

# 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.

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# **Chapter 1**

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

0% done.



# **The TiO<sub>2</sub>/Ti Interface System**

## **Initial Attempts to Model the TiO<sub>2</sub>/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 Nonequilibrium Statistical Mechanics**

12.5 % done.

#### **Equilibrium Statistical Mechanics**

25% done.

#### **Exact Solutions**

50% done.

#### **Approximations**

0% done.

## **Nonequilibrium Statistical Mechanics**

### **Exact Solutions**

0% done.

### **Approximations**

0% done.

### **Similarities and Differences Between Nonequilibrium 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.