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

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July 15, 2025

* A \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**

Part II

CHARACTERIZATION AND IMPROVEMENTS OF A MILLIKELVIN CONFOCAL MICROSCOPE

Part III

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

Introduction

6



The mjolnir measurement framework

7

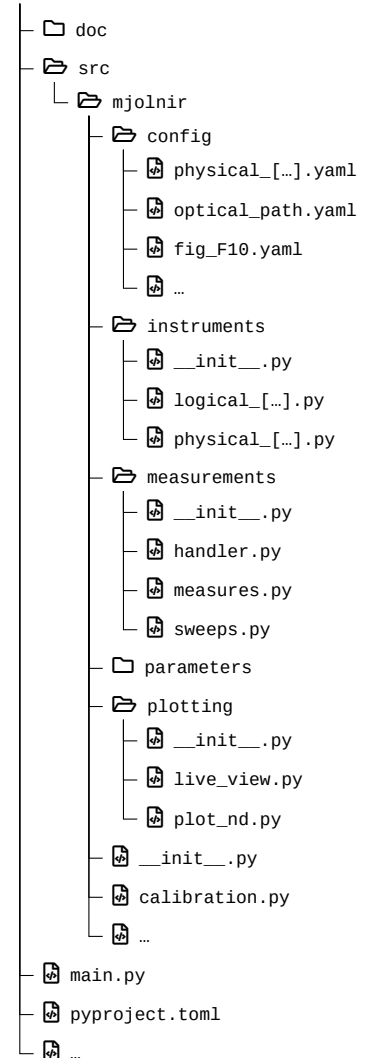


Figure 7.1: Source tree structure of the mjolnir package. Logical QCoDeS instruments and parameters are defined in the instruments and parameters modules, respectively. Instruments are configured using yaml files located in the config directory. The measurements module provides classes for the abstraction 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.

8.1 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 [1] to elucidate the observed quenching of photoluminescence (PL) when illuminating gate electrodes as well as the overall optical efficiency.¹ I will first briefly recap the simulation method following Reference 1. 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 $\epsilon_{r,i}$.² The electric field component along y of an electromagnetic wave transverse electric (TE) mode originating in some far away point satisfies the Helmholtz equation

$$\frac{\partial^2 E_y}{\partial z^2} + \gamma_i^2 E_y = 0, \quad (8.1)$$

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 8.1 may be written as a superposition of plane waves incident and reflected on the lower and upper interfaces [1],

$$\begin{cases} E_{y,i}(z) = A_i^+ \exp\{i\gamma_i[z - z_i]\} + B_i^+ \exp\{-i\gamma_i[z - z_i]\}, \\ E_{y,i}(z) = A_i^- \exp\{i\gamma_i[z - z_{i+1}]\} + B_i^- \exp\{-i\gamma_i[z - z_{i+1}]\}, \end{cases} \quad (8.2)$$

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

$$\begin{pmatrix} A_{i+1}^+ \\ B_{i+1}^+ \end{pmatrix} = T_{i,i+1} \begin{pmatrix} A_i^- \\ B_i^- \end{pmatrix} \quad (8.3)$$

with

$$T_{i,i+1} = \frac{1}{2\gamma_{i+1}} \begin{pmatrix} \gamma_i + \gamma_{i+1} & \gamma_i - \gamma_{i+1} \\ \gamma_i - \gamma_{i+1} & \gamma_i + \gamma_{i+1} \end{pmatrix} \quad (8.4)$$

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,

$$\begin{pmatrix} A_i^- \\ B_i^- \end{pmatrix} = C_i \begin{pmatrix} A_i^+ \\ B_i^+ \end{pmatrix}, \quad (8.5)$$

with

$$C_i = \exp \{ \text{diag}(-i\gamma_i h_i, i\gamma_i h_i) \}. \quad (8.6)$$

Iterating Equations 8.4 and 8.6, the total transfer matrix $T = T_{0,N+1}$ then reduces to the matrix product

$$T = T_{N,N+1} \prod_{i=0}^{N-1} T_{i,i+1} C_i. \quad (8.7)$$

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.* Equation 3.18) at the top of layers i and $i+1$. In the TE case considered here, Equation 3.18 reduces to [1]

$$S_i = \text{Re} \left[\frac{\gamma_i^*}{\gamma_0} (A_i^+ - B_i^+) (A_i^+ + B_i^+) \right] \quad (8.8)$$

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

Equation 8.7 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 8.6 can lead to instabilities for evanescent waves ($\gamma_i \in \mathbb{C}$) due to finite-precision floating point arithmetic [2]. Rewriting Equation 8.4 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,³

$$E_{y,i}(x, z) = \exp(ik_x x) \rightarrow \int \frac{dk_x}{2\pi} \mathcal{E}_0(k_x) E_{y,i}(k_x, z) \exp(ik_x x), \quad (8.9)$$

with (*cf.* Equation 4.6)

$$\mathcal{E}_0(k_x) = \frac{w_0}{2\sqrt{\pi}} \exp \left\{ -ik_x x_0 - \left[\frac{w_0 k_x}{2} \right]^2 \right\} \quad (8.10)$$

and

$$E_{y,i}(k_x, z) = A_i^- \exp\{i\gamma_i(k_x)[z - z_{i+1}]\} + B_i^+ \exp\{-i\gamma_i(k_x)[z - z_i]\}, \quad (8.11)$$

and where we considered only normal incidence for simplicity.

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

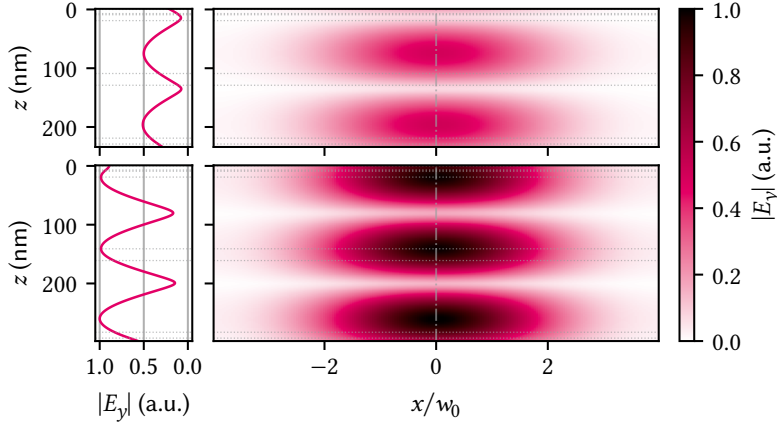


Figure 8.1: Absolute value of the electric field inside the double-gated heterostructure under illumination with a Gaussian beam at $\lambda = 825$ nm from the top. Top (bottom) panels show the structure with the default (optimized) barrier thickness of 90 nm (122 nm), respectively. Dotted horizontal 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 ~ 120 nm (~ 150 nm), leading to enhanced absorption.

In the second case, Langevin et al. [1] consider an AC current I flowing through a translationally invariant, one-dimensional wire along y at $x = x_s$. This introduces a source term into the Helmholtz equation Equation 8.1 which, upon Fourier transforming in x direction, leads to

$$\frac{\partial^2 \hat{E}_y}{\partial z^2} + \gamma_i^2 \hat{E}_y = -i\omega\mu_0 I \delta(z) \exp(ik_x x_s). \quad (8.12)$$

The electric field $\hat{E}_{y,i}(k_x, z)$ is thus proportional to the Green's function of Equation 8.12 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 8.9 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 8.1

	\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

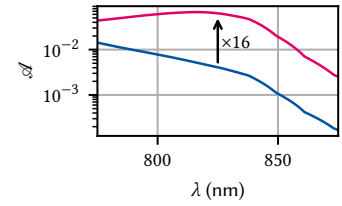


Figure 8.2: QW absorptance \mathcal{A} in a heterostructure with default (blue) and optimized (magenta) barrier thickness and top and bottom gates as function of wavelength. Optimization was performed at 825 nm using the differential evolution algorithm implemented in PyMoosh, resulting in a barrier thickness of 122 nm and an absorptance better by a factor of 16 at 6.3%.

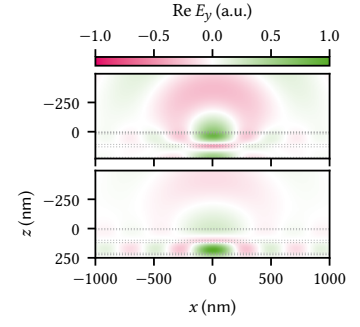


Figure 8.3: Real part of the electric field emitted by a current line located in the QW (black point) for different cases of the unoptimized structure. From top to bottom: bare heterostructure, top gate, bottom gate, top and bottom gate. The half space $z < 0$ is the air above the membrane in the direction 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.

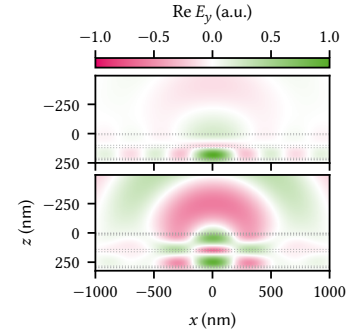


Figure 8.4: Real part of the electric field emitted by a current line located in the QW (black point) for the default (top) and optimized (bottom) structures with top and bottom gates. Optimizing the barrier thickness for absorption in the QW evidently also drastically improves the outcoupling efficiency into the half-space $z < 0$.

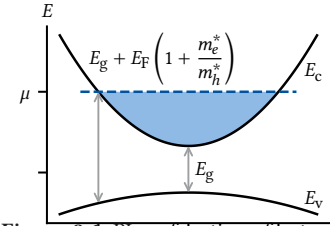
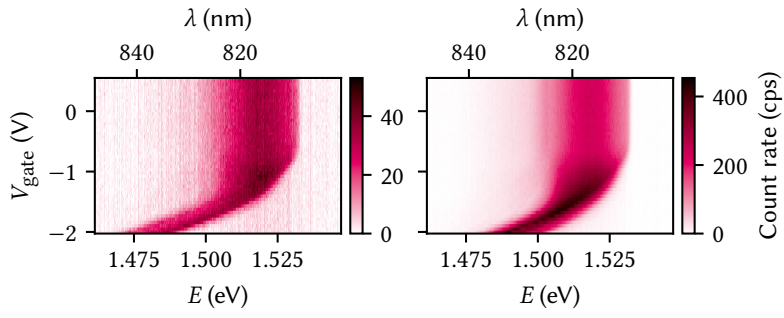


Figure 8.6: PL as function of gate voltage on a single fan-out gate on the bottom (left) and top (right) side of the membrane. The behavior is qualitatively similar but the overall quantum efficiency lower by an order of magnitude for gates on the bottom (as-grown buried) side.

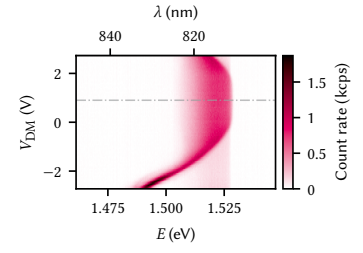


Figure 8.7: PL as function of difference-mode voltage on a large exciton trap. The observed Stark shift follows the expected quadratic dispersion, but is offset by 0.9 V with respect to zero bias (dash-dotted gray line). Remnant PL of the two-dimensional electron gas (2DEG) from outside the trap region is faintly visible below -1 V.

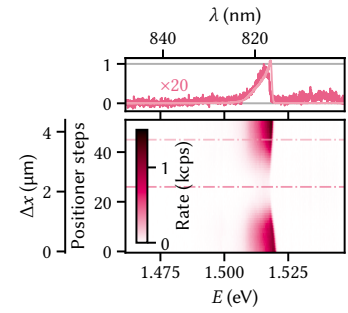


Figure 8.8

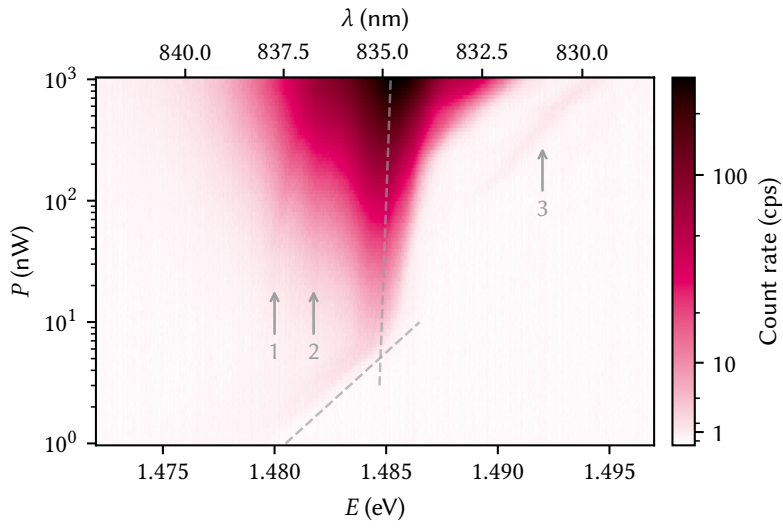


Figure 8.9

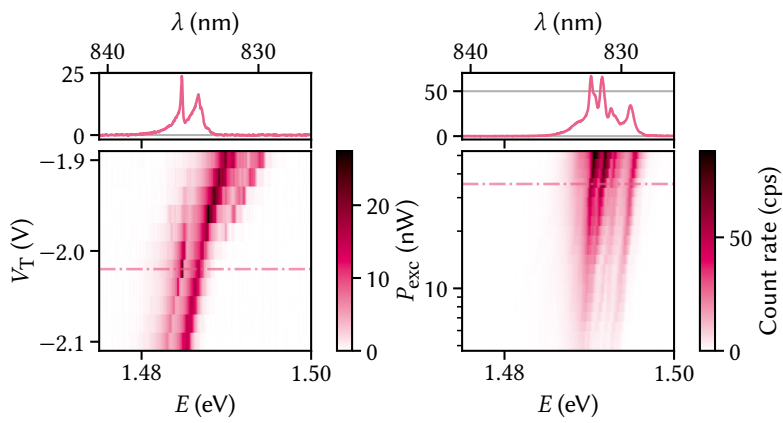


Figure 8.10

Conclusion & outlook

9

D^{OGS}

Part IV

A FILTER-FUNCTION FORMALISM FOR UNITAL QUANTUM OPERATIONS

APPENDIX

Additional TMM simulations



C.1 Dependence on epoxy thickness

C.2 Optimization of the barrier thickness

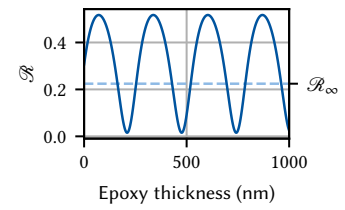


Figure C.1

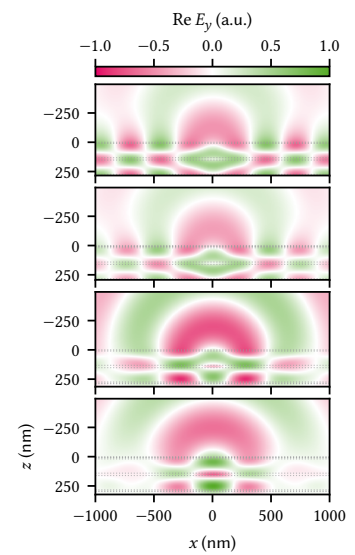


Figure C.2

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Special Terms

Numbers

2DEG two-dimensional electron gas. 39

C

CCD charge-coupled device. 33

P

PL photoluminescence. 34, 38, 39

PSD power spectral density. iii

Q

QW quantum well. 36, 37

T

TE transverse electric. 34, 35

TMM transfer-matrix method. iv, 34, 35, 39

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 15, 2025.