# On Interacting Particles in 1D and 2D (Skeleton Edition) (Completeness and Scheduling Estimates in Contents)

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# Abstract

This is the skeleton of the thesis, in terms of the chapters etc planned. The Conclusions are still a little fluid, and the Results will consist of a large number of graphs, so I'll probably arrange that in a little more detail when I get to it. Underneath the chapter headings I have put the percentage of completion, and where I have written stuff I have broken this down by section, subsection etc. As of now I have written just under half of the Analytics chapter; I suspect that that chapter will constitute a little over a quarter of the finished thesis. According to my current estimates, I need a further 9 weeks to complete the thesis, which would imply completion in mid-August. However, this might be an underestimate and is partially dependent upon obtaining decent 2d data soon, which might not happen as my calculations keep failing. Thus, I think an extension of one month might be a good idea, just to make absolutely sure it's finished.

# Contents

# List of Figures

# List of Tables

# Chapter 1

# Preliminary Work, Background and Motivation (0% done) (Needs 3 weeks)

0% done.

## The $TiO_2$/Ti Interface System

## Initial Attempts to Model the $TiO_2$/Ti Interface System

### The Difficulties of Nonequilibrium Statistical Mechanics

### Dynamics of Ionic Crystals

### Initial Work Done with MD

### The Problems with MD

## Simple Large-Scale Models of the Ti/O/Nb Interacting System

### Proposed Linear System

### Attempts to create a Suitable Nonlinear System

### Parametrisation from a Microscopic Model

## The Sticky Particle Model

### Model Motivation

### Model Definition

### Model Properties

### Relation to Existing Literature

### Generalisation to Higher Dimensions



## Implications of Initial Work for the PhD Direction

# Chapter 2

# Analytical Results about the SPM (45% done) (Needs 2 more weeks)

45% done.

## Solving Problems in Nonequlibrium Statistical Mechanics

12.5 % done.

### Equilibrium Statistical Mechanics

25% done.

#### Exact Solutions

50% done.

#### Approximations

0% done.

## Nonequlibrium Statistical Mechanics

### Exact Solutions

0% done.

### Approximations

0% done.

### Similarities and Differences Between Nonequlibrium and Equilibrium Statistical Mechanics

## Where does the SPM stand?

0% done.

# Similarities between the SPM and Established Models in 1D

80% done.

## Relationship with the Ising Model

90% done.

## Correlation Functions

100% done.

### Equivalence with the Misanthrope Process

100% done.

### Differences Between SEP and the SPM

0% done.

## Using the Mean-Field Approximation on the SPM

40% done.

### Lattice MFT Derivation

100% done.

### Continuum Limit MFT Derivation

90% done.

### Negative Diffusion Coefficients

0% done.

### Continuum Limit MFT Solutions

0% done.

### Continuum MFT Breakdown

0% done.

# The SPM in Higher Dimensions

0% done.

# Chapter 3

# Numerical Results about the SPM (0% done) (Needs 2 weeks)

0% done.

## Numerical Simulations of Continuous-Time Markov Processes

### Known Methods

`KMCLib`

### Running `KMCLib` on `Eddie3`

## Calculation Results

### 1D

### 2D

# Chapter 4

# Conclusions (0% done) (Needs unknown amount of time, probably 2 weeks)

0% done.

# Appendix A

# Code Listings (25% done) (Doesn't need much time, is done as the other chapters are made)

25 % done.

## 1d Ising Correlation Functions

100% done.