

On Interacting Particles in 1D

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Abstract

Interface growth, and in particular the prediction of its rate, has long been a tough problem in statistical physics. In this thesis, I will outline my personal take on the matter, and will showcase a possible approach to it consisting of constructing a microscopic model on a lattice and using this to parametrise a large-scale model of the phenomenon. I will then discuss how to do this with multiple interacting particle species in play.

Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

Parts of this work have been published in [1].

(Joshua DM Hellier, July 2018)

Acknowledgements

Insert people you want to thank here.

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Chapter 1

Preliminary Work, Background and Motivation

Here we need to talk about the original intent of the project.

The TiO_2/Ti Interface System

A description of the initial problem upon which the project was based.

Initial Attempts to Model the TiO_2/Ti Interface System

The Difficulties of Nonequilibrium Statistical Mechanics

Dynamics of Ionic Crystals

Maybe mention Ewald sums, and the other issues with computations about materials.

Initial Work Done with MD

I used some LAMMPS code to try to work with MD initially; melts and things.

The Problems with MD

Need to explain why issues with using MD, and why I eventually decided it was not a useful technique for this problem; in particular, why MD is fundamentally flawed as a concept.

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

I had a think about various methods I could use to tackle the system in question, and decided that the approach would be most likely to bear fruit would be a continuum-modelled bulk PDE system with appropriate boundary conditions between phases.

Proposed Linear System

Simplest possible model, and why it failed.

Attempts to create a Suitable Nonlinear System

Talk about why nonlinearity is necessary (as in, it just spits out the previous system again), and the difficulties of parametrising it.

Parametrisation from a Microscopic Model

Talk about the Dresden conference and what I learned from it.

The Sticky Particle Model

Model Motivation

As in, why this is a good start in 1d.

Model Definition

Model Properties

Including Detailed Balance, symmetry, “locality”. Also mention that it is a Markov process.

Relation to Existing Literature

Generalisation to Higher Dimensions

Including a proof of detailed balance in arbitrary dimensions (on square lattice).

Implications of Initial Work for the PhD Direction

Why the Change of Direction?

Essentially, why trying to solve this particular problem is actually kind of silly, and why having a better theory of driven lattice flows would be more useful.

Why Investigate Flow in the SPM?

Talk about how boundary-condition-induced flow on systems that would otherwise obey detailed balance hasn’t really been done before. Bring it around to the question: “Can we have interesting dynamics in a model which is symmetric and obeys detailed balance?”

Chapter 2

Analytical Results about the SPM

Existing Approaches to Nonequilibrium Statistical Mechanics

Mean-Field Theory

Quick history of this, how to use it, when it might work.

Exact Solutions

Talk about stuff like ASEP. Remember to mention that only very specific models seem to be analytically solveable, in particular you can't have interactions and range in the current models.

Where does the SPM stand?

Basically, why we can't analytically solve it, and so why performing mean-field approximation is a decent start.

Analytic Derivations from the SPM in 1D

This stuff is kinda self-explanatory.

Lattice MFT Derivation

Continuum Limit MFT Derivation

Negative Diffusion Coefficients

When do they happen? What do they mean?

Continuum Limit MFT Solutions

There's a bunch of these.

Continuum MFT Breakdown

The SPM in Higher Dimensions

Kinda repeat the earlier stuff in higher dimensions, particularly 2 where we actually have data. Maybe less need for elaborate sections structure here; just write freely and see how it goes.

Chapter 3

Numerical Results about the SPM

Numerical Simulations of Continuous-Time Markov Processes

Known Methods

Discuss commonly-used methods, and how they work. Eventually, talk about why we are using the n-fold way.

KMCLib

Talk about how it works, why I picked it over other implementations.

Running KMCLib on Eddie3

How calculations are managed day-to-day.

Calculation Results

1D

2D

Chapter 4

Conclusions

Need to summarise the key results of the research here, and give an overview.

Appendix A

The First Appendix

Not sure what I would put in appendices; this might become more clear when I start writing the thing. Code, perhaps?

Bibliography

- [1] Conway, D. *Object Oriented Perl: A comprehensive guide to concepts and programming techniques*. Connecticut, USA: Manning Publications Co., 2000.