PHD Thesis

Something something something SABRE

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Declaration

I hereby declare, that I am the sole author and composer of my thesis and that no other sources or learning aids, other than those listed, have been used. Furthermore, I declare that I have acknowledged the work of others by providing detailed references of said work.
I hereby also declare, that my Thesis has not been prepared for another examination or assignment, either wholly or excerpts thereof.

Place, Date

Signature

Abstract

foo bar

Contents

List of Figures

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1 Introduction

This is a template for an undergraduate or master's thesis. The first sections are concerned with the template itself. If this is your first thesis, consider reading Section 1.3. Of course, the structure of this thesis is only an example. Discuss with your adviser what structure fits best for your thesis.

1.1 Template Structure

- To compile the document either run the makefile or run your compiler on the file 'thesis_main.tex'. The included makefile requires latexmk which automatically runs bibtex and recompiles your thesis as often as needed. Also it automatically places all output files (aux, bbl, ...) in the folder 'out'. As the pdf also goes in there, the makefile copies the pdf file to the parent folder. There is also a makefile in the chapters folder, to ensure you can also compile from this directory.

- The file 'setup.tex' includes the packages and defines commands. For more details see Section 1.2.

- Each chapter goes into a separate document, the files can be found in the folder chapters.

- The bib folder contains the .bib files, I'd suggest to create multiple bib files for different topics. If you add some or rename the existing ones, don't forget to also change this in thesis_main.tex. You can then cite as usual [1, 2, 3].

- The template is written in a way that eases the switch from scrbook to book class. So if you're not a fan of KOMA you can just replace the documentclass in the main file. The only thing that needs to be changed in setup.tex is the caption styling, see the comments there.

1.2 setup.tex

Edit setup.tex according to your needs. The file contains two sections, one for package includes, and one for defining commands. At the end of the includes and commands there is a section that can safely be removed if you don't need algorithms or tikz. Also don't forget to adapt the pdf hypersetup!!
setup.tex defines:

- some new commands for remembering to do stuff:
  - `\todo{Do this!}`: **(TODO: Do this!)**
  - `\extend{Write more when new results are out!}`: **(EXTEND: Write more when new results are out!)**
  - `\draft{Hacky text!}`: **(DRAFT: Hacky text!)**
- some commands for referencing, 'in `\chapref{chap:introduction}`' produces 'in Chapter 1'
  - `\chapref{}`
  - `\secref{sec:XY}`
  - `\eqref{}`
  - `\figref{}`
  - `\tabref{}`
- the colors of the Uni's corporate design, accessible with `{\color{UniX} Colored Text}`
  - UniBlue
  - UniRed
  - UniGrey
- a command for naming matrices `\mat{G}`, $\mathbf{G}$, and naming vectors `\vec{a}`, $\mathbf{a}$. This overwrites the default behavior of having an arrow over vectors, sticking to the naming conventions normal font for scalars, bold-lowercase for vectors, and bold-uppercase for matrices.
- named equations:

```
\begin{align}
    d(a,b) &= d(b,a)\\ \eqname{symmetry}
\end{align}
```

$$d(a, b) = d(b, a) \quad (1)$$

symmetry

1.3 Advice

This section gives some advice how to write a thesis ranging from writing style to formatting. To be sure, ask your advisor about his/her preferences.
For a more complete list we recommend to read Donald Knuth's paper on mathematical writing. (At least the first paragraph). `http://jmlr.csail.mit.edu/reviewing-papers/knuth_mathematical_writing.pdf`

- Don't use passive voice. It's harder to read, more likely to produce errors, and most of the times less precise. Of course there are situations where the passive voice fits but in scientific papers they are rare. Compare the sentence: 'We created the wheel to solve this.' to 'The wheel was created to solve this', you don't know who did it, making it harder to understand what is your contribution and what is not.
- If you use formulas pay close attention to be consistent throughout the thesis!
- Usually in a thesis you don't write 'In [24] the data is..'. You have more space than a paper has, so write 'AuthorXY et al. prepare the data... [24]'. Also pay attention to the placement: The citation is at the end of the sentence before the full stop with a no-break space. `... last word~\cite{XY}.`
- Pay attention to comma usage, there is a big difference between English and German. '...the fact that bla...' etc.
- Do not write 'don't ', 'can't' etc. Write 'do not', 'can not'.
- If an equation is at the end of a sentence, add a full stop. If it's not the end, add a comma: $a = b + c \quad (1),$
- Avoid footnotes if possible.

- Use ‘ ‘ ’ ’ for citing, not " ".

2 Theory

2.1 Nuclei and Spin

2.2 NMR

Nuclear Magnetic Resonance (NMR) is a technique that emerged in 1946 with the discovery of the absorption properties of nuclei irradiated with electromagnetic waves resonant to their larmor frequencies.**??** The subsequent observation of signal from those previously excited nuclei, known as free induction decay (FID) paved the road to the now well established method which in the beginning was primarily used in chemistry for structural analysis of Molecules and chemical kinetics.

2.2.1 Flip angle

An external, on-resonant magnetic field will cause the magnetization of an ensemble of spins to flip by an angle α known as the flip angle (FA). An FA of $n \cdot 180\,\mathrm{deg} + 90\,\mathrm{deg}$ will rotate the magnetization to the transverse plane perpendicular to the magnetic field resulting in an FID. Pulses of $n \cdot 180\,\mathrm{deg}$ will keep the magnetization aligned with the magnetic field or invert it, therefore not resulting in a FID. All other FAs will produce a linear combination of the two cases.

2.2.2 Relaxation

After being deflected from its equilibrium, z-magnetization tends to relax towards its thermal equilibrium. That process is called T1 relaxation or spin-lattice relaxation and is an exponential decay. In addition, the transverse magnetization decays - usually much faster - because of different magnetic fields experienced by the individual spins leading to a dephasing of the signal.

h **(TODO: T1/T2 figure)**

2.2.3 A simple NMR experiment

The most basic experiment in NMR is the reaction of a spin ensemble to an

2.2.4 Field Gradients

2.2.5 2D-NMR

2.3 MRI

2.3.1 MRI in Medicine

2.3.2 Frequency encoding

2.3.3 Phase encoding

2.4 Hyperpolarization

The main limitation of NMR and MRI is the low thermal polarization. For each energy state E_i the Boltzmann distribution dictates

$$N_i = \exp \frac{E_i}{k_B T} \tag{2}$$

For energy differences between two states that are small compared to the thermal Energy, the polarization can be expressed as follows:

$$P = N_+ - N_- N = \tanh \left(\frac{\hbar \gamma B}{2kT} \right) \tag{3}$$

2.4.1 DNP

2.4.2 Hyperpolarization of Noble Gases

2.4.3 Brute Force Hyperpolarization

2.4.4 Parahydrogen induced Hyperpolarization

3 Materials and Methods

3.1 Low field NMR

To achieve NMR spectra at fields where SABRE is feasible **(TODO: Ref sabre)**, a low field NMR spectrometer was built **(TODO: ref niels)**. Its main field is genrated by a resisitve solenoid coil. Inside that coil, there is a saddle coil generating a B_1 field perpendicular to B_0. Perpendicular to and inside both, a third coil, also a solenoid, is used to detect the signal generated by the spins.

3.1.1 Static Magnetic Field

The B_0 coil is wound around an acrylic tube in two full layers. In addition, at the tube's ends compensation windings are installed to homogenize the field inside the coil. The length of these windings was optimized in matlab simulations **(TODO: figure of whole setup)**

3.1.2 Radiofrequency Excitation

To irradiate samples with radiofrequency pulses, a saddle coil **(TODO: dimensions)** wsa used. It was operated untuned and unmatched as a broadband resonator. The pulse generation was performed using a National Instruments data acquisition crate (NI **(TODO: which?)**).

3.1.3 Data Readout

All readout was done using a NI **(TODO: name)**

3.1.4 Shim System

For homogenization of the field, a shim system was built according to Biot Savart simulations. It features linear shim coils for all three spatial dimensions mounted to a .**(TODO: cm)** acrylic tube. The x and y shims are made of four saddle coils respectively that were plainly manufactured individually and bent to fit the tube. The z shims, which are basically a pair of maxwell coils, were added on top of these saddle coils. All shims are driven by a **(TODO: H&U)** programmable power supply providing up to 10 A of current.

3.2 Magritek Low Field MRI

To acquire images at low fields, a Magritek Terranova **(TODO: ref)** was used. It features similar hardware as the low field spectrometer, but uses its B_0 coil only for prepolarization while signal is read out at earth magnetic field. **(TODO: subsections)**

3.3 Bruker Low Field MRI

3.3.1 Gradient Coil Setup

(TODO: subsections)

3.4 High field MRI

The most well known application of NMR is the high field MRI of human antomy with its widespread use in clinics around the world. Not as common, but equally important are preclinical scanners for research purposes. These preclinical scanner, primarily built for animal experiments, were used in most of the high field experiments shown in this work.

3.4.1 MRI Hardware

3.4.2 Paravision Software

3.4.3 Custom High Field Coils

Most commercially available coils are for proton imaging and spectroscopy. Coils for other nuclei are obtainable, but usually expensive and not necessarily tailored to the specific purpose in mind. Therefore, we built single and dual tune coils for different nuclei and different fields.

^{15}N coil

A solenoid of thick, stable copper wire was wound to fit the experimental setup of the shuttling system described in 3.5. The solenoid was attached to a circuit board via clamped and soldered connections. On the board, a high voltage tune capacitor as well as two symmetric matching capacitors were installed. Coaxial cable was used to make the connection to the scanner and the whole setup was mounted to a teflon holder for precise positioning. The tune capacitor was chosen so that it can be tuned to both a 7 T and a 9.4 T field at 300 MHz and 400 MHz respectively. **(TODO: image coil)**

3.5 Shuttling system

3.5.1 Magnetic Shielding

3.5.2 Low Field Reactor

3.5.3 High Field Probe

3.5.4 Fluid Handling System

3.6 Fluxgate Field Probe

3.6.1 Arduino Shield

3.6.2

(TODO: fill with stories of my life)

4 Simulations

(TODO: fill with stories of my life)

5 Results

5.1 Low field NMR

5.2 Sabre in water

5.3 Sabre in cell solution and blood

5.4 15N Sabre

5.5 High field Sabre

6 Conclusion

7 Acknowledgments

First and foremost, I would like to thank...

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Bibliography

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