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

Perliminary Work and Motivation

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

1.1 The TiO_2/Ti Interface System

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

1.2 Molecular Dynamics

1.2.1 Initial Work Done with MD

I used some LAMMPS code to try to work with MD initially.

1.2.2 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.

1.3 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 would be most likely to bear fruit would be a continuum-modelled bulk PDE system with appropriate boundary conditions between phases.

1.3.1 Proposed Linear System

Simplest possible model, and why it failed.

1.3.2 Attempts to create a Suitable Nonlinear System

Talk about why nonlinearity is necessary, and the difficulties of parametrising it.

1.3.3 Parametrisation from a Microscopic Model

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

Chapter 2

The Sticky Particle Model

Here we will talk about the SPM, which I have (mostly) written a paper about.

2.1 Definition and Motivation

2.1.1 Interacting Diffusion through Lattices

Here we describe why the assumptions of periodic potential + short-range interaction + hard core repulsion are reasonable assumptions for small particles moving through a metal lattice.

2.1.2 Model Definition

We put those assumptions together in 1D, and get the SPM.

2.2 Analytic Derivations from the SPM

This stuff is kinda self-explanatory.

2.2.1 Continuum Limit MFT Derivation

2.2.2 Continuum Limit MFT Solutions

2.2.3 Continuum MFT Self-Downfall predictions

2.3 Numerical Calculations using the SPM

2.3.1 Code Setup Used

2.3.2 The Types of Calculation Performed

2.3.3 The Quantities Measured

Or rather, the various quantities we could measure, and why we couldn't measure the other ones we wanted to measure.

2.4 Numerical Results

And their comparisons with related analytics. We should just chuck all the results we have in here. Inc. discussion about the spacetime flow patterns.

2.5 Building a Full Continuum Model

As in, tweaking the MFT to give correct bulk predictions, as well as boundary condition information, to get a recipe for prediciting large-scale stuff about the SPM.

Chapter 3

Multispecies Generalisation of the SPM

Would like this to structurally mirror the previous chapter. Intend to use essentially the same methodology to analyse the generalisation as the original model, with a few tweaks here and there. Of course, this is stuff I haven't done yet, so can't say with much more certainty than that!

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.