

SIMULATING ULTRACOLD ATOMS

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From classical to quantum gases

December 2013 – version 0.0.1

Christopher Jon Watkins: *Simulating Ultracold Atoms*, From classical to quantum gases, © December 2013

Ohana means family.
Family means nobody gets left behind, or forgotten.
— Lilo & Stitch

Dedicated to the loving memory of Rudolf Miede.
1939 – 2005

ABSTRACT

Short summary of the contents...

PUBLICATIONS

Some ideas and figures have appeared previously in the following publications:

Put your publications from the thesis here. The packages `multibib` or `bibtopic` etc. can be used to handle multiple different bibliographies in your document.

*We have seen that computer programming is an art,
because it applies accumulated knowledge to the world,
because it requires skill and ingenuity, and especially
because it produces objects of beauty.*

— ? [?]

ACKNOWLEDGEMENTS

Put your acknowledgements here.

Many thanks to everybody who already sent me a postcard!

Regarding the typography and other help, many thanks go to Marco Kuhlmann, Philipp Lehman, Lothar Schlesier, Jim Young, Lorenzo Pantieri and Enrico Gregorio¹, Jörg Sommer, Joachim Köstler, Daniel Gottschlag, Denis Aydin, Paride Legovini, Steffen Prochnow, Nicolas Repp, Hinrich Harms, Roland Winkler, and the whole L^AT_EX-community for support, ideas and some great software.

Regarding L^yX: The L^yX port was initially done by Nicholas Mariette in March 2009 and continued by Ivo Pletikosić in 2011. Thank you very much for your work and the contributions to the original style.

¹ Members of GuIT (Gruppo Italiano Utilizzatori di T_EX e L^AT_EX)

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ACRONYMS

DRY Don't Repeat Yourself

API Application Programming Interface

UML Unified Modeling Language

Part I

INTRO MATERIAL

You can put some informational part preamble text here. Illo principalmente su nos. Non message occidental angloromanic da. Debitas effortio simplicate sia se, auxiliar summarios da que, se avantiate publicationes via. Pan in terra summarios, capital interlingua se que. Al via multo esser specimen, campo responder que da. Le usate medical addresses pro, europa origine sanctificate nos se.

INTRODUCTION

This template for \LaTeX has two goals:

1. Provide students with an easy-to-use template for their Master's or PhD thesis (though it might also be used by other types of authors for reports, books, etc.).
2. Provide a classic, high-quality typographic style that is inspired by ?'s "The Elements of Typographic Style" [?].

The bundle is configured to run with a full MiKTeX or TeXLive installation right away and, therefore, it uses only freely available fonts.

People interested only in the nice style and not the whole bundle can now use the style stand-alone via the file `classicthesis.sty`. This works now also with "plain" \LaTeX .

As of version 3.0, `classicthesis` can also be easily used with LyX¹ thanks to Nicholas Mariette and Ivo Pletikosić. The LyX version of this manual will contain more information on the details.

This should enable anyone with a basic knowledge of \LaTeX or LyX to produce beautiful documents without too much effort. In the end, this is my overall goal: more beautiful documents, especially theses, as I am tired of seeing so many ugly ones.

The whole template and the used style is released under the GNU General Public License.

If you like the style then I would appreciate a postcard:

Andre Miede
Detmolder Strasse 32
31737 Rinteln
Germany

The postcards I received so far are available at:

<http://postcards.miede.de>

IMPORTANT NOTE: Some things of this style might look unusual at first glance, many people feel so in the beginning. However, all things are intentionally designed to be as they are, especially these:

- No bold fonts are used. Italics or spaced small caps do the job quite well.
- The size of the text body is intentionally shaped like it is. It supports both legibility and allows a reasonable amount of information to be on a page. And, no: the lines are not too short.

¹ <http://www.lyx.org>

- The tables intentionally do not use vertical or double rules. See the documentation for the booktabs package for a nice discussion of this topic.²
- And last but not least, to provide the reader with a way easier access to page numbers in the table of contents, the page numbers are right behind the titles. Yes, they are not neatly aligned at the right side and they are not connected with dots that help the eye to bridge a distance that is not necessary. If you are still not convinced: is your reader interested in the page number or does she want to sum the numbers up?

Therefore, please do not break the beauty of the style by changing these things unless you really know what you are doing! Please.

1.1 ORGANIZATION

A very important factor for successful thesis writing is the organization of the material. This template suggests a structure as the following:

*You can use these margins
for summaries of the text
body...*

- `Chapters/` is where all the “real” content goes in separate files such as `Chapter01.tex` etc.
- `FrontBackMatter/` is where all the stuff goes that surrounds the “real” content, such as the acknowledgments, dedication, etc.
- `gfx/` is where you put all the graphics you use in the thesis. Maybe they should be organized into subfolders depending on the chapter they are used in, if you have a lot of graphics.
- `Bibliography.bib`: the Bib_TE_X database to organize all the references you might want to cite.
- `classicthesis.sty`: the style definition to get this awesome look and feel. Bonus: works with both L^AT_EX and PDF_LA_TE_X... and L_XY.
- `ClassicThesis.tcp` a T_EXnicCenter project file. Great tool and it’s free!
- `ClassicThesis.tex`: the main file of your thesis where all the content gets bundled together.
- `classicthesis-config.tex`: a central place to load all nifty packages that are used. In there, you can also activate backrefs in order to have information in the bibliography about where a source was cited in the text (i. e., the page number).

Make your changes and adjustments here. This means that you specify here the options you want to load `classicthesis.sty` with. You

² To be found online at
<http://www.ctan.org/tex-archive/macros/latex/contrib/booktabs/>.

also adjust the title of your thesis, your name, and all similar information here. Refer to [Section 1.3](#) for more information.

This had to change as of version 3.0 in order to enable an easy transition from the “basic” style to L^AT_EX.

In total, this should get you started in no time.

1.2 STYLE OPTIONS

There are a couple of options for `classicthesis.sty` that allow for a bit of freedom concerning the layout:

- General:
 - `drafting`: prints the date and time at the bottom of each page, so you always know which version you are dealing with. Might come in handy not to give your Prof. that old draft.
- Parts and Chapters:
 - `parts`: if you use Part divisions for your document, you should choose this option. (Cannot be used together with `nochapters`.)
 - `nochapters`: allows to use the look-and-feel with classes that do not use chapters, e.g., for articles. Automatically turns off a couple of other options: `eulerchapternumbers`, `linedheaders`, `listsseparated`, and `parts`.
 - `linedheaders`: changes the look of the chapter headings a bit by adding a horizontal line above the chapter title. The chapter number will also be moved to the top of the page, above the chapter title.
- Typography:
 - `eulerchapternumbers`: use figures from Hermann Zapf’s Euler math font for the chapter numbers. By default, old style figures from the Palatino font are used.
 - `beramono`: loads Bera Mono as typewriter font. (Default setting is using the standard CM typewriter font.)
 - `eulermath`: loads the awesome Euler fonts for math. (Palatino is used as default font.)
 - `pdfspacing`: makes use of `pdftex`’ letter spacing capabilities via the `microtype` package.³ This fixes some serious issues regarding math formulæ etc. (e.g., “ß”) in headers.
 - `minionprospacing`: uses the internal `textssc` command of the MinionPro package for letter spacing. This automatically enables the `minionpro` option and overrides the `pdfspacing` option.

*...or your supervisor
might use the margins for
some comments of her own
while reading.*

³ Use `microtype`’s `DVIoutput` option to generate DVI with `pdftex`.

- Table of Contents:
 - `tocaligned`: aligns the whole table of contents on the left side. Some people like that, some don't.
 - `dottedtoc`: sets pagenumbers flushed right in the table of contents.
 - `manychapters`: if you need more than nine chapters for your document, you might not be happy with the spacing between the chapter number and the chapter title in the Table of Contents. This option allows for additional space in this context. However, it does not look as "perfect" if you use `\parts` for structuring your document.
- Floats:
 - `listings`: loads the `listings` package (if not already done) and configures the List of Listings accordingly.
 - `floatperchapter`: activates numbering per chapter for all floats such as figures, tables, and listings (if used).
 - `subfigure`: is passed to the `tocloft` package to enable compatibility with the `subfigure` package. Use this option if you want use `classicthesis` with the `subfigure` package.

The best way to figure these options out is to try the different possibilities and see, what you and your supervisor like best.

In order to make things easier in general, `classicthesis-config.tex` contains some useful commands that might help you.

1.3 CUSTOMIZATION

This section will give you some hints about how to adapt `classicthesis` to your needs.

The file `classicthesis.sty` contains the core functionality of the style and in most cases will be left intact, whereas the file `classicthesis-config.tex` is used for some common user customizations.

The first customization you are about to make is to alter the document title, author name, and other thesis details. In order to do this, replace the data in the following lines of `classicthesis-config.tex`:

Modifications in classicthesis-config.tex

```
1 \newcommand{\myTitle}{A Classic Thesis Style\xspace}
  \newcommand{\mySubtitle}{An Homage to ... \xspace}
  \newcommand{\myDegree}{Doktor-Ingenieur (Dr.-Ing.)\xspace}
```

Further customization can be made in `classicthesis-config.tex` by choosing the options to `classicthesis.sty` (see [Section 1.2](#)) in a line that looks like this:

```
\PassOptionsToPackage{eulerchapternumbers,listings,drafting,
  pdfspacing, subfigure,beramono,eulermath,parts}{classicthesis}
```

If you want to use backreferences from your citations to the pages they were cited on, change the following line from:

```
\setboolean{enable-backrefs}{false}
```

to

```
\setboolean{enable-backrefs}{true}
```

Many other customizations in `classicthesis-config.tex` are possible, but you should be careful making changes there, since some changes could cause errors.

Finally, changes can be made in the file `classicthesis.sty`, although this is mostly not designed for user customization. The main change that might be made here is the text-block size, for example, to get longer lines of text.

*Modifications in
classicthesis.sty*

1.4 ISSUES

This section will list some information about problems using `classicthesis` in general or using it with other packages.

Beta versions of `classicthesis` can be found at the following Google code repository:

<http://code.google.com/p/classicthesis/>

There, you can also post serious bugs and problems you encounter.

Compatibility with the glossaries Package

If you want to use the `glossaries` package, take care of loading it with the following options:

```
\usepackage[style=long,nolist]{glossaries}
```

Thanks to Sven Staehs for this information.

Compatibility with the (Spanish) babel Package

Spanish languages need an extra option in order to work with this template:

```
\usepackage[spanish,es-lcroman]{babel}
```

Thanks to an unknown person for this information (via Google Code issue reporting).

Compatibility with the pdfsync Package

Using the `pdfsync` package leads to linebreaking problems with the `graffito` command. Thanks to Henrik Schumacher for this information.

1.5 FUTURE WORK

So far, this is a quite stable version that served a couple of people well during their thesis time. However, some things are still not as they should be. Proper documentation in the standard format is still missing. In the long run, the style should probably be published separately, with the template bundle being only an application of the style. Alas, there is no time for that at the moment. . . it could be a nice task for a small group of L^AT_EXnicians.

Please do not send me email with questions concerning L^AT_EX or the template, as I do not have time for an answer. But if you have comments, suggestions, or improvements for the style or the template in general, do not hesitate to write them on that postcard of yours.

1.6 LICENSE

GNU GENERAL PUBLIC LICENSE: This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 2 of the License, or (at your option) any later version.

This program is distributed in the hope that it will be useful, but without any warranty; without even the implied warranty of merchantability or fitness for a particular purpose. See the GNU General Public License for more details.

EXAMPLES

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetur id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

2.1 A NEW SECTION

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Examples: *Italics*, ALL CAPS, SMALL CAPS, LOW SMALL CAPS¹.

2.1.1 Test for a Subsection

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Note: The content of this chapter is just some dummy text.

¹ Footnote example.

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2.1.2 *Autem Timeam*

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2.2 ANOTHER SECTION IN THIS CHAPTER

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Sia ma sine svedese americas. Asia ? [?] representantes un nos, un altere membros qui.² Medical representantes al uso, con lo unic vocabulos, tu peano esencialmente qui. Lo malo laborava anteriormente uso.

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² De web nostre historia angloromanic.

aliquet odio. Integer vitae justo. Aliquam vestibulum fringilla lorem. Sed neque lectus, consectetur at, consectetur sed, eleifend ac, lectus. Nulla facilisi. Pellentesque eget lectus. Proin eu metus. Sed porttitor. In hac habitasse platea dictumst. Suspendisse eu lectus. Ut mi mi, lacinia sit amet, placerat et, mollis vitae, dui. Sed ante tellus, tristique ut, iaculis eu, malesuada ac, dui. Mauris nibh leo, facilisis non, adipiscing quis, ultrices a, dui.

LABEL TEST 2: Morbi luctus, wisi viverra faucibus pretium, nibh est placerat odio, nec commodo wisi enim eget quam. Quisque libero justo, consectetur a, feugiat vitae, porttitor eu, libero. Suspendisse sed mauris vitae elit sollicitudin malesuada. Maecenas ultricies eros sit amet ante. Ut venenatis velit. Maecenas sed mi eget dui varius euismod. Phasellus aliquet volutpat odio. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Pellentesque sit amet pede ac sem eleifend consectetur. Nullam elementum, urna vel imperdiet sodales, elit ipsum pharetra ligula, ac pretium ante justo a nulla. Curabitur tristique arcu eu metus. Vestibulum lectus. Proin mauris. Proin eu nunc eu urna hendrerit faucibus. Aliquam auctor, pede consequat laoreet varius, eros tellus scelerisque quam, pellentesque hendrerit ipsum dolor sed augue. Nulla nec lacus.

This statement requires citation ? [?].

2.2.1 *Personas Initialmente*

Suspendisse vitae elit. Aliquam arcu neque, ornare in, ullamcorper quis, commodo eu, libero. Fusce sagittis erat at erat tristique mollis. Maecenas sapien libero, molestie et, lobortis in, sodales eget, dui. Morbi ultrices rutrum lorem. Nam elementum ullamcorper leo. Morbi dui. Aliquam sagittis. Nunc placerat. Pellentesque tristique sodales est. Maecenas imperdiet lacinia velit. Cras non urna. Morbi eros pede, suscipit ac, varius vel, egestas non, eros. Praesent malesuada, diam id pretium elementum, eros sem dictum tortor, vel consectetur odio sem sed wisi.

2.2.1.1 *A Subsubsection*

Sed feugiat. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Ut pellentesque augue sed urna. Vestibulum diam eros, fringilla et, consectetur eu, nonummy id, sapien. Nullam at lectus. In sagittis ultrices mauris. Curabitur malesuada erat sit amet massa. Fusce blandit. Aliquam erat volutpat. Aliquam euismod. Aenean vel lectus. Nunc imperdiet justo nec dolor.

A PARAGRAPH EXAMPLE Etiam euismod. Fusce facilisis lacinia dui. Suspendisse potenti. In mi erat, cursus id, nonummy sed, ullamcorper eget, sapien. Praesent pretium, magna in eleifend egestas, pede pede pretium

LABITUR BONORUM PRI NO	QUE VISTA	HUMAN
fastidii ea ius	germano	demonstratea
suscipit instructor	titulo	personas
quaestio philosophia	facto	demonstrated ?

Table 2.1: Autem timeam deleniti usu id. ?

lorem, quis consectetur tortor sapien facilisis magna. Mauris quis magna varius nulla scelerisque imperdiet. Aliquam non quam. Aliquam porttitor quam a lacus. Praesent vel arcu ut tortor cursus volutpat. In vitae pede quis diam bibendum placerat. Fusce elementum convallis neque. Sed dolor orci, scelerisque ac, dapibus nec, ultricies ut, mi. Duis nec dui quis leo sagittis commodo.

- A. Enumeration with small caps
- B. Second item

Another statement requiring citation ? [?] but this time with text after the citation.

2.2.2 Figure Citations

Veni introduction es pro, qui finalmente demonstrate il. E tambien anglese programma uno. Sed le debitas demonstrate. Non russo existe o, facite linguistic registrate se nos. Gymnasios, e.g., sanctificate sia le, publicate [Figure 2.1](#) methodicamente e qui.

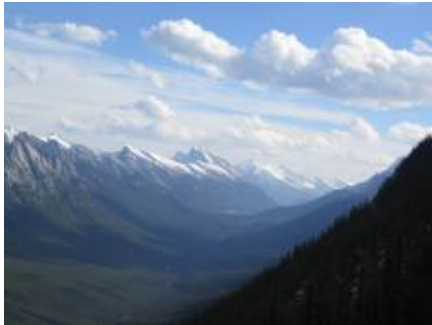
Lo sed apprende instruite. Que altere responder su, pan ma, i.e., signo studio. [Figure 2.1b](#) Instruite preparation le duo, asia altere tentation web su. Via unic facto rapide de, iste questiones methodicamente o uno, nos al.



(a) Asia personas duo.



(b) Pan ma signo.



(c) Methodicamente o uno.



(d) Titulo debitas.

Figure 2.1: Tu duo titulo debitas latente.

Aliquam lectus. Vivamus leo. Quisque ornare tellus ullamcorper nulla. Mauris porttitor pharetra tortor. Sed fringilla justo sed mauris. Mauris tellus. Sed non leo. Nullam elementum, magna in cursus sodales, augue est scelerisque sapien, venenatis congue nulla arcu et pede. Ut suscipit enim vel sapien. Donec congue. Maecenas urna mi, suscipit in, placerat ut, vestibulum ut, massa. Fusce ultrices nulla et nisl.

3.1 SOME FORMULAS

Due to the statistical nature of ionisation energy loss, large fluctuations can occur in the amount of energy deposited by a particle traversing an absorber element¹. Continuous processes such as multiple scattering and energy loss play a relevant role in the longitudinal and lateral development of electromagnetic and hadronic showers, and in the case of sampling calorimeters the measured resolution can be significantly affected by such fluctuations in their active layers. The description of ionisation fluctuations is characterised by the significance parameter κ , which is proportional to the ratio of mean energy loss to the maximum allowed energy transfer in a single collision with an atomic electron:

$$\kappa = \frac{\xi}{E_{\max}} \quad (3.1)$$

E_{\max} is the maximum transferable energy in a single collision with an atomic electron.

$$E_{\max} = \frac{2m_e\beta^2\gamma^2}{1 + 2\gamma m_e/m_x + (m_e/m_x)^2},$$

where $\gamma = E/m_x$, E is energy and m_x the mass of the incident particle, $\beta^2 = 1 - 1/\gamma^2$ and m_e is the electron mass. ξ comes from the Rutherford scattering cross section and is defined as:

$$\xi = \frac{2\pi z^2 e^4 N_{\text{Av}} Z \rho \delta x}{m_e \beta^2 c^2 A} = 153.4 \frac{z^2}{\beta^2} \frac{Z}{A} \rho \delta x \quad \text{keV},$$

where

You might get unexpected results using math in chapter or section heads. Consider the pdfspacing option.

¹ Examples taken from Walter Schmidt's great gallery:
<http://home.vrweb.de/~was/mathfonts.html>

z charge of the incident particle

N_{Av} Avogadro's number

Z atomic number of the material

A atomic weight of the material

ρ density

δx thickness of the material

κ measures the contribution of the collisions with energy transfer close to E_{max} . For a given absorber, κ tends towards large values if δx is large and/or if β is small. Likewise, κ tends towards zero if δx is small and/or if β approaches 1.

The value of κ distinguishes two regimes which occur in the description of ionisation fluctuations:

1. A large number of collisions involving the loss of all or most of the incident particle energy during the traversal of an absorber.

As the total energy transfer is composed of a multitude of small energy losses, we can apply the central limit theorem and describe the fluctuations by a Gaussian distribution. This case is applicable to non-relativistic particles and is described by the inequality $\kappa > 10$ (i.e., when the mean energy loss in the absorber is greater than the maximum energy transfer in a single collision).

2. Particles traversing thin counters and incident electrons under any conditions.

The relevant inequalities and distributions are $0.01 < \kappa < 10$, Vavilov distribution, and $\kappa < 0.01$, Landau distribution.

3.2 VARIOUS MATHEMATICAL EXAMPLES

If $n > 2$, the identity

$$t[u_1, \dots, u_n] = t[t[u_1, \dots, u_{n-1}], t[u_n, \dots, u_n]]$$

defines $t[u_1, \dots, u_n]$ recursively, and it can be shown that the alternative definition

$$t[u_1, \dots, u_n] = t[t[u_1, u_2], \dots, t[u_{n-1}, u_n]]$$

gives the same result.

INTRODUCTION

I am going to need to introduce the different trapping potentials in here some where I think.

4.1 MAGNETIC TRAPPING

Ioffe Pritchard trap

$$\mathbf{B}_{\text{IP}}(x, y, z) = B_0 \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} + B' \begin{bmatrix} x \\ -y \\ 0 \end{bmatrix} + \frac{1}{2} B'' \begin{bmatrix} -xz \\ -yz \\ z^2 - \frac{1}{2}(x^2 + y^2) \end{bmatrix} \quad (4.1)$$

the magnitude of this field can be approximated as the following for small position

$$|\mathbf{B}_{\text{IP}}| = \frac{1}{2} (B''_\rho (x^2 + y^2) + B'' z^2), \quad (4.2)$$

where

$$B''_\rho = \frac{B'^2}{B_0} - \frac{B''}{2}.$$

Quadrupole trap

$$\mathbf{B}_{\text{Q}}(x, y, z) = \frac{1}{2} B_z \begin{bmatrix} x \\ y \\ -2z \end{bmatrix} \quad (4.3)$$

Part II

DSMC

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SIMULATING COLLISIONS IN THERMAL GASES

Need to introduce the usefulness of the method here. References to many kinds of applications and such things. I also need to perform a literature review of all DSMC used in cold atoms physics.

Compare to molecular dynamic approaches, when is DSMC appropriate / good? When does it fail?

Find out the knudsen number for typical cold atom conditions. Wade has numbers for stamper kern and shvatchuck.

DSMC - Birds Book [1]

Evaporative Cooling and Expansion Dynamics: [2–4]

Bosonic Collective-Mode dynamics: [5–9], Can't find Jackson Zaremba 2002 Laser Physics, 12, 93

Fermion Dynamics: [10–13] (see also [14–17])

Sympathetic Cooling: [18, 19]

Applications - Rayleigh Bernard Flow: [20]

Spacecraft aerodynamics: [21]

Chemical reactions: [22] Goldsworthy?

Microfluidics: [23]

Acoustics on Earth, Mars and Titan: [24]

Volcanic plumes on Jupiter: [25]

Read: [26], [45]

Refer to cuda section 10 Should also discuss the development of this parallel implementation of the code. Compare to CPU implementations. Goldsworthy has a few references for other CUDA codes.

The heart of the DSMC method is to simplify the simulation of inter-particle interactions in the form of two body collisions. In this sense there are two aspects we need to ensure are modelled accurately; the number and frequency of collisions (collision rate) and the collisions themselves, whether or not they are correctly distributing the kinetic energy. In the following sections I carefully analyse these two aspects to ensure the utmost accuracy in our simulations.

5.1 COLLISION RATES IN THERMAL GASES

Overall collision rate, spatial collision rate, talk about number of cells, the occupancy of cells and the effect of inhomogeneity.

One of the most basic tests for the application of the DSMC method to cold atom physics is to investigate the collision rate for a thermal gas. Using the Boltzmann equation we can derive [29] the thermally averaged collision rate per unit density for a single species atomic gas bound by the potential $\mathcal{U}(\mathbf{r})$,

Maybe say something about the Boltzmann equation here and give some references.

$$\tau_c^{-1} = \frac{1}{2} n_0 \langle v \sigma \rangle \frac{V_{2e}}{V_e}, \quad (5.1)$$

where $n_0 = N/V_e$ is the central density of the gas, $\langle v \sigma \rangle$ is the thermally averaged product of the atomic velocity and collision cross section, $V_e = \int \exp[-\mathcal{U}(\mathbf{r})/kBT] d\mathbf{r}$ is the effective volume of the gas, and $V_{2e} = \int \exp[-2\mathcal{U}(\mathbf{r})/kBT] d\mathbf{r}$ is the effective volume corresponding to the distribution of pairs. For the bulk of this work we will consider collisions in three unique trapping potentials: no trapping potential, i.e. a homogeneous gas, an Ioffe Pritchard trap (cite) and a spherical quadrupole trap (cite - is it really spherical?)¹. The simplest scenario we can use to investigate the effects of changing the free parameters is that of a homogeneous gas. In this case the collision rate simply reduces to

$$\tau_{c,\text{box}}^{-1} = \frac{1}{\sqrt{2}} n_0 \bar{v} \sigma,$$

where $\bar{v} = \sqrt{8k_B T/\pi m}$, is the average speed of the atoms². In this case the effective volume, V_e , is simply the volume of the box, V .

If we use the expression, (4.2), for the magnetic field produced by an Ioffe Pritchard trap from section 4.1 we find the collision rate to be

$$\tau_{c,\text{IP}}^{-1} = \frac{1}{4} n_0 \bar{v} \sigma.$$

However this time the expression for the effective volume is a little more complex

$$V_{e,\text{IP}} = \frac{1}{\sqrt{B''} B''_\rho} \left(\frac{4\pi k_B T}{g_s \mu_B} \right)^{3/2}.$$

We can combine these two equations to form an expression explicit in the temperature and trapping parameters

$$\tau_{c,\text{IP}}^{-1} = \sqrt{B''} B''_\rho \frac{N (g_s \mu_B)^{3/2} \sigma}{8\pi^2 \sqrt{2} m k_B T}. \quad (5.2)$$

The interesting thing to note here is that the collision rate increases as the temperature decreases, which is the converse to the homogeneous gas. This is because for a trapped gas the density

5.2 DSMC SIMULATIONS OF COLLISIONS

The DSMC method offers some free parameters which we can optimise to balance the accuracy and efficiency, namely the number of cells, n_c , and the number of test particles, N_p . We wish to see the effect of varying these parameters on the results of the simulation.

- ¹ We have a more in depth discussion of magnetic trapping in appendix B.
- ² It is interesting to note that the average velocity of the atoms depends only on the temperature of the gas. It is completely independent of position and trapping potential. In appendix A we have carefully derived this expression for the average velocity of atoms.

The effective volume, V_e , of an inhomogeneous gas equals the volume of a homogeneous gas with the same number of atoms and density.

TRAPPING POTENTIAL	TRAP POWER	EFFECTIVE VOLUME, V_e	COLLISION RATE, τ_c^{-1}
Homogeneous Gas	0	V	$\frac{1}{\sqrt{2}} n_0 \bar{v} \sigma$
Spherical Quadrupole	1	$256 \left(\frac{\pi k_B T}{9_s \mu_B B_z} \right)^3$	$\frac{1}{8\sqrt{2}} n_0 \bar{v} \sigma$
Ioffe Pritchard	2	$\frac{1}{\sqrt{B''} B''_\rho} \left(\frac{4\pi k_B T}{9_s \mu_B} \right)^{3/2}$	$\frac{1}{4} n_0 \bar{v} \sigma$
Power Law	$3/\gamma$	$\frac{4}{3} \pi r_e^3 \Gamma[\gamma + 1] \left(\frac{k_B T}{u_0} \right)^\gamma$	$\frac{1}{2^{\gamma+0.5}} n_0 \bar{v} \sigma$

Table 5.1: Collision rates for different trapping potentials.

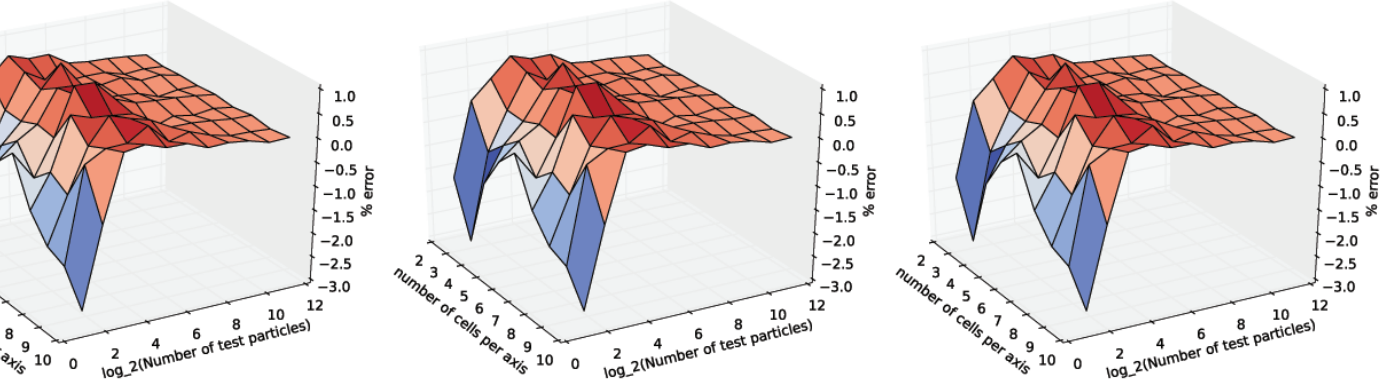


Figure 5.1: Error of DSMC method as a function of test particle number and cell number.

**Include a surface plot of the collision rate as a function of cell number and test particle number. Should make the z axis percentage error. See fig 14. in wade. **

Figure 5.5a shows how well the DSMC method performs over a wide range of test particle and cell numbers. We can see in the corner the method beginning to fail. This is the region where, on average, we have less than two test particles per cell. This means that there is not enough atoms to perform a collision within a cell. One way to avoid this (which has not been implemented here) is to search neighbouring cells for collision pairs when a partner can not be found in the current cell. The main thing to observe here is the increase in the error as the number of test particles is reduced.

5.3 THERMALISATION

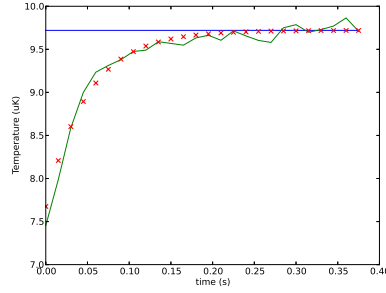
[27], [28]

5.3.1 Walraven Thermalisation

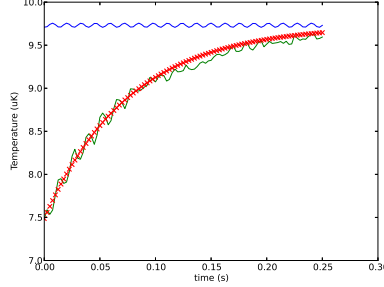
In [29] we are shown that if we perturb the energy of a small fraction of atoms in a single component gas then the rethermalisation time is given by

$$\tau_{\text{th}}^{-1} = \frac{1}{2(\gamma + 3/2)} \tau_c^{-1}, \quad (5.3)$$

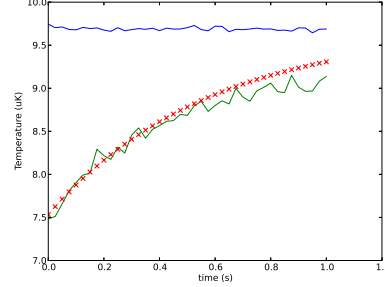
where γ describes the geometry of the trap. For a homogeneous, harmonic and linear trap γ is equal to 0, 3/2 and 3 respectively. Thus we would expect these traps to thermalise in 3, 6 and 9 collision times.



(a) Walraven homogeneous gas thermalisation. $\tau_c^{-1}/\tau^{-1} = 1.2$ should equal 3?



(b) Walraven ip gas thermalisation. $\tau_c^{-1}/\tau^{-1} = 1.6$ should equal 6?



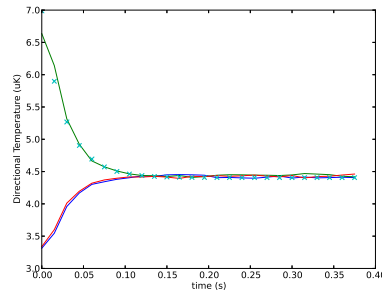
(c) Walraven quad gas thermalisation. $\tau_c^{-1}/\tau^{-1} = 10.45$ should equal 9?

Figure 5.2: Error of DSMC method as a function of test particle number and cell number.

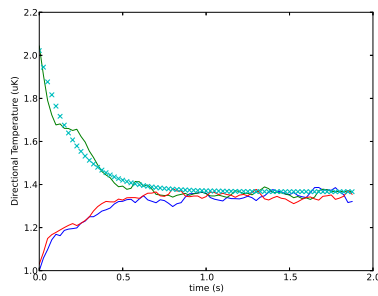
5.3.2 Monroe Thermalisation

Also simulations of Monroe et al. I need to somehow think about this problem analytically. Is there anyway to find an analytic expression for this directional thermalisation?

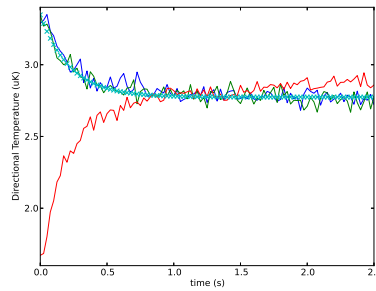
Also do it for different temperatures or trap numbers.



(a) Monroe homogeneous gas thermalisation. $\tau_c^{-1}/\tau^{-1} = 0.77$



(b) Walraven homogeneous gas thermalisation. $\tau_c^{-1}/\tau^{-1} = 2.21$



(c) Walraven quad gas thermalisation. $\tau_c^{-1}/\tau^{-1} = 6.09$

Figure 5.3: Error of DSMC method as a function of test particle number and cell number.

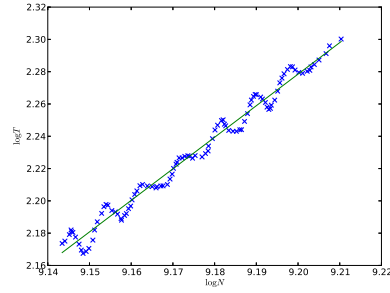
*** MUST REDO ALL OF THESE SIMULATIONS WITH COLLISIONS WORKING CORRECTLY (I.E. WITH THE NEW SORTING FIX IMPLEMENTED). ***

5.4 EVAPORATION

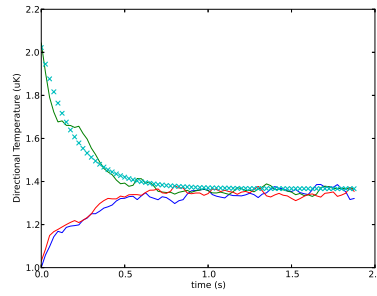
Compare some results to those predicted by the theory of walraven and the other guy.

5.5 ADIABATICITY

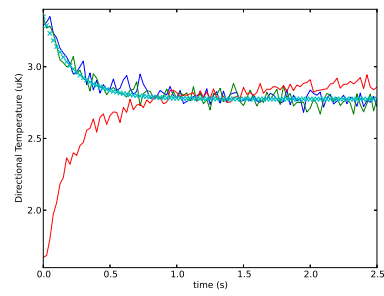
Have a look at squeezing the magnetic trap both diabatically and adiabatically.



(a) η should equal 7, here it is equal to 7.86

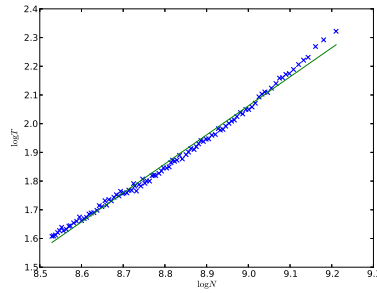


(b) I want this to be a plot of n_0 vs N .

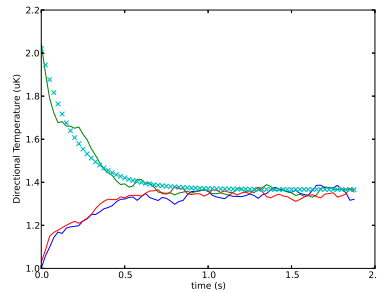


(c) Not sure what plot tp put here

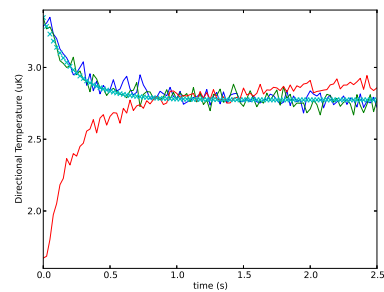
Figure 5.4: IP trap evaporation.



(a) η should equal ?(check the paper), here it is equal to 5



(b) I want this to be a plot of n_0 vs N .



(c) Not sure what plot tp put here

Figure 5.5: Quadrupole trap evaporation.

MAJORANA INTERULDE

6.1 MAJORNAN SPIN FLIPS

Talk about Majorana problem, history, derive formula etc

6.2 LANDAU ZENER FORMULA

Content

DSMC WITH SPIN - EHRENFEST

7.1 SCHRÖDINGER SIMULATIONS

Content

7.1.1 *Simulating Schrödinger Equation*

Content

7.1.2 *Single Atom Spin Flips*

Content

7.2 FULL GAS SIMULATIONS

Content

7.2.1 *Ioffe Pritchard Trap*

Content

7.2.2 *Quadrupole Trap*

Content

DSMC WITH SPIN - MCWF

8.1 SCHRÖDINGER SIMULATIONS

Content

8.1.1 *Simulating Schrödinger Equation*

Content

8.1.2 *Single Atom Spin Flips*

Content

8.2 FULL GAS SIMULATIONS

Content

8.2.1 *Ioffe Pritchard Trap*

Content

8.2.2 *Quadrupole Trap*

Content

Part III

FEMDVR

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FEMDVR

9.1 1D FEMDVR

Content

9.1.1 *Scaling Comparison to CPU*

Content

9.1.2 *Real Simulation*

Content

9.2 3D FEMDVR

Content

9.2.1 *Knots*

Content

Part IV

CUDA

You can put some informational part preamble text here. Illo principalmente su nos. Non message occidental angloromanic da. Debitas effortio simplicate sia se, auxiliar summarios da que, se avantiate publicationes via. Pan in terra summarios, capital interlingua se que. Al via multo esser specimen, campo responder que da. Le usate medical addresses pro, europa origine sanctificate nos se.

CUDA DSMC

10.1 CUDA

Content

10.1.1 *Parallelisation*

Content

10.2 SPEED UP

Content

10.2.1 *Some simulations*

Content

Part V

APPENDIX

MOTION INTEGRATION

A.1 COLLISION RATES IN THERMAL GASES

MOTION INTEGRATION

In this appendix we will explain in detail the different methods of integrating the Newtonian motion of particles and specifically how we have gone about it.

C.1 EULER METHOD

$$x_{n+1} = x_n + v_n \Delta t, \quad (\text{C.1})$$

$$v_{n+1} = v_n + a_n \Delta t. \quad (\text{C.2})$$

C.2 SEMI-IMPLICIT EULER METHOD

$$x_{n+1} = x_n + v_n \Delta t, \quad (\text{C.3})$$

$$v_{n+1} = v_n + a_{n+1} \Delta t. \quad (\text{C.4})$$

C.3 VERLET ALGORITHM

Sometimes referred to as the Störmer-Verlet method (see wikipedia page it's pretty good), it was made popular by Verlet in 1976 [30]. The Verlet algorithm can be derived from the Taylor series expansions for position as follows,

$$\mathbf{r}(t_{n+1}) = \mathbf{r}(t_n) + \mathbf{k}\mathbf{v}(t_n) + \frac{1}{2}\mathbf{k}^2\mathbf{a}(t_n) + \mathcal{O}(\mathbf{k}^3), \quad (\text{C.5a})$$

$$\mathbf{r}(t_{n-1}) = \mathbf{r}(t_n) - \mathbf{k}\mathbf{v}(t_n) + \frac{1}{2}\mathbf{k}^2\mathbf{a}(t_n) + \mathcal{O}(\mathbf{k}^3), \quad (\text{C.5b})$$

we can now add equations (C.5a) and (C.5b) together to get

$$\begin{aligned} \mathbf{r}(t_{n+1}) + \mathbf{r}(t_{n-1}) &= 2\mathbf{r}(t_n) + \mathbf{k}^2\mathbf{a}(t_n) + \mathcal{O}(\mathbf{k}^4), \\ \Rightarrow \mathbf{r}(t_{n+1}) &= 2\mathbf{r}(t_n) - \mathbf{r}(t_{n-1}) + \mathbf{k}^2\mathbf{a}(t_n) + \mathcal{O}(\mathbf{k}^4),. \end{aligned} \quad (\text{C.6})$$

We can see from equation (C.6) that the leap frog method is fourth order in time. However, we can also note that the velocities do not explicitly appear in the method, this means we need to derive them from positions. A simple approximation would be to use the midpoint method

$$\mathbf{v}(t_n) = \frac{1}{2}\mathbf{k}(\mathbf{r}(t_{n+1}) - \mathbf{r}(t_{n-1})) \quad (\text{C.7})$$

C.4 LEAP FROG METHOD

[31]

$$x_n = x_{n-1} + v_{i-1/2} \Delta t, \quad (\text{C.8})$$

$$v_{n+1/2} = v_{n-1/2} + a_n \Delta t. \quad (\text{C.9})$$

C.5 VELOCITY VERLET

[32]

$$x_{n+1} = x_n + v_i \Delta t + \frac{1}{2} a_n \Delta t^2, \quad (\text{C.10})$$

$$v_{n+1} = v_n + \frac{1}{2} (a_n + a_{n+1}) \Delta t. \quad (\text{C.11})$$

C.6 BEEMAN'S ALGORITHM

[33]

$$x_{n+1} = x_n + v_n \Delta t + \frac{1}{6} (4a_n - a_{n-1}) \Delta t^2, \quad (\text{C.12})$$

$$v_{n+1} = v_n + \frac{1}{6} (2a_{n+1} + 5a_n - a_{n-1}) \Delta t. \quad (\text{C.13})$$

DIRECT SIMULATION MONTE CARLO

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D.1 APPENDIX SECTION TEST

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quaestio philosophia	facto	demonstrated

Table D.1: Autem usu id.

Listing D.1: A floating example

```

4 for i:=maxint to 0 do
  begin
    { do nothing }
  end;
```

D.2 ANOTHER APPENDIX SECTION TEST

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NON-DIMENSIONALISATION

E.1 QUASI - 1D GPE

Let's just start with writing out the full quasi-one-dimensional three component equation in a harmonic potential

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} f_+ = & \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \frac{1}{2} m \omega_z^2 z^2 + E_+ + E_\perp + c_0 N \eta \rho \right. \\ & \left. + c_2 N \eta (\rho_+ + \rho_0 - \rho_-) \right) f_+ + c_2 N \eta f_0^2 f_-^*, \end{aligned} \quad (\text{E.1a})$$

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} f_0 = & \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \frac{1}{2} m \omega_z^2 z^2 + E_0 + E_\perp + c_0 N \eta \rho \right. \\ & \left. + c_2 N \eta (\rho_+ + \rho_-) \right) f_0 + 2c_2 N \eta f_+ f_- f_0^*, \end{aligned} \quad (\text{E.1b})$$

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} f_- = & \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \frac{1}{2} m \omega_z^2 z^2 + E_- + E_\perp + c_0 N \eta \rho \right. \\ & \left. + c_2 N \eta (\rho_- + \rho_0 - \rho_+) \right) f_- + c_2 N \eta f_0^2 f_+^*, \end{aligned} \quad (\text{E.1c})$$

$$\rho \frac{\partial E_\perp}{\partial \chi} + \left(\frac{c_0 N}{2} \rho^2 + \frac{c_2 N}{2} S_2 \right) \frac{\partial \eta}{\partial \chi} = 0. \quad (\text{E.1d})$$

If we make the Thomas Fermi ansatz then the transverse mode energy and the scaling factor are given by

$$E_\perp = \frac{\hbar \omega_\perp}{6} \frac{\chi^2}{a_\perp^2}, \quad (\text{E.2})$$

$$\eta = \frac{4}{3\pi\chi^2}, \quad (\text{E.3})$$

where $a_\perp = \sqrt{\hbar/m\omega_\perp}$. If we substitute (E.2) and (E.3) into (E.1d) then we find

$$\chi = \left(\frac{4c_0 N \rho^2 + c_2 N S_2}{m\pi\rho\omega_\perp^2} \right)^{\frac{1}{4}}. \quad (\text{E.4})$$

Now substituting (E.4) back into (E.2) and (E.3) and simplifying we have

$$E_\perp = \sqrt{\frac{mN\omega_\perp^2 (c_0\rho^2 + c_2 S_2)}{9\pi\rho}}, \quad (\text{E.5})$$

$$\eta = \frac{2}{3} \sqrt{\frac{m\rho\omega_\perp^2}{\pi N (c_0\rho^2 + c_2 S_2)}}. \quad (\text{E.6})$$

Now we can begin to non-dimensionalise the equations. Let us only consider the non-dimensionalisation of the positive component since the procedure will be exactly the same for all components. We begin by making the substitutions

$$\begin{aligned} t &\rightarrow t_c \tau, \\ z &\rightarrow z_c \zeta, \\ f_+ &\rightarrow f_c u_+. \end{aligned}$$

Equation (E.1a) now becomes

$$\begin{aligned} i\hbar \frac{f_c}{t_c} \frac{\partial}{\partial \tau} u_+ &= \left(-\frac{\hbar^2}{2mz_c^2} \frac{\partial^2}{\partial \zeta^2} + \frac{1}{2} m\omega_z^2 z_c^2 \zeta^2 + f_c E_+ + f_c E_\perp + c_0 f_c N\eta\rho \right. \\ &\quad \left. + c_2 f_c N\eta (\rho_+ + \rho_0 - \rho_-) \right) f_c u_+ + c_2 f_c^2 N\eta u_0^2 u_-^*, \\ i \frac{mz_c^2}{\hbar t_c} \frac{\partial}{\partial \tau} u_+ &= \left(-\frac{1}{2} \frac{\partial^2}{\partial \zeta^2} + \frac{1}{2} \frac{m^2 \omega_z^2 z_c^4}{\hbar^2} \zeta^2 + \frac{mz_c^2}{\hbar^2} f_c [E_+ + E_\perp + c_0 N\eta\rho \right. \\ &\quad \left. + c_2 N\eta (\rho_+ + \rho_0 - \rho_-)] \right) u_+ + \frac{mz_c^2}{\hbar^2} c_2 f_c N\eta u_0^2 u_-^*. \end{aligned}$$

Looking at the coefficient of the ζ^2 term we can see that if we set it to $1/2$ we will be able to solve for z_c ,

$$\begin{aligned} 1 &= \frac{m^2 \omega_z^2 z_c^4}{\hbar^2}, \\ \Rightarrow z_c &= \sqrt{\frac{\hbar}{m\omega_z}}, \end{aligned} \tag{E.7}$$

which is the harmonic oscillator length along the z axis, a natural length scale for the z dimension. Now we can turn our attention to the coefficient of the time derivative, and set it to i ,

$$\begin{aligned} 1 &= \frac{mz_c^2}{\hbar t_c}, \\ &= \frac{m\hbar}{m\hbar\omega_z t_c}, \\ \Rightarrow t_c &= \frac{1}{\omega_z}, \end{aligned} \tag{E.8}$$

which is the angular period of the oscillator, again a natural length scale. Finally we can consider the energy terms. With these we need to choose f_c such that the dimension of the energy term is one. To cut a long story short, this makes a suitable choice for f_c to be $1/\sqrt{z_c}$. Giving us the final form of the non-dimensionalised equation

$$\begin{aligned} i \frac{\partial}{\partial \tau} u_+ &= \left(-\frac{1}{2} \frac{\partial^2}{\partial \zeta^2} + \frac{1}{2} \zeta^2 + \frac{m}{\hbar^2} \left(\frac{\hbar}{m\omega_z} \right)^{\frac{3}{4}} [E_+ + E_\perp + c_0 N\eta\rho \right. \\ &\quad \left. + c_2 N\eta (\rho_+ + \rho_0 - \rho_-)] \right) u_+ + \frac{m}{\hbar^2} \left(\frac{\hbar}{m\omega_z} \right)^{\frac{3}{4}} c_2 N\eta u_0^2 u_-^*. \end{aligned} \tag{E.9}$$

E.2 MAJORANA PROBLEM SPIN HALF

The potential energy operator [?] for a magnetic dipole in a field is given by

$$\hat{V} = -\hat{\boldsymbol{\mu}} \cdot \mathbf{B}, \quad (\text{E.10})$$

where $\hat{\boldsymbol{\mu}}$ is the magnetic dipole operator and \mathbf{B} is the magnetic field. Which for a spin half particle is

$$\hat{V} = \frac{1}{2} \mu_B g_s \begin{bmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{bmatrix},$$

where μ_B is the Bohr magneton [?] and g_s is the Landé g-factor of the spin- $\frac{1}{2}$ particle. Now we can write the time dependant Schrödinger equation for our system (need to introduce kinetic energy operator as well)

$$i\hbar \partial_t \psi_{\uparrow} = -\frac{\hbar^2}{2m} \partial_{zz} \psi_{\uparrow} + \frac{1}{2} \mu_B g_s B_z \psi_{\uparrow} + \frac{1}{2} \mu_B g_s (B_x - iB_y) \psi_{\downarrow}, \quad (\text{E.11})$$

$$i\hbar \partial_t \psi_{\downarrow} = -\frac{\hbar^2}{2m} \partial_{zz} \psi_{\downarrow} - \frac{1}{2} \mu_B g_s B_z \psi_{\downarrow} + \frac{1}{2} \mu_B g_s (B_x + iB_y) \psi_{\uparrow}. \quad (\text{E.12})$$

Maybe before we non-dimensionalise we will insert or actual values for the magnetic field, $\mathbf{B} = (B_x, 0, -dB_z z)$. Now to non-dimensionalise. We make the substitutions

$$z \rightarrow z_c \zeta,$$

$$t \rightarrow t_c \tau,$$

$$\psi_i \rightarrow \psi_c \phi.$$

From here we will only consider the equation for the spin up component as the two will have the same non-dimensionalisation. After making these substitutions the above equation becomes

$$i\hbar \frac{\psi_c}{t_c} \partial_{\tau} \phi_{\uparrow} = -\frac{\hbar^2}{2m z_c^2} \partial_{\zeta\zeta} \phi_{\uparrow} - \frac{1}{2} \mu_B g_s dB_z z_c \zeta \psi_c \phi_{\uparrow} + \frac{1}{2} \mu_B g_s \psi_c B_x \phi_{\downarrow},$$

rearranging so that the coefficient of the highest derivative is dimensionless

$$i \frac{m z_c^2}{\hbar t_c} \partial_{\tau} \phi_{\uparrow} = -\frac{1}{2} \partial_{\zeta\zeta} \phi_{\uparrow} - \frac{1}{2} \frac{\mu_B g_s m dB_z z_c^3}{\hbar^2} \zeta \phi_{\uparrow} + \frac{1}{2} \frac{\mu_B g_s m z_c^2}{\hbar^2} B_x \phi_{\downarrow}.$$

From here we can see

$$z_c = \frac{B_x}{dB_z}, \quad (\text{E.13})$$

$$t_c = \frac{\hbar}{B_x g_s \mu_B}, \quad \text{1 / Larmor frequency around Bx} \quad (\text{E.14})$$

$$\psi_c = \frac{dB_z^2 \hbar^2}{B_x^3 g_s m \mu_B}. \quad (\text{E.15})$$

Leaving us with the non-dimensionalised equation

$$\partial_{\tau} \phi_{\uparrow} = \frac{1}{2} \partial_{\zeta\zeta} \phi_{\uparrow} + \frac{1}{2} \zeta \phi_{\uparrow} - \frac{1}{2} \phi_{\downarrow}.$$

More dummy text

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Table E.1: Autem usu id.

Listing E.1: A floating example

```

1 for i:=maxint to 0 do
  begin
    { do nothing }
  end;

```

E.3 ANOTHER APPENDIX SECTION TEST

Curabitur tellus magna, porttitor a, commodo a, commodo in, tortor. Donec interdum. Praesent scelerisque. Maecenas posuere sodales odio. Vivamus metus lacus, varius quis, imperdiet quis, rhoncus a, turpis. Etiam ligula arcu, elementum a, venenatis quis, sollicitudin sed, metus. Donec nunc pede, tincidunt in, venenatis vitae, faucibus vel, nibh. Pellentesque wisi. Nullam malesuada. Morbi ut tellus ut pede tincidunt porta. Lorem ipsum dolor sit amet, consectetur adipiscing elit. Etiam congue neque id dolor.

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