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Colophon

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The source code of this book is available at:

<https://github.com/fmarotta/kaobook>

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The harmony of the world is made manifest in Form and Number, and the heart and soul and all the poetry of Natural Philosophy are embodied in the concept of mathematical beauty.

– D'Arcy Wentworth Thompson

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Part I

**A FLEXIBLE PYTHON TOOL FOR
FOURIER-TRANSFORM NOISE
SPECTROSCOPY**

The `python_spectrometer` software package

1

In this chapter, I will lay out the design and functionality of the `python_spectrometer` Python package.¹

1.1 Package design and implementation

The `python_spectrometer` package provides a central class, `Spectrometer`, that users interact with to perform data acquisition, spectrum estimation, and plotting. It is instantiated with an instance of a child class of the DAQ base class that implements an interface to various data acquisition device (DAQ) hardware devices. New spectra are obtained by calling the `Spectrometer.take()` method with all acquisition and metadata settings.

In the following, I will go over the the design of these aspects of the package in more detail.

1.1.1 Data acquisition

The `daq` module contains on the one hand the declaration of the DAQ abstract base class and its child class implementations, and on the other the `settings` module, which defines the `DAQSettings` class. This class is used in the background to validate data acquisition settings both for consistency (c.f. ??) and hardware constraints.

To better understand the necessity of this functionality, consider the typical scenario of a physicist² in the lab. Alice has wired up her experiment, performed a first measurement, and to her dismay discovered that the data is too noisy to see the sought-after effect. She sets up the `python_spectrometer` code to investigate the noise spectrum of her measurement setup. From her noisy data she could already estimate the frequency of the most harrowing noise, so she knows the frequency band $[f_{\min}, f_{\max}]$ she is most interested in. But because she is lazy,³ she does not want to do the mental gymnastics to convert f_{\min} to the parameter that her DAQ device understands, L (see Table 1.1), especially considering that L depends on the number of Welch averages and the overlap. Furthermore, while she could just about do the conversion from f_{\max} to the other relevant DAQ parameter, f_s , in her head, her device imposes hardware constraints on the allowed sample rates she can select! The `DAQSettings` class addresses these issues. It is instantiated with any subset of the parameters listed in Table 1.1⁴ and attempts to resolve the parameter interdependencies lined out in ?? upon calling `DAQSettings.to_consistent_dict()`.⁵ This either infers those parameters that were not given from those that were or, if not possible, uses a default value. Child classes of the DAQ class can subclass `DAQSettings` to implement hardware constraints such as a finite set of allowed sampling rates or a maximum number of samples per data buffer.

1: The package repository is hosted on [GitLab](#). Its documentation is automatically generated and hosted on [GitLab](#) as well. Releases are automatically published to [PyPI](#) and allow the package to be installed using `pip install python-spectrometer`.

Table 1.1: Variable names used in ?? and their corresponding parameter names as used in `python_spectrometer` and `scipy.signal.welch()` [1].

Variable	Parameter
L	<code>n_pts</code>
f_s	<code>fs</code>
K	<code>noverlap</code>
N	<code>nperseg</code>
M	<code>n_seg</code>
f_{\min}	<code>f_min</code>
f_{\max}	<code>f_max</code>

2: Let's call her Alice.

3: Physicists generally are.

4: `DAQSettings` inherits from the builtin `dict` and as such can contain arbitrary other keys besides those listed in Table 1.1. However, automatic validation of parameter consistency is only performed for these special keys.

5: Since the graph spanned by the parameters is not acyclic, this only works *most* of the time.

6: Settings are automatically parsed when passed to the `take()` method of the `Spectrometer` class.

Listing 1.1: `DAQSettings` example showcasing automatic parameter resolution. `n_avg` determines the number of outer averages, *i.e.*, the number of data buffers acquired and processed individually.

```
>>> from python_spectrometer.daq import DAQSettings
>>> settings = DAQSettings(f_min=1.5, f_max=7.2e4)
>>> settings.to_consistent_dict()
{'f_min': 1.5,
 'f_max': 72000.0,
 'fs': 144000.0,
 'df': 1.5,
 'nperseg': 96000,
 'noverlap': 48000,
 'n_seg': 5,
 'n_pts': 288000,
 'n_avg': 1}
```

```
{'f_min': 14.30511474609375,
 'f_max': 72000.0,
 'fs': 234375.0,
 'df': 14.30511474609375,
 'nperseg': 16384,
 'noverlap': 0,
 'n_seg': 1,
 'n_pts': 16384,
 'n_avg': 1}
```

Listing 1.2: Resolved settings for the same input parameters as in Listing 1.1 but for the `ZurichInstrumentsMFLIScope` backend with hardware constraints on `n_pts` and `fs`.

[2]: (n.d.), *Scope Module - LabOne API User Manual*

7: And issued a warning to inform the user their requested settings could not be matched.

8: Which might differ from the requested settings as outlined above.

For instance, Alice might want to measure the noise spectrum in the frequency band [1.5 Hz, 72 kHz]. Although she would not have to do this explicitly,⁶ she could inspect the parameters after resolution using the code shown in Listing 1.1.

If the instrument she'd chosen for data acquisition had been a Zurich Instruments MFLI's "Scope" module [2], the same requested settings would have resolved to those shown in Listing 1.2.⁷ This is because the Scope module constrains $L \in [2^{12}, 2^{14}]$ and $f_s \in 60 \text{ MHz} \times 2^{[-16, 0]} \approx \{915.5 \text{ Hz}, \dots, 30 \text{ MHz}, 60 \text{ MHz}\}$.

As already mentioned, the `DAQ` base class implements a common interface for different hardware backends, allowing the `Spectrometer` class to be hardware agnostic. That is, changing the instrument that is used to acquire the data does not necessitate adapting the code used to interact with the instrument. To enable this, different instruments require small wrapper drivers that map the functionality of their actual driver onto the interface dictated by the `DAQ` class. This is achieved by subclassing `DAQ` and implementing the `DAQ.setup()` and `DAQ.acquire()` methods. Their functionality is best explained at hand of the internal workflow. When acquiring a new spectrum, all settings supplied by the user are first fed into the `setup()` method where instrument configuration takes place. The method returns the actual device settings,⁸ which are then forwarded to the `acquire()` generator function. Here, the instrument is armed (if necessary) and subsequently data is fetched from the device and yielded to the caller `n_avg` times, where `n_avg` is the number of outer averages. Listing 1.3 represents the data acquisition workflow as pseudocode.

Listing 1.3: `DAQ` workflow pseudocode. A `SomeDAQ` object (representing the instrument `Some`) is instantiated with a driver object (for instance a `QCoDeS Instrument`). The instrument is configured with the given `user_settings`. Calling the generator function `daq.acquire()` with the actual device settings returns a generator, iterating over which yields one data buffer per iteration. The data buffers can then be passed to further processing functions (the power spectral density (PSD) estimator in our example).

```
daq = SomeDAQ(driver)
parsed_settings = daq.setup(**user_settings)
acquisition_generator = daq.acquire(**parsed_settings)
for data_buffer in acquisition_generator:
    do_something_with(data_buffer)
```

1.1.2 Data processing

Once time series data has been acquired using a given DAQ backend, it could in principle immediately be used to estimate the PSD following ???. However, it is often desirable to transform, or process, the data in some fashion. This can include simple transformations such as accounting for the gain of a transimpedance amplifier (TIA) to convert the voltage back to a current⁹ or more complex ones such as calibrations.

9: Although it is of course less than trivial to discriminate between current and voltage noise in a TIA.

1.2 Feature overview

Part II

CHARACTERIZATION AND IMPROVEMENTS OF A MILLIKELVIN CONFOCAL MICROSCOPE

Part III

ELECTROSTATIC TRAPPING OF EXCITONS IN SEMICONDUCTOR MEMBRANES

Part IV

A FILTER-FUNCTION FORMALISM FOR QUANTUM OPERATIONS

APPENDIX

Bibliography

- [1] *Welch — SciPy v1.15.2 Manual*. URL: <https://docs.scipy.org/doc/scipy/reference/generated/scipy.signal.welch.html> (visited on 03/31/2025) (cited on page 3).
- [2] *Scope Module - LabOne API User Manual*. URL: https://docs.zhinst.com/labone_api_user_manual/modules/scope/index.html (visited on 04/02/2025) (cited on page 4).

Special Terms

D

DAQ data acquisition device. 3, 4

P

PSD power spectral density. 4, 5

T

TIA transimpedance amplifier. 5