

PHYSICAE AUSCULTATIONES

A Dissertation Presented

by

D. W. BLAIR

Submitted to the Graduate School of the
University of Massachusetts Amherst in partial fulfillment
of the requirements for the degree of

DOCTOR OF PHILOSOPHY

September 2010

Physics Department

TABLE OF CONTENTS

	Page
CHAPTER	
1. MELTING: PART A (SCIENCE PAPER)	1
1.1 Background	1
1.1.1 theory of 2-D melting	1
1.2 Experiments by Savage et. al	2
1.3 Depletion potential	2
1.3.1 range $\sim 10\%$ of particle diameter	2
1.3.2 observation: sublimation at steady rate until characteristic size, then enhanced melting	2
1.3.3 Figure: N vs t (Fig 2. from savage et. al)	2
1.3.4 Figure: Q_6 vs t (Fig 3. from savage et. al)	2
1.4 Simulations	2
1.5 Motivation	2
1.5.1 confirm that odd hydrodynamics didn't play a role	2
1.5.2 explore role of range of potential on melting	2
1.6 Simulation algorithm / details	2
1.6.1 brownian dynamics simulation	2
1.6.2 phase diagram exploration	3
1.7 Results	3
1.7.1 short-range potential ($\sim 10\%$)	3
1.7.2 longer-range potential ($\sim 80\%$)	3
1.8 Discussion	3
1.9 Future work	3

1.9.1	3D	3
1.9.2	curved surfaces	3
1.9.3	non-spherical molecules	3
2.	MELTING: PART B (MOUMITA)	4
2.1	Background	4
2.1.1	Reference to experimental work and theory work in melting A chapter	4
2.1.2	Theory: range of potential controls brittle/ductile transition	4
2.1.3	When crystallites are sufficiently brittle, melting is mediated by defects	4
2.2	Theory	5
2.2.1	Determine energy cost, E , of creating a disclination on flat 2D Membrane	5
2.2.2	For thermally-activated disclinations, $K_B T \sim E$	5
2.2.3	Disclinations create internal stresses: relieved by cracking	5
2.2.4	potential energy penalty, V , of crack in 2D sheet	5
2.2.5	minimize V to find critical crack length, $l_c(Y, \gamma)$	5
2.2.6	estimate Y, γ for simulations	5
2.2.7	use these to find a , critical average interparticle separation	5
2.2.8	this allows us to find a critical potential range, a	5
2.3	Simulations	5
2.3.1	Brownian dynamics background (refer to previous)	5
2.3.2	My code (include in thesis) vs. Gromacs	5
2.3.3	New form of the interparticle potential	5
2.3.4	Phase behavior / melting temperature	5
2.3.5	Results	5
2.4	Discussion	6
2.5	Code	6
3.	DIAMETER OF RANDOM CLUSTERS	7
3.1	Background	7
3.1.1	Applications and physical realizations of the potts model	7
3.1.2	Interesting properties of potts model clusters	7
3.1.3	Review of potts model	8
3.2	Simulations	8

3.2.1	swendsen wang algorithm	8
3.2.2	method: determining chemical distance	8
3.2.3	simulation details	9
3.3	Results	9
3.3.1	2D $q=1,2,3,4$	9
3.3.2	3D $q=1,2$	9
3.3.3	4D $q=2$	9
4.	PHASE TRANSITIONS IN COMPUTATIONAL COMPLEXITY	10
4.1	Background	10
4.1.1	Constraint Satisfaction Problems (CSP)	10
4.1.2	Proposal: study complexity of percolation model	11
4.2	Percolation	11
4.2.1	The Model	11
4.2.2	Background / applications	11
4.3	PRAM	11
4.3.1	Applications in comp sci	11
4.3.2	PRIORITY CRCW	11
4.4	Parallel Algorithm for Percolation	11
4.5	Results	11
4.5.1	D_2 vs. p for several system sizes L	11
4.5.2	$\log(D_2)$ vs. $\log(L)$	11
4.5.3	Distribution of cluster sizes	11

CHAPTER 1

MELTING: PART A (SCIENCE PAPER)

1.1 Background

1.1.1 theory of 2-D melting

- bulk: hexatic, two-stage
- for finite crystallites: melting dominated by surface
- range of potential as issue
- imaging small crystallites difficult before savage's technique

1.2 Experiments by Savage et. al

1.3 Depletion potential

1.3.1 range ~ 10 % of particle diameter

1.3.2 observation: sublimation at steady rate until characteristic size, then enhanced melting

1.3.3 Figure: N vs t (Fig 2. from savage et. al)

1.3.4 Figure: Q_6 vs t (Fig 3. from savage et. al)

1.4 Simulations

1.5 Motivation

1.5.1 confirm that odd hydrodynamics didn't play a role

1.5.2 explore role of range of potential on melting

1.6 Simulation algorithm / details

1.6.1 brownian dynamics simulation

- theory

- algorithm

- form of the interaction potential used
 - A-O depletion model

 - 'Blairium' – A-O, but avoid infinite Brownian dynamics force

1.6.2 phase diagram exploration

1.7 Results

1.7.1 short-range potential (~10%)

- N vs. t

- Q_6 vs. t

- Q_6 vs. N

1.7.2 longer-range potential (~80%)

1.8 Discussion

1.9 Future work

1.9.1 3D

1.9.2 curved surfaces

1.9.3 non-spherical molecules

CHAPTER 2

MELTING: PART B (MOUMITA)

2.1 Background

2.1.1 Reference to experimental work and theory work in melting A chapter

2.1.2 Theory: range of potential controls brittle/ductile transition

- brittle / ductile theory

2.1.3 When crystallites are sufficiently brittle, melting is mediated by defects

- alternative melting models

2.2 Theory

2.2.1 Determine energy cost, E , of creating a disclination on flat 2D Membrane

2.2.2 For thermally-activated disclinations, $K_B T \sim E$

2.2.3 Disclinations create internal stresses: relieved by cracking

2.2.4 potential energy penalty, V , of crack in 2D sheet

2.2.5 minimize V to find critical crack length, $l_c(Y, \gamma)$

2.2.6 estimate Y , γ for simulations

2.2.7 use these to find a , critical average interparticle separation

2.2.8 this allows us to find a critical potential range, a

2.3 Simulations

2.3.1 Brownian dynamics background (refer to previous)

2.3.2 My code (include in thesis) vs. Gromacs

2.3.3 New form of the interparticle potential

- plot for short-range, longer-range

2.3.4 Phase behavior / melting temperature

- brittle

- ductile

2.3.5 Results

- For Brittle and Ductile cases:

– N vs. t

- Q_6 vs. $(N-N^*)$
- Q_6 vs. $(N-N^*)$
- Ave. topological charge vs. $(N-N^*)$

- Alternative theories: e.g. Lacoste

2.4 Discussion

2.5 Code

CHAPTER 3

DIAMETER OF RANDOM CLUSTERS

3.1 Background

3.1.1 Applications and physical realizations of the potts model

3.1.2 Interesting properties of potts model clusters

- mass
- perimeter
- chemical distance
 - literature review
 - * applications
 - current understanding
 - no established relationship to other scaling exponents
- diameter
 - graph theoretic definition

- applications
 - * relevant to efficiency of simulations
 - * communication on a potts network
- mean field expectations

3.1.3 Review of potts model

- overview
- phase behavior for $q=1,2,3,4$, $D=1,2,3,4,\text{infinite}$

3.2 Simulations

3.2.1 swendsen wang algorithm

3.2.2 method: determining chemical distance

- review methods in literature
- proposed trick
- our method (useful when periodic boundaries)
- estimated algorithmic complexity

3.2.3 simulation details

- autocorrelation time / independence
- scaling methods

3.3 Results

3.3.1 2D $q=1,2,3,4$

3.3.2 3D $q=1,2$

3.3.3 4D $q=2$

CHAPTER 4

PHASE TRANSITIONS IN COMPUTATIONAL COMPLEXITY

4.1 Background

4.1.1 Constraint Satisfaction Problems (CSP)

- Examples
 - kSAT
 - Graph-coloring
 - Spin models
 - error-correcting codes
- Observation of threshold behavior in CSP
- Difficulties in tackling phase behavior of CSP

4.1.2 Proposal: study complexity of percolation model

4.2 Percolation

4.2.1 The Model

4.2.2 Background / applications

4.3 PRAM

4.3.1 Applications in comp sci

4.3.2 PRIORITY CRCW

4.4 Parallel Algorithm for Percolation

4.5 Results

4.5.1 D_2 vs. p for several system sizes L

4.5.2 $\log(D_2)$ vs. $\log(L)$

4.5.3 Distribution of cluster sizes

- logarithmic or power law? (power law \rightarrow algorithm will often fail)