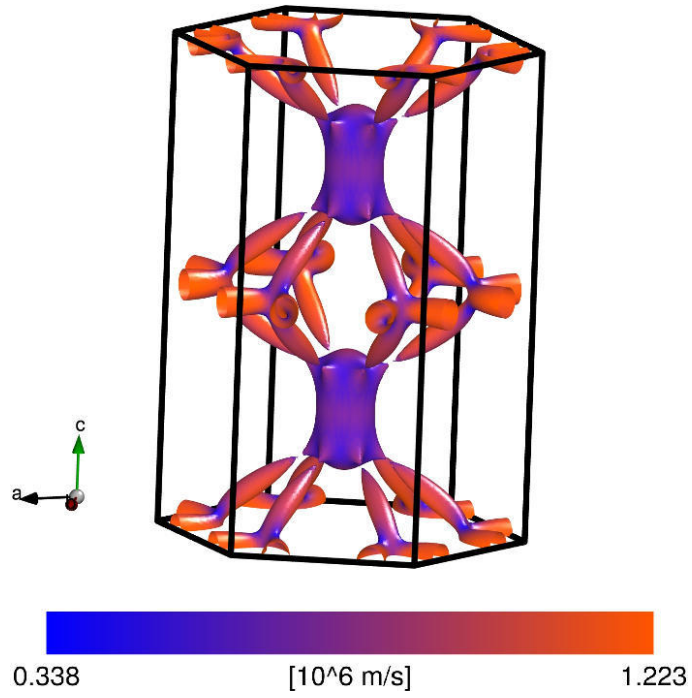


Figure 8: The ZrFe₂ tree.

A remark on file sizes. It is possible to reduce the size of the cache file by using the following options in the `bandplot` submenu: set `Lower energy bound` and `Upper energy bound` and switch on `Restrict bands to window`.