On Interacting Particles in 1D and 2D

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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 .

(*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 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 whose bulk motion is symmetric and obeys detailed balance?"

Chapter 2

Analytical Results about the SPM

We now have a model, the SPM, which should represent the kind of behaviour we are interested in. In this chapter we will attempt to derive analytic results about how material flows in the model. Initially this was all done with the aim of producing an approximation to the behaviour in the hydrodynamic limit and thus informing us about the surface layer formation; however, as you will see the analytic predictions suggest that the flows could be quite interesting in their own right.

Solving Problems in Nonequlibrium Statistical Mechanics

Models in nonequlibrium statistical mechanics which contain nontrivial interactions between components often produce interesting behaviour, hence the wide interest in these models. However, they usually prove to be difficult to "solve" in any concrete sense. In this section I will give a brief overview of solution methods in equilibrium statistical mechanics, why nonequilibrium statistical mechanics problems tend to be harder to solve, and how this affects the way we approach the SPM.

Equilibrium Statistical Mechanics

Equilibrium statistical mechanics is a bread and butter part of undergraduate physics, and there are a great many texts on the subject [1]. When we speak of "solving" an equilibrium statistical mechanics system, the gold standard is to be able to calculate relationships between the statistics of large-scale quantities as a function of the system constraints or their conjugates. This allows one to classify the system's behaviour by making equations of state and identifying phase transitions (situations where at least some large-scale quantity statistics vary with respect to each other in a discontinuous manner). As you will see, the SPM itself is isomorphic to an equilibrium statistical mechanics model so long as we do not drive the system using boundary conditions (e.g. particle reservoirs with different concentrations).

Exact Solutions

A quantity of key interest in equilibrium statistical mechanics is the partition function, usually denoted by Z. Say we have a closed classical mechanical system maintained at constant temperature T by a heat bath, so only energy can enter and leave the system (the canonical ensemble). Let its state space be Ξ, and denote an individual microstate (specific configuration of the system) by ξ. Such a system must of course have a Hamiltonian $H : \Xi \to \mathbb{R}$. The canonical partition function for this system is defined to be

$$Z(\beta) = \int_{\Xi} \mathrm{d}\xi \;\; e^{-\beta H(\xi)}, \tag{2.1}$$

with $\beta T = 1$, where the integrand on the right hand side is the familiar Boltzmann weighting. This quantity is extremely useful, because itself and its derivatives are directly related to the statistics of large-scale quantities. For example, the ensemble-averaged total energy $\langle E \rangle$ satisfies

$$\langle E \rangle = -\frac{\partial \log Z}{\partial \beta} \tag{2.2}$$

If one is able to obtain an expression for the canonical partition function by analytic means, you can calculate essentially any statistical moment of any large-scale quantity you desire, and thus the system is "solved" in the sense we used above.

Approximations

Nonequlibrium Statistical Mechanics

Exact Solutions

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

Approximations

Approximations in noneq statmech

Similarities and Differences Between Nonequlibrium and Equilibrium Statistical Mechanics

Where does the SPM stand?

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

Similarities between the SPM and Established Models in 1D

In the previous section we have discussed the various approaches one might use when attempted to derive properties of a nonequilibrium statistical mechanical system. We will now try to put these ideas into practise on the SPM.

Relationship with the Ising Model

If we implement the rules of the SPM on a periodic domain, we no longer have to deal with boundary conditions. In this special circumstance, we can find an

isomorphism between this model and the Ising model with fixed magnetisation. One does this by associating the Ising spins $\sigma_i \in \{-1, 1\}$ with $\rho_i \in \{0, 1\}$ via

$$\rho_i = \frac{1}{2}\left(1 + \sigma_i\right). \tag{2.3}$$

Recalling our proof that the SPM obeys detailed balance, we saw that the equilibrium probability of finding the SPM in a state containing N particle-particle adjacencies is proportional to λ^{-N}. If our Ising Hamiltonian is defined via

$$H = \frac{1}{2}\sum_{i=1}^{L} J\sigma_i\sigma_{i+1} \pmod{L}, \tag{2.4}$$

the probability of finding ourselves in a state with N paired spins is $e^{-\beta N J}$, with $\beta T = 1$. The comparison with the SPM is now obvious; we set $\log\lambda = \beta J$. Thus λ in the SPM is simultaneously playing the of the binding energy and temperature in the Ising model. !Try to compute average energy!

Correlation Functions

For relatively small systems, given a system size L and a number of particles N, we can analytically compute the pairwise correlation function $C(l) = \langle\rho_i\rho_{i+l}\rangle$ (as the system is clearly homogeneous in i). The following `Python` code does this:

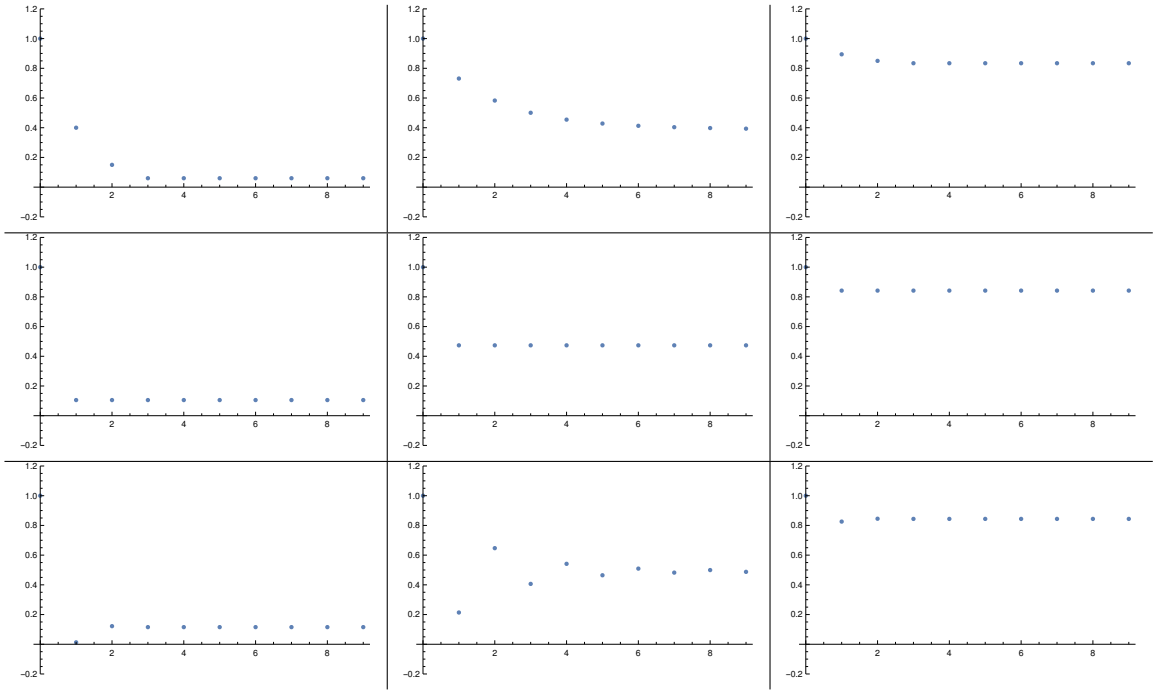
```
import copy
import sys

def configMake(L, N, prevList, totList):
    if L==1:
        endList = [copy.deepcopy(prevList), N]
        totList.append(unfold(endList))
        return [N]
    if N==0:
       return configMake(L-1, 0, [copy.deepcopy(prevList), 0], totList)
    if L==N:
        return configMake(L-1, N-1, [copy.deepcopy(prevList), 1], totList)
    return [configMake(L-1, N, [copy.deepcopy(prevList), 0], totList), configMake(L-1, N-1, [co

def adjSum(candList):
    listLen = len(candList)
    total = 0
    for index in range(0, listLen):
        total += candList[index-1]*candList[index]
    return total

def unfold(candList):
    if isinstance(candList, list):
        if len(candList)==2:
```

```
            return unfold(candList[0])+unfold(candList[1])
        if len(candList)==1:
            return candList
        if len(candList)==0:
            return []
    return [candList]

def listCollate(candList):
    maxItem = 0
    for index in candList:
        if index > maxItem:
            maxItem = index
    outPut = []
    for size in range(0, maxItem+1):
        numCounts = 0
        for index in candList:
            if index == size:
                numCounts += 1
        outPut.append((size, numCounts))
    return outPut

def genCorrFn(L, N):
    totList = []
    allStates = configMake(L, N, [], totList)
    restStates = []
    weightList = []
    maxAdj = 0
    for state in totList:
        if state[0]==1:
            restStates.append((state, adjSum(state)))
            if restStates[-1][1]>maxAdj:
                maxAdj = restStates[-1][1]
            weightList.append(restStates[-1][1])
    partFnList = listCollate(weightList)
    print(partFnList)
    partitionFn = "("
    for pair in partFnList:
        partitionFn += str(pair[1])+"␣Exp["+str(pair[0]-maxAdj)+"b]␣+␣"
    partitionFn += "0)"
    print(partitionFn)
    finalOut = "{"
    for shift in range(0, L-L/2):
        tempList = []
        for config in restStates:
            if config[0][shift] == 1:
                tempList.append(config[1])
        stateDist = listCollate(tempList)
        outSum = "{"+str(shift)+",␣("
        for pair in stateDist:
            outSum += str(pair[1])+"␣Exp["+str(pair[0]-maxAdj)+"b]␣+␣"
        outSum += "0)/"+partitionFn+"}"
        finalOut += outSum
        if shift != L-L/2-1:
            finalOut += ",␣"
    finalOut+="}"
    return finalOut
```

```
L = int(sys.argv[1])

with open("corrFnResults.m", 'w') as f:
    f.write("{")
    for n in range(2, L-2):
        f.write("{"+str(n)+"/"+str(L)+",␣"+genCorrFn(L, n)+"},␣")
    f.write(genCorrFn(L, L-2) + "}")
```

This is quite a nice result, as we can use simple recursion to perform a calculation which would otherwise be quite difficult to code. Unfortunately the time complexity of the calculation grows exponentially in and L, so the largest L I can reasonably run for is 20. In the table below I have plotted the occupation probability of sites shifted from the origin (assuming the origin is occupied) for a selection of $\lambda = e^{-b}$ and particle densities.

Figure 2.1



!write some more about this sometime!

Equivalence with the Misanthrope Process

- show the equivalence
- show lack of explosive condensation
- discuss limits of this (e.g. doesn't really clue us in to how flow works etc)

Using the Mean-Field Approximation on the SPM

Lattice MFT Derivation

From here we will be assuming that there isn't a way to solve the SPM exactly, so we will attempt to use approximation. MFT is, as always, and option.

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] Landau, L. D., E. M. Lifshitz, and L. Pitaevskii. "Statistical physics, part I.", 1980.