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# **Millikelvin Confocal Microscopy of Semiconductor Membranes and Filter Functions for Unital Quantum Operations**

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\* A  $\text{\LaTeX}$  lover/hater

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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# Software

The following open-source software packages were developed (at least partially) during the work on this thesis.

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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 introduce the `python_spectrometer` Python package<sup>1</sup> [1] and lay out its design and functionality. This software package was developed to make it easier for experimentalists to transfer the mathematical machinery introduced in ?? to the lab. While in principle the entire process of spectrum estimation from a given array of time series data is already covered by the `welch()` routine in SciPy [2], obtaining the data array is not standardized. Different data acquisition (DAQ) instruments have different capabilities, both on the hardware and the software level, and different driver interfaces to communicate with them. This implies custom data acquisition code is required for every instrument, introducing a significant entry barrier to spectral analysis. The `python_spectrometer` package implements a simple interface to different hardware instruments that allows for changing the hardware backend without having to adapt the user-facing code and also incorporates different hardware constraints.

What is more, noise spectroscopy tends to be a visual endeavor in practice; it is hard to compare different noise spectra based on quantitative reasoning alone. Data visualization is hence an integral part of noise spectroscopy, but plotting is not just plotting. Do we want the data to be shown on a log-log scale?<sup>2</sup> Do we want to show the relative magnitude of different data sets? Do we want to inspect the time traces as well? The `python_spectrometer` package addresses these questions by allowing users to interactively change features of the main plot window to adapt it to the form best suited to the situation at hand.

Moreover, when concerned with noise spectrum estimation, we are typically more interested in specifying parameters of the resulting power spectral density (PSD) rather than parameters of the underlying time series data. The `python_spectrometer` package approaches data acquisition from the inverse direction: rather than inferring the spectrum properties from the time series data, users specify the properties they would like the resulting spectrum to have and the package chooses the correct parameters for data acquisition accordingly.

## 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 DAQ hardware devices.<sup>3</sup> 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.

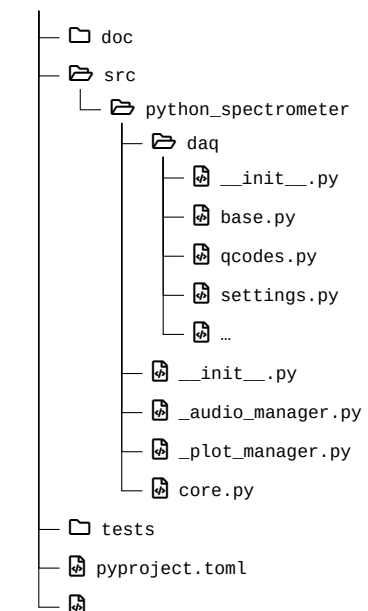
### 1.1.1 Data acquisition

Figure 1.1 shows the directory structure of the source code. The `daq` subpackage contains on the one hand the declaration of the DAQ abstract base class (`base.py`) and its child class implementations (`qcodes.py`, *etc.*), and on the other the `settings.py` module, which defines the `DAQSettings`

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

[2]: (n.d.), *welch* — SciPy v1.15.2 Manual

2: The short answer is yes, but it comes with visual side-effects that demand other ways of plotting data at times. The long answer is therefore yes, and ...



**Figure 1.1:** Source tree structure of the `python_spectrometer` package. Driver wrappers are placed in the `daq` subpackage. `core.py` exports the `Spectrometer` class.

3: Actually *drivers* to be more precise.

class. This class is used in the background to validate data acquisition settings both for consistency (see ??) and hardware constraints.

To better understand the necessity of this functionality, consider the typical scenario of a physicist<sup>4</sup> 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,<sup>5</sup> 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 1.1<sup>6</sup> and attempts to resolve the parameter interdependencies laid out in ?? and depicted in ?? upon calling `DAQSettings.to_consistent_dict()`.<sup>7</sup> 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.

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,<sup>8</sup> she could inspect the parameters after resolution using the code shown in Listing 1.1.

```
>>> 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}
```

If the instrument she'd chosen for data acquisition had been a Zurich Instruments MFLI's Scope module,<sup>9</sup> the same requested settings would have resolved to those shown in Listing 1.2.<sup>10</sup> 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 `Spectrometer`. 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()` meth-

**Table 1.1:** Variable names used in ?? and their corresponding parameter names as used in `python_spectrometer` and `scipy.signal.welch()` [2].

VARIABLE	\protect\textsc{Parameter}
$L$	<code>n_pts</code>
$N$	<code>nperseg</code>
$K$	<code>noverlap</code>
$M$	<code>n_seg</code>
$O$	<code>n_avg</code>
$f_s$	<code>fs</code>
$f_{\max}$	<code>f_max</code>
$f_{\min}$	<code>f_min</code>

4: Let's call her Alice.

5: Physicists generally are.

6: `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.

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

8: 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.

```
{'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`.

9: [https://docs.zhinst.com/labone\\_api\\_user\\_manual/modules/scope/index.html](https://docs.zhinst.com/labone_api_user_manual/modules/scope/index.html)

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

ods. Their functionality is best illustrated by the internal workflow as representatively shown in Listing 1.3.

```
daq = MyDAQ(driver_handle)

parsed_settings = daq.setup(**user_settings)
acquisition_generator = daq.acquire(**parsed_settings)

for data_buffer in acquisition_generator:
    estimate_psd(data_buffer)
```

**Listing 1.3:** DAQ workflow pseudocode. A MyDAQ object (representing the instrument My) 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 PSD estimator in our example).

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,<sup>11</sup> 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.<sup>12</sup> An exemplary implementation of a DAQ subclass for a fictitious instrument is shown in Listing 1.4. In addition to the methods to configure the instrument and perform data acquisition, it is possible to override the DAQSettings property to implement instrument-specific hardware constraints such as, in this example, the number of samples per buffer being constrained to the discrete interval [1, 2048]. Leveraging the qutil.domains module, more complex constraints such as sample rates restricted to an internal clock rate divided by a power of two<sup>13</sup> can be specified.

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

12: I.e., the number of time series data batches acquired, as opposed to the number of Welch averages n\_seg within one batch.

13: See for example the implementation of the AlazarTech ATS9440 digitizer card.

### 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) and convert the voltage back to a current,<sup>14</sup> or more complex ones such as applying calibrations. In particular, since the process of computing the PSD already involves Fourier transformation, the processing can also be performed in frequency space.

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

In python\_spectrometer, this can be done using procfn (in the time domain) or fourier\_procfn (in the Fourier domain). The former is specified as an argument directly to the Spectrometer constructor. It is a callable with signature (x, \*\*kwargs) -> xp, that is, takes the time series data as its first (positional) argument and arbitrary settings that are passed through from the take() method as keyword arguments, and returns the processed data. Listing 1.5 shows a simple function that accounts for the gain of an amplifier. The latter is specified in the psd\_estimator argument of the Spectrometer constructor. This argument allows the user to specify a custom estimator for the PSD, in which case a callable is expected. Otherwise, it should be a mapping containing parameters for the default PSD estimator, scipy.signal.welch() [2]. Here, the keyword fourier\_procfn should be a callable with signature (xf, f, \*\*kwargs) -> (xfp, fp).<sup>15</sup> That is, it should take the frequency-

[2]: (n.d.), welch — SciPy v1.15.2 Manual

15: I.e., the psd\_estimator argument would be {"fourier\_procfn": fn}.

```
# daq/mydaq.py
import dataclasses
from qutil.domains import DiscreteInterval
from .base import DAQ
from .settings import DAQSettings

@dataclasses.dataclass
class MyDAQ(DAQ):
    handle: mydriver.DeviceHandle

    @property
    def DAQSettings(self) -> type[DAQSettings]:
        class MyDAQSettings(DAQSettings):
            ALLOWED_NPERSEG = DiscreteInterval(1, 2048)
        return MyDAQSettings

    def setup(self, **settings) -> dict:
        settings = self.DAQSettings(settings)
        parsed_settings = settings.to_consistent_dict()
        self.handle.configure(parsed_settings)
        return parsed_settings

    def acquire(self, n_avg: int, *, **settings) -> Generator:
        self.handle.arm(n_avg)
        for _ in range(n_avg):
            self.handle.wait_for_trigger()
            yield self.handle.fetch()
        return self.handle.metadata
```

**Listing 1.4:** Exemplary code for a DAQ implementation of some instrument with given driver class `DeviceHandle` in the package `mydriver`. The `MyDAQ` class is instantiated with a `DeviceHandle` instance. Optionally, the `DAQSettings` property can be overridden to implement hardware constraints or default values for data acquisition parameters. For this, the `qutil.domains` module provides several classes that represent bounded domains and sets. The `setup()` method parses the given acquisition settings and configures the instrument through the external driver interface `handle.configure()`. The `acquire()` method arms the instrument (if necessary) and loops over the number of outer averages, `n_avg`. In the body of the loop, it can wait for external triggers (or send software triggers) before yielding a batch of data fetched from the external driver interface. Once acquisition is done, the method can return arbitrary metadata to the `Spectrometer` object to attach to the stored data.

space data, the corresponding frequencies, and arbitrary keyword arguments and return a tuple of the processed data and the corresponding frequencies.

A simple example for a processing function in Fourier space is shown in Listing 1.6, which computes the (anti-)derivative of the data using the fact that

$$\frac{\partial^n}{\partial t^n} \xrightarrow{\text{F.T.}} (i\omega)^n \quad (1.1)$$

under the Fourier transform. In ??, I discuss more complex use-cases of the processing functionality included in `python_spectrometer` in the context of vibration spectroscopy.

## 1.2 Feature overview

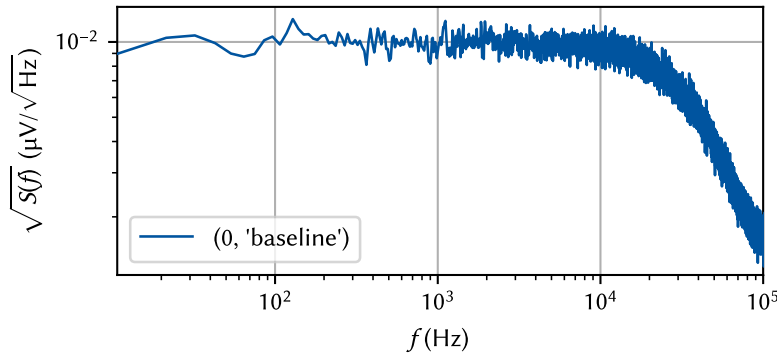
Now that we have a basic understanding of the design choices underlying `python_spectrometer`, let us discuss the typical workflow of using the package. Two modes of operation are to be distinguished: first, “serial” mode, in which users record new spectra manually, and second, “live” mode, in which new data is continuously being acquired. The former is well suited to a structured approach to noise spectroscopy where data is retained persistently and discrete changes are made to the system in between subsequent data acquisitions. The latter is aimed at a more fluent workflow in which data is not retained and data acquisition runs in the background.

```
def comp_gain(x, gain=1.0, **_):
    return x / gain
```

**Listing 1.5:** A simple procfn, which converts amplified data back to the level before amplification. Note the token `**_` variable keyword argument that ensures no errors arise from other parameters being passed to the function. More complex processing chains can concisely be defined with `qutil.functools.FunctionChain` that pipes the output of one function into the input of the next.

```
def derivative(xf, f, n=0, **_):
    return xf / (2j * pi * f)**n
```

**Listing 1.6:** A simple `fourier_procfn`, which calculates the (anti-)derivative.



**Figure 1.2:** The python\_spectrometer plot after acquiring the (here: synthetic) baseline spectrum. By default, the amplitude spectral density (ASD) =  $\sqrt{\text{PSD}}$  is displayed in the main plot. Each spectrum is assigned a unique identifier key consisting of an incrementing integer and the user comment, and can be referred to by either (or both) when interacting with the object.

### 1.2.1 Serial spectrum acquisition

The default mode for spectrum acquisition using python\_spectrometer revolves around the `take()` method. Key to this workflow is the idea that each acquired spectrum be assigned a comment that allows to easily identify it in the main plot. For instance, this comment could contain information about the particular settings that were active when the spectrum was recorded, or where a particular cable was placed.

Consider as an example the procedure of “noise hunting”, *i.e.*, debugging a noisy experimental setup. The experimentalist,<sup>16</sup> having discovered that his data is noisier than expected, sets up the Spectrometer class with an instance of the DAQ subclass for the DAQ instrument connected to his sample, a Zurich Instruments MFLI.<sup>17</sup> Choosing to work with the demodulated data to benefit from the corresponding DAQ module’s larger flexibility, he recognizes that the resulting PSD will be the two-sided version because the data returned by the lock-in amplifier (LIA) is complex. Since he is interested in the physical frequencies<sup>18</sup> he sets the lock-in’s modulation frequency to 0 Hz and disables plotting the negative part of the frequency spectrum as it contains only redundant data in this case. Selecting the frequency bounds, say  $f_{\min} = 10$  Hz and  $f_{\max} = 100$  kHz, and using the sensible defaults for the remaining spectrum parameters, Bob first grounds the input of his DAQ to record a *baseline* spectrum. Thus far, his code would hence look something like that shown in Listing 1.7, which produces the plot shown in Figure 1.2.

```
from python_spectrometer import Spectrometer, daq
from qutil.functools import scaled

mfli_daq = daq.ZurichInstrumentsMFLIDAQ(session, device)
spect = Spectrometer(mfli_daq, procfn=scaled(1e6),
                    plot_negative_frequencies=False,
                    processed_unit='uV')

settings = {'f_min': 1e1, 'f_max': 1e5, 'freq': 0}
spect.take('baseline', daq='grounded', **settings)
```

The noise spectrum he obtains is white up until approximately 20 kHz where it starts falling off  $\propto f^{-n}$ . This is because the LIA low-pass filters the signal to suppress aliasing.<sup>19</sup> After acquiring the baseline, he next ungrounds the DAQ to obtain a representative spectrum of the noise in an actual measurement. He then proceeds by tweaking things on his setup, testing out different parameters, *etc.* Every time he changes something, he acquires another spectrum using `take()`, labeling each with a

16: Let’s call him Bob.

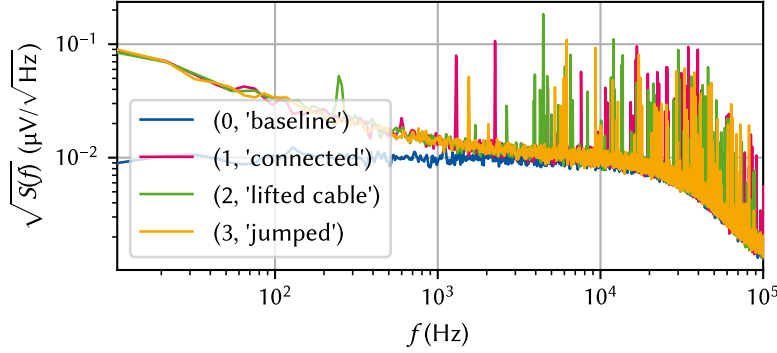
17: For the MFLI, DAQ subclasses for both the [Scope](#) and the [DAQ](#) module are implemented. The former gives access to the signal before and the latter to the signal after demodulation.

18: A discussion of lock-in amplification is beyond the scope of this chapter. Here I will simply note that, for finite modulation frequencies  $f_m$ , LIAs will measure the PSD in the up-converted frequency band  $[-f_{\max} + f_m, f_m + f_{\max}]$  rather than the baseband.

**Listing 1.7:** Setup and serial workflow using the python\_spectrometer package. `session` and `device` are Application Programming Interface (API) objects of the `zhinst.toolkit` driver package. It is therefore possible to simply use the driver objects that are already in use in the measurement setup. The `procfn` and `processed_unit` arguments help converting raw data into a more human-friendly unit.

19: Aliasing effects arise from finite sampling according to the Nyquist-Shannon sampling theorem [3–5]. It states that for a given physical bandwidth, the sampling rate  $f_s$  must be at least twice as large to faithfully reconstruct the signal in order to avoid aliasing, *i.e.*, the reverse of the argument we have made for the largest resolvable frequency  $f_{\max}$ . Some DAQ devices perform internal aliasing rejection while others do not.





**Figure 1.3:** The python\_spectrometer plot after acquiring additional (synthetic) spectra. Each spectrum is uniquely identified by a two-tuple of (index, comment).

meaningful comment for identification. The code shown in Listing 1.8 would then leave him with the spectrometer plot as shown in Figure 1.3. While working, Bob realizes he'd like see the signal in the time domain as well. He easily achieves this by setting `spect.plot_timetrace = True`, which adds an oscilloscope subplot to the spectrometer figure as shown in Figure 1.4. Since his DAQ returns complex data, the absolute value  $R = X + iY$  is plotted.

```
settings['daq'] = 'connected'
spect.take('connected', **settings)
spect.take('lifted cable', cable='lifted', **settings)
spect.take('jumped', **settings)
```

**Listing 1.8:** Code to acquire additional spectra. Arbitrary key-value pairs can be passed to the `take()` method, which are stored as metadata if they do not apply to any functions downstream in the data processing chain.

Bob now observes that the noise spectra he has recorded display many sharp peaks in particular at high frequencies while the  $1/f$  noise floor seems pretty consistent across different measurements. This makes it harder for him to evaluate whether any of his changes are actually an improvement or not. The python\_spectrometer package allows addressing this by plotting the integrated spectra in another subplot. Bob's spectrometer figure after setting `spect.plot_cumulative = True` is shown in Figure 1.5. In the case that `spect.plot_amplitude == True`, this new subplot shows the root mean square (RMS) in the band  $[f_{\min}, f]$ ,

$$\text{RMS}_S(f) \equiv \text{RMS}_S(f_{\min}, f), \quad (1.2)$$

and the band power (??) otherwise.

The cumulative RMS plot already helps, but Bob would like a more quantitative comparison of relative spectral powers. Therefore, he rescales the spectra in terms of their relative powers expressed in dB<sup>20</sup> by applying the following settings, which changes the plot to the layout shown in Figure 1.6:

```
spect.plot_dB_scale = True
spect.plot_amplitude = False
spect.plot_density = False
```

The attribute `plot_density` controls whether the *power spectral density* or the *power spectrum* is plotted.<sup>21</sup> Scaling the data to the power spectrum instead of the density, Bob can get an estimate of the RMS at a single frequency by reading off the peak height. Additionally displaying the data in dB then gives insight into relative noise powers of different spectra.

Bob carries on with his enterprise and continues to acquire spectra until, finally, he finds the source of his noise! Alas, his spectrometer plot is

20: Recall that the decibel is defined by the ratio  $L_P$  of two powers  $P_1, P_2$  as [6]

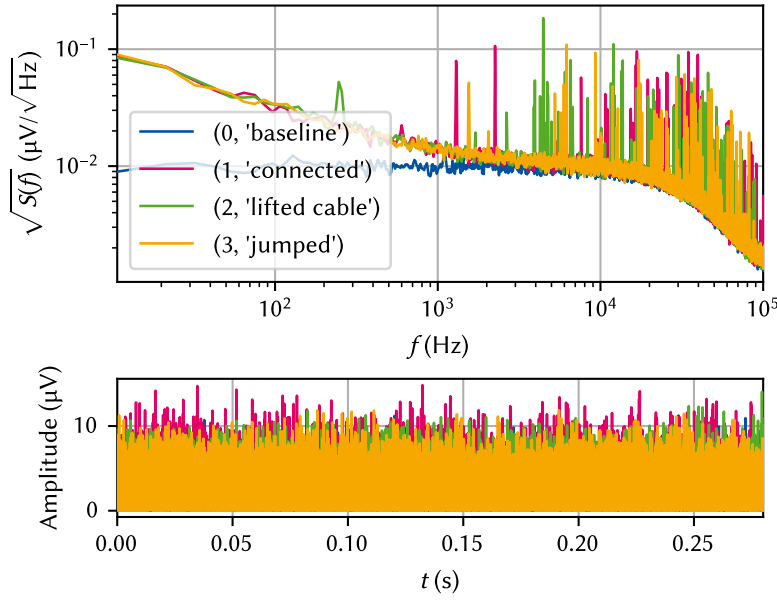
$$L_P = 10 \log_{10} \left( \frac{P_1}{P_2} \right) \text{ dB}.$$

21: At this point, we *do* need to distinguish between the PSD and the power spectrum counter to ?? in ???. The PSD and power spectrum are related by the equivalent noise bandwidth (ENBW),

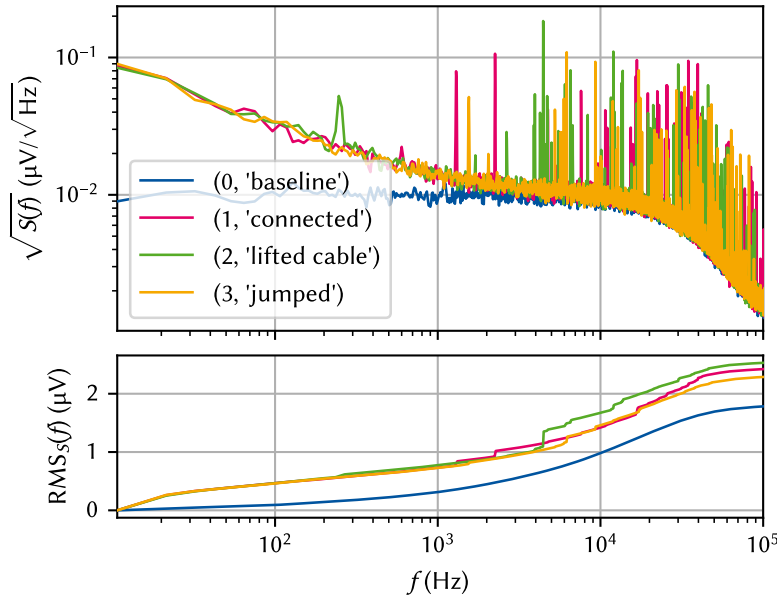
$$\text{Spectral density} \xrightarrow{\times \text{ENBW}} \text{Spectrum},$$

which is itself a function of the sampling rate and the properties of the spectral window [7],

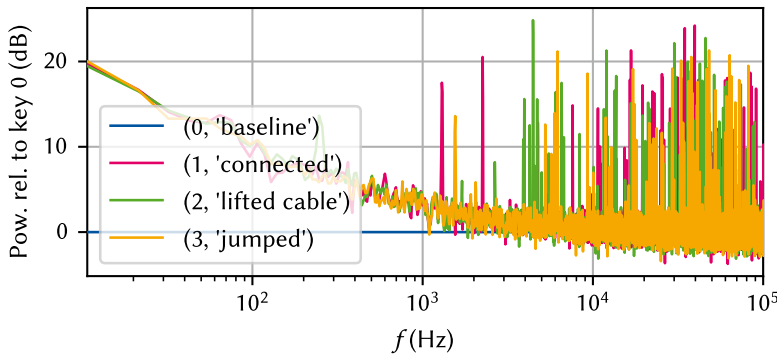
$$\text{ENBW} = f_s \frac{\sum_n \hat{w}_n^2}{\left[ \sum_n \hat{w}_n \right]^2}. \quad (1.3)$$



**Figure 1.4:** The python\_spectrometer plot shown in Figure 1.3 when setting `spect.plot_timetrace = True`. This adds a subplot that shows the time series data from which the PSD was computed akin to what an oscilloscope would show. For complex time series, the absolute value  $R = X + iY$  is plotted. Note that this is the entire time series, *i.e.*, the data of length  $L$ , which is (by default, using Welch's method) segmented for spectrum estimation.



**Figure 1.5:** The python\_spectrometer plot shown in Figure 1.3 when setting `spect.plot_cumulative = True`. This adds a subplot that shows the RMS (see ??) which can be helpful in evaluating the contribution of individual peaks in the spectrum to the total noise power. Both the oscilloscope subplot (Figure 1.4) and the RMS subplot can also be shown at the same time.



**Figure 1.6:** The python\_spectrometer plot in relative mode. Starting from the state in Figure 1.3, we set `spect.plot_dB_scale = True` as well as `spect.plot_amplitude = False` and `spect.plot_density = False` to compare the relative noise powers with respect to the baseline.

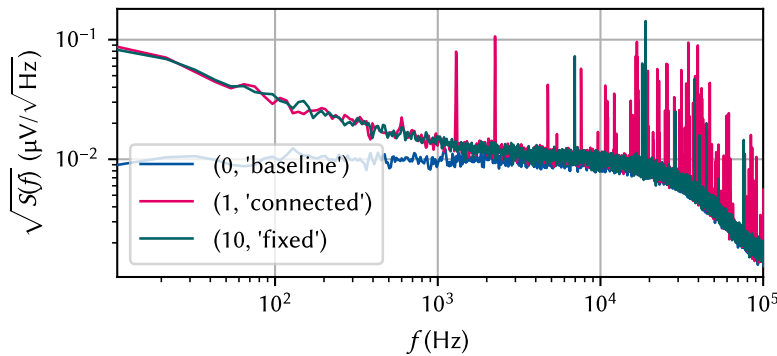


Figure 1.7: The python\_spectrometer plot after multiple additional spectra were acquired and hidden. Hiding spectra that one is not interested in anymore is achieved through `spect.hide(*range(2, 10))`. This is reversed by `spect.show(*range(2, 10))`. Data can also be dropped (`spect.drop(key)`) or deleted (`spect.delete(key)`) from the internal cache and disk, respectively.

now overflowing with plotted data when really he just wants to compare the baseline, the original, noisy state, and the final, clean spectrum. He simply calls

```
| spect.hide(*range(2, 10))
```

to hide the eight spectra of unsuccessful debugging, leaving him with a plot as shown in Figure 1.7.

Finally, happy with the results, Bob serializes the state of the spectrometer to disk, allowing him to pick up where he left off at a later point in time:

```
| spect.serialize_to_disk('2032-12-24_noise_hunting')
```

The next week, Bob is asked by his team about his progress on debugging the noise in their setup. Even though he is working from home that day and does not have access to the lab computer, Bob simply uses his laptop computer and pulls up the Spectrometer session stored on the server, allowing them to interactively discuss the spectra:

```
| file = '2032-12-24_noise_hunting'
| # Read-only instance because no DAQ attached
| spect = Spectrometer.recall_from_disk(savepath / file)
```

This opens up the plot shown in Figure 1.7 again. While they cannot acquire new spectra in this state,<sup>22</sup> they can still use all the plotting features like showing or hiding spectra, or changing plot types as discussed above.

22: They could of course always attach a DAQ instance to the spectrometer and continue as they were.

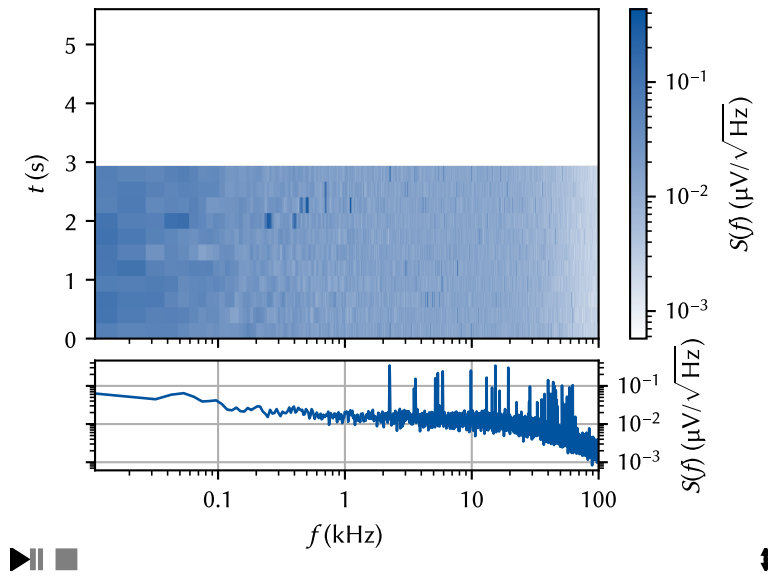
## 1.2.2 Live spectrum acquisition

Manually recording spectra in the workflow outlined in 1.2.1 becomes tedious at some point, and experimenters tend to become negligent with keeping metadata and comments up to date as they continue to change settings. Once a certain number of spectra has been obtained, the spectrometer plot also becomes crowded, and hiding old spectra manually is cumbersome. Moreover, each time a spectrum is captured, data is saved to disk, potentially accruing large amounts of storage space. For these reasons, the python\_spectrometer package also offers a non-persistent live mode for displaying spectra continuously.

This mode is facilitated by the `util.plotting.live_view` module that provides asynchronous plotting functionality based on `matplotlib`. The `live_view` module supports both the multithreading and multiprocessing paradigms for concurrency in order to keep the interpreter responsive.<sup>23</sup> In the former case, the window hosting the figure runs in the

23: Note that technically, data is also recorded in a background thread in serial mode by default.





**Figure 1.8:** Spectrometer live view. The bottom plot shows the most recently acquired spectrum, while the top plot shows a waterfall plot of the most recent ones. Data acquisition runs in a background thread, keeping the interpreter responsive and available to interact with instruments, for example. The icons in the bottom left and right corners allow interacting with the live view.

main thread and is kept responsive using `matplotlib`'s GUI event loop mechanisms. In the latter, the plotting takes place in a separate process, resulting in true parallelism.

The live mode is started with the `Spectrometer.live_view()` method. Data is continuously acquired<sup>24</sup> in a background thread using the same DAQ interface as the serial mode. Instead of saving the data on disk and managing plotting from `python_spectrometer`, however, the data is fed into a queue.<sup>25</sup> A `live_view.IncrementalLiveView2D` object then retrieves the data from the queue and handles plotting in the graphical user interface (GUI) event loop. To start a spectroscopy session with the same parameters as in 1.2.1 with a given `Spectrometer` object (see Listing 1.7), we would call

```
| view = spect.live_view(f_min=1e1, f_max=1e5, in_process=True)
```

which would open a figure window such as that shown in Figure 1.8. Similar to `take()`, the data acquisition parameters are passed to `live_view()` as keyword arguments.<sup>26</sup> The `in_process` argument specifies if multiprocessing (`True`) or multithreading (`False`) is used. Dictionaries with customization parameters for the `live_view` object can further be passed to the method.

24: Technically, a very large `n_avg` is used.

25: A queue is a concurrency mechanism for exchanging data between multiple threads or processes.

26: The difference is, of course, that we do not need to specify a comment since no data is retained.

## **Part II**

# **CHARACTERIZATION AND IMPROVEMENTS OF A MILLIKELVIN CONFOCAL MICROSCOPE**

**Part III**

**OPTICAL MEASUREMENTS OF  
ELECTROSTATIC EXCITON TRAPS IN  
SEMICONDUCTOR MEMBRANES**

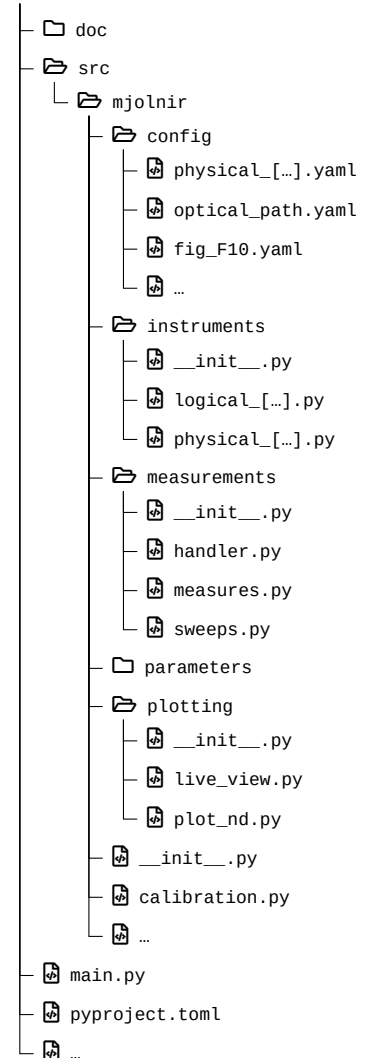
# Introduction

2



# The mjolnir measurement framework

# 3



**Figure 3.1:** Source tree structure of the mjolnir package. Logical QCoDeS instruments and parameters are defined in the instruments and parameters modules, respectively. Instruments are configured using yaml files located in the config directory. The measurements module provides classes for the abstraction of measurements using QCoDeS underneath. Live plots of instrument data as well as a plot function for multidimensional measurement data are defined in the plotting module. calibration.py contains routines for power, CCD, and excitation rejection calibrations. The main.py file is a code cell-based script that serves as the entrypoint for measurements.

## 4.1 Transfer-matrix method simulations of the membrane structure

The transfer-matrix method (TMM) is a computationally efficient method of obtaining the electric field in layered structures. In this section, I perform simulations of the heterostructure membranes investigated in this part of the present thesis using the PyMoosh package [8] to elucidate the observed quenching of photoluminescence (PL) when illuminating gate electrodes as well as the overall optical efficiency.<sup>1</sup> I will first briefly recap the simulation method following Reference 8. For more details, refer to *ibid.* and references therein.

Consider a layered structure along  $z$  with interfaces at  $z_i, i \in \{0, 1, \dots, N+1\}$  that is translationally invariant along  $x$  and  $y$ . Each layer  $i$  may consist of a different dielectric material characterized by a (complex) relative permittivity  $\epsilon_{r,i}$ .<sup>2</sup> The electric field component along  $y$  of an electromagnetic wave transverse electric (TE) mode originating in some far away point satisfies the Helmholtz equation

$$\frac{\partial^2 E_y}{\partial z^2} + \gamma_i^2 E_y = 0, \quad (4.1)$$

where  $\gamma_i = \sqrt{\epsilon_{r,i} k_0^2 - k_x^2}$  with  $k_0 = \omega/c$  the wave vector in vacuum and  $k_x$  the component along  $x$ . In layer  $i$  of the structure, the solution to Equation 4.1 may be written as a superposition of plane waves incident and reflected on the lower and upper interfaces [8],

$$\begin{cases} E_{y,i}(z) = A_i^+ \exp\{i\gamma_i[z - z_i]\} + B_i^+ \exp\{-i\gamma_i[z - z_i]\}, \\ E_{y,i}(z) = A_i^- \exp\{i\gamma_i[z - z_{i+1}]\} + B_i^- \exp\{-i\gamma_i[z - z_{i+1}]\}, \end{cases} \quad (4.2)$$

where the coefficients with superscript  $+$  ( $-$ ) are referenced to the phase at the upper (lower) interface, respectively. Matching these solutions at  $z = z_i$  for all  $i$  to satisfy the interface conditions imposed by Maxwell's equations gives rise to a linear system of equations, the solution to which can be obtained through several different methods.

A particularly simple method is the transfer-matrix method ( $T$ -matrix formalism), which corresponds to writing the interface conditions at  $z = z_i$  as the matrix equation

$$\begin{pmatrix} A_{i+1}^+ \\ B_{i+1}^+ \end{pmatrix} = T_{i,i+1} \begin{pmatrix} A_i^- \\ B_i^- \end{pmatrix} \quad (4.3)$$

with

$$T_{i,i+1} = \frac{1}{2\gamma_{i+1}} \begin{pmatrix} \gamma_i + \gamma_{i+1} & \gamma_i - \gamma_{i+1} \\ \gamma_i - \gamma_{i+1} & \gamma_i + \gamma_{i+1} \end{pmatrix} \quad (4.4)$$

the transfer matrix for interface  $i$ . Connecting the coefficients for adjacent interfaces within a layer of height  $h_i = z_{i+1} - z_i$  requires propagating

1: Strictly speaking, the term TMM only refers to one of the several formalisms implemented in the PyMoosh package. While fast, it not the most numerically stable, and other methods may be preferred if wall time is not a limiting issue.

2: We disregard magnetic materials with relative permeability  $\mu_r \neq 1$  for simplicity.

the phase,

$$\begin{pmatrix} A_i^- \\ B_i^- \end{pmatrix} = C_i \begin{pmatrix} A_i^+ \\ B_i^+ \end{pmatrix}, \quad (4.5)$$

with

$$C_i = \exp \{ \text{diag}(-i\gamma_i h_i, i\gamma_i h_i) \}. \quad (4.6)$$

Iterating Equations 4.4 and 4.6, the total transfer matrix  $T = T_{0,N+1}$  then reduces to the matrix product

$$T = T_{N,N+1} \prod_{i=0}^{N-1} T_{i,i+1} C_i. \quad (4.7)$$

From  $T$ , the reflection and transmission coefficients can be obtained as  $r = A_0^- = -T_{01}/T_{00}$  and  $t = B_{N+1}^+ = rT_{10} + T_{11}$ . Taking the absolute value square of reflection and transmission coefficients then yields the reflectance  $\mathcal{R}$  and the transmittance  $\mathcal{T}$ , which correspond to the fraction of total incident power being reflected and transmitted, respectively. To obtain the absorptance  $\mathcal{A}$ , the fraction of power being absorbed, in layer  $i$ , one can compute the difference of the  $z$ -components of the Poynting vectors (*cf.* ??) at the top of layers  $i$  and  $i+1$ . In the TE case considered here, ?? reduces to [8]

$$S_i = \text{Re} \left[ \frac{\gamma_i^*}{\gamma_0} (A_i^+ - B_i^+)^* (A_i^+ + B_i^+) \right] \quad (4.8)$$

and is hence straightforward to extract from the calculation of either the  $S$  or  $T$  matrices.

Equation 4.7 is simple to evaluate on a computer, making this method attractive for numerical applications. However, the opposite signs in the argument of the exponentials in Equation 4.6 can lead to instabilities for evanescent waves ( $\gamma_i \in \mathbb{C}$ ) due to finite-precision floating point arithmetic [9]. Rewriting Equation 4.4 to have incoming and outgoing fields on opposite sides of the equality alleviates this issue while sacrificing the simple matrix-multiplication composition rule in what is known as the scattering matrix ( $S$ -matrix) formalism.

Beyond the calculation of the aforementioned coefficients, the TMM formalism also allows to compute the full spatial dependence of the fields. Two cases are implemented in PyMoosh: irradiation of the layered structured with a Gaussian beam rather than plane waves of infinite extent, and a current line source inside the structure. In the first case, the previously assumed translational invariance along  $x$  leading to a plane-wave spatial dependence is replaced by a superposition of plane waves weighted with a normally distributed amplitude,<sup>3</sup>

$$E_{y,i}(x, z) = \exp(ik_x x) \rightarrow \int \frac{dk_x}{2\pi} \mathcal{E}_0(k_x) E_{y,i}(k_x, z) \exp(ik_x x), \quad (4.9)$$

with (*cf.* ??)

$$\mathcal{E}_0(k_x) = \frac{w_0}{2\sqrt{\pi}} \exp \left\{ -ik_x x_0 - \left[ \frac{w_0 k_x}{2} \right]^2 \right\} \quad (4.10)$$

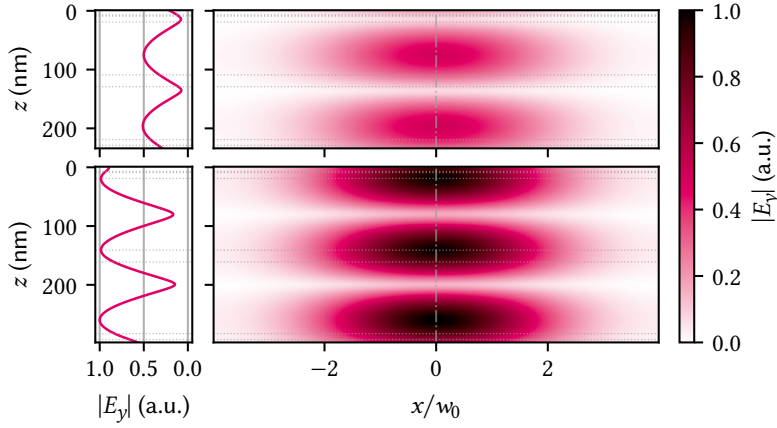
and

$$E_{y,i}(k_x, z) = A_i^- \exp\{i\gamma_i(k_x)[z - z_{i+1}]\} + B_i^+ \exp\{-i\gamma_i(k_x)[z - z_i]\}, \quad (4.11)$$

and where we considered only normal incidence for simplicity.

In the second case, Langevin et al. [8] consider an AC current  $I$  flow-

3: *I.e.*, the inverse Fourier transform of  $\mathcal{E}_0(k_x) E_{y,i}(k_x, z)$ .



**Figure 4.1:** Absolute value of the electric field inside the double-gated heterostructure under illumination with a Gaussian beam at  $\lambda = 825$  nm from the top. Top (bottom) panels show the structure with the default (optimized) barrier thickness of 90 nm (122 nm), respectively. Dotted horizontal lines indicate interfaces between different materials while the vertical dash-dotted line indicates the position of the line cuts shown in the left column. Increasing the thickness of the barrier has two beneficial effects; first, the overall field intensity inside the structure is higher by a factor of two, and second, there is a peak rather than a knot in the quantum well (QW) at a depth of  $\sim 120$  nm ( $\sim 150$  nm), leading to enhanced absorption.

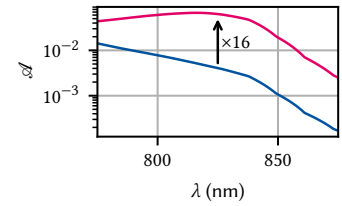
ing through a translationally invariant, one-dimensional wire along  $y$  at  $x = x_s$ . This introduces a source term into the Helmholtz equation Equation 4.1 which, upon Fourier transforming in  $x$  direction, leads to

$$\frac{\partial^2 \hat{E}_y}{\partial z^2} + \gamma_i^2 \hat{E}_y = -i\omega\mu_0 I\delta(z) \exp(ik_x x_s). \quad (4.12)$$

The electric field  $\hat{E}_{y,i}(k_x, z)$  is thus proportional to the Green's function of Equation 4.12 and can be obtained using a similar procedure as in the case of a distant source incident on the structure by matching the interface conditions. Performing the inverse Fourier transform by means of Equation 4.9 with constant weights,  $\mathcal{E}_0(k_x) \equiv 1$ , then yields the two-dimensional spatial distribution of the electric field,  $E_{y,i}(x, z)$ .

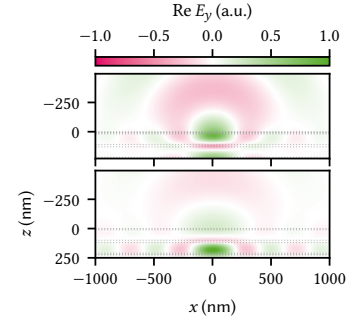
**Table 4.1**

	$\mathcal{A}$ (%)	$\mathcal{R}$ (%)
Bare	2.93	22.43
TG	1.79	41.98
BG	0.50	82.72
TG+BG	0.41	84.78

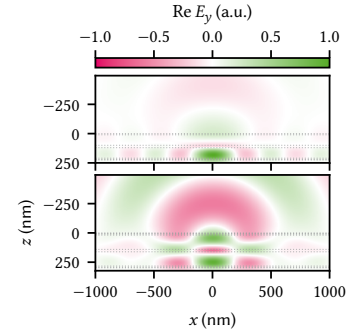


**Figure 4.2:** QW absorptance  $\mathcal{A}$  in a heterostructure with default (blue) and optimized (magenta) barrier thickness and top and bottom gates as function of wavelength. Optimization was performed at 825 nm using the differential evolution algorithm implemented in PyMoosh, resulting in a barrier thickness of 122 nm and an absorptance better by a factor of 16 at 6.3 %.

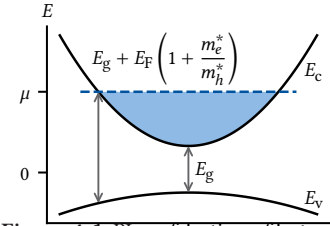
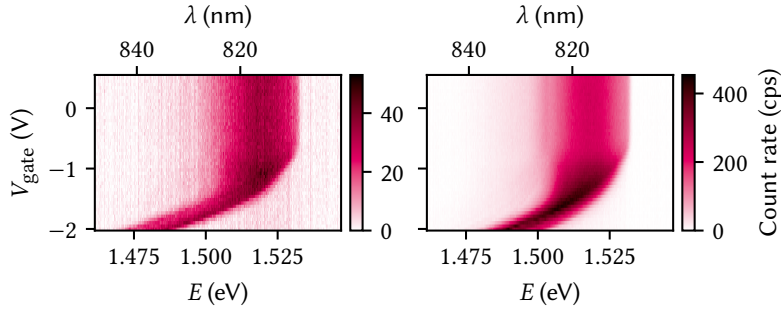




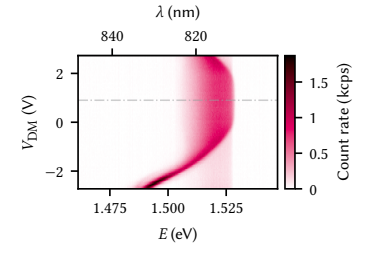
**Figure 4.3:** Real part of the electric field emitted by a current line located in the QW (black point) for different cases of the unoptimized structure. From top to bottom: bare heterostructure, top gate, bottom gate, top and bottom gate. The half space  $z < 0$  is the air above the membrane in the direction of the objective lens and the dotted lines indicate interfaces between materials. Evidently, the bottom gate reduces the amplitude in the upper half of the membrane and thereby the outcoupling efficiency compared to the structures with just a top gate, consistent with what is observed in the experiment.



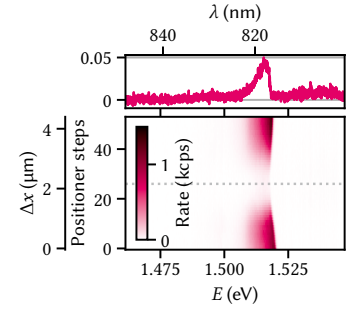
**Figure 4.4:** Real part of the electric field emitted by a current line located in the QW (black point) for the default (top) and optimized (bottom) structures with top and bottom gates. Optimizing the barrier thickness for absorption in the QW evidently also drastically improves the outcoupling efficiency into the half-space  $z < 0$ .



**Figure 4.6:** PL as function of gate voltage on a single fan-out gate on the bottom (left) and top (right) side of the membrane. The behavior is qualitatively similar but the overall quantum efficiency lower by an order of magnitude for gates on the bottom (as-grown buried) side.



**Figure 4.7:** PL as function of difference-mode voltage on a large exciton trap. The observed Stark shift follows the expected quadratic dispersion, but is offset by 0.9 V with respect to zero bias (dash-dotted gray line). Remnant PL of the two-dimensional electron gas (2DEG) from outside the trap region is faintly visible below  $-1$  V.



**Figure 4.8**

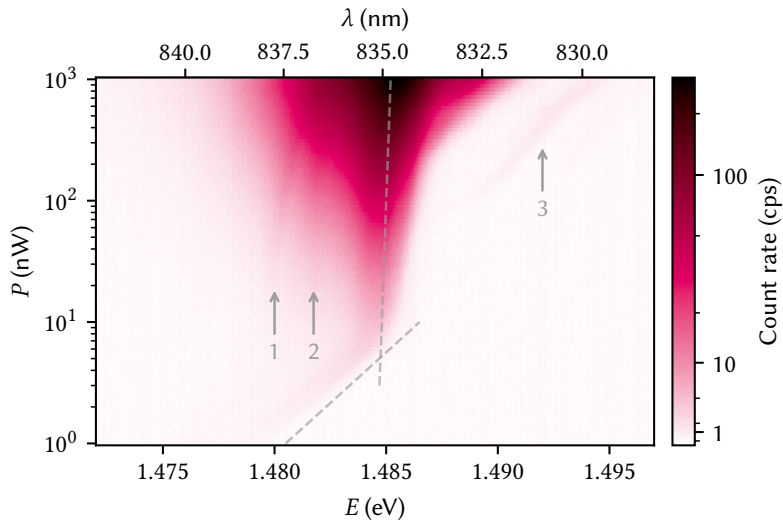


Figure 4.9

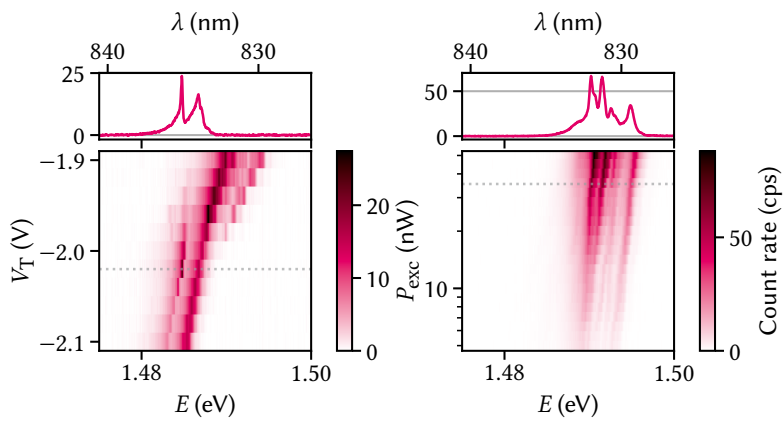


Figure 4.10

## Conclusion & outlook

5



## **Part IV**

# **A FILTER-FUNCTION FORMALISM FOR UNITAL QUANTUM OPERATIONS**

# **APPENDIX**

# Additional TMM simulations



## A.1 Dependence on epoxy thickness

## A.2 Optimization of the barrier thickness

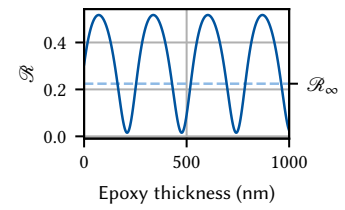


Figure A.1

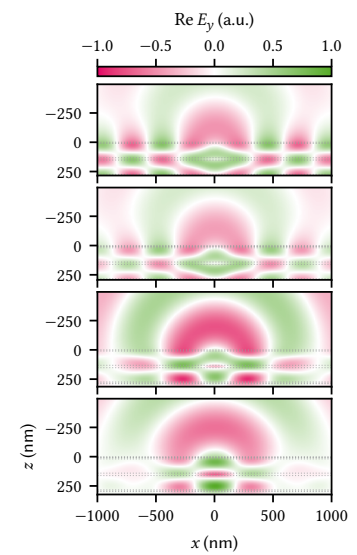


Figure A.2



# Bibliography

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# Special Terms

## Numbers

**2DEG** two-dimensional electron gas. 20

## A

**API** Application Programming Interface. 6

**ASD** amplitude spectral density. 6

## C

**CCD** charge-coupled device. 14

## D

**DAQ** data acquisition. 2–4, 6, 7

## E

**ENBW** equivalent noise bandwidth. 7

## G

**GUI** graphical user interface. 10

## L

**LIA** lock-in amplifier. 6

## P

**PL** photoluminescence. 15, 19, 20

**PSD** power spectral density. 2, 4, 6–8

## Q

**QW** quantum well. 17, 18

## R

**RMS** root mean square. 7, 8

## T

**TE** transverse electric. 15, 16

**TIA** transimpedance amplifier. 4

**TMM** transfer-matrix method. iii, 15, 16, 25

# Declaration of Authorship

I, Tobias Hangleiter, declare that this thesis and the work presented in it are my own and has been generated by me as the result of my own original research.

I do solemnly swear that:

1. This work was done wholly or mainly while in candidature for the doctoral degree at this faculty and university;
2. Where any part of this thesis has previously been submitted for a degree or any other qualification at this university or any other institution, this has been clearly stated;
3. Where I have consulted the published work of others or myself, this is always clearly attributed;
4. Where I have quoted from the work of others or myself, the source is always given. This thesis is entirely my own work, with the exception of such quotations;
5. I have acknowledged all major sources of assistance;
6. Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself;
7. Parts of this work have been published before as:

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Aachen, July 14, 2025.