

FieldOptic



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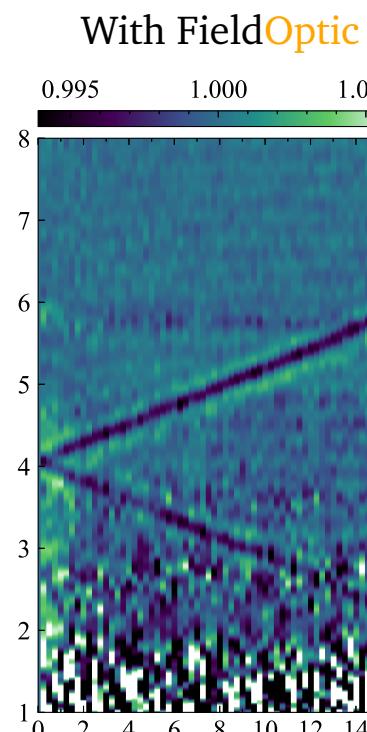
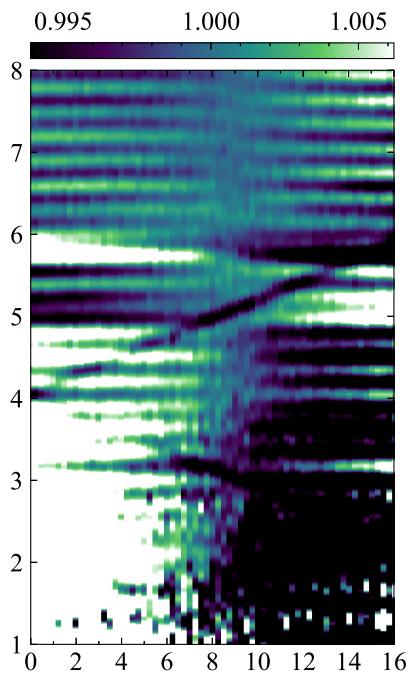
I | Introduction

I.1 Preface

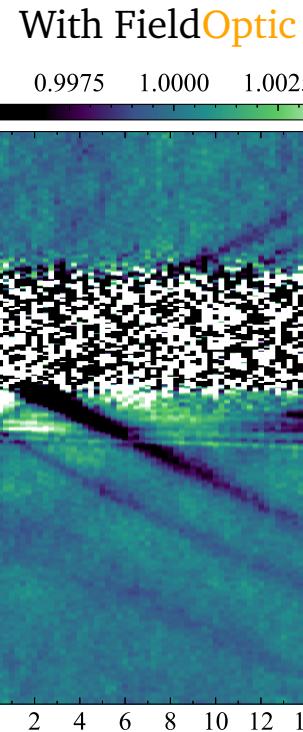
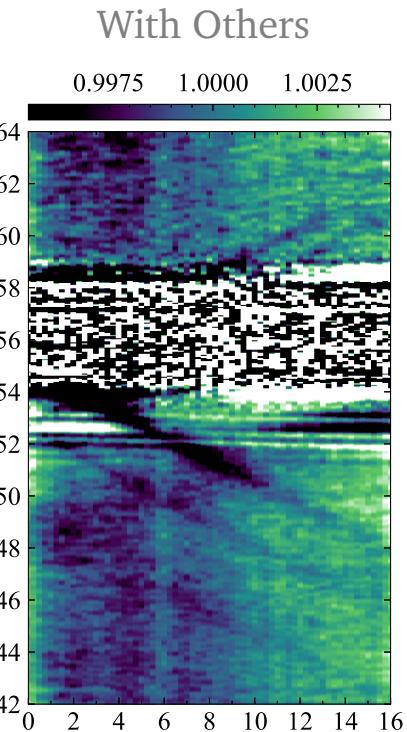
FieldOptic was designed to assist condensed matter physicists in plotting and manipulating data, primarily from magneto-optical measurements, and has the potential to extend its utility to other disciplines involving two-dimensional mapping. It serves as an intuitive platform for interacting with stack plots and provides precise control over 2-dimensional maps. The software introduces innovative approaches to background subtraction, offering a novel method for noise cancellation to maximize measurement signal quality. Currently, FieldOptic functions as a data-processing software with key modeling capabilities. Future updates may expand its features to include more sophisticated data analysis.

FieldOptic is the culmination of 2-3 years of simultaneous effort during my former Ph.D. study and my current first Postdoc. I owe a debt of gratitude to those who made this work possible. Special thanks to Bing Xu and Premysl Marsik for introducing me to Qt Designer. Jan Wyzula deserves acknowledgement for sharing the PyQt Graph package and providing a valuable starting point with his software. I am grateful to David Santos Cottin and Ivan Mohelsk'y for their numerous ideas that have contributed to enhancing the software. Lastly, a big thank you to Seul-Ki Bac for designing all the logos incorporated into this software.

I.2 Highlight With Others



(a) Noise Cancelling From the Measurements



(b) Noise Cancelling From the Reference

Figure I.1: Different map pictures at the loading stage and after some data processing (part 1).

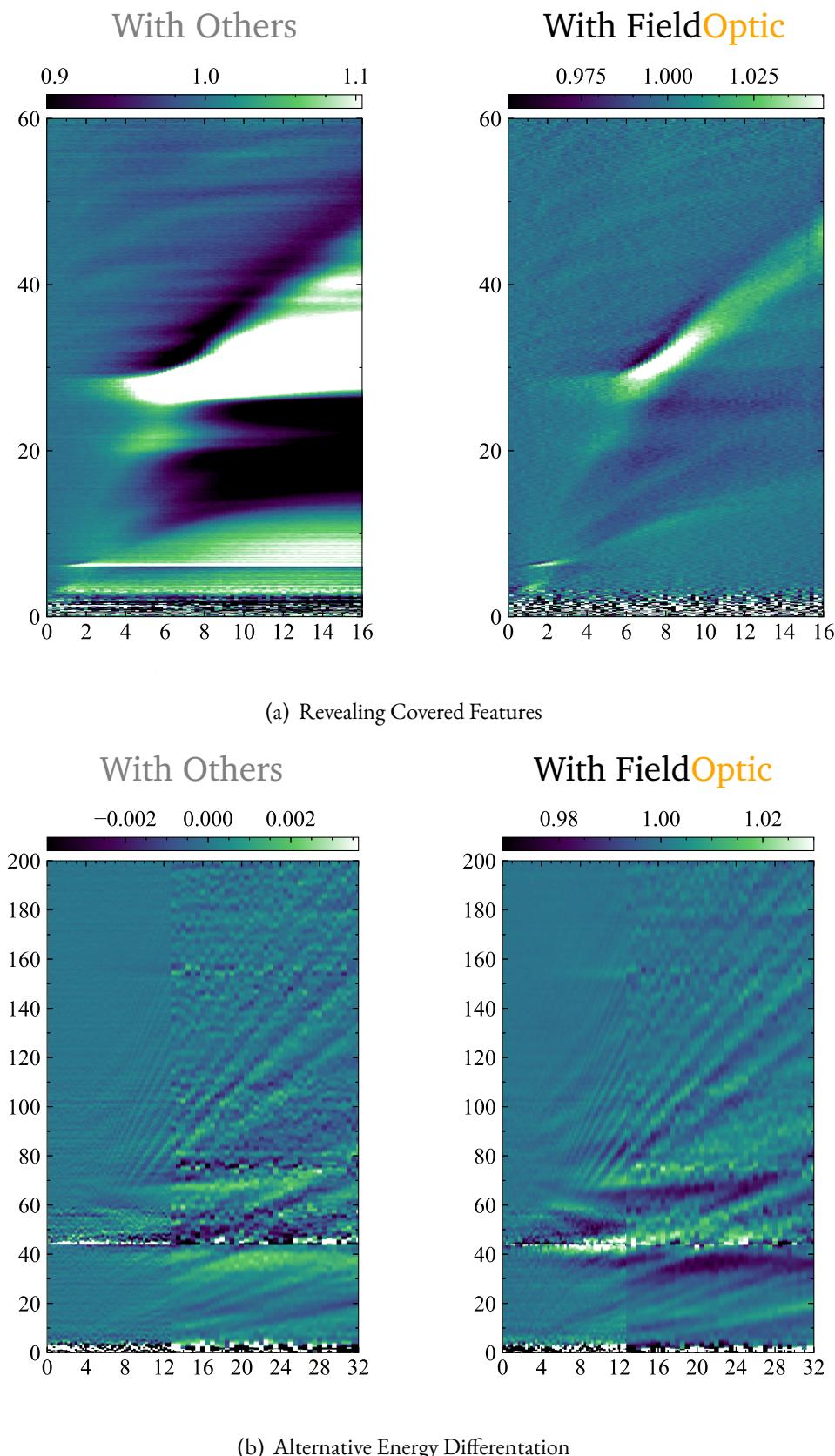


Figure I.2: Different map pictures at the loading stage and after some data processing (part 2).

I.3 Credits

This software was built and designed via Python thanks to amazing packages:

- PyQt5 [1].
- Qt designer [2].
- PyQtGraph [3].
- SciencePlots [4].
- PyInstaller [5].

I.4 Getting help

If you find any bugs or have questions on FieldOptic software or even manual, you can contact me via:

fieldoptic.hmf@gmail.com.

You are encouraged to propose any enhancements, potential expansion of the dataset, or additional fitting methods for FieldOptic. I would gladly incorporate valuable suggestions into the current version if they prove beneficial to a broader audience. Specific requests can also be discussed for further consideration. Your input is highly appreciated!

II | Importing data

This section is dedicated to loading data into the software. It's important to note that the software exclusively operates with equal spacing on both the x and y-axes. Thus, for optimal usage, it is recommended to establish a regular step during measurements, even in test scenarios. For illustrative purposes, a sample data set is included in the download folder of the executable.

Originally tailored for magneto-optical data, the provided data will consist of optical spectra in energy at varying magnetic fields.

II.1 Overview



Figure II.1: Main window

Before delving into the software's usage, a brief overview of the main window can provide a useful glimpse of its core mechanics (see Fig. II.1). The main window is segmented into various parts, each delineated by distinct color rectangles.

Let's be slightly explicit and give an overview of this different part:

- *Importing data:*

This section occupies the top left and center bottom of the main window, serving as the primary data-loading interface. The data must follow a two-column format, with the first column representing energy (in reverse centimeters), and the second column capturing the optical response.

- *Data table:*

Located at the bottom left of the main window, this section functions as a repository for storing data matrices in the form of items, providing a platform for later interaction. Additionally, you can utilize this area for basic modeling and point-picking on your data.

- *Graph:*

In the center of the main window, a series of four graphs is arranged as a tab window, enabling you to visualize the data. There are two visualization options: the first is the **[Stack]** tab, presenting the raw plot of curves with a defined offset. The second visualization involves color maps. The **[Fan Chart]** tab displays the color map of your data from the **[Stack]** tab. In the **[Derivative E]** tab, a color map of the energy derivative of the data is shown. Lastly, in the **[Derivative B]** tab, the field derivative of the data is presented.

- *Command Buttons:*

On the right side of the main window, a set of **[Command Buttons]** is arranged in the form of icon buttons. These buttons represent functions for interacting with the data, graphs, and other functionalities. A more detailed explanation of each button's function will be provided later.

- *Unit:*

An essential feature includes a straightforward **[Unit Converter]** interactive tool, serving as a secondary means for a secondary way of uploading data.

- *Project:*

At the bottom left, a set of three buttons **[Load]**, **[Save]**, and **[New]** projects are positioned. These buttons enable you to preserve the states of your data manipulation for future interactions.

II.2 Main Loading - Auto load on

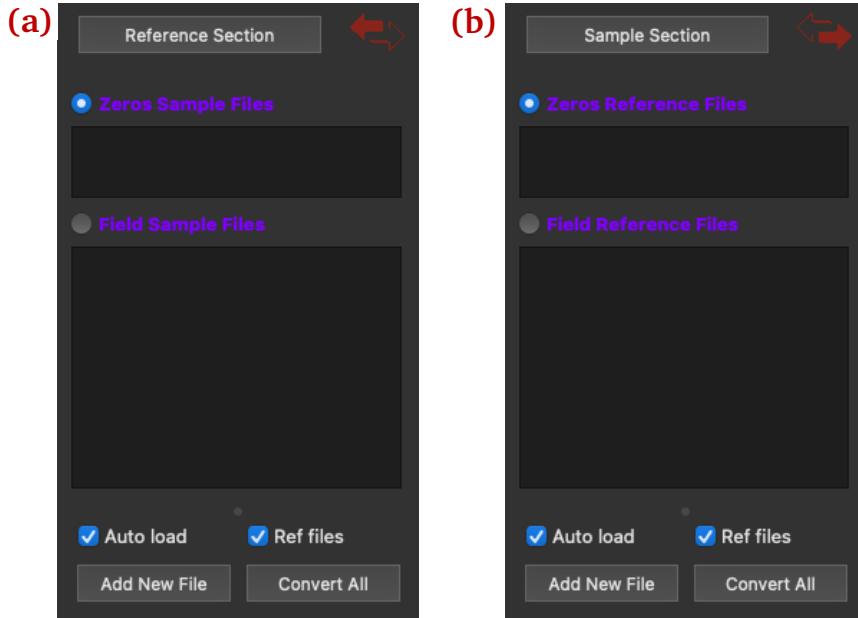


Figure II.2: Loading sections for sample and reference data

To understand the loading process, let's consider an example together. In the "PracticeData" folder, locate the "TIBiSeS" folder, which contains two subfolders named "Transmission" and "Reflection" representing the two possible configurations in magneto-optic measurements.

Let's begin with the transmission case. Open the "Transmission" folder, and within it, find two subfolders labeled "FIR" and "MIR," representing different energy ranges. Start with the "FIR" case. Inside this folder, you'll see "Reference" and "Sample" folders. In the case of transmission, measuring a reference is essential to account for the field dependence of the detector response, hence the "Reference" folder. Begin by opening the "Sample" folder.

Inside, you'll find a set of "txt" files with specific names. The specific naming, particularly the end part, plays a crucial role in the software, simplifying the data loading process. It's highly recommended to adhere to this naming convention for your own data. If your data follows this naming format, you can keep the software in **[Auto Load]** mode; otherwise, disable it.

In typical magneto-optic measurements, zero-field files are often recorded at the start, possibly in the middle, and likely at the end of the measurements to address and compensate for any drift over time in the zero-field response of the sample. These zero-field files should follow a specific naming convention outlined as follows:

- **For the Zeros:**

(Name)_a00p000T_a00p000T.txt – measured at the beginning
 (Name)_a00p000T_a**p***T.txt – measured after a specific field

while any field measurements will be written as:

- **For the Field:**

(Name)_a**p***T.txt – measured at a certain field

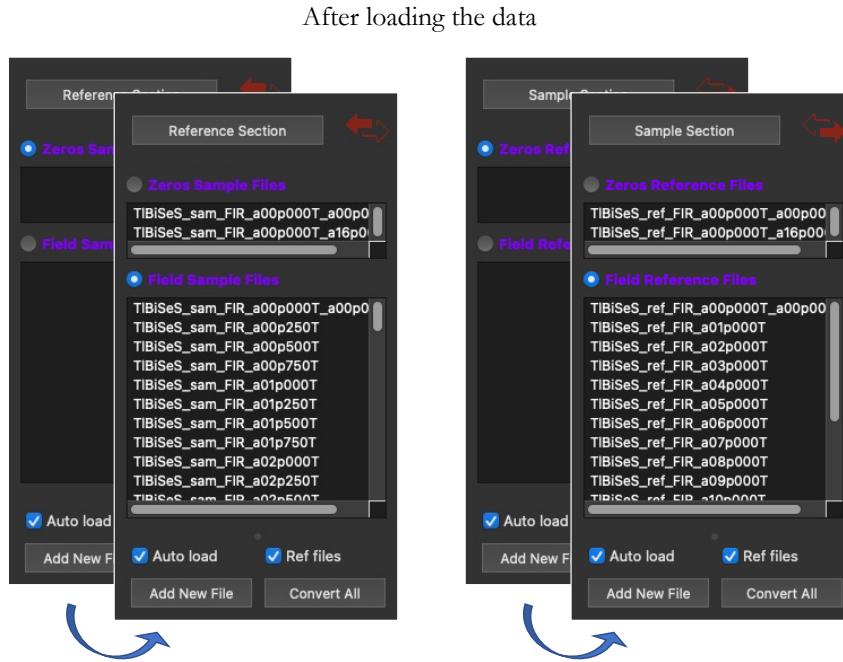


Figure II.3: Loading sections for sample and reference data

Now that the process is hopefully clear, let's proceed with loading the data! The zero-field data mentioned earlier should be loaded into the list named **[Zeros Sample Files]** by clicking on the name (or the small blue circle before it) as shown in Fig. II.3(a). A file dialog will open, allowing you to navigate to the correct folder and select all the zero-field files. Similarly, the field response of the sample should be loaded into the list named **[Field Sample Files]**.

In transmission measurements, there is also a set of reference data that needs to be loaded. Clicking on the button **[Reference Section]** will replace the two previous lists with two others for reference data, namely **[Zeros Reference Files/Field Reference Files]** (see Fig. II.3(b)). The loading process follows the same logic as before. Populate both lists with the reference measurements.

It's worth noting that this reference section can also be used for substrate reference if your sample, for instance, is a layer on top of a substrate. If no reference was measured, this section can remain empty. Additionally, the top button will change its name to **[Sample Section]**, allowing you to revert to the previous lists by clicking on it again.

Now that both sets of data (sample and reference) are loaded, your files should be populated as shown in the image in Fig. II.3. Before clicking on the **[Add New Files]** button, you may have noticed the small checkbox above it in figures II.2 & II.3, labeled **[Auto load]**. If this checkbox is selected, you are in the

main loading with auto-load configuration. If not, some specifications will need to be set beforehand to read these data files.

Finally, you can press the [**Add New Files**] button. A pop-up window should appear, asking for the name of the item that you will create.

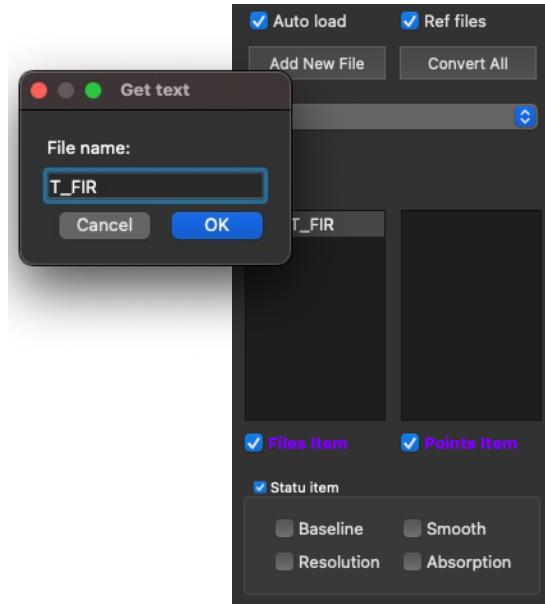
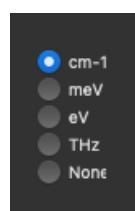


Figure II.4: Get Text

Enter a name, "T_FIR" for transmission in FIR as an example, and press the [**Ok**] button. An item should appear in the list named [**Files Item**]. All data should be plotted in all the graphs of all the different tabs, as mentioned before. If everything went well, your main window should look like this (see Fig. II.5). Now you can repeat this process and add several items that cover different ranges of energy or different ranges of magnetic fields.

The data set in Figure II.5 is plotted in cm^{-1} . This is a good moment for a brief digression on the available units in the software, as it might be useful in the next section. At the right bottom of the main window, you'll find a few circular buttons in the [**Unit Converter**] section, which can be clicked to automatically change the unit of the data.

As discussed in the loading section, the expected units for the data are in cm^{-1} . The software can automatically recognize the unit and convert the data before plotting. However, in case your data is in a unit different from cm^{-1} , you can load them with the radio button [**None**] active. This means that no energy transformation will be applied to the data during loading. If your data still belongs to one of the units supported by the software (cm^{-1} , meV, eV, and THz), you can, after loading in the [**None**] mode, click on the appropriate unit without any energy change. This allows your data to re-enter the software's mechanism and be converted again if needed. Nevertheless, if your data is in nm, you can either operate in [**None**] mode or load them in a CSV manner.



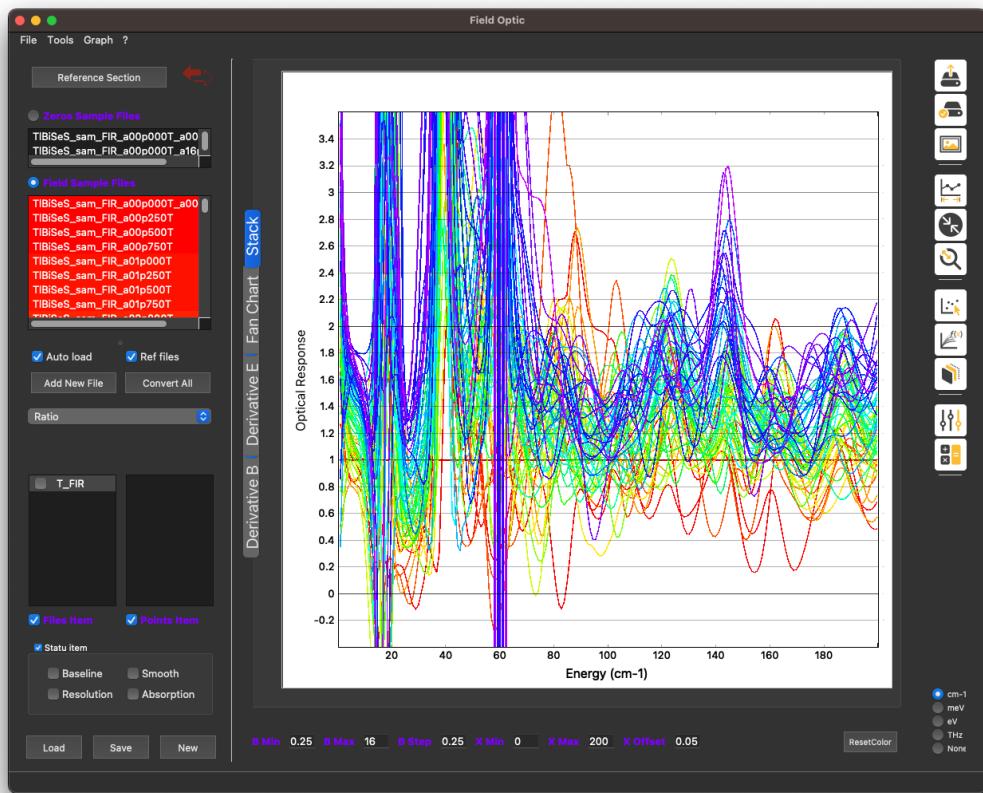


Figure II.5: Main window after loading the FIR data of TlBiSeS. To continue from here click here [III.1](#)

Shape of the files:

As this software was mainly done to visualize infrared spectroscopy in field, the data shape in this loading section has to be in two columns the first one in energy and the second the optical response.

Infrared spectroscopy is made by a Fourier transform spectrometer that is given with a software name OPUS that should save the data in OPUS file format ".0, .1, .2 ..." or in txt, dat or dpt depending on how you define the macro inside. All these file formats are allowed inside the software.

In the case of a repeat measurement, via OPUS, each file of the same field will see an increment on the OPUS format name, measure 1: "name.0", measure 2 "name.1". The software allows you to load all these files at once and to make an automatic averaging on them.

As OPUS measure in reverse centimeter (cm^{-1}) the energy expected during the loading is cm^{-1} .

Zeros interpolation:

One has to be precise about why those names are important. The main way to visualize those data is to plot the ratio of your signal in field over the signal at zero field $S(BT)/S(0T)$. The zero field response $S(0T)$ might vary through time (if the sample slightly moves) hence the need to measure more than one zero throughout the measurement. Therefore, the ratio $S(BT)/S(0T)$ will depend on the zero closest to each measurement in the field. For example, if you measure your sample from 1T to 16T by a step of 1T, with two zero fields made at the beginning and at the end of the measurement. The response at 1T will have to be divided by the zeros made at the beginning

$$\frac{S(BT = 1T)}{S(0T)_{a00p000T}} \quad (\text{II.1a})$$

with $S(0T)_{a00p000T}$ referring to the first zero, while the response at 16T will have to be divided by the zeros made at the end:

$$\frac{S(BT = 16T)}{S(0T)_{a16p000T}} \quad (\text{II.2a})$$

with $S(0T)_{a16p000T}$ referring to the last zero. All the other fields will have to be divided by a linear combination of those two zeros, weighted by the number of curves in your measurement. Thus the software needs to know at which field the zero was made in order to make this zeros interpolation.

Those interpolations will also play a role in the reference measurements in case you measure the reference with a lower magnetic step than the sample (for example up to 16T with 2T steps). The software will generate some linear interpolation to simulate all the "missing" curves in the ratio:

$$\frac{S(BT)}{S(0T)} / \frac{R(BT)}{R(0T)} \quad (\text{II.3a})$$

with $R(BT), R(0T)$ representing the signal of the reference.

II.3 Main Loading - Auto load off

In the case of different file naming, the data can still be loaded in the main loading section, but the process will be a bit more meticulous as additional information will need to be provided. To do this, first, uncheck the checkbox **[Auto load]** and specify in the parameter lines, shown in Figure II.6, some measurement parameters. These parameter lines are located in the bottom center of the main window (see Figure III.1) and are alternatively visible depending on the section you are in (see Figure II.2).

On the **[Sample Section]** the line (a) "Sample Parameters" will be visible, while on the **[Reference Section]** the line (b) "Reference parameters" will be shown.

(a) Sample Parameters



(b) Reference Parameters



Figure II.6: sample load

- **For (a) "Sample Parameters":**

The range of the magnetic field will have to be precise from the minimum and maximum field placed in the **[Field Sample Files]** list. Plus, the magnetic step is used.

- **For (b) "Reference Parameters":**

By lack of space, the information for the **[Zero Sample Files]** list will be put here. In the line **[Sam Zeros]** the last closest magnetic field before the zero measurement will have to be put in the line and each field will have to be separated by a "space" as visible in the fig. II.2(b).

In the example picture, one zero was measured at the beginning "0 15.5 35.5". Another after 15.5 T "0 15.5 35.5". And the last one after 35.5 T "0 15.5 35.5".

In the same way, now the zeros field and the field of the reference will have to be placed in their respective line **[Ref Zeros]** and **[Ref Files]**. Obviously, if no reference measurements are made those lines don't need to be modified.

As this process can be annoying I advise using the specific naming to not have to deal with this.

Nonetheless, I provide some simplification within this process. For **[Sam Zeros]** and **[Ref Zeros]**, if only one curve is provided, it will obviously be used for all the fields, and there's no need to fill those lines. If two curves are provided, the software will assume that one zero was taken at the beginning and the other at the end of the measurement (as it should be the case if only two zeros are made). Thus, the software will make a linear interpolation based on the number of fields measured, and those lines don't need to be filled. Above two curves, no simplification was possible.

And for the [Ref Files] lines, if the same number of fields were measured for the reference, the software doesn't need to make any interpolation and this line doesn't need to be filled, otherwise it has to be precise.

Finally, you may have noticed three additional lines visible in Fig. II.6(a): [X Min], [X Max], and [X Offset]. The first two determine the energy range displayed during the loading of the data (modifiable later). The last line represents the offset of the curves, depending on the magnetic field, used for plotting in the [Stack] tab mentioned earlier (also adjustable later on). This offset is designed to be universal, ensuring proper stacking of data from different measurements, such as 0T-16T from one measurement and 17T-35T from another.

II.4 Second Loading – CSV or different data files



In this section, we will explore an alternative method for loading data that are stored in a structured manner. This involves having a first column for energy followed by a series of columns for each magnetic field. Once again, it's crucial for the step between the fields to be uniform for successful loading into the software.

At the top of the [Commands Buttons] section, you'll notice a logo of a hard drive with an arrow (as seen in the left picture). Clicking on it will open a secondary window named [CSVload], which should appear in front of the main window (see Fig. II.7).

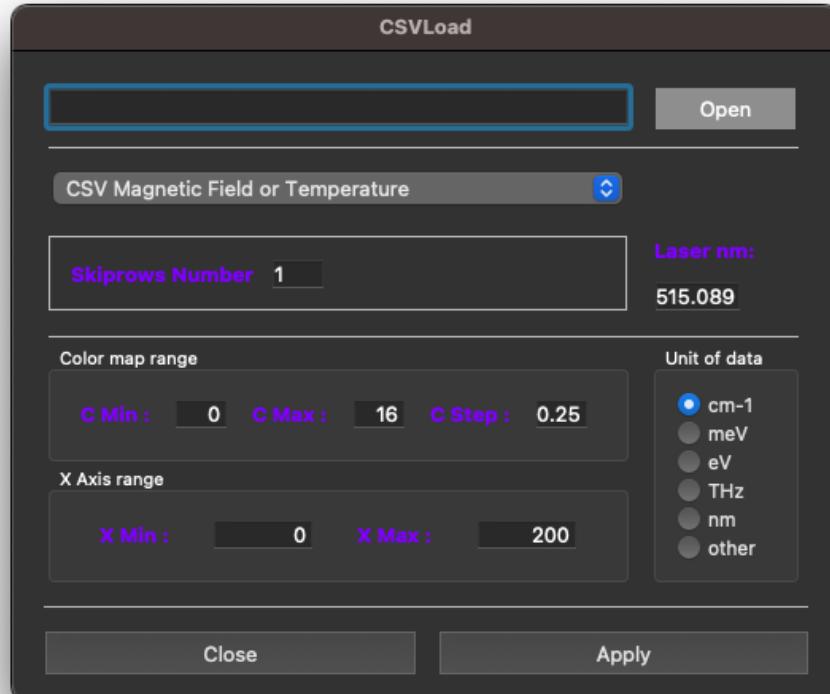


Figure II.7: CSV

The operation is quite straightforward. Click on the [Open] button to load your CSV file. The files can also have the "txt" or "dat" extension, as long as they are organized in a table shape.

You will find two group boxes named [**Color Map Range**] and [**X Axis Range**]. In the same process as before, these lines need to be filled with the parameters of your data. Additionally, you'll find a line named [**Skiprow Number**] in case your data has a defined number of header lines.

On the right side, there is also a box named [**Unit of Data**]. In contrast to the main loading, which assumes data with a unit of cm^{-1} , in this CSV loading section, I assume no unit upon entry. Therefore, it needs to be specified in order to match the unit system of the software, in case any conversion needs to be done. I allow the loading of data with nanometer units and have added a line for the laser value on top of the [**Unit box**], enabling conversion into one of the units allowed in the software. This addition was mainly implemented to facilitate the loading of Raman data in the field.

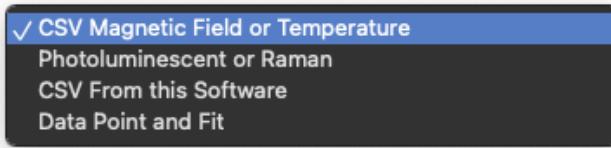


Figure II.8: Several loading options.

You may have noticed the option to switch between loading options, presented in the form of a combo list, as depicted in Fig. II.8. The first option is named [**CSV Magnetic Field or Temperature**], and all the explanations before were based on this option. I want to emphasize again that this software was primarily designed for a *Magnetic* external perturbation applied to the sample. However, you can still load data that depend on *Temperature* or even *Mechanical Pressure*, as long as the steps are evenly spaced (for example, from 5K to 305K with a step of 20K, to be overly precise).

The second option, named [**Photoluminescent or Raman**], was designed for a specific data-saving format used in my current lab. It may not be useful for most cases, and therefore, it will not be further described here.

The two final options are made to re-load some specific data saving from this software and will be explained later in the section – Saving data III.3.

III | Manipulating data

In this part, we will continue from the loading of TlBiSeS when we end up with one item "T_FIR" in the [Files item] list of the main window, see fig II.5. Please stay on the [Stack] tab.

III.1 One item interaction

In this figure, we mainly observe the noise in the data as we are examining a small part of the full energy range. The reason for this noise is that during the loading, **X Min 0 X Max 200 X Offset 0.05** the energy range lines were set with a minimum at 0 cm^{-1} and a maximum at 200 cm^{-1} with an offset of 0.05 (a special unit to have an absolute offset depending on the field). The energy range only applies during the loading process.

To interact with the energy range of those curves again, you can simply right-click on the item. A [menu item] should appear with several possible options. One of these options is [Interactive], composed of [Energy Trim] and [Magnetic Trim]. By clicking on one of them, another window for each possibility should open on top of the main window. All this procedure is summarized in the picture III.1. On both new windows, you will find lines that can be edited with the preferred parameters or modified by clicking on one of the double arrows on their right. Modifying one of those lines will automatically change the item in question without any need to validate. It's important to specify that the unit of these lines depends on the unit of the software, and any change of unit should also convert the boundaries defined in those windows.

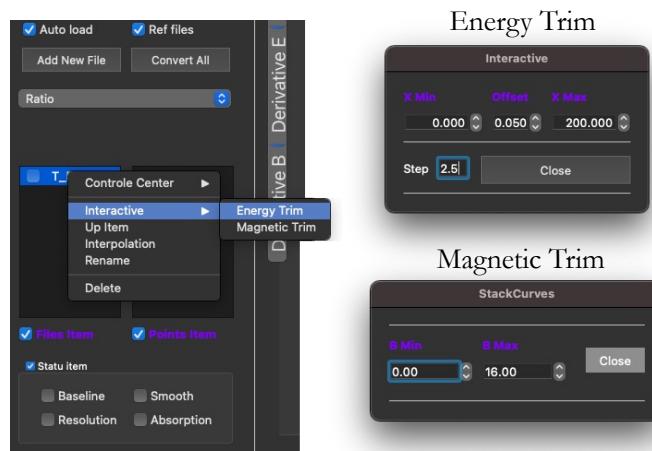


Figure III.1: Interactive windows, in the menu item.

Now let's change the energy range of the item "T_FIR" and set a maximum value of 1200 (cm^{-1} in our case). I also advise changing the [**X offset**] line for 0.5, as the modulation of this measurement is quite significant. If you have followed those indications, you should have noticed that the graph doesn't re-scale by itself. It is intended in case of multiple item connection, for example. This precision allows me to speak about one [**Icon button**] functionality (left in text). If you click on this button the graph should auto scale to visualize all the data present. For all the graph tabs, except the [**Stack**] tab, this function is based on the one from PyQt5. For the [**Stack**] tab, I try to improve it, to not take into account noise spikes inside the scaling.

If everything went well you should obtain a main window that looks like the fig III.2:

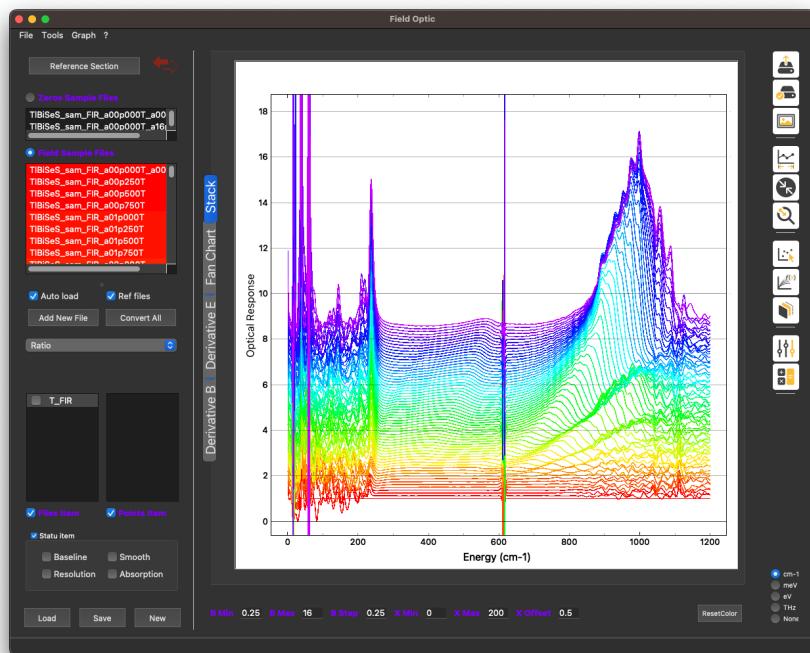


Figure III.2: Main window

You may have noticed that the value in the [**X Offset**] line on the main window changes when we modify it. This value has to be absolute if you have multiple items with different energy or magnetic ranges for the same compound. Therefore, modifying the offset for one item will also affect all the other items (after the window closes). For the sake of simplicity, if you only want to change the offset, you can modify the number in the [**X Offset**] line of the main window and then press the [**Convert All**] button or simply press [**Enter**]. However, we will discuss the main function of the [**Convert All**] button later on.

In specific cases, the use of reference correction may not actually enhance the visualization of a given signal or transition. An example could be the injection of noise by the reference into the data, obscuring a weak modulation. To address this, you can find another check button named [**Ref Files**] to the right of the [**Auto Load**] check button. This button allows you to interactively apply or remove the reference correction. I encourage you to try it and observe the modifications it brings to all graphs. For multiple items, this will interact with all the items having a reference correction. If the item doesn't have one, nothing will change.

III.2 Several item interaction

III.2.1 Isolation

In the previous figure III.2, we can observe that above $\sim 800 \text{ cm}^{-1}$, the transitions become more noisy. Another measurement was performed to improve the data at higher energies. Let's load the data in the "MIR" folder, following the same procedure as we did in the previous section II.2, and name it "T_MIR". Remember to define the energy range from 0 to 1200 cm^{-1} .

By following this process, you should observe in the [Stack] tab the curves from both items overlapping. In the other tabs, where we have color maps, the last item on the list (in this case, "T_MIR") should be on top of the other items (in this case, "T_FIR").

I provide the option to isolate one map from another by clicking on the little [Check] box placed to the left of the item name. A checked item will make all the unchecked items become invisible. You can check more than one item at a time. This allows you to deal with a lot of different items and still visualize the one you desire. I illustrate an example of this effect in figure III.3. The left graph shows the isolation of the "T_FIR" item, while the right one demonstrates the isolation of "T_MIR". If your color scheme differs from the picture, it's because I unchecked the [Ref Files].

The [Check] box will also be important in point picking on maps, providing an easy and intuitive way for the software to know which map to consider. You may also notice a [Check] box near the list names [Files Item]. If this box is unchecked, all the items will become invisible. This functionality might be more useful for the [Points Item] list, where the point picking and modeling will occur, as they might overload the maps.

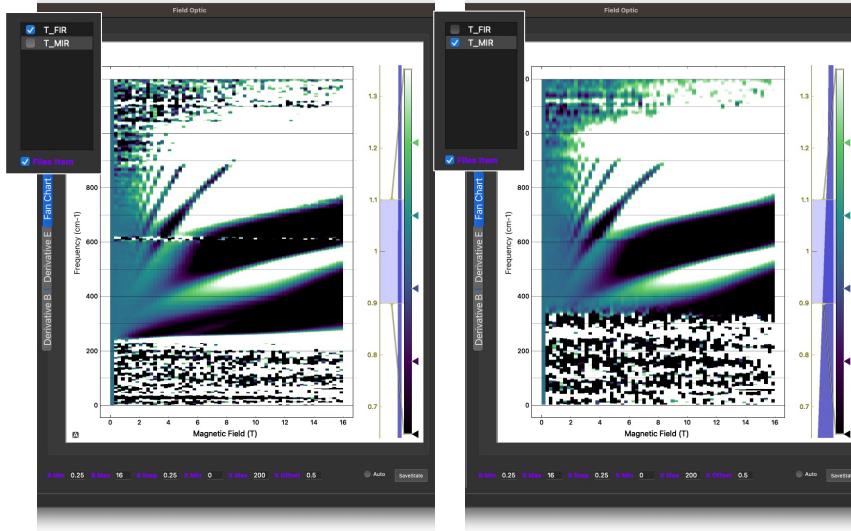


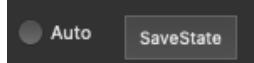
Figure III.3: Map isolation depending on the clicked item.

From figure III.3, it is evident that the low energy is better resolved with "T_FIR" and the high energies with "T_MIR". Therefore, it might be a good idea to trim the high energies of "T_FIR" from 0 to 600 cm^{-1} and trim "T_MIR" from 590 to 1200 cm^{-1} . This slight overlap in energy will be important later, so please retain those values.

III.2.2 Color bar mechanic

After this small adjustment, we can begin to manipulate the color scheme of each item with the interactive color bar. This color bar is provided by **PyQtGraph**. Now, let's understand how the color bar works inside this software. The color bar will always be connected to one item at a time, as you may have already noticed if you try to play with it. If you want to redefine the color bar for another item, you should just double-click on that item.

I am introducing a special mechanism here to save a desired color scheme for one item. If, after some adjustment of the color bar, you like the color scheme on the map, you have to press, before switching



items, the button named: **[SaveState]**, located underneath the color bar. It may seem a bit intricate, but it turns out to be more effective than saving by adjusting the color bar. Adjusting the color bar directly may sometimes degrade your color scheme in the process of improvement. If you find a good color scheme, save it. If you wish to experiment further, save it first, then try adjustments. If adjustments don't work out, double-click on the same item, and the previous color scheme should reappear.

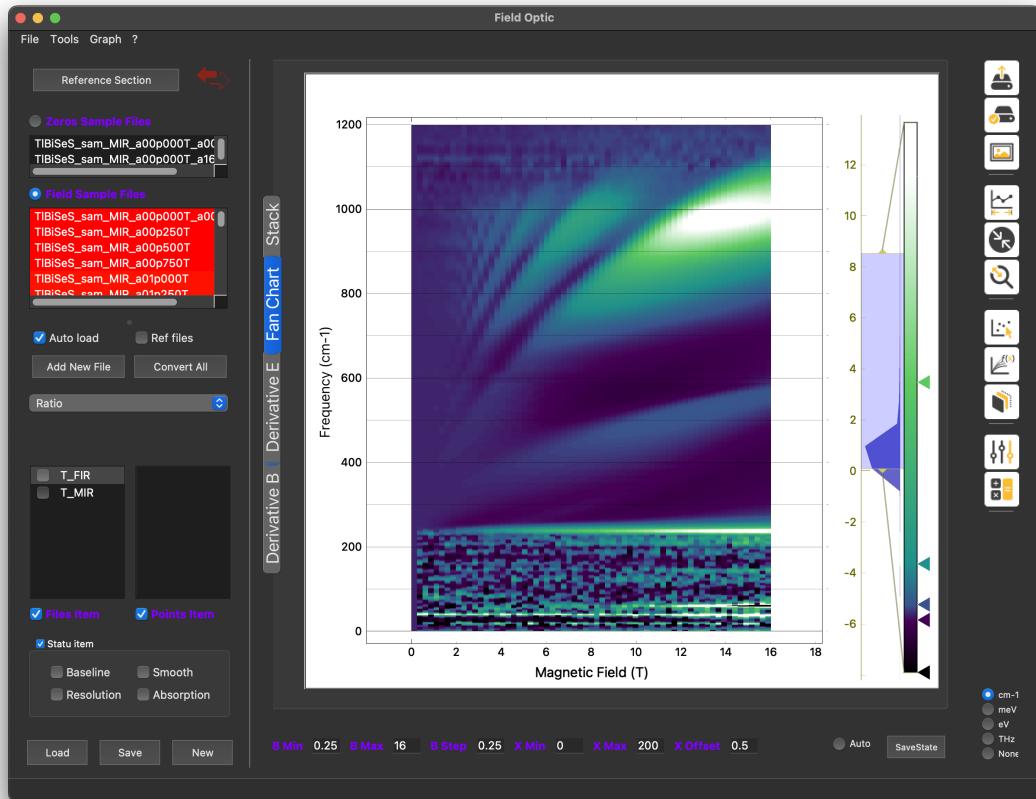


Figure III.4: Main window

Next to the **[SaveState]** button, you will find a button named **[Auto]**. This button can be activated to transfer the color scheme from one item to another. In our example with TlBiSeS, this **[Auto]** button is quite useful as the modulation of the two ranges is very similar. If you find a good color scheme for one range, save it, turn on the **[Auto]** button, and then double-click on the other item. This can save time in

finding a matching color scheme between items. Remember to turn off the **[Auto]** button if the color schemes are different between items; otherwise, it may overwrite your previous work.

Now, let's try to create the best color map possible for the two energy ranges. After some experimentation, you may have found something like the one shown in Figure III.4. I hope you found an even better result. If you observe carefully, you'll notice that the positions of the ticks in the color bar are no longer equidistant. This is one of the functionalities provided by **PyQtGraph**. However, one needs to be cautious with this, as strong modulations, like in TlBiSeS, can saturate the color scheme quickly. Nevertheless, in the **[Derivative E]** and **[Derivative B]** tabs, these modulations are attenuated, allowing for a better visualization of the transitions.

I want to emphasize that the mechanism for saving a color scheme is the same for each map tab. This means that double-clicking on an item will interact with the color bar of the tab, and nothing should happen in the other tab.

III.2.3 Introduction to Status item

As I highlight the strong modulations in the sample, I would like to introduce a feature in this software called **[Status Item]**, which can help enhance the visualization. **[Status Item]** was designed to maximize interactivity within this software. It is located beneath the list of items in the bottom left of the main window, as shown in Fig. III.5.

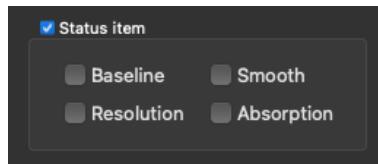


Figure III.5: Status item

Each item in the software will have a designated **[Status Item]**, accessible in that box by simply clicking on the item in question. In the **[Status Item]**, four modifications of the item are possible.

- **Baseline correction:**

In magneto-optics, which examines magnetic field variations, the ratio of a field to the zero field should ideally be "1" if no modulations are visible. However, there are cases where this baseline or "1" of the measurement may differ. Baseline correction enables you to align all the curves to this "1" reference point.

- **Smooth correction:**

As previously mentioned, a reference measurement is sometimes necessary. However, since it is still a measurement, it can introduce noise that may affect the sample data. Smooth correction involves utilizing the ratio $R(B)/R(0T)$ of the reference acquisition to minimize noise injection and enhance the visualization of potential transitions.

- **Resolution correction:**

In case you acquire an excessive number of data points, causing lag in the **[Stack]** tab, you have the option to plot one point out of every n , where n is a user-defined number. This feature may not be particularly useful but is still available.

- **Absorption:**

This option enables you to visualize your signal with a logarithmic transformation. In the case of transmission, this transformation corresponds to the absorption of your sample, hence the name "Absorption."

It should be noted that some of these modifications cannot be directly applied by clicking the [Check] box near the name. They need to be set elsewhere before. The [Status item] will indicate whether any modifications have already been made to the item and if they are currently applied. You can easily remove these modifications by clicking on the check button. This feature is powerful, allowing you to interactively and visually observe these changes on the color map, with or without these options, and decide whether they enhance the map visualization.

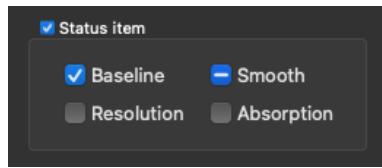


Figure III.6: Status item

In Figure III.6, I illustrate a case where an item has undergone several transformations. The [Baseline] checkbox is active, indicating that this correction is applied to the data. However, the [Smooth] checkbox is in a "standby" or inactive mode, signifying that this correction was previously configured but not yet applied to the data. Consequently, you can click on the [Smooth] checkbox and instantly observe the difference on the map between the two scenarios.

In summary, you begin with an item in which all the statuses are turned off. Subsequently, you apply various modifications or transformations, causing the corresponding [check] boxes to become activated. If you wish to eliminate a specific modification, you click on the corresponding [check] box, and it enters standby mode, allowing you to reapply it as needed.

Returning to the strong modulations in our data, these can be attenuated by applying a logarithmic transformation. The [Absorption] check box is the only button that can apply a transformation without any settings beforehand, as it simply involves a logarithmic change. Later on, you can also adjust the thickness of your sample to obtain an "absolute" absorption.

So, let's transform the signal using "log" by first selecting one item – "T_FIR" or "T_MIR" – and then clicking on the [Check] box of the [Absorption] status. Repeat this process for the other item. During this process, the color map in the [Fan Chart] tab will drastically change, as the baseline of a logarithmic ratio will be "0". We can try to adjust the color map again to achieve a decent color scheme. If everything goes well, you may obtain something like the figure III.7, where the need for a nonlinear color bar thickness is no longer necessary (once again, my [Ref files] check box is off).

III.2.4 Modeling the data

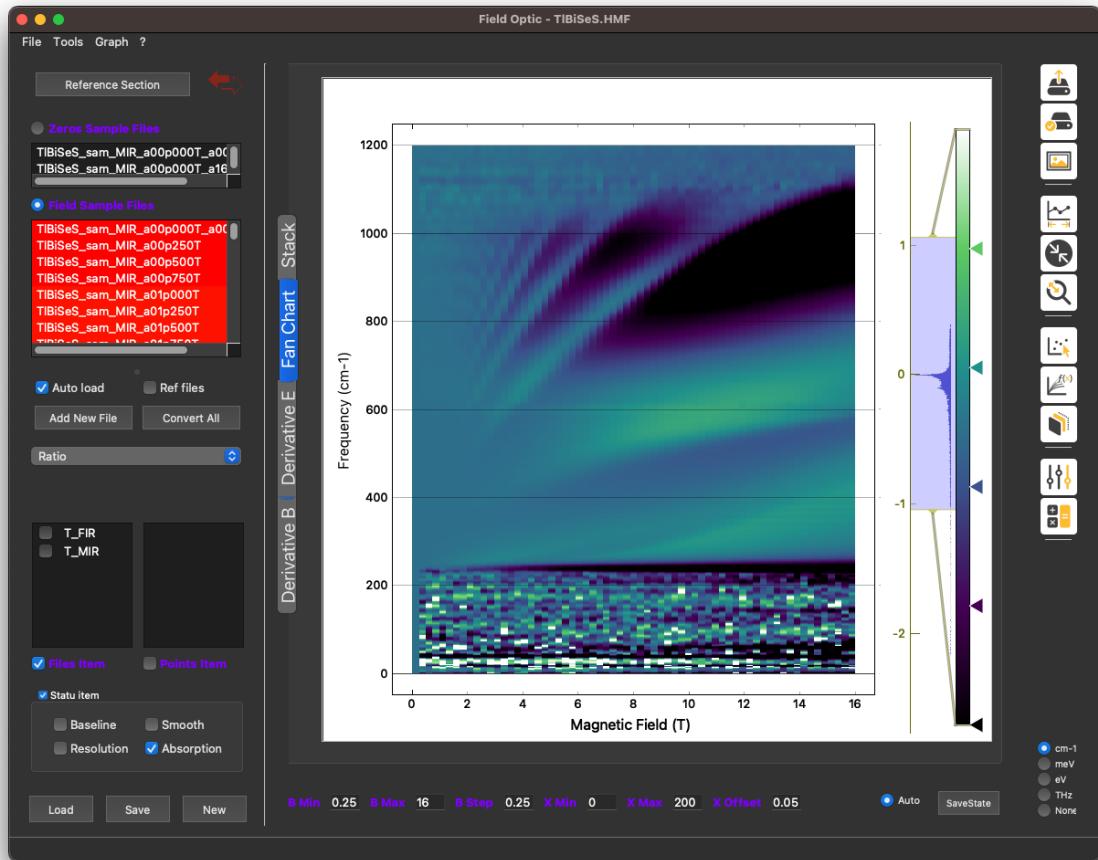


Figure III.7: Statu item



If we delve into the physics behind it, those predominant transitions visible in the color maps can be related to inter-Landau level transitions. They even arise from linear bands and follow the "basic" theoretical model of a 3D Dirac dispersion quite well. In that sense, I find it interesting to provide some theoretical modeling in one of the **[Icon buttons]** in the command section of the main window (left in the text).

Clicking on this **[Icon button]** should open a new window named **[Fit]** (see fig. III.8). This window will allow you to manually set the parameters of your modeling and visually interact with the outcome on all the color maps. The interactivity is based on the same principle as the **[Energy Trim]** view mentioned earlier. A set of double arrows allows you to increment or decrease the parameters with a defined step on the same line. This step will surely depend on the unit of the software. As you can see, on the top left, a list of options is possible. In this software version, it is composed of **[Landau level]** and **[Magnon]** modeling. Any other suggestions are always welcome.

In our case, I have already preset the appropriate parameters in figure III.8. We are dealing with **[Linear]** bands, observing $[n = 7]$ transitions of **[Inter LL level]**, with a **[Velocity]** of $4 \cdot 10^5$ m/s and a **[Gap]** of 258 cm^{-1} .

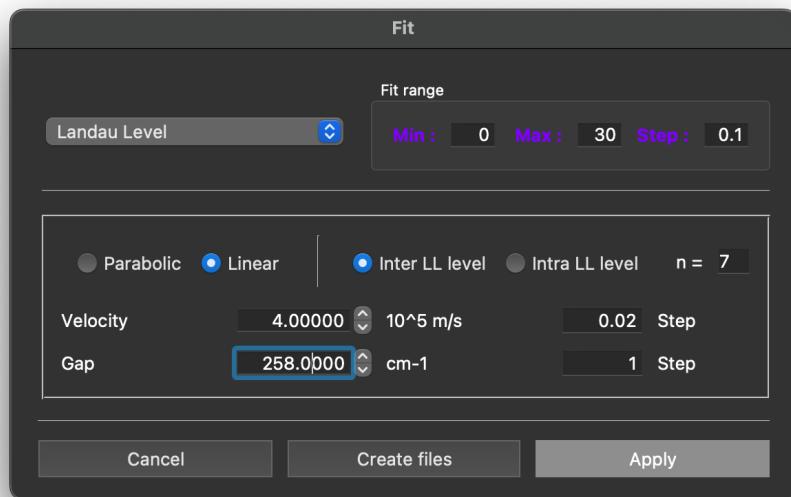


Figure III.8: Fit window

The initial concept was to specify the number of transitions " n " in the example of Landau levels, generate the lines using the **[Create files]** button, and then interact with the double arrows. However, it turns out that modifying a value is enough to generate the lines. Nevertheless, to change the number of transitions, merely modifying the line is not sufficient; you have to press **[Create files]** again or interact with the data. The current selection rule is $n \rightarrow n + 1$. In a future update, I may allow for more flexibility in this regard.

Additionally, it's worth noting that the **[Fit range]** box determines the magnetic field range for the modeling.

Once the desired modeling is completed, you need to confirm by pressing the **[Apply]** button. If everything is successful, the resulting window should resemble the one shown in Figure III.9.

The seven inter-Landau level transitions should be generated as separate items within the **[Points item]** list. I'm not sure if it would have been better to create only one item with the seven transitions inside. Nevertheless, here, you can easily isolate one item from the others or delete only one.

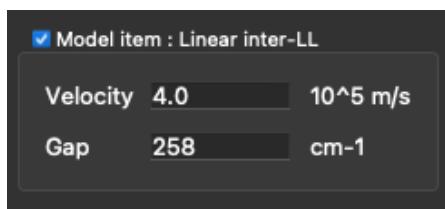


Figure III.10: Model item – information box

For those items, if you select them by clicking on them, you should see the **[Status Item]**, mentioned before, switch to a **[Model item]** that will contain all the information of the modeling. It goes without saying that modifying the units will convert those parameters if needed. This line can be edited but will not currently affect anything. I might allow this interaction in the future.

One problem is that, in the case of separating all transitions, modifying one also has to affect the other transitions from the same "family". Therefore, it is slightly more complex to program. This provides a good argument for having only one item containing all transitions.

Anyway, any feedback on what will be more intuitive and interactive is, again, more than welcome.

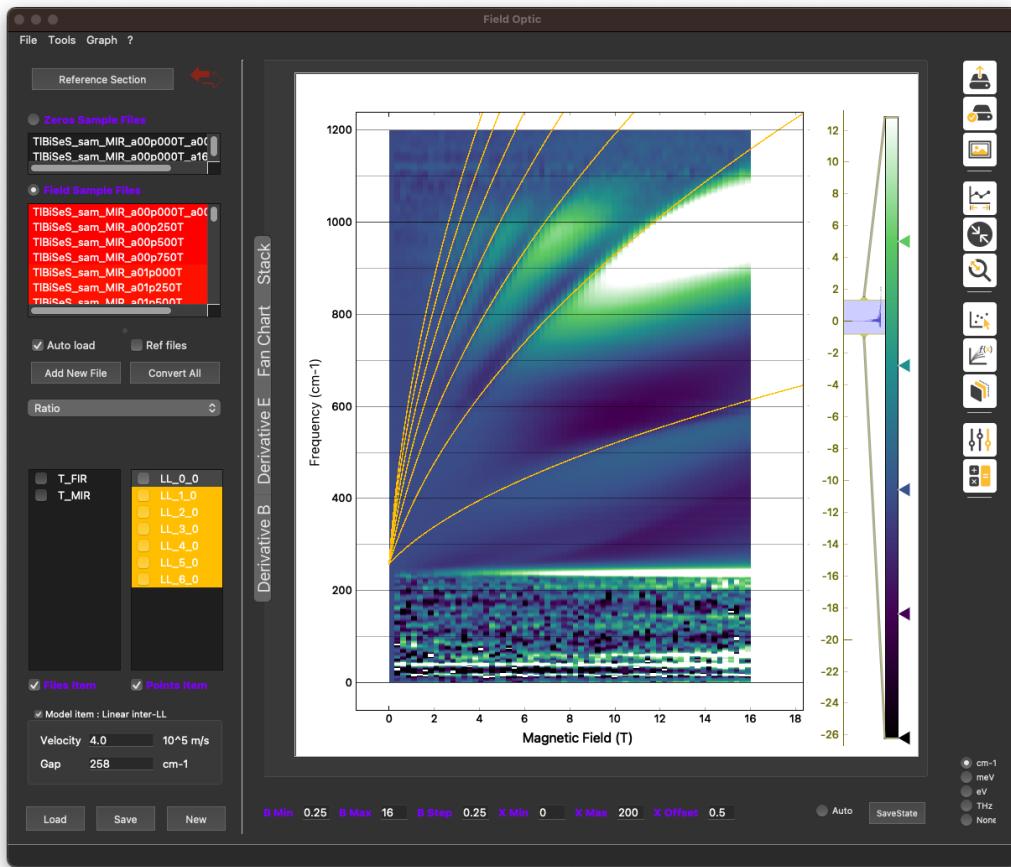


Figure III.9: Fit window

III.2.5 Map point picking



It is highly probable that your transitions don't follow a perfect theoretical, textbook-like prediction. In that case, the common procedure could be to pick some points coming from your transitions and fit them with a specific equation that could describe your system. I hence provide a map point picking tool in the **[Icon button]** command section, as shown in the left figure. I emphasize "map" as this function only works on the color maps. Nonetheless, those points will still be plotted on the stack curves after validation.

In the same process as the modeling, clicking on the **[Icon button]** will open a new window called **[Map Points]** (see Fig. III.11). As soon as this window is open, you can already interact with the map(s) by clicking on the coordinate where you want to put a point. You will also notice, by trying, that you can't have two points at the same field, and therefore, the first picking point will be erased. The boundary of the picking points is defined by the map. Sadly, as it is possible to hide some energies and magnetic fields, the picking point still remembers them and can pick points outside the visible range. This is also one feature to improve.

On the **[Map Points]** window, two main options are present in the shape of circular buttons: **[Add Point]** and **[Remove Point]**. For the sake of a detailed explanation, if you want to remove one point, you have to switch options. After some point picking, if you change your mind and don't want them

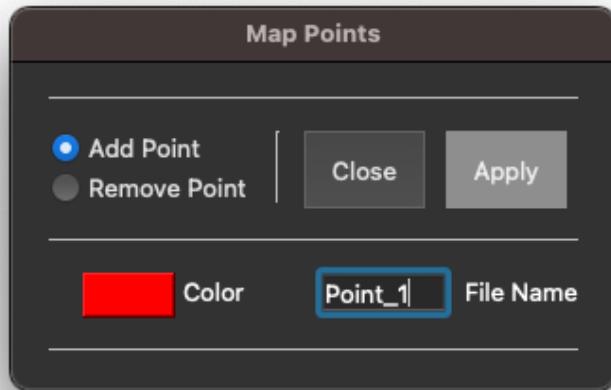


Figure III.11: Picking point window

anymore, you can just click on the [Close] button. If you are satisfied, just press the [Apply] button, and an item should appear in the [Points Item] list. Note that you have to define a name in the [File Name] line of the [Map Points] window. You can also choose a specific color by clicking on the [Color] button, see Figure III.11.

Let's continue the initiation by picking up some points and generating an item. If everything goes well, you should have a main window that looks like Figure III.13. You can observe that the previous inter-Landau level transitions are no longer visible. This is because I checked the [Check] box of the item named "Point_1"; hence, only this one is visible. It works in the same way as the [Files Item] list.

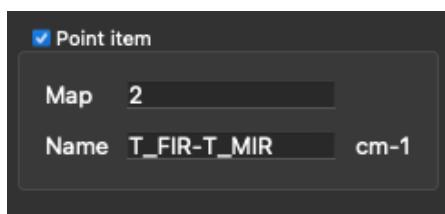


Figure III.12: Point item – information box

Here comes something important with the point-picking item. If you select that item, you should see on the information box in the bottom left of the Main window a [Point item] status with two lines named [Map] and [Name], see Figure III.12. [Map] will refer to the number of [Files Item] used to pick up the points, and the [Name] will be, obviously, the name of the [Files Item] used. Here we see 2 maps and the items "T_FIR" & "T_MIR", which makes sense. Now I would like you to double-click again on the point item "Point_1".

You should see the [Map Points] window open again, and the two items "T_FIR" & "T_MIR" will become checked. This feature is very important as it is a way to not lose the information of which map(s) belong to those points. Let's take the example that you measure the magneto-optical response of a sample in temperature (or pressure, etc.). You could load all those maps inside the software to see their differences. Then, if you want to pick up points on one map at a certain temperature, you should just select this map to isolate it and pick the points. Now if you do this process for all maps, you will end up with several Point items on the graph but maybe not associated with the correct map (if you didn't make them invisible). So, if you try to interact again with the [Point item] by double-clicking, the software will automatically isolate the correct map(s) with respect to those points. All of this is done to maintain a certain coherence.

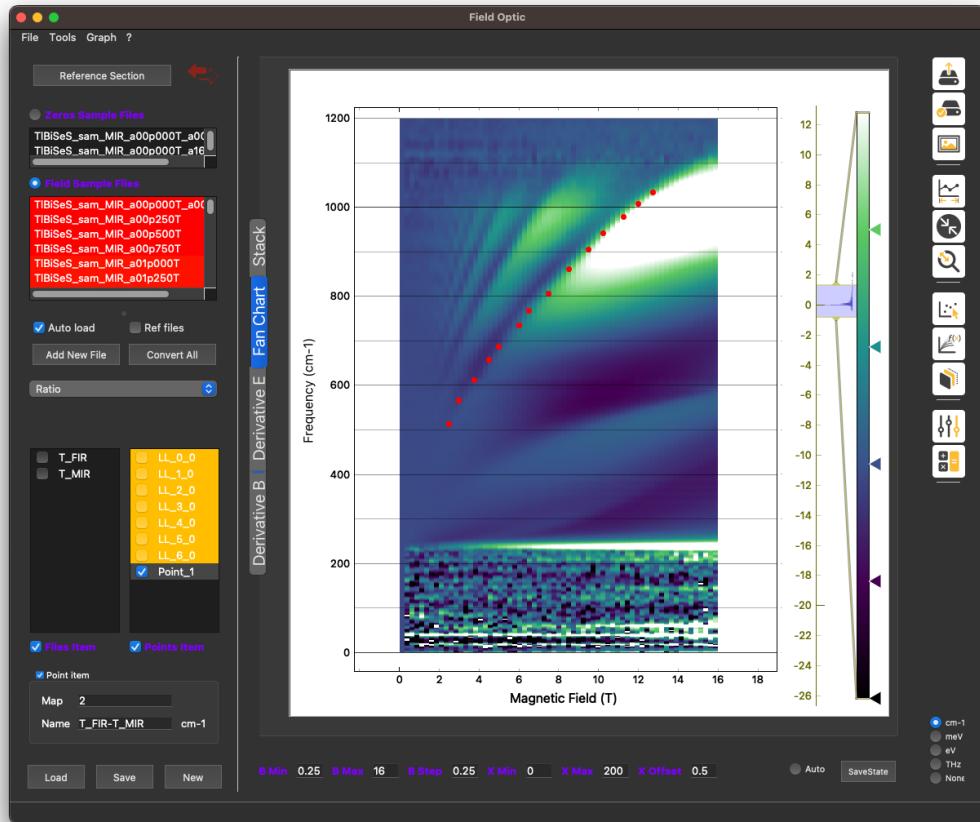


Figure III.13: Picking point window

To be very clear, when picking up points on map(s), you can specify which one you want by checking the **[Check]** box of the item in the **[Files item]** list. If no checking is done, the software will consider all the maps inside the **[Files Item]**. When a points item is created, it will include information about the map(s) used. If you double-click on them to interact again, to remove or add new points, the software will isolate the map(s) on which those points were taken.

Finally, if we go back to the **[Stack]** tab, we should see the previously picked points overlaid on the curves of the map taken during the picking. If there's a small mismatch, meaning that some points are off the curves, please press the button **[Convert All]**; it should correct this issue.

III.2.6 Save Project

As we have made significant progress, it would be beneficial to create a saved state for this TlBiSeS analysis. In the bottom left corner of the main window, you will find a set of three buttons that allow you to load, save, or create a new project, as shown in Fig. III.14. Each save operation will store two "documents": one **folder** and one **save state file**. Therefore, it is recommended to organize these save states in one location. The **save state file** contains the parameters of the main window, while the **folder** holds the data of the item(s). These saved projects can take up space on your computer, depending on the amount of data they

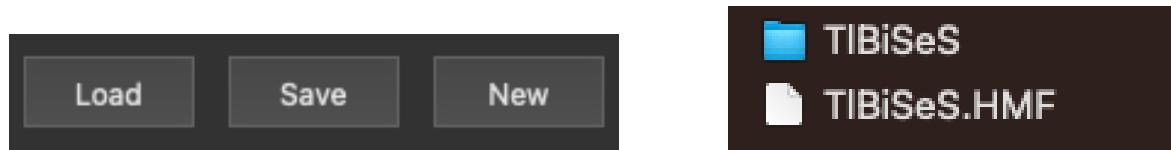


Figure III.14: Loading, saving or creating project – Data folder and save state file from a Save project

contain. Please note that the **folder** and the **save state file** share the same name, so you cannot modify one without the other; otherwise, the loading process will not work. Modifying both with the same name should be fine, except for the inclusion of special characters ".", "\", or "/".

To load a project, click on the **[Load]** button and open the **save state file** with the extension "HMF". Alternatively, you can drag and drop this file into the main window.

The button **[New]** allows you to erase everything inside this software and start a new project.

III.2.7 Introduction to tools and calculator – icon button

Tools



The previous content indicates that it would be helpful to provide some tools for performing operations or combinations on the data matrices. One of the **Icon buttons** in the command section, depicted on the left, offers functions related to matrices. If you recall, I advised you to maintain some overlap between the "T_FIR" and "T_MIR" items; now, I'll explain the reason behind this recommendation.

Now, click on the "Tools" icon button. A window titled "Tools" will appear, featuring a "combo" list containing various options, including **[Merge Energy]**. If everything is proceeding as expected, you should see a result similar to the one shown in Figure III.16.

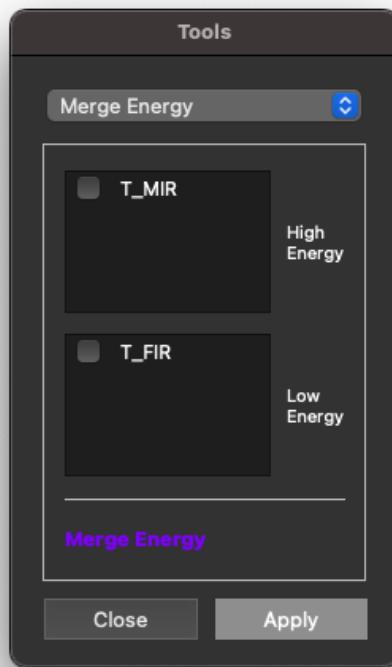


Figure III.15: tools window

As depicted in the figure, you can observe that I've populated the two lists with items from the main window. This can be accomplished by a simple drag-and-drop of the items. The upper list is designated for the item with the highest energy, while the lower list is for the item with the lowest energy. In the case of **[Merge Energy]**, the merging operation will be applied to the visible ratio within the window, signifying that the trim energies will be permanently altered. For other options, the process may vary, and each will be explained in detail later.

The merging operation will be successful if the curves of the two items share a common energy range. Upon switching to the **[Merge Energy]** option, you may have observed a **[Report]** box appearing in the middle bottom of the main window, with the following information:

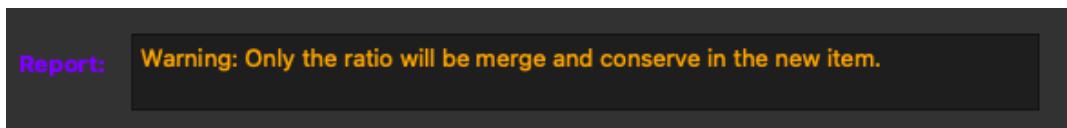


Figure III.16: Report tools

This **[Report]** box is designed to provide information about the operation, guiding you through any issues that may arise. Detailed explanations for these messages will be provided later. For now, let's proceed with the merge. Arrange the items as shown in Fig. III.16, then click on **[Apply]**. A pop-up window will prompt you to enter the name for the new item; let's name it "T_Merge."

Now, you should have a new item named "T_Merge" that covers the full range of energy. You'll need to set up the color scheme again, but using the **[Auto]** button should simplify the process. Note that the new item inherits the logarithmic transformation from the original items, so you may choose to revert to a non-logarithmic transformation if desired. Keep in mind that if you had defined a thickness for the original items, this information will be lost in the merged item. While merging in either field or energy may not be recommended in all cases, it can be a useful function in specific scenarios, especially when dealing with independent maps.

Primarily, the **[Tools]** functionality is designed to perform operations on all the datasets within the item(s), taking into account the reference data if present. For example, in the **[Interpolation]** options, the interpolation will be applied to all the spectral curves, enhancing the interactivity of the new item.

In the **[Tools]** section, there are certain restrictions. I don't allow energy interpolation for all options. In **[Average]**, for example, if you measure the same energy range multiple times, you can average each run of measurements here. Unfortunately, if the matrices don't have the same energy range, it might not work. I block this because the average should be prioritized for measurements done under the same conditions. Since I aim to average every spectrum, I want all the spectra to be "equivalent," so to speak.

Nonetheless, if you are still interested in those operations, I also provide you with a calculator.

Calculator



If you are familiar with OPUS software, the **[Calculator]** that I provide is highly based on and designed after their calculator. It allows reasonable operations on matrices in the common region. In other words, if your matrices have the same Tesla step and a common energy range, some computations should work, with some energy interpolation.

By clicking on the **[Icon button]** (left in text), a window, see Fig. III.17, should appear. An example of how to compute is already displayed in the **[Console input]** of the calculator window. Each line will be dedicated to one of the elements of the equation that you want to proceed. These elements can be placed by clicking on the different **[Button]** of the **[Calculator]** window or by dragging and dropping the **[Files Items]**. The operation made in the example (fig. III.17) has no physical meaning and is just there to remind us that we are still in a Python shell, and the use of common functions such as Logarithm, Exponential, etc. will have to be followed by a ")" at the end. To compute, just press the equal button [=] and enter a name for the new item.

Warning: This calculator will compute the visible spectra. If you are already in an **[Absorption]** mode, this modification will be preserved in the new computed item. Furthermore, as this software can perform different background subtractions, you can really change the data and may not be able to recover

the original one, as we have seen in the previous section when using [Tools]. So, be careful. However, the calculator can be useful for Faraday rotation analysis, for example.

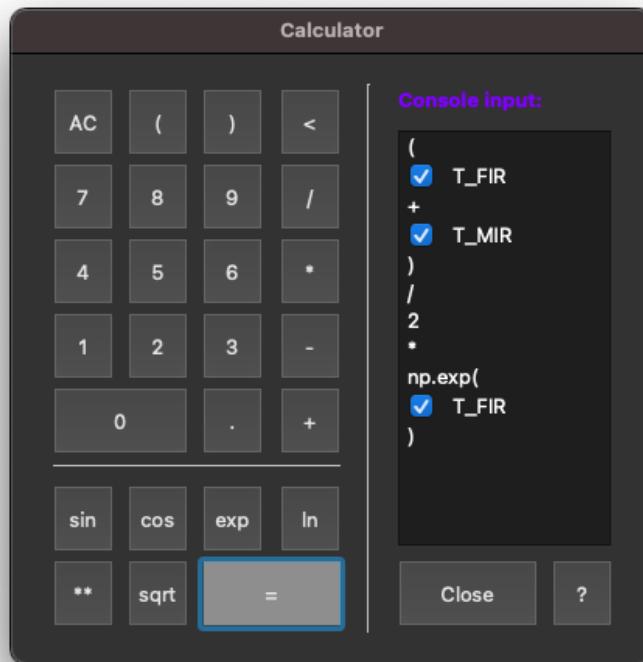


Figure III.17: Calculator window

III.3 Data Saving and reload



After performing some data treatment inside this software, the curves visible in the [Stack] tab can be saved in the form of a CSV file (meaning table files). It is also possible to save the modeling items and the point-picking items.

The data-saving process is quite simple and straightforward. Click on the [Save] icon button, represented by a checked hard drive (see image), in the command section. A window named [Save Window] will appear. Then, drag and drop the item of your choice, as shown in Fig. III.18, into the right list.

The left list, labeled [Stack Files], corresponds to the [Files item] list of the main window. There are three different ways to save this data.

- Visible ratio:

It will save only the data visible in the graphs, cutting off the energies not plotted for the item. If you have interacted with the magnetic field range and some of them were not visible, those will still be saved.

- Full ratio range:

This option saves the full energy and magnetic range of the ratio data, even if it's not visible on the graphs.

- All data (6D):

This option saves the full data set of the item, including the ratio, the raw sample, and reference curves. It also saves all the information on the modifications made on this item. This special saving was designed to transfer an item from one Save state of the software to another, without losing any information (except the color scheme).

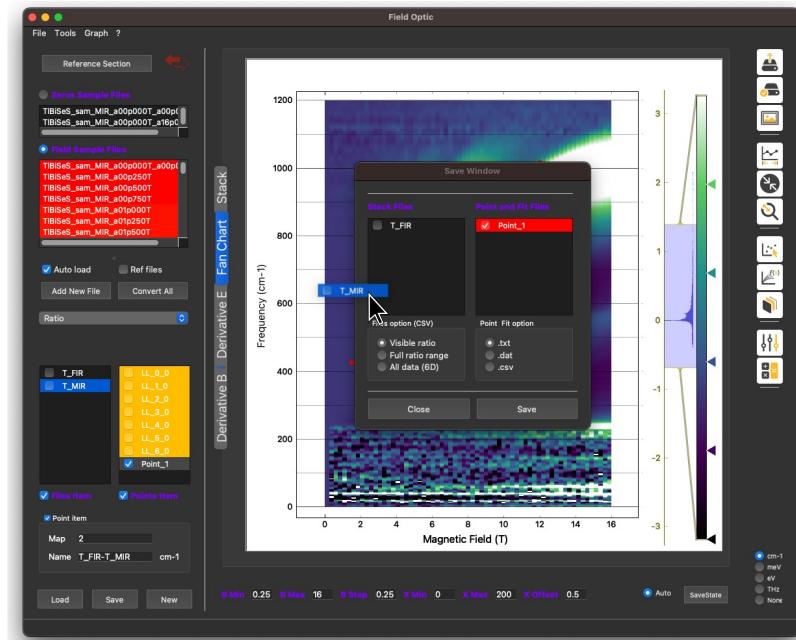


Figure III.18: Data saving window

The right list of the saving window, named **[Point and Fit Files]**, is for the **[Points Item]** list of the main window. In the same process, you just drag and drop from one list to the other. You can choose from different saving formats that were added for symmetry within the window.

When all the items that you want to save are placed inside their respective list, you press the button **[Save]** and choose a folder destination where you want to store those data. After validating, the data files inside the **[Save Window]** list should disappear and be inside the chosen folder.

The data will be saved with the same name. If you want a different one, you can double-click on each item in the list. A pop-up window will appear, asking for a new name. Redefine the name and press **[Ok]** to apply the new name.

Now that we have covered how to save data within this software, we can discuss the two other options in the **[Load Data]** icon button that we previously explored. I have illustrated the two different **[CSV Load]** windows possible, depending on the two last options in the list, in Fig. III.19.

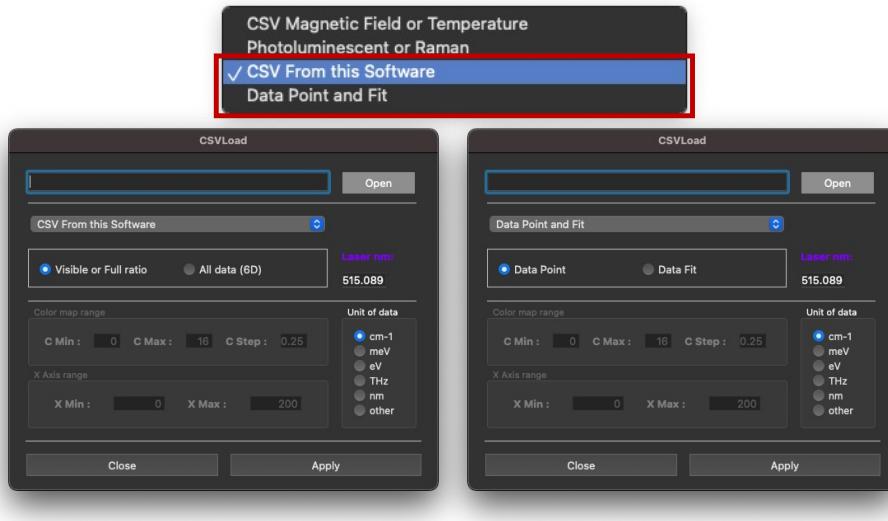


Figure III.19: CSVload window

The options provided in these **[CSV Load]** windows are exclusively designed for data saved using this software. In the displayed figure, you can observe that the **[Color map range]** and **[X axis range]** fields are disabled. This is because all relevant information should be embedded in the header of the previously saved data file. However, it's important to note that the energy information is not retained during the saving process and needs to be specified again.

For both options, you are required to accurately indicate the type of data being loaded, such as **[Fit]**, **[Points]**, **[Visible or Full ratio]**, or **[All Data (6D)]**. This information is crucial for the software to appropriately store and handle the data. Future updates may aim to simplify this process further.

One drawback of this loading is only one file at a time can be loaded. Has to be improved too.

IV | Normalization and background subtraction

In this chapter, we will explore various methods for visualizing data, encompassing different normalization techniques to observe the relative changes in spectra, as well as the presentation of raw spectra without normalization. Using the reflection measurement of TlBiSeS as an illustrative example, we will compare different color maps, examine what can be extracted and identified, and discuss the mathematical expressions employed.

All the various options will be organized in a "conbow" list, positioned at the left center of the main window, beneath the two buttons [**Add New File**] and [**Convert All**], as depicted in Fig. IV.1. There are a total of seven ways to visualize the data, each serving a different purpose, and they can be derived in terms of energy or magnetic field (or x and y axes if your data is not magneto-optical). To switch between these options, you need to select one and then press the [**Convert All**] button. The special case of [**Raw data**] will not be addressed, as it pertains to straightforward curves without any normalization.

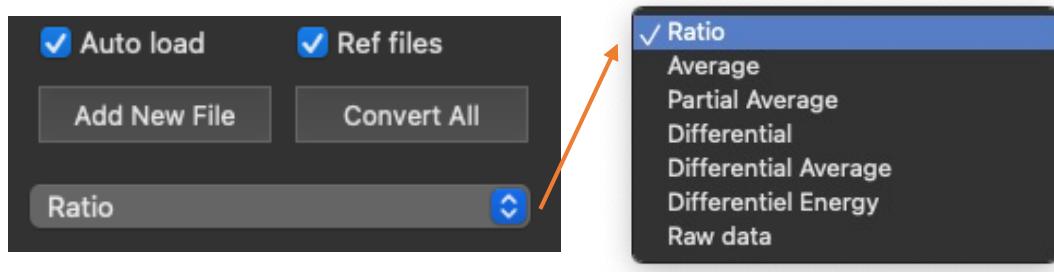


Figure IV.1: Several options to normalize the data

IV.1 Ratio

Let's begin with the most common way of plotting, the [**Ratio**] option, and observe the reflection of TlBiSeS. Locate a folder named **Reflection** containing the relevant data. Load this data into the software as described in Chapter II, and navigate to the [**Fan Chart**] tab. You should obtain a visualization similar to what is shown in Figure IV.2.

The formula for the "Ratio" option is simply:

$$\frac{S(B)}{S(B = 0T)} \quad (\text{IV.1})$$

With $S(B)$ representing the reflectivity signal at magnetic field B and $S(B = 0T)$ denoting the reflectivity at zero field, the quantity $S(B = 0T)$ can be a linear interpolated curve between the actual data

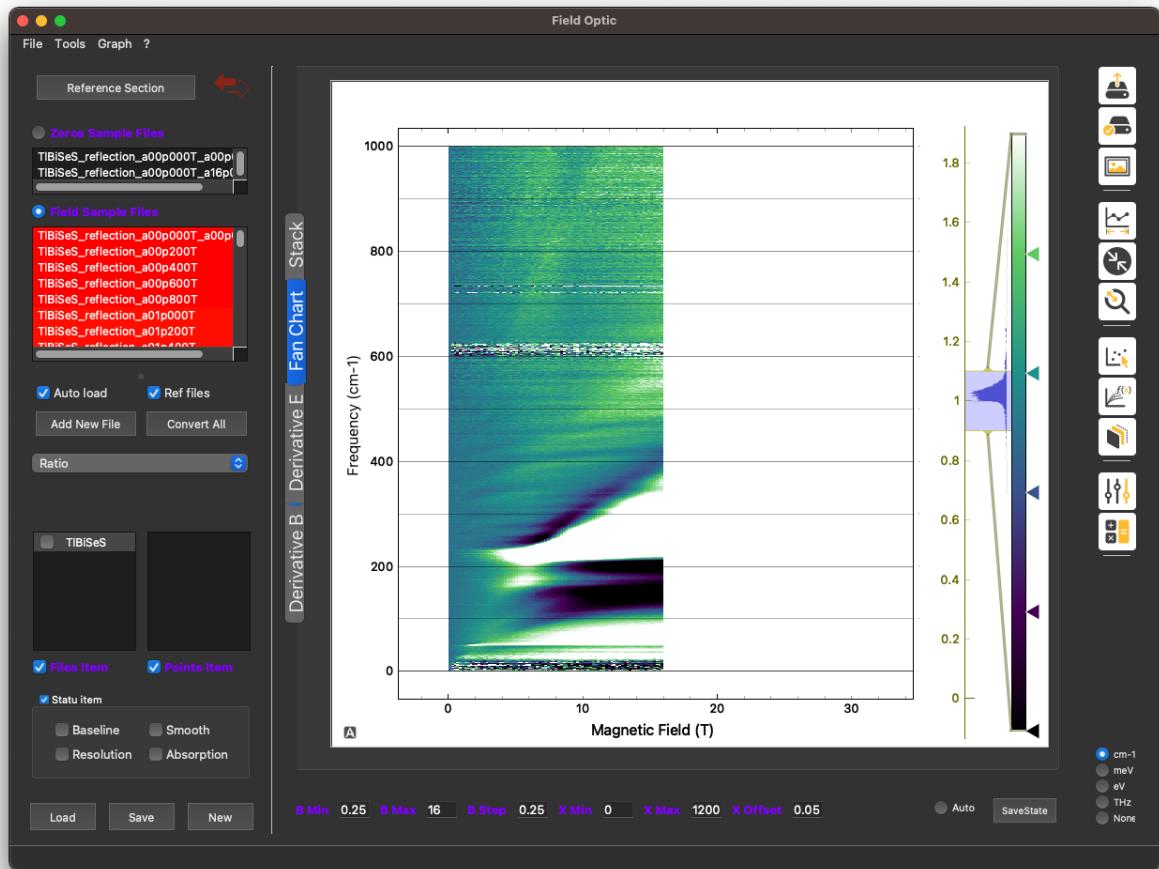


Figure IV.2: Fan chart of the ratio option for the reflection measurement of TlBiSeS

measurements, depending on the number of zero-field spectra conducted. In our case, with two zero-field measurements performed at the start and end of the measurement, at k Tesla, $S(B = 0T)_{kT}$ will be equal:

$$S(B = 0T)_{kT} = \frac{(n - k)S(B = 0T)_{First} + kS(B = 0T)_{Last}}{n} \quad (\text{IV.2})$$

where n is the total number of measurements and k is the k^{th} measure, representing a weighted average of the zero fields. In other words, it takes into account the proximity of the zero field measurement to the specific magnetic field value k Tesla.

The **[Ratio]** option serves as the common and conventional method for plotting the picture. While it may seem straightforward, it plays a foundational role, as all other options can be derived from it through the **[Ratio]**. This software occasionally prioritizes the ratio over other considerations, especially when utilizing the **[Tools]** icon button.

To elaborate, in the previous chapter, we explored the **[Report]** output generated by the **[Tools]** button, as shown in Figure III.16. The report contained the statement "**Warning: Only the ratio will be merged and conserved in the new item**" when attempting to merge two items in energy. Given the various

ways data can be visualized, attempting to merge them in an option other than [Ratio] would result in curves that could no longer seamlessly transition between different modes in the list of options. Therefore, the software is designed to restrict merging to the [Ratio] mode to preserve overall interactivity.

The optical response of TlBiSeS, as displayed in Fig. IV.2, exhibits strong modulation at low energy stemming from multiple contributions. The overlap of these contributions makes it challenging to identify them accurately. Given that we are dealing with a Dirac system and have previously observed intra-Landau level transitions, it is reasonable to assume that some of the contributions may be intra-Landau level.

To address this, let's generate a model using the [Fit] icon button, as discussed in the previous chapter (see Section III.2.4). Ensure that the parameters remain the same as before, and be sure to click [intra-LL level] with $[n = 3]$. The resulting figure should resemble what is shown in Fig. IV.3.

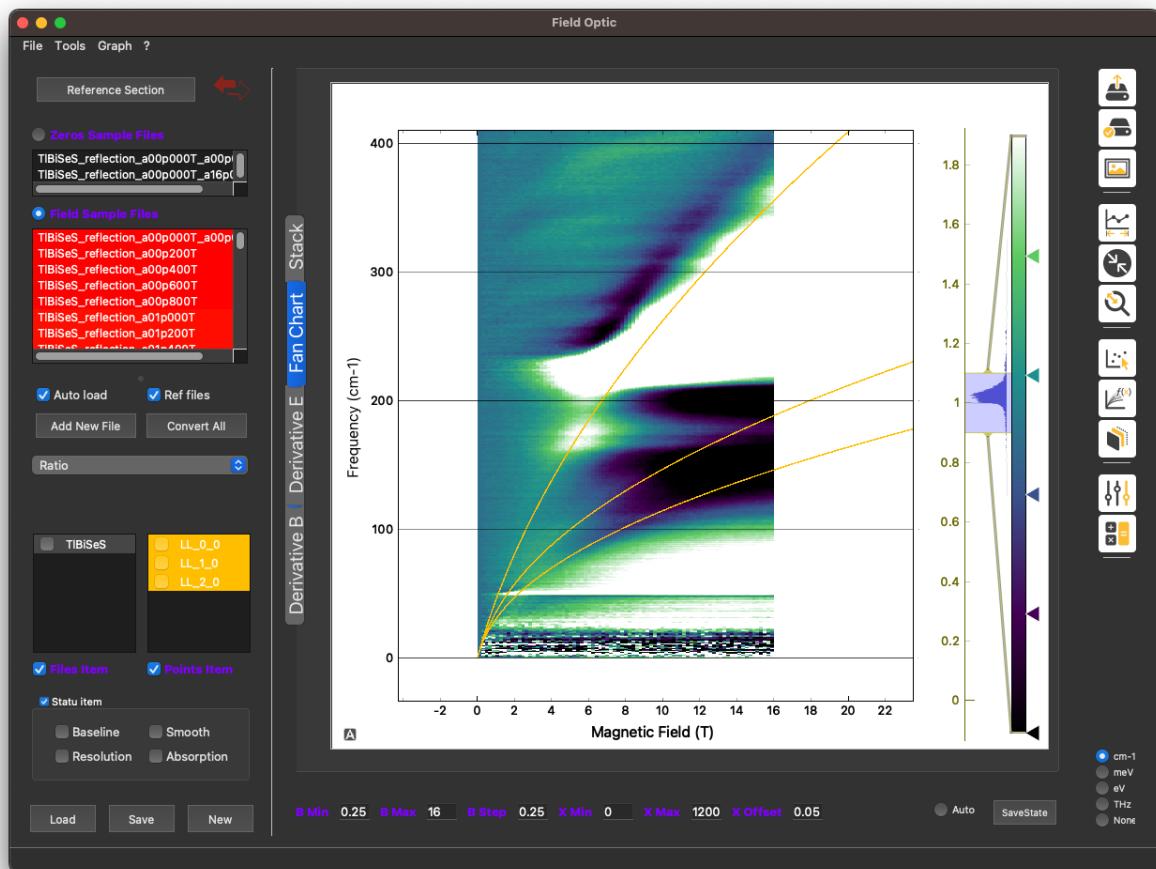


Figure IV.3: Intra Landau level model

The overall model doesn't appear to be bad; the electronic background on the map seems to evolve similarly. However, it might be beneficial to eliminate other contributions and isolate those within the intra-Landau levels. Feel free to explore other options while I continue explaining the remaining steps until we arrive at the optimal one.

IV.2 Average and Partial Average

These two options are quite similar and can be explained together. The [**Average**] option will employ the averaging of all the fields as a normalizing curve instead of the zero field. The formula for this option can be expressed as follows:

$$\frac{S(B)}{\text{Average}(S [:])} = \frac{S(B)}{S [:]} \quad (\text{IV.3})$$

where $S [:]$ will correspond to all the measurement curves present in the item.

The [**Partial Average**] option, on the other hand, will average all the curves below the corresponding field. The mathematical expression for this option is:

$$\frac{S(B)}{\text{Average}(S [:B])} = \frac{S(B)}{S [:B]} \quad (\text{IV.4})$$

with $S [:B]$ are all the curve before the magnetic field B .

The [**Average**] option enables you to eliminate a constant feature that may arise from the zero field curve when a transition is already present but varies with the magnetic field, as seen in the case of a magnon, for example. In Figure IV.4, I have plotted the top three panels to illustrate examples of the three options for a magnetic sample exhibiting an easy-axis magnon dispersion.

In the [**Ratio**] case, a constant transition in energy at approximately ~ 15 meV is observable. This originates from the original position of the magnon before its energy shift with the application of the magnetic field. Since we are only dividing by the zero field, it is not possible to ratio out this contribution, making it visible in the color map.

However, in the [**Average**] mode, we can effectively blur out this contribution. A milder blurring effect is also noticeable in [**Partial Average**]. Unfortunately, [**Average**], in contrast to [**Partial Average**] (and [**Ratio**]), can introduce some folding back of the transition into the data, potentially significantly affecting the curves. You may have observed this if you experimented with the TlBiSeS reflection data. In Figure IV.4, we can observe this effect with the transition at ~ 13.5 meV. This is also faintly visible in the slightly brighter color below the two dispersing branches.

It's important to note that one of the primary advantages of this averaging method is noise cancellation from the data itself. In the presence of a very weak signal, characterized by a weak modulation and low intensity, this averaging technique can be instrumental in revealing otherwise "hidden" transitions. In Figure IV.4, the noise cancellation effect is evident in the non-transmissive line at ~ 17.5 meV, which is less noisy in the averaging cases. However, it's worth mentioning that in cases where the signal is already sufficiently strong, the noise canceling may not be as pronounced.

The [**Average**] option has been documented in the literature, but I introduced the [**Partial Average**] option to extend its applicability to Landau-level dispersions without significant disruption. It's crucial to clarify that there is also, understandably, a folding forward into the data. However, since, in most cases, the intensity of Landau level transitions increases with the magnetic field, this folding is less noticeable and doesn't disturb the signal significantly. You can verify this by testing with the transmission data of TlBiSeS

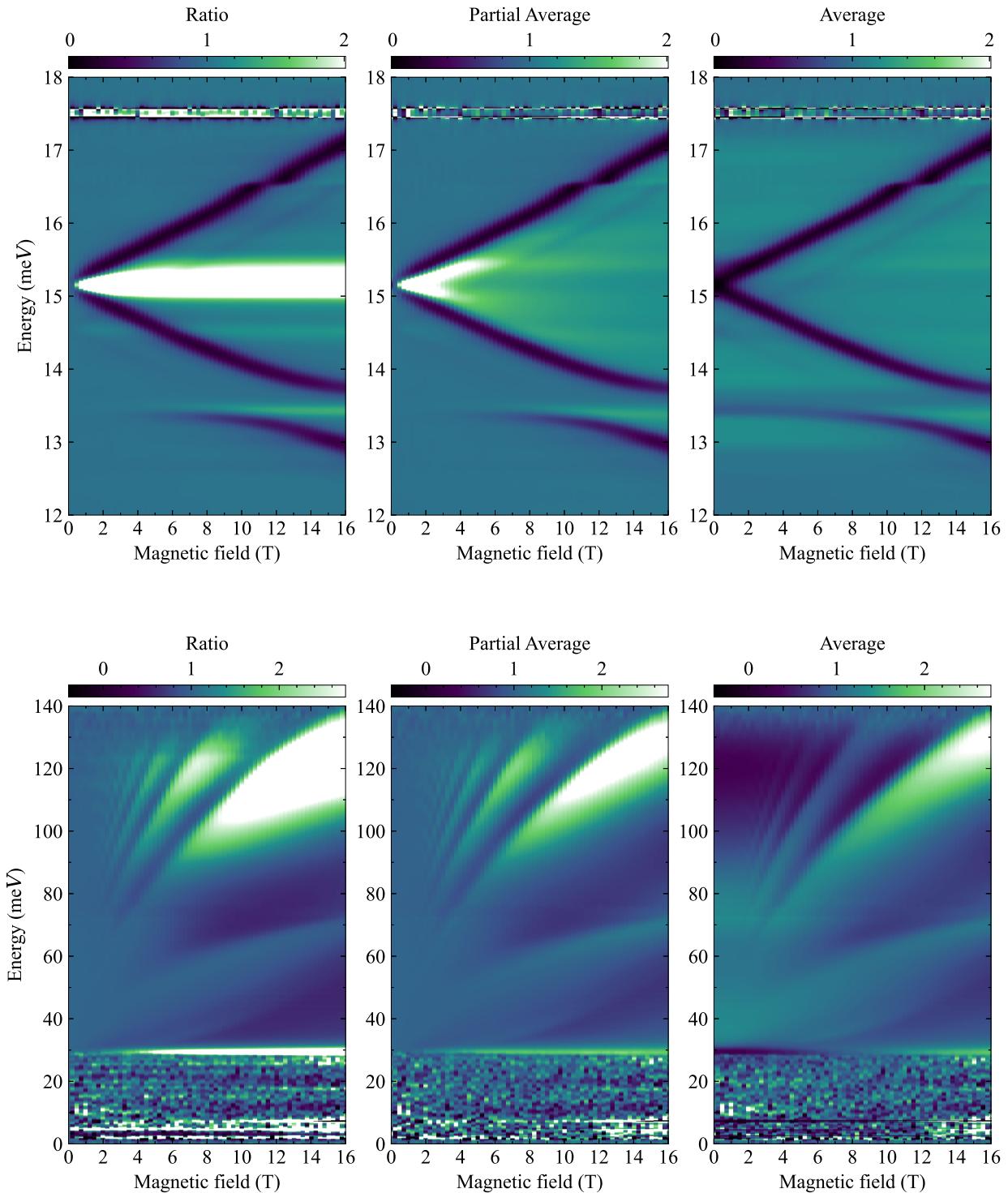


Figure IV.4: Comparison between "Ratio" "Average" "Partial Average"

or examining the three bottom panels in Fig IV.4. It's evident that the [Average] option has degraded the baseline in lower magnetic fields, particularly at energies where intense transitions are present at higher fields. In contrast, [Partial Average] preserves the integrity of the curves.

IV.3 Differential, Differential Average and Differential Energy

With these options, we can effectively eliminate the background contribution in TlBiSeS and isolate the intra-Landau level transitions. The **[Differential]** option is also well-established and can be expressed mathematically as:

$$\frac{S(B)}{S(B - 1)}. \quad (\text{IV.5})$$

In this case, we use the previous magnetic field as the normalizing curve. If you apply this option to the TlBiSeS data and adjust the color bar, you can generate a refined color map, as shown in Fig. IV.5.

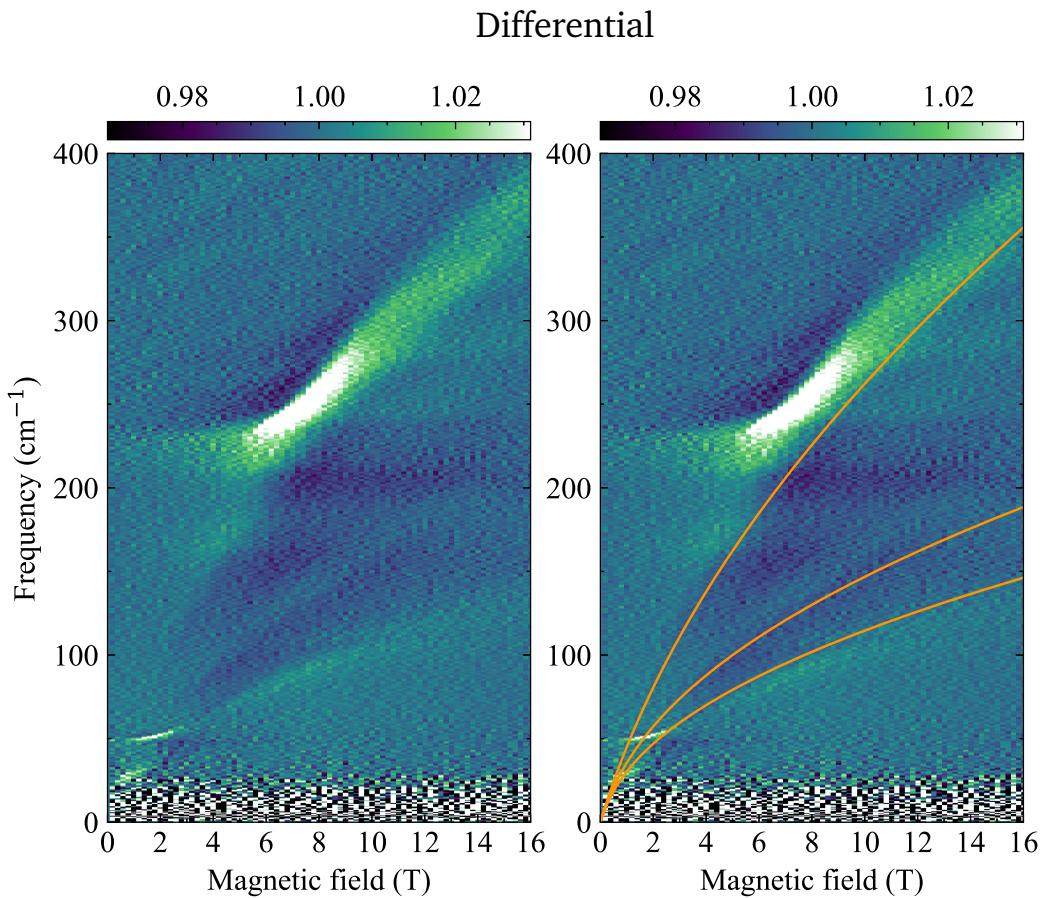


Figure IV.5: Differential option

The **[Differential]** option also enables the cancellation of constant features in energy, such as phonon modes. However, it can also eliminate certain electronic backgrounds that other treatments may not. Nonetheless, the signal modulation becomes significantly attenuated, leading to increased noise in the data. To address this, I introduced the idea of combining averaging and differential treatments in the **[Differential Average]** mode. The formula for this mode is as follows:

$$\frac{S(B)}{\text{Average}(S[B - k : B + k])} = \frac{S(B)}{S[B - k' : B + k]} \quad (\text{IV.6})$$

Here, k and k' represent a variable number of curves that can be selected within the software, centered around the magnetic response $S(B)$. The term $\overline{S[B - k' : B + k]}$ denotes the average of all the curves within the range $B - k'$ to $B + k$. In the software, the parameters k and k' will be visible below the "combo" list of options when the **[Differential Average]** mode is selected. Two lines named "Min" and "Max" will appear. Although I allow for asymmetry around B , I recommend keeping this option symmetric, meaning $k = k'$. Let's take, for example, $k = k' = 7$. The result should resemble something like this:

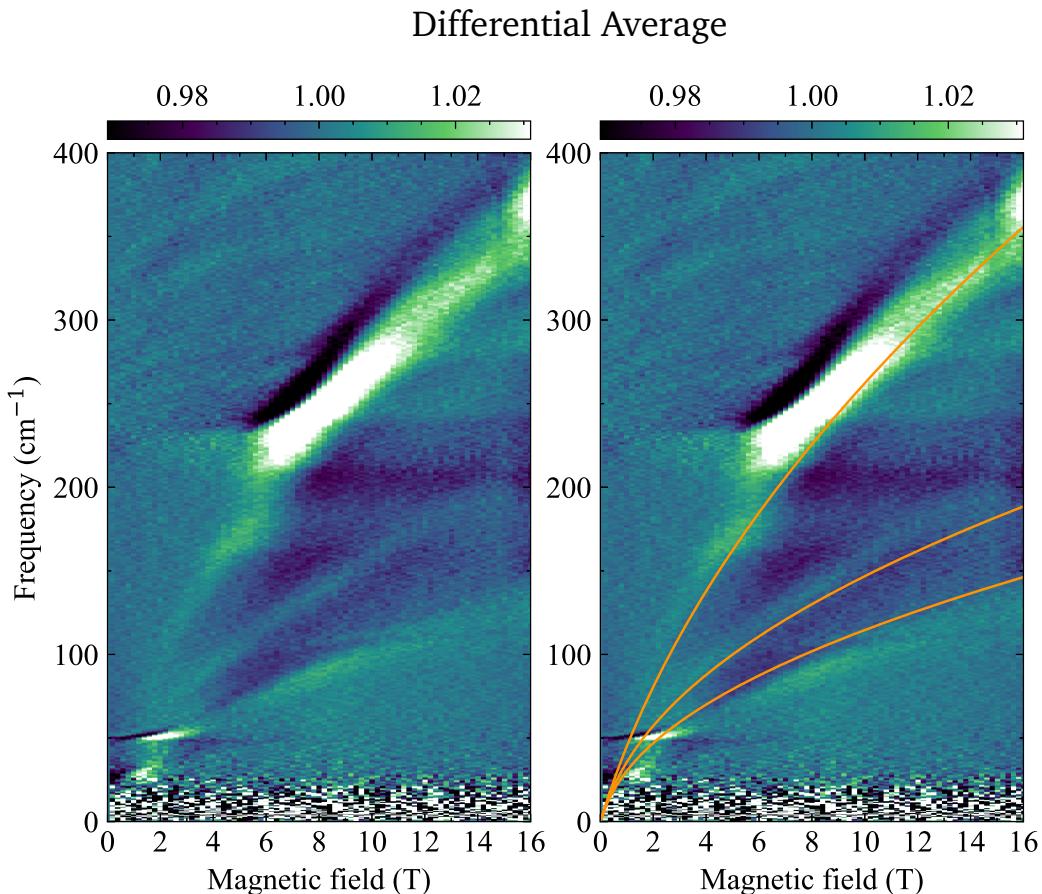


Figure IV.6: Differential option

This normalization technique proves to be powerful as it effectively magnifies the signal. The **[Differential Average]** option, in particular, offers a finer tuning in the averaging process, enhancing its overall effectiveness.

It's important to note the boundary condition used in Equation IV.6. When k or k' exceeds the number of remaining curves, there are two possible options. I experimented with a smooth approach that reduces the number of curves k' below B to maintain symmetric averaging around B' . Alternatively, I kept the same number of curves k' before B , introducing a slight asymmetry at the edges. After practical considerations, I opted for the second case (asymmetric), as it consistently provided more reliable color maps.

In a parallel approach, mirroring the concept of averaging slices along the y-axis (magnetic field), we can apply a similar technique along the x-axis (energy). This led to the addition of the **[Differential**

Energy] mode to the various normalization options. The mathematical expression for this mode is:

$$\frac{S(E)}{\text{Average}(S [E - k : E + k])} = \frac{S(E)}{S [E - k' : E + k]} \quad (\text{IV.7})$$

Interestingly, in the case of **[Differential Energy]**, having an asymmetric averaging around E is not as critical. However, it should be employed for a specific reason, which is also the drawback of this function: noise injection. The noise injection into the data originates from the edges of the measurement window, and the averaging process can fold this noise back into the data. Additionally, in transmission measurements, the Reststrahlen band can contribute to this noise injection effect. I recommend exercising caution when using this option, despite its potential for improving data visualization, as shown in Fig. I.2(b). This is particularly relevant in reflection measurements where a large energy range is accessible without noise.

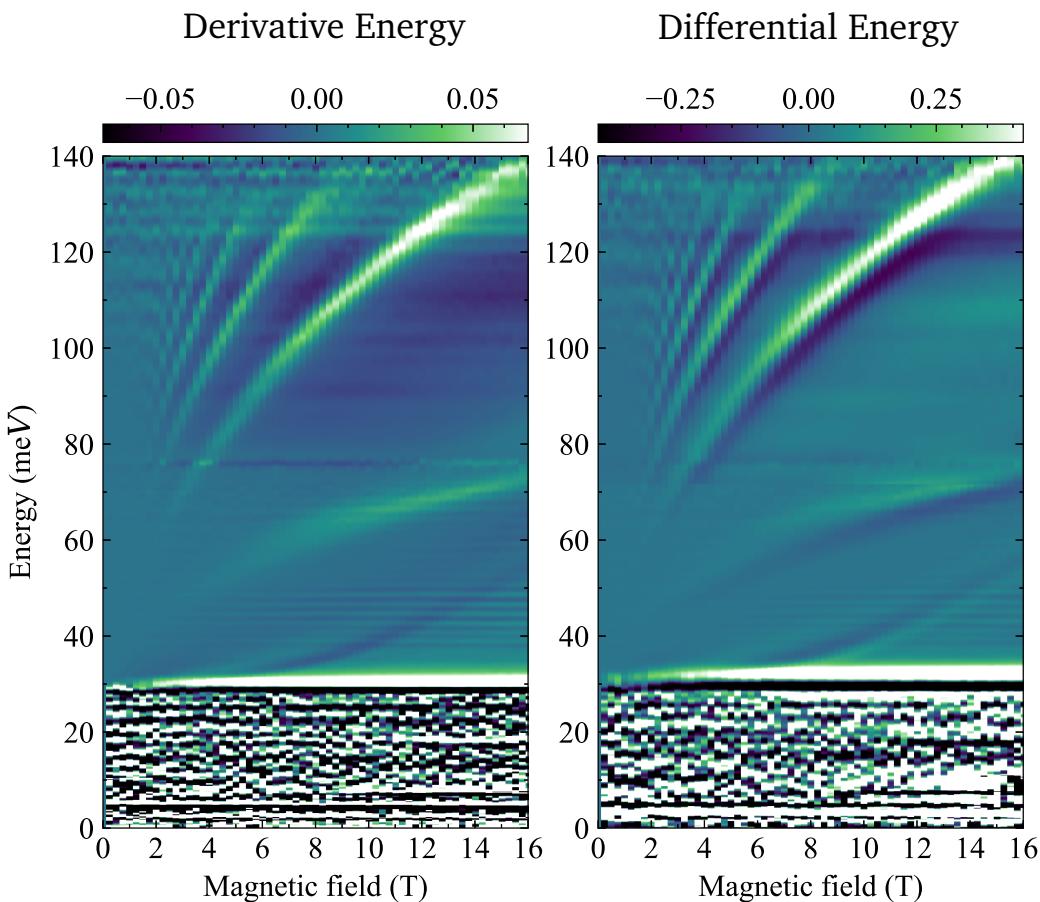


Figure IV.7: Differential option

Nevertheless, it is still feasible to apply the **[Differential Energy]** option to transmission data, as demonstrated in Fig. IV.7. In this comparison, I illustrate the difference between a normal energy derivative using the "gradient" function in Python and the **[Differential Energy]** option. The number of curves used, as per Equation IV.7, was $k = k' = 5$. This analysis was conducted after the logarithm transformation on the TlBiSeS transmission data from the previous chapter.

IV.4 Absolute and RawData

For this option, there isn't much to elaborate on. The normalization performed here depends on whether the check button [**Ref Files**] is selected or not. If you have reference files, you will plot:

$$\frac{S(B)}{R(B)} \quad (\text{IV.8})$$

Here, $S(B)$ represents the sample signal, and $R(B)$ represents the reference. In cases of well-acquired reference data, this equation can be considered as the absolute transmission or reflection.

If you don't have a reference or choose not to use them (unchecked [**Ref Files**] button), the [**Absolute/RawData**] option will plot the raw sample data without normalization.

V | Control center and Map evolution

In this chapter, we will explore how to interact with the complete data set of an item and apply certain data corrections to enhance color maps. Additionally, we will examine a function within the software that enables us to observe the evolution of features between maps.

V.1 Control center

As discussed in Chapter III, you can right-click on an item in the [Files item] list. The first option should be named [Control center], offering two possibilities: [Open] and [Fast Baseline]. If you choose [Open], a new window should appear, as depicted in Fig. V.1.

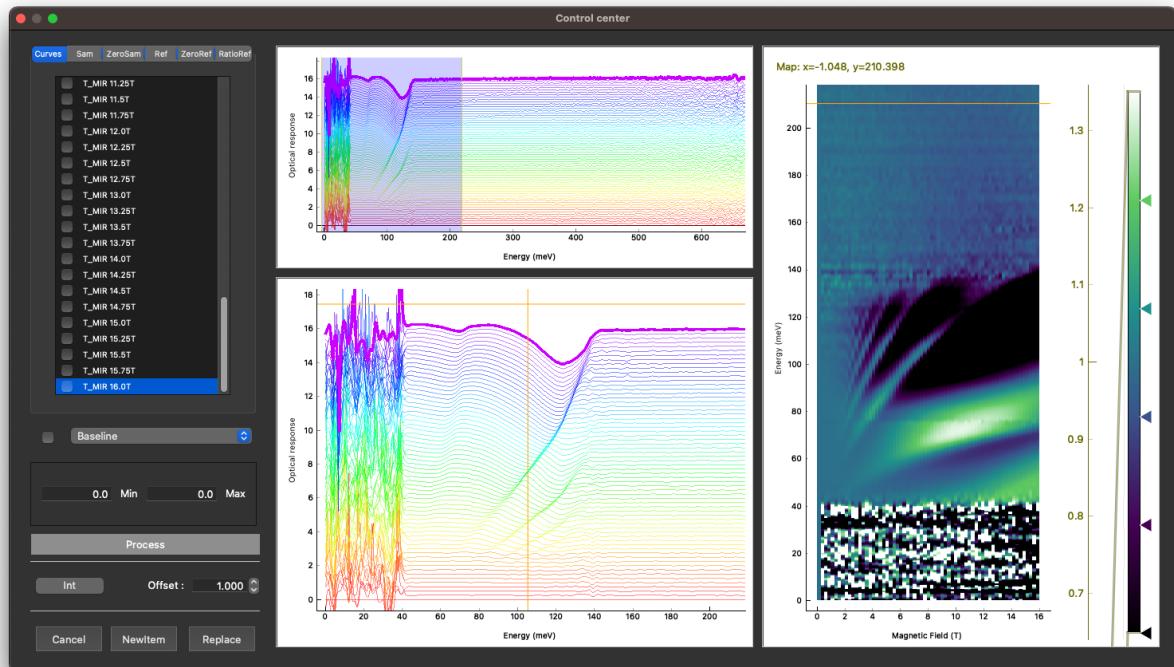


Figure V.1: Window page of the control center

This window consists of three graphs: two stacked plots and one color map. The top-left graph displays the full range of the data set with an interactive blue-shaded region. The bottom-left graph provides a magnified view of the stack plot within the blue-shaded region. The same region is also highlighted in

the color map.

On the far left side of the [Control center] window, six different [tabs] of data are arranged:

Curves – In this tab, you will find the current normalization used in the main window.

Sam – Here, you will find the raw curves of your sample field data.

ZeroSam – This tab contains both the raw curves and interpolated ones for the zero sample field measurements.

Ref – In this tab, you will find the raw curves and interpolated (if needed) data for the reference field measurements.

ZeroRef – In this tab, you can access the raw curves and interpolated data (if needed) for the zero reference field measurements.

RatioRef – This tab will display the ratio of your reference field over the zero reference.

Switching from one tab to another will alter the content on the graph, optimizing the visualization of the entire item.

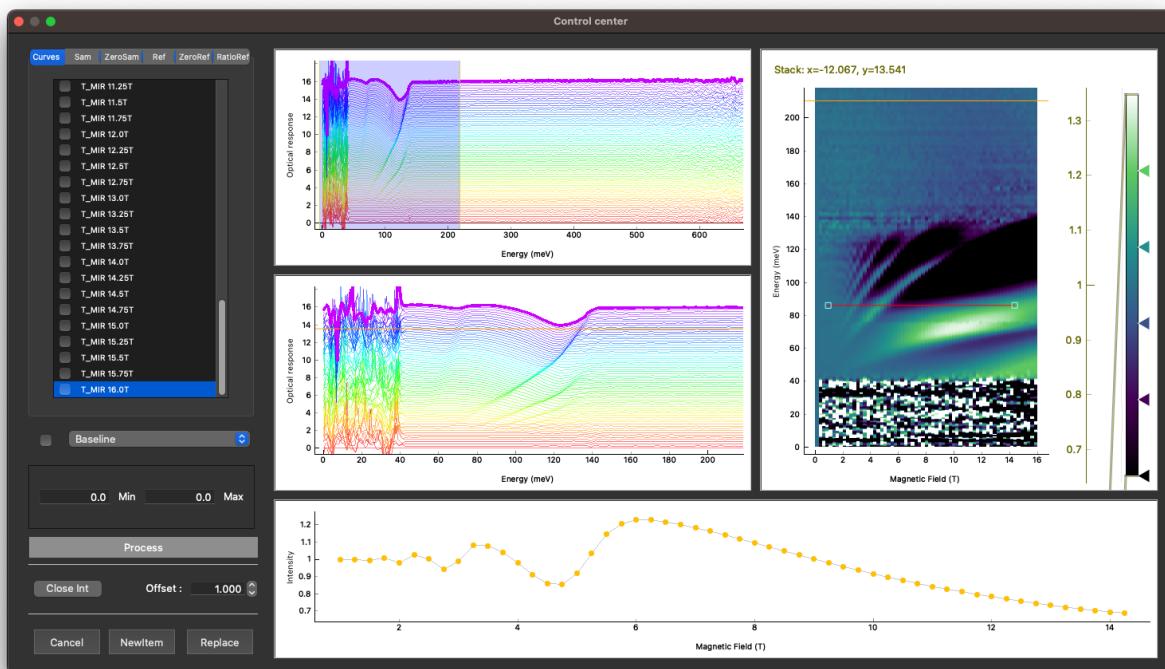


Figure V.2: Window page of the control center, with the intensity graph

Another graph, positioned at the bottom of the page (see Fig. V.2), becomes available after clicking on the button [Int]. This graph illustrates the intensity dependence in the magnetic field of a defined line cut from the color map. After clicking, a red line should appear on the color map at the (0,0) to (1,1) coordinate. You can freely move it in height and length, but diagonal cuts may be less accurate, and you cannot go beyond the bounds of the color map. This function is still evolving, and any good ideas for its use are welcome. The button name [Int] changes to [Close Int] to remove the graph.

V.1.1 Baseline correction

A quick reminder: the relative change of a sample in a magnetic field should be equal to "1" if no changes are observed. Therefore, all the curves should align with this value, regardless of the field. However, it might happen that this is not the case, and some curves are slightly off. A baseline correction will add or subtract a constant to compensate for any drift.

Just below the tabs, there should be a region (depicted in Fig V.3) reserved for applying modifications to the current item. The first option on the list is the **[Baseline]**. To proceed, check the box on the right of the "combo" list and define a range of the x-axis (here energy) region, depending on the unit. This region should mostly contain no transitions or features. Once selected, click the button **[Process]** to observe the change in the graphs.

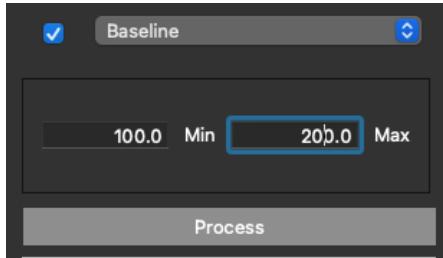


Figure V.3: Baseline correction

The software will calculate the average value of this selected region and find the appropriate constant to bring all the curves back to "1". It's important to note that, for now, this is just a constant shift of the spectra; a baseline correction may work well in one region of energy but not across the entire range. I hope to implement a "background" correction in the future that could take the full range of energy into account, if you find it of interest.

The baseline correction is indeed very useful and widely used. I've added a way to apply a **[Fast Baseline]** correction without entering the **[Control center]** window. You can right-click on the item and select "Control center" → "Fast Baseline". Alternatively, uncheck the box on the left of the **[Status item]** (see Fig. V.4). In both cases, a small window should pop up with two lines to define the spectral region with which the baseline correction will be performed.



Figure V.4: Fast Baseline window

V.1.2 Smooth correction

It's important to clarify that smoothing will be applied to the reference data, not the sample data. Therefore, if you don't have a reference measurement, the smoothing will have no effect.

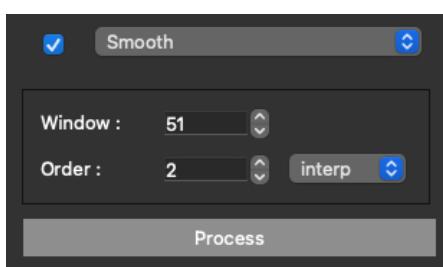


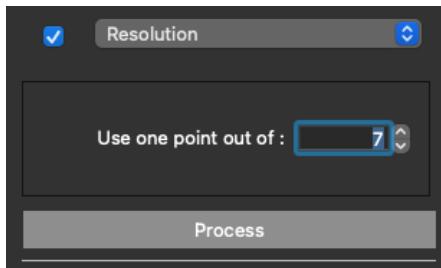
Figure V.5: Smooth correction

It's generally not advisable to smooth data that exhibits features, and such an operation is not permitted within this software. However, sample data can be corrected by a reference measurement, which might introduce some noise into the sample measure. To mitigate this, you can smooth the reference curves. Optical spectra, with their abrupt changes in response, can be challenging to smooth. In such cases, the ratio $R(B)/R(0T)$ will be used instead, as indicated by the last **[tab]**.

The process to apply the [Smooth] correction is similar to before. You begin by checking the small box on the left of the list, as displayed in Fig. V.5. Afterward, you define a mode of smoothing, here [interp], and modify the [Window/Order] lines. Changing one of the three last options will automatically smooth the reference and alter the curves on the graphs.

V.1.3 Resolution correction

This data correction is arguably the least significant and may be replaced by something more useful in the future.



Essentially, this correction allows you to plot one point out of every n points, a value you can define (here set to 7 in Fig. V.6). This can be applied if you have too much resolution or data points within the curves, causing the software to lag, especially in the [Stack] tab.

Figure V.6: Smooth correction

V.1.4 Absorption–log

As mentioned in Chapter III, the [Absorption–log] transformation can be applied directly in the [Status item] of an item by clicking on the checkbox.

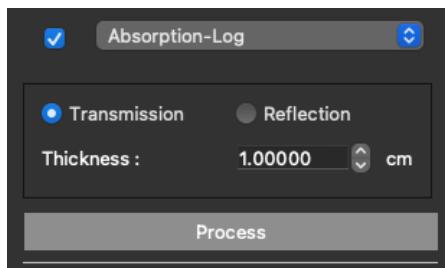


Figure V.7: Absorption–log transformation

The mathematical expression used will be:

$$A = -\log(S) \quad (\text{V.1})$$

where A is the absorbance and S is the current normalization used within the software. This transformation is applicable if you have transmission data; for reflection data, you would simply apply a logarithm transformation. In the case of transmission, most of the normalizations discussed here focus on the relative change in the magnetic field. Therefore, Equation V.2 will give you the relative absorbance of the system.

However, in the [Absolute/RawData] option with proper reference files you should obtain the "real" absorbance of your system.

In the case of one thin layer, with two symmetrical boundaries, we can express the transmission as:

$$T = \frac{[(1 - R)^2 + 4R \sin^2 \phi_T] e^{\alpha d}}{(1 - Re^{\alpha d})^2 + 4R \sin^2(\beta + \phi_T) e^{\alpha d}} \quad (\text{V.2})$$

With R being the bulk reflectivity, ϕ the phase change upon transmission, α is the absorption, β to be continue

V.2 Map Evolution



In the command section, you will find an icon button named **[Map evolution]**, as shown in the image on the left. Clicking on it should open a new window, as displayed in Fig. V.8. It's important to note that this function can only be activated if you are in one of the color map **[tabs]**; if you are in the stack tab, nothing will happen. This function was designed to observe the evolution of a color map concerning a third external parameter. To be more precise, you could measure the magneto-optical response of a sample at different temperatures. Since you can load multiple items in the main window, you can upload all the temperatures (in order) and use **[Map evolution]** to see how your transition may evolve. The third external parameter could also be pressure or chemical doping.

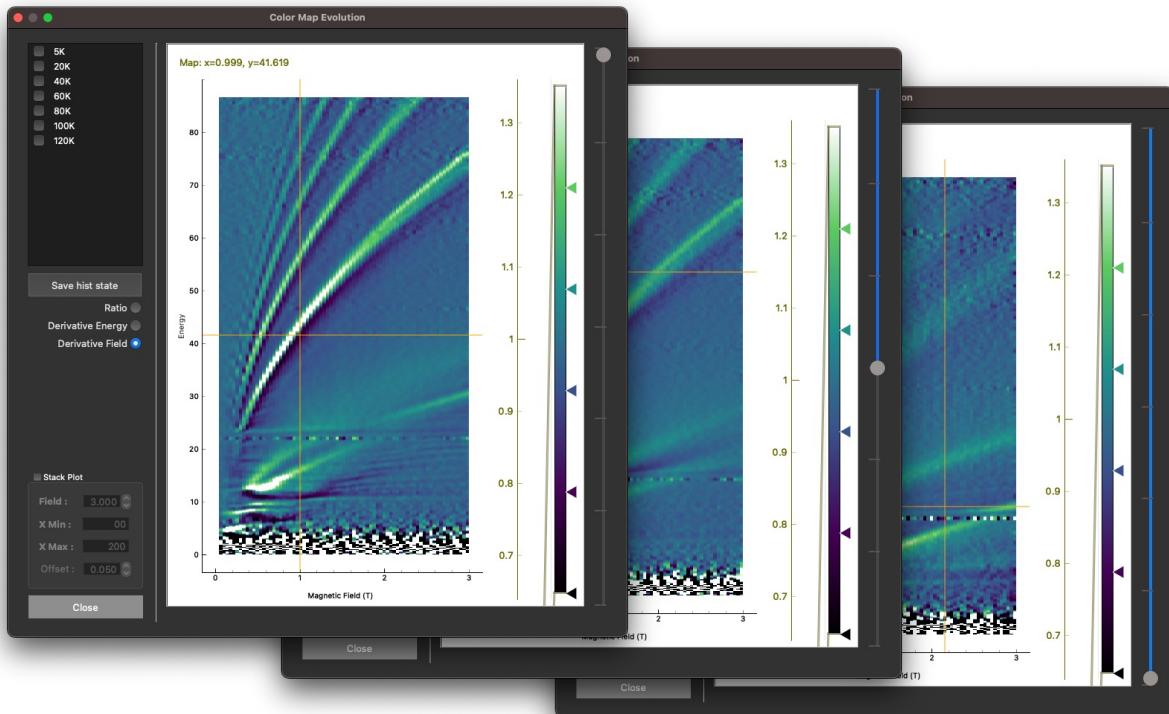


Figure V.8: Window page of the Color Map Evolution

The **[Map evolution]** window, as seen in Figure V.8, is comprised of a list on the left containing all the items from the main window. In the middle is a graph of the color map, and on the full right is a **[Slider]**. The **[Slider]** will be subdivided into steps corresponding to one item in the list. By moving the slider along all the steps, a progressive shading of all the items will be made to observe any evolution of the features as smoothly as possible.

On the left part of the **[Map evolution]** window, you can find a button named **[Save hist state]**. The color scheme for each map will be the same as in the main window, but with this button, you can save the state of a modified map by simply clicking on it. To interact again with one item, you need to double-click on it. The slider should automatically go to the correct steps, although there is an unfixed

bug that may occasionally prevent it from working as expected.

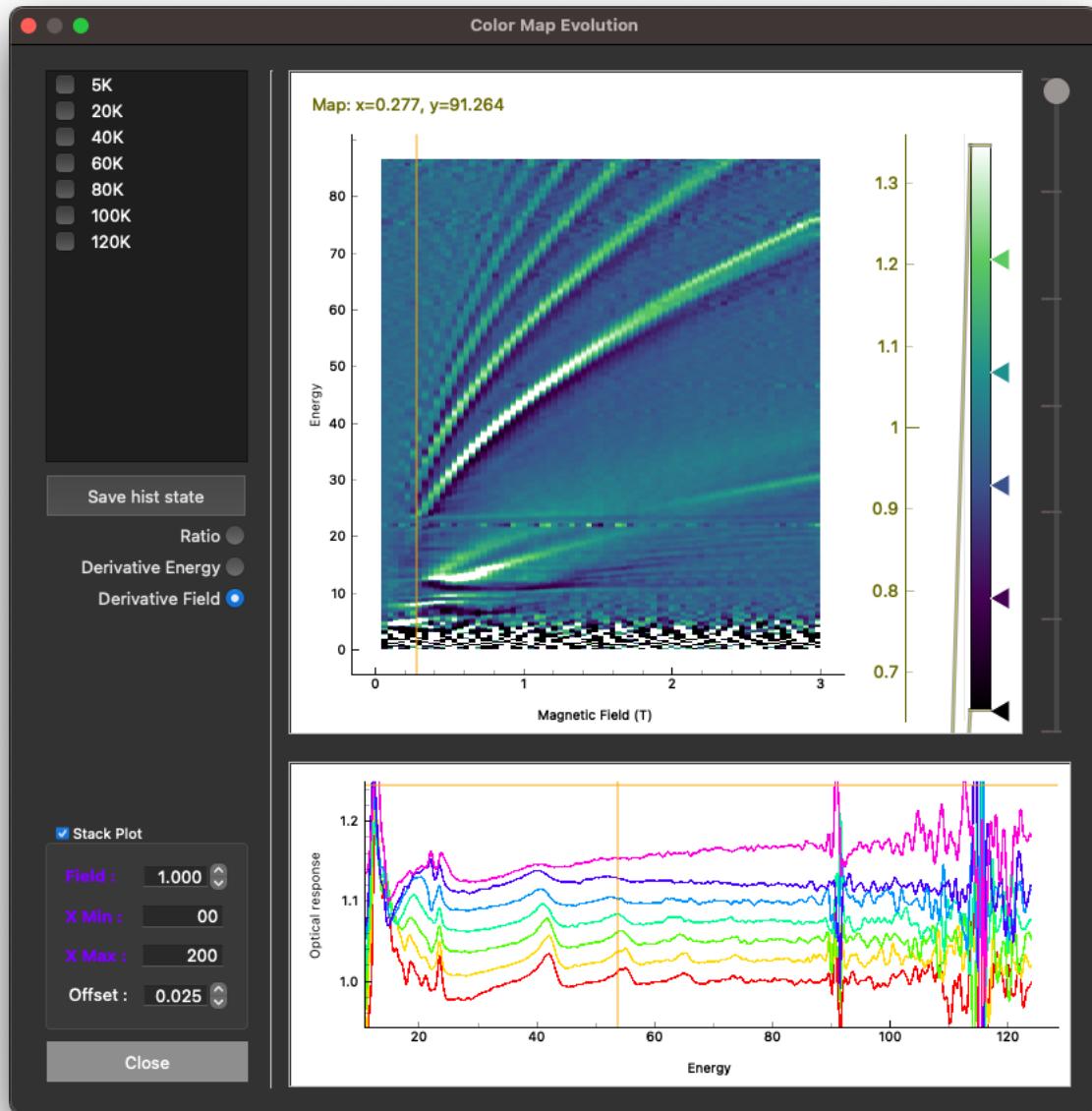


Figure V.9: Window page of the Color Map Evolution, with the stack plot section

The [Map evolution] window also features a stack plot graph that can be accessed when you click on the group box named [**Stack Plot**] (bottom left), as shown in Fig. V.9. The stack plot will depict the evolution of one magnetic field, in this case, 1T, for all the color maps.

VI | Color Map and Stack exportation

This chapter will cover the extraction of the stack curves or the color map in the form of a figure for possible inclusion in an article. Given that this software enables fine-tuning of the color scheme and offers an intuitive way to modify and enhance these color shades to maximize the visualization of features, it would be unfortunate not to be able to generate images of them.



You may find an icon named **[Export]** in the **[Commands icons]** section, with the logo depicted above. This icon is linked to two different windows that will open depending on which **[tab]** of the main window you are in. One of the new windows will be dedicated to the extraction of stacking curves, and the other for the extraction of the map(s). They are very similar and only differ in a few options.

You can collect a lot of data inside the software, but you may choose to plot only a specific subset. Only the item checked in the **[Files item]** or **[Points item]** will be plotted. If none of them are checked, all the data will be plotted.

The image formats available for saving a picture are "jpg," "png," and "pdf." This software was developed on Mac, and it is also possible on this OS to extract in the formats "ps" and "eps" (not possible on Windows, but hopefully, this will be corrected in an update).

VI.1 Stack exportation

Let's start with the Stack case and understand the mechanics behind plotting a figure. To reach the **[GraphStack]** window, you should be in the **[Stack]** tab and click on the **[Export]** icon button. A window of the shape, as shown in Fig. VI.1, should appear. In this example, I've already plotted the stacks of TLBiSeS in transmission, without logarithmic transformation. In Fig. VI.1, I've also labeled a few important steps to help you produce an image.

(a) – The first step is to define a name and a path inside your computer for the image to be saved. Click on **[Path]**, choose a name, and press **[Ok]**. A line of the path should appear; without this line, no image can be printed, it's a common mistake that can be made.

– The default format will be "jpg." To use another format, just change the extension name to "png" or "pdf." Note that in the "pdf" case, if you are running on Windows, the image may not appear (for some reason) but will still be saved inside the folder. On Mac, the "pdf" should appear, but with a low quality that is not actually the quality of the image saved. On Mac, if you save with "ps" or "eps," the image will not be displayed in the **[GraphStack]** window. Therefore, it is better to build the image in "jpg" and save it in another format when you are satisfied with it. I'll try to find a better way in an update.

(b) – You can define your labels for the x and y axes in the line at the bottom of the window, or use the shortcut [button] on the left side of the window. This shortcut is also there to remind us that we are in a Python shell, so we have to use the Python language to write, such as "\$" for exponentiation.

(c) – The bottom of the window will be composed of parameter lines for the image, such as font size or figure resolution.

– You can notice a line named [Label Stack], which will define the legend regarding the Tesla in our case. You have to write the increment number, here "2" and the unit, here "T". Both pieces of information should be separated by one space. If you don't want any legend, just uncheck the [Check] button on the right side or write "0 T".

– You will find a [Gradient] list with different colors, along with an [Inverse] check button to change, obviously, the order of the colors. This check button should be off for color schemes such as "Blue–Red."

– The [Offset] line is the same as the main window. The [LW] line is the Line Width of the curves.

– Warning: the image inside the [GraphStack] window will be scaled according to the [Fig X size/Fig Y size] line; thus, if this number is too large, it will enlarge the window excessively.

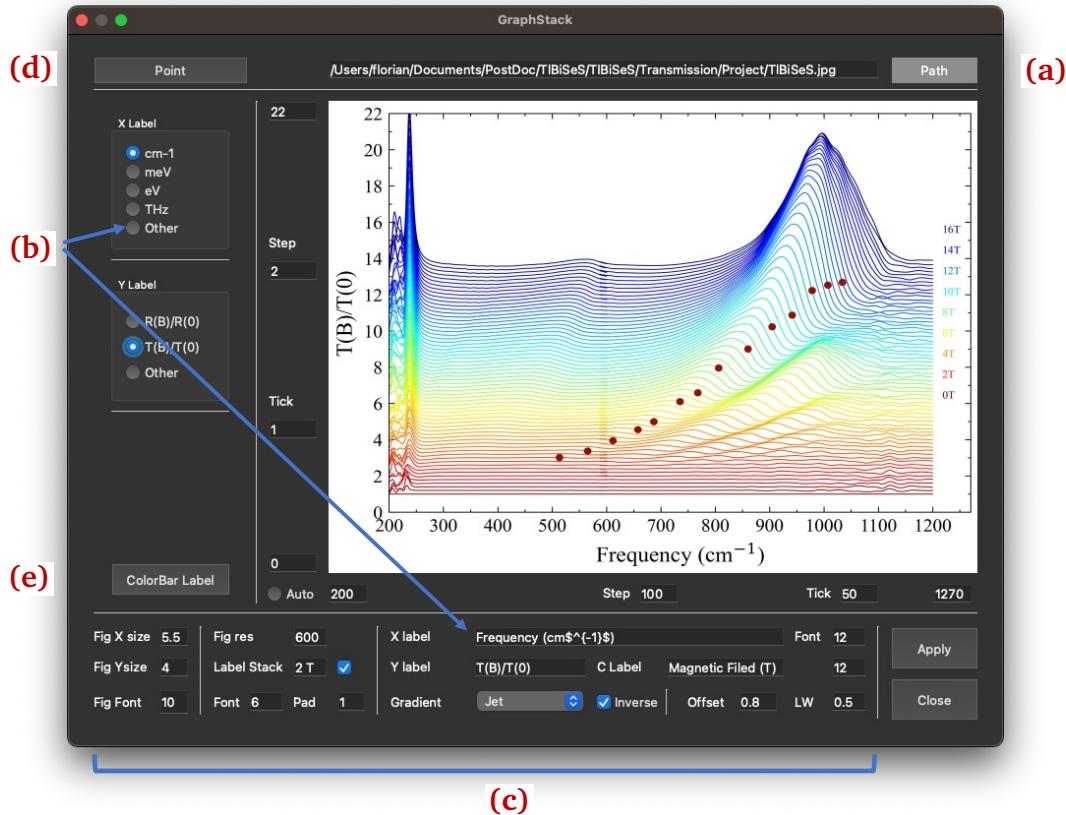


Figure VI.1: GraphStack window to export stack figures.

(d) – As you can see in the image in Fig. VI.1, the points we picked are plotted. To interact with those

points, click on the button **[Point]** in the top-left corner of the **[GraphStack]** window. A section, as shown in Fig. VI.5, should appear. The default color of those points is black. To change them, double-click on the item and select a new color. The item's background color should change.

- If you **[Check]** the item, the points will become a line. You can define a dot line or not with the **[Marker]** section, and a line style in the **[LineStyle]**. The **[Point size]** line will also affect the line width. It should have some reasonable proportion between the line and points.

- The **[Clear]** button is used to remove the points if you don't want them on the figure.

- Warning: All modifications to the points (colors mainly) will be erased if you close the **[GraphStack]** window.

- Instead of the normal legend, you can have a color bar legend. This is a bit tedious, but you should first uncheck the **[Label stack]** checkbox. Click on the button **[ColorBar label]**. A new section will appear, as represented in Fig. VI.3.

The **[Color label]** will refer to the position of the color bar. **[Right]** will take the full size of the Y length of the picture and be outside of the image. If you choose **[Custom]**, as in Fig. VI.3, the color bar will be inside the image, and you could define the position, length, height, etc. The section **[Range]** will allow you to control the ticks of the color bar. And finally, in Fig. VI.1 (c), the **C label line** will be the legend of the color bar if you use it.

Finally, The button **[Auto]** is there to find an automatic scaling range in the X and Y axis of the figure.

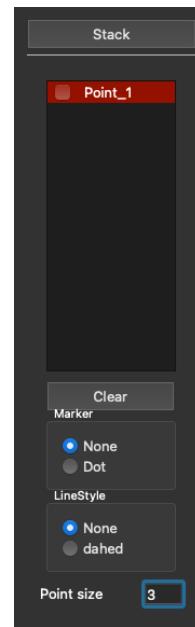


Figure VI.2: Point section

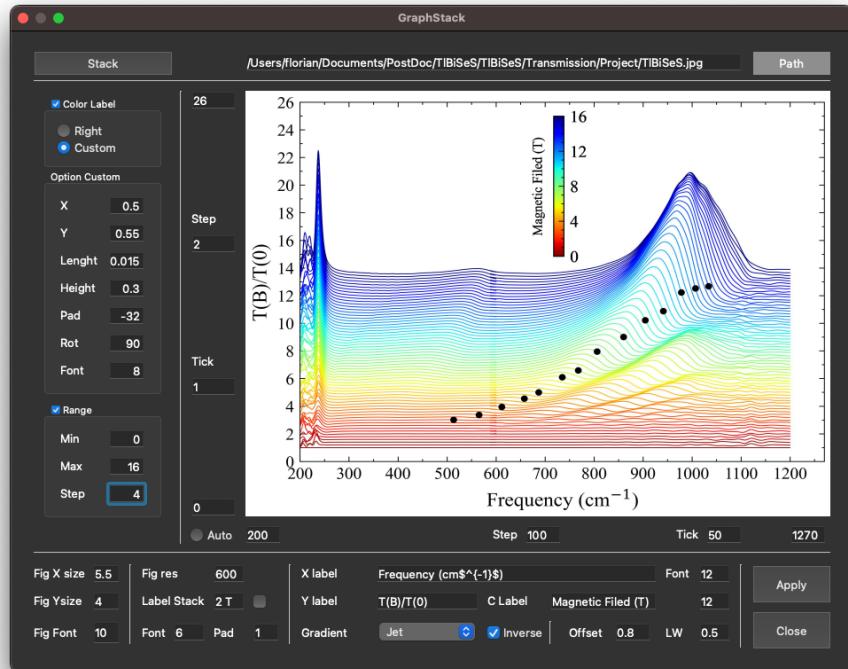


Figure VI.3: GraphStack window to export stack figures, with the color bar option.

VI.2 Map exportation

In the same manner as the stack, to export a map, you need to be on the [Tab] that you want and click on the icon button [Export]. A window named [Graph] should appear, as shown in Fig. VI.4. Its structure is basically the same as what we have seen previously.

It will operate the same way. One difference will be the button [T] (Top), [R] (Right), and [N] (None), for the position of the color bar. The little line with the number "1" in it will be the width of the color bar.

On the map picture in Fig. VI.4, I also plot the modeling so here is how the Point section looks like in this case.

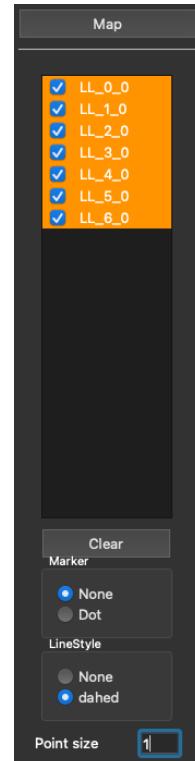


Figure VI.5: Point section 2

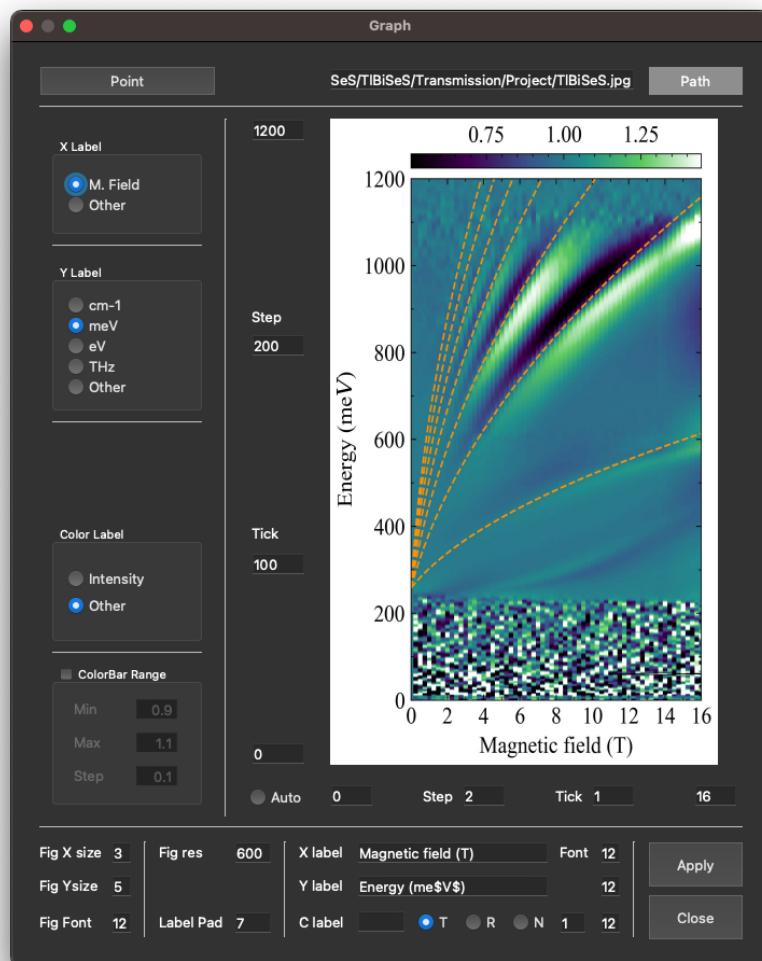


Figure VI.4: Graph window to export map(s) figures.

Appendices

A | Command summary

Table A.1:

Name	Icon Button	Description
Load Data		Allow to load CSV shape or data from this software
Save Data		Save the data present in the software
Export Graph		Allow to extract the in an image the graph seen in the software. Format available are: jpg, png, pdf and for Mac eps (and ps)
Change Range		Can specify the X or Y limit of your stack and map, depending on which graph is visible when you click on it. Allow also to change the color bar range.
Auto Range		Automatically magnify the graph to visualize the full set of data. This function is mainly based on the PyQt Graph auto range function for the color map, but is slightly improved for the Stack curves when large spike noise signals are present.
Zoom or Drag		This button is made to simplify the change of the mouse mode in the graph made by PyQt Graph. If you click on this Icon button you could zoom inside the graph by clicking in one point and draw a yellow rectangle of the region of interest.

Continued on next page

Table A.1: (Continued)

Zoom or Drag		This button is made to simplify the change of the mouse mode in the graph made by PyQt Graph. If you click on this Icon button the graph become "interactive" like with the mouse (default settings).
Points		Allow to pick points inside the color maps only. it will automatically found the intensity of that point and draw it on the "Stack" tab curves.
Fitting		This Icon button provide a simple basic modeling tools to "Fit" your data.
Map Evolution		You can visualize a evolution of all your map present in the software, by a gradual shade gradient between them. (Can be use for temperature dependence of the magnetic response of a sample in a define energy region)
Tool		Some useful operating tool for the "Files Item" only.
Calculator		Calculatrice that can do some matrix operation on the "Files Item" only.

B | Model used in the Fit window

In this appendix, I just give the equations of the model used in the [Fit] window. All the parameters put in red are the free parameters that can be interactively modified for a fine-tuning of the model.

Landau levels for parabolic band

$$E_n^{Inter} = \frac{\hbar e B}{\textcolor{red}{m_{eff}} * m_e} | n + \frac{1}{2} | + \frac{\hbar e B}{\textcolor{red}{m_{eff}} * m_e} | n + \frac{3}{2} | + 2\Delta. \quad (\text{B.1a})$$

$$E_n^{Intra} = \frac{\hbar e B}{\textcolor{red}{m_{eff}} * m_e} | n | \quad (\text{B.1b})$$

E_n^{Inter} , E_n^{Intra} are the energy of the inter/intra Landau level transition, \hbar Planck constant, e is the electric charge, B is the magnetic field, m_e is the bare mass of electron, $\textcolor{red}{m_{eff}}$ is the effective mass, Δ is the gap.

Landau levels for linear band

$$E_n^{Inter} = \sqrt{2\hbar e \textcolor{red}{v}^2 B | n + 1 | + \Delta^2} + \sqrt{2\hbar e \textcolor{red}{v}^2 B | n | + \Delta^2}. \quad (\text{B.2a})$$

$$E_n^{Intra} = \sqrt{2\hbar e \textcolor{red}{v}^2 B | n + 1 | + \Delta^2} - \sqrt{2\hbar e \textcolor{red}{v}^2 B | n | + \Delta^2}. \quad (\text{B.2b})$$

E_n^{Inter} , E_n^{Intra} are the energy of the inter/intra Landau level transition, \hbar Planck constant, e is the electric charge, B is the magnetic field, Δ is the gap, $\textcolor{red}{v}$ is the in-plane velocity.

Magnon dispersion – easy axis

$$E \pm = \textcolor{red}{E}_\Delta \pm \textcolor{red}{g} \mu_B B. \quad (\text{B.3})$$

$E \pm$ are the upper and lower magnon branches, $\textcolor{red}{E}_\Delta$ is the magnon gap energy, $\textcolor{red}{g}$ is the g-factor, μ_B is the Bohr magneton, B is the magnetic field

Magnon dispersion – hard axis

$$E = \sqrt{\textcolor{red}{E}_\Delta^2 + (\textcolor{red}{g} \mu_B B)^2}. \quad (\text{B.4})$$

$\textcolor{red}{E}_\Delta$ is the magnon gap energy, $\textcolor{red}{g}$ is the g-factor, μ_B is the Bohr magneton, B is the magnetic field.

VI | Bibliography

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