# UNIVERSITÄT LEIPZIG

**REPORT** Institute für Physik The Physics Institutes



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Front cover

Back covers

Institut für Experimentelle Physik I Institut für Experimentelle Physik II Institut für Theoretische Physik

Fakultät für Physik und Geowissenschaften

Universität Leipzig

Institute for Experimental Physics I Institute for Experimental Physics II Institute for Theoretical Physics

**Faculty of Physics and Earth Sciences** 

Universität Leipzig

Report 2012

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Leipzig, Month 2010

Director 1 Director 2 Director 3 Directors

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## 1

# Structure and Staff of the Institutes

## **1.1 Institute for Experimental Physics I**

1.1.1 Office of the Director

## 1.1.2 Molecular Nano-Photonics, Molekulare Nanophotonik [MON]

Prof. Dr. Frank Cichos

Secretary

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.1.3 Molecular Physics, Molekülphysik [MOP]

Prof. Dr. F. Kremer

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.1.4 Physics of Interfaces, Grenzflächenphysik [GFP]

Prof. Dr. Jörg Kärger

#### Secretary

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.1.5 Soft Matter Physics, Physik der weichen Materie [PWM]

Prof. Dr. Josef A. Käs

Secretary

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.1.6 Biological Physics, Biologische Physik [BIP]

Prof. Dr. Claudia Mierke

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.1.7 Molecular Biophysics, Molekulare Biophysik [MBP]

Prof. Dr. Ralf Seidel

Secretary

**Technical staff** 

Academic staff

PhD candidates

Students

## **1.2 Institute for Experimental Physics II**

#### **1.2.1** Office of the Director

Prof. Dr. Marius Grundmann (director) Prof. Dr. Tilman Butz (vice director)

## 1.2.2 Magnetic Resonance of Complex Quantum Solids, Magnetische Resonanz Komplexer Quantenfestkörper [MQF]

Prof. Dr. Jürgen Haase

Secretary

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.2.3 Nuclear Solid State Physics, Nukleare Festkörperphysik [NFP]

Prof. Dr. Tilman Butz

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.2.4 Semiconductor Physics, Halbleiterphysik [HLP]

Prof. Dr. Marius Grundmann

Secretary

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.2.5 Solid State Optics and Acoustics, Festkörperoptik und -akustik [FKO]

Prof. Dr. Wolfgang Grill

Secretary

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.2.6 Superconductivity and Magnetism, Supraleitung und Magnetismus [SUM]

Prof. Dr. Pablo Esquinazi

**Technical staff** 

Academic staff

PhD candidates

Students

## **1.3 Institute for Theoretical Physics**

#### 1.3.1 Office of the Director

Secretary

### 1.3.2 Computational Quantum Field Theory, Computerorientierte Quantenfeldtheorie [CQT]

Prof. Dr. Wolfhard Janke

#### **Technical staff**

—

#### Academic staff

Dr. Stefan Schnabel Dr. Jonathan Gross Dr. Suman Majumder

#### PhD candidates

M.Sc. Johannes Bock M.Sc. Henrik Christiansen M.Sc. Momchil Ivanov M.Sc. Stanislav Kazmin M.Sc. Ravinder Kumar ("co-tutelle" with Coventry University, UK) Dipl.-Phys. Martin Marenz Dipl.-Phys. Marco Müller Dipl.-Phys. Hannes Nagel Dipl.-Phys. Andreas Nußbaumer M.Sc. Philipp Schierz

#### Students

Kieran Austin Thomas Els Lisa Fiedler Hans-Joachim Lange Fabio Müller David Oberthür Simon Schneider Franz Paul Spitzner Ronja St $\tilde{A}_4^1$ bel Dimitrij Tschodu Tobias Weiss Chris Allen Jakob Bürgermeister Adrian Häußler Michel Michalkow

## 1.3.3 Molecular Dynamics / Computer Simulation, Moleküldynamik / Computersimulation [MDC]

PD Dr. H.L. Vörtler (Speaker) PD Dr. S. Fritzsche

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.3.4 Quantum Field Theory and Gravity, Quantenfeldtheorie und Gravitation [QFG]

Prof. Dr. Gerd Rudolph (Speaker) Prof. Dr. Rainer Verch

**Technical staff** 

Academic staff

PhD candidates

Students

## 1.3.5 Statistical Physics, Statistische Physik [STP]

Prof. Dr. Bernd Rosenow

**Technical staff** 

#### Academic staff

#### PhD candidates

Students

#### 1.3.6 Theory of Condensed Matter, Theorie der kondensierten Materie [TKM]

Prof. Dr. Ulrich Behn (Speaker) Prof. Dr. Klaus Kroy

Prof. Dr. Dieter Ihle (retired) Prof. Dr. Adolf Kühnel (retired)

**Technical staff** 

Academic staff

PhD candidates

Students

### **1.3.7** Theory of Elementary Particles, Theorie der Elementarteilchen [TET]

Prof. Dr. Klaus Sibold

**Technical staff** 

Academic staff

PhD candidates

Students

# I Institute for Experimental Physics I

2

# **Molecular Nano-Photonics**

## 2.1 Introduction

Introductory text ...

Group Leader

## 2.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

Table 2.1: Test table – example of column alignment types.

left	right	center	page (width 60 mm)
abc	abc	abc	The quick brown fox jumps over
			the lazy dog.
de	de	de	Six big devils from Japan quickly
			forgot how to waltz.
fghi	fghi	fghi	Oh, welch Zynismus, quiekte
2	9	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

## 2.3 Contribution 2

J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 2.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

- [1] Akiyoshi's illusion pages, www.ritsumei.ac.jp/ akitaoka/index-e.html
- [2] Reference 2

## 2.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

## 2.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

## 2.6 External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

## 2.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

Posters

Poster 1

Poster 2

## 2.8 Graduations

### Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

### Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## 2.9 Guests

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

3

# **Molecular Physics**

## 3.1 Introduction

Introductory text ...

Group Leader

## 3.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

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2	9	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

## 3.3 Contribution 2

J. Doe, M. Mustermann

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- [2] Reference 2

## 3.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

## 3.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

## 3.6 External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

## 3.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

Posters

Poster 1

Poster 2

## 3.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date
- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

4

# **Physics of Interfaces**

### 4.1 Introduction

Introductory text ...

Group Leader

### 4.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

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5	9	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

### 4.3 Contribution 2

J. Doe, M. Mustermann

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Figure 4.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

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- [2] Reference 2

# 4.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

# 4.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

- Duty 1
- Duty 2

# 4.6 External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

### 4.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

Posters

Poster 1

Poster 2

# 4.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

5

# **Soft Matter Physics**

### 5.1 Introduction

Introductory text ...

Group Leader

### 5.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

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2	9	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

### 5.3 Contribution 2

J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 5.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

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- [2] Reference 2

# 5.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

# 5.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

- Duty 1
- Duty 2

### 5.6 External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

### 5.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

Posters

Poster 1

Poster 2

# 5.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

6

# **Biological Physics**

### 6.1 Introduction

Introductory text ...

Group Leader

### 6.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

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fghi	fghi	fghi	Oh, welch Zynismus, quiekte
5	5	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

### 6.3 Contribution 2

J. Doe, M. Mustermann

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Figure 6.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

- [1] Akiyoshi's illusion pages, www.ritsumei.ac.jp/ akitaoka/index-e.html
- [2] Reference 2

### 6.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

# 6.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

- Duty 1
- Duty 2

## 6.6 External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

### 6.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

Posters

Poster 1

Poster 2

# 6.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

Institute for Experimental Physics II

# Magnetic Resonance of Complex Quantum Solids

```
7.1 Introduction
```

Introductory text ...

Group Leader

### 7.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 †Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

**Table 7.1:** Test table – example of column alignment types.

left	right	center	page (width 60 mm)
abc	abc	abc	The quick brown fox jumps over
			the lazy dog.
de	de	de	Six big devils from Japan quickly
			forgot how to waltz.
fghi	fghi	fghi	Oh, welch Zynismus, quiekte
0	U	U	Xavers jadegrüne Bratpfanne.
abc de fghi	abc de fghi	abc de fghi	The quick brown fox jumps over the lazy dog. Six big devils from Japan quickly forgot how to waltz. Oh, welch Zynismus, quiekte Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

# 7.3 Contribution 2

#### J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 7.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

- [1] Akiyoshi's illusion pages, www.ritsumei.ac.jp/ akitaoka/index-e.html
- [2] Reference 2

### 7.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

# 7.5 Organizational Duties

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

### 7.6 External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

### 7.7 Publications

Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

Talks

Talk 1

Talk 2

#### Posters

Poster 1

Poster 2

### 7.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

# **Nuclear Solid State Physics**

### 8.1 Introduction

Introductory text ...

Group Leader

### 8.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

**Table 8.1:** Test table – example of column alignment types.

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			the lazy dog.
de	de	de	Six big devils from Japan quickly
			forgot how to waltz.
fghi	fghi	fghi	Oh, welch Zynismus, quiekte
5	9	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

### 8.3 Contribution 2

J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 8.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

- [1] Akiyoshi's illusion pages, www.ritsumei.ac.jp/ akitaoka/index-e.html
- [2] Reference 2

### 8.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

# 8.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

- Duty 1
- Duty 2

## 8.6 External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

### 8.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

Posters

Poster 1

Poster 2

# 8.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

9

# **Semiconductor Physics**

### 9.1 Introduction

Introductory text ...

Group Leader

### 9.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

Table 9.1: Test table – example of column alignment types.

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fghi	fghi	fghi	Oh, welch Zynismus, quiekte
5	9	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

### 9.3 Contribution 2

J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 9.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

- [1] Akiyoshi's illusion pages, www.ritsumei.ac.jp/ akitaoka/index-e.html
- [2] Reference 2

### 9.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

# 9.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

- Duty 1
- Duty 2
## 9.6 External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

## 9.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

Posters

Poster 1

Poster 2

## 9.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## 9.9 Guests

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

## **Solid State Optics and Acoustics**

## 10.1 Introduction

Introductory text ...

Group Leader

## **10.2** Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

**Table 10.1:** Test table – example of column alignment types.

left	right	center	page (width 60 mm)
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			forgot how to waltz.
fghi	fghi	fghi	Oh, welch Zynismus, quiekte
5	5	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

## 10.3 Contribution 2

J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 10.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

- [1] Akiyoshi's illusion pages, www.ritsumei.ac.jp/ akitaoka/index-e.html
- [2] Reference 2

## 10.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

## **10.5** Organizational Duties

Person 1

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

## **10.6** External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

## 10.7 Publications

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Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

Posters

Poster 1

Poster 2

## 10.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
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## Diploma

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- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## 10.9 Guests

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

## **Superconductivity and Magnetism**

## 11.1 Introduction

Introductory text ...

Group Leader

## 11.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor $^*$ , A. Uthor $^{\dagger}$ , A.U.T. Hor $^*$ 

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

 Table 11.1: Test table – example of column alignment types.

left	right	center	page (width 60 mm)
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			forgot how to waltz.
fghi	fghi	fghi	Oh, welch Zynismus, quiekte
5	5	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

## 11.3 Contribution 2

J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 11.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

- [1] Akiyoshi's illusion pages, www.ritsumei.ac.jp/ akitaoka/index-e.html
- [2] Reference 2

## 11.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

## 11.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

## **11.6** External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

## 11.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

Posters

Poster 1

Poster 2

## 11.8 Graduations

## Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## 11.9 Guests

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

## **Institute for Theoretical Physics**

## **Computational Quantum Field Theory**

## 12.1 Introduction

The Computational Physics Group performs basic research into classical and quantum statistical physics with special emphasis on phase transitions and critical phenomena. In the centre of interest are the physics of spin glasses, diluted magnets and other materials with quenched, random disorder, soft condensed matter physics with a focus on fluctuating paths and interfaces, biologically motivated problems such as polymer collapse/folding, adsorption and aggregation as well as related properties of proteins, and the intriguing physics of low-dimensional quantum spin systems.

The methodology is a combination of numerical and analytical techniques. The numerical tools are mainly Monte Carlo (MC) and Molecular Dynamics (MD) computer simulations, chain-growth algorithms, and exact enumeration techniques. The computational approach to theoretical physics is expected to gain more and more importance with the future advances of massively parallel computer technologies, and is likely to become the third cornerstone of physics besides experiment and analytical theory as sketched in Fig. 12.1. Already now it often helps to bridge the gap between experiments and the often necessarily approximate calculations in analytic approaches. To achieve the desired high efficiency of the numerical studies we develop new algorithms and, to guarantee the flexibility required by basic research, all computer codes are implemented by ourselves. The technical tools are Fortran, C, C++, and Python programs running under Unix or Linux operating systems and computer algebra using Maple or Mathematica. The software is developed and tested at the Institute on a cluster of PCs and workstations, where also most of the numerical analyses are performed. Currently we are also exploring the possibilities of the rapidly developing graphics card computing, that is computer simulations on general purpose graphics processing units (GPGPUs) with a very large number of cores. High-performance simulations requiring vast amounts of computer time are carried out at the Institute on quite powerful compute servers, at the parallel computers of the Saxon computing centre in Dresden, and, upon successful grant application, at the national supercomputing centres in Jülich, Stuttgart and München on parallel high-capability computers. This hierarchy of various platforms gives good training and qualification opportunities for the students, which offers promising job perspectives in many different fields for their future careers.

Our research activities are closely integrated into the Graduate School "Build-MoNa": Leipzig School of Natural Sciences – Building with Molecules and Nano-



**Figure 12.1:** Sketch of the "triangular" relationship between experiment, analytical theory and computer simulation.

objects, the International Max Planck Research School (IMPRS) *Mathematics in the Sciences*, and the International Doctoral College *Statistical Physics of Complex Systems* with Université de Lorraine in Nancy, France, supported by the Deutsch-Französische Hochschule (DFH-UFA). In the second funding period 2011–2013, Coventry University in England has been integrated as an associated partner, and in the third funding period 2014–2016, also the National Academy of Sciences of Ukraine in Lviv has joined as an other associated partner institution, offering our PhD students now several interesting options for secondments. For instance, in 2014, one PhD student started a "co-tutelle de thèse" jointly supervised with a colleague from Coventry University. Currently the DFH-UFA Doctoral College under the acronym "L<sup>4</sup>" is in its fourth funding period 2017–2020. The three Graduate Schools are all "Classes" of the Research Academy Leipzig (RALeipzig), providing the organizational frame for hosting visiting students and senior scientists, offering language courses, organizing childcare and for many other practical matters.

At a more post-graduate level our research projects are embedded into the Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility* together with Halle University. Our group also actively contributes to two of the top level research areas ("Profillinien") and the Centre for Theoretical Sciences (NTZ) of the University. Beside "BuildMoNa" the latter structures are particularly instrumental for our cooperations with research groups in experimental physics and biochemistry on the one hand and with mathematics and computer science on the other.

On an international scale, our research projects are carried out in a wide net of collaborations which are currently mainly funded by the Deutsch-Französische Hochschule (DFH-UFA) through the Doctoral College "L<sup>4</sup>" and the EU IRSES Network DIONICOS: *Dynamics of and in Complex Systems*, a consortium of 6 European and 12 non-European partners, including sites in Austria, England, France and Germany as well as in Armenia, Russia, Ukraine, India, the United States and Venezuela. Further close contacts and collaborations are established with research groups in Armenia, Austria, China, France, Great Britain, India, Israel, Italy, Japan, Poland, Russia, Spain,

Sweden, Taiwan, Turkey, Ukraine, and the United States. These contacts are refreshed and furthered through topical Workshops, Advanced Training Modules and Tutorials, and our International Workshop series *CompPhys: New Developments in Computational Physics*, taking annually place at the end of November just before the first advent weekend.

Wolfhard Janke

## 12.2 Monte Carlo simulations of poly(3-hexylthiophene) (P3HT): Comparison of three coarse-grained models

J. Gross, M. Ivanov, N. Oberthür, F. Müller, W. Janke



**Figure 12.2:** Hairpin conformations of poly(3-hexylthiophene) for a degree of polymerization  $DP_n = 20$  in three different models. (a) One-particle coarse-grained model (one bead per monomer), (b) three-particle coarse-grained model, and (c) fully atomistic model.

Regioregular poly(3-hexylthiophene) (P3HT) is a very interesting conjugated polymer due to its electronic and optical properties [1]. One of its applications is the use as semiconducting layer in organic photovoltaics [2]. Studies of P3HT on the microscopic level are of great importance for a fundamental understanding of the tuneability of electronic properties and their dependence on external constraints, e.g., the adsorption on electrode surfaces. Hence a number of experimental studies addressed for example the influence of structure formation by polymer self-assembly on ideal surfaces on the electronic properties of oligo- and polythiophenes [3]. Due to the complexity of these macromolecules many of the experimental findings have not been supported with simulations so far, which in contrast is well-established for studies of small organic molecules. Our previous study [4] reported on an collaborative effort within the DFG SFB/TRR 102 project to combine the experimental observation of polymer chain conformations adsorbed on a metal surface with Monte Carlo simulations of a coarsegrained P3HT model developed by Huang et al. [5]. Based on our previous work on a three beads per monomer coarse-grained model, we expanded our studies in two directions. We focused our interest on the polymer itself and, firstly, investigated an even coarser model with one bead per monomer [6] using Monte Carlo simulations.

Secondly, we simulated a fully atomistic representation of P3HT using molecular dynamics. The different levels of resolution are illustrated in Fig. 12.2. We pursue these two routes to gauge the level of detail that is necessary to reproduce experimental findings more accurately. Another interest is the development of our own simplified model by systematically performing the coarse-graining procedure ourselves. For this we looked at the iterative Boltzmann inversion method [7]. A comparative analysis of all three models regarding structural observables, but also the computational effort is discussed in Ref. [8]. Recently we extended our simulations with the three-particle coarse-grained P3HT model to the case where the polymers are entirely adsorbed on a two-dimensional substrate with a striped pattern, modeling for instance the modulation pattern of a surface-reconstructed Au(001) gold substrate [9]. Our results show that the shape of the stripe pattern has a substantial effect on the obtained conformations of the polymer and can be tailored to promote either more stretched out or more compact configurations. In the compact phases we observe different structural motifs, such as hairpins, double-hairpins, and interlocking "zipper" states, cf. Fig. 12.3.



**Figure 12.3:** Snapshots of coarse-grained P3HT polymers of length N = 65 in different structural phases on a modulated surface with stripe-distance parameter m = 3.5, resembling the modulation pattern of a surface-reconstructed Au(001) gold substrate.

 X. Bai, S. Holdcroft: Macromolecules 26, 4457 (1993); Z. Bao et al.: Appl. Phys. Lett. 69, 4108 (1996); M.R. Andersson et al.: J. Mater. Chem. 9, 1933 (1999); B.W. Boudouris et al.: Macromolecules 44, 6653 (2011)

- [2] J.M. Frost et al.: Nano Letters 6, 1674 (2006); M. Campoy-Quiles et al.: Nat. Mater.
   7, 158 (2008); A.M. Ballantyne et al.: Adv. Funct. Mater. 18, 2373 (2008)
- [3] Z.Y. Yang et al.: ACS Nano 2, 743 (2008); Y.F. Liu et al.: Nanoscale 5, 7936 (2013)
- [4] S. Förster et al.: J. Chem. Phys. 141, 164701 (2014)
- [5] D.M. Huang et al.: J. Chem. Theory Comput. 6, 526 (2010)
- [6] C.K. Lee et al.: Energy Environ. Sci. 4, 4124 (2011)
- [7] D. Reith et al.: J. Comput. Phys. 24, 1624 (2003); Macromolecules 36, 5406 (2003)
- [8] J. Gross et al.: J. Phys.: Conf. Ser. 750, 012009 (2016); Eur. Phys. J. Special Topics 226, 667 (2017)
- [9] N. Oberthür et al.: J. Chem. Phys. 149, 144903 (2018)

#### **12.3** Adsorption of semiflexible polymers

K.S. Austin, J. Zierenberg<sup>\*</sup>, W. Janke

\*Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany

The conformational properties of a semiflexible polymer in the vicinity of an attractive surface is of relevance for a wide range of applications from material design to catalysis to DNA sequencing through nanopores. If the polymer adsorbs, which is not always desired in applications, there may occur different structural conformations. Often, the discussion of semiflexible polymer adsorption considers polymers under good solvent conditions with purely *repulsive* monomer-monomer interactions [1, 2]. Finitesize scaling analyses of computer simulation data show that the adsorption transition temperature increases linearly with persistence length for stiff polymers as predicted [2]. This may be expected to be maintained under poor solvent conditions. However, additional short-range *attractive* monomer-monomer interactions will lead to a rich conformational phase space as a result of the competition of polymer stretching and collapse close to an attractive surface.

In general, there has been an extensive theoretical and numerical effort towards the study of flexible polymers near attractive surfaces. Under poor solvent conditions, the final adsorbed states range from partially adsorbed to fully flat conformations, demonstrated for an entire class of flexible polymers [3]. Similar observations were made for the adsorption of specific lattice proteins [4]. If the surface shows complex attractive motifs, one observes in addition pattern recognition effects [4, 5].

Semiflexible, *self-attractive* polymers undergoing a collapse transition exhibit a rich variety of structural phases already in the case of an isolated chain [6, 7]. These include collapsed, toroidal, hairpin, and knotted conformations, partially depending on the geometric and energetic constraints of the model. This plays a crucial role for practical purposes, since semiflexibility is a common property of biopolymers such as DNA. The question arises how semiflexibility influences the structural and thermal adsorption properties of dilute self-attractive polymers. A detailed study of the interplay of (effective) polymer stiffness and surface adsorption for the full range of self-attracting polymer models was so far lacking and in Ref. [8] we intended to fill this gap.



**Figure 12.4:** Structural phase diagram for a semiflexible polymer of length N = 40 grafted to a weakly attractive surface ( $\epsilon_s = 0.7$ ). The background color encodes the average fraction of surface contacts  $n_s = N_s/N$ . Dotted lines indicate that signals are found only in a small subset of observables. Representative conformations from the respective conformational regimes are shown below. They comprise globule-like (G), compact (C), and random coil-like (R) conformations, as well as folded bundles ( $D_m$ ), desorbed and adsorbed weakly bent rods (R\* and AR\*, respectively), and hairpins ( $E_H$ ). The (blue-red) rhombus at  $\kappa \approx 15$  marks the crossover from a second-order-like to a first-order-like collapse transition.

This study comprises sophisticated Monte Carlo computer simulations of a linear homopolymer consisting of N = 40 monomers connected by anharmonic springs fluctuating around an "equilibrium" bond length  $r_0$ . We consider the cases of a completely free polymer and a polymer grafted to a non-interacting as well as an attractive substrate (i.e., the first monomer remains at a fixed location on the surface). Our polymer description is intended to model a full class of (grafted) semiflexible polymers in a range of solvent conditions. The resulting coarse-grained model incorporates four energy terms: bond-vibrational energy, non-neighboring 12-6 Lennard-Jones interactions, bending energy parametrized by the bending stifness  $\kappa$ , and 9-3 Lennard-Jones surface interaction parametrized by the interaction strength  $\varepsilon_s$ . As a typical example of our results, Fig. 12.4 shows the  $\kappa$ -T phase diagram for a weakly attractive surface with  $\varepsilon_s = 0.7$ . For a recent overview see Ref. [9].

- [1] T. Sintes et al.: Macromolecules **34**, 1352 (2001)
- [2] H.-P. Hsu, K. Binder: Macromolecules 46, 2496 (2013)
- [3] J. Luettmer-Strathmann et al.: J. Chem. Phys. **128**, 064903 (2008); M. Möddel et al.: Phys. Chem. Chem. Phys. **12**, 11548 (2010)
- [4] A.D. Swetnam, M.P. Allen: Phys. Chem. Chem. Phys. 11, 2046 (2009); Phys. Rev. E 85, 062901 (2012)
- [5] M. Möddel et al.: Phys. Rev. Lett. 112, 148303 (2014)
- [6] D.T. Seaton et al.: Phys. Rev. Lett. **110**, 028103 (2013)
- [7] M. Marenz, W. Janke: Phys. Rev. Lett. 116, 128301 (2016)
- [8] K.S. Austin et al.: Macromolecules 50, 4054 (2017)
- [9] W. Janke: Generalized ensemble computer simulations of macromolecules, invited Ising Lecture Notes 2016, in Order, Disorder and Criticality: Advanced Problems of Phase Transition Theory, Vol. 5, ed. Y. Holovatch (World Scientific, Singapore, 2018), pp. 173–225

# 12.4 Computer simulations of semiflexible polymers in disordered environments

J. Bock, W. Janke



(a) Weighting histogram



(b) Semiflexible polymer in 3D disorder

**Figure 12.5:** (a) Histogram used for the guiding field in 3D and (b) an examplary configuration of a polymer with N = 30 and  $\xi = 1$ .

Single-molecule experiments have established the wormlike chain (WLC) as a standard model for semiflexible polymers [1]. Exploiting the analogy of the WLC with a one-dimensional Heisenberg ferromagnet, it can be shown that the equilibrium tangent-tangent correlation function decays exponentially. The decay rate defines the thermal persistence length  $l_p$ . When the same polymer is embedded in a quenched, disordered environment in three dimensions, this property may change quantitatively or even qualitatively. We addressed this problem by performing extensive numerical simulations of



**Figure 12.6:** End-to-end distance distributions for (a) free polymers and (b) polymers in gaseous disorder, both in 3D.

semiflexible polymers in a simple lattice disorder and in a gaseous disorder constructed by microcanonical Lennard-Jones gas simulation which represents the disordered environment. Further plans are to simulate the polymers in algebraically correlated disorder. Only the space between the spheres is accessible to the polymer. The extreme strength and density of the environmental constraints are a great challenge to conventional Monte Carlo simulation schemes, which we found hard to overcome even with a sophisticated multicanonical histogram reweighting procedure [2]. We have therefore adopted a breadth-first chain-growth algorithm [3] that resolves this difficulty by circumventing energy barriers instead of trying to cross them [2, 4], see examples in Fig. 12.5. Therefore the already existing procedures were expanded to the third dimension to investigate the behaviour of the tangent-tangent correlation length, the mean square end-to-end distance and the end-to-end probability distribution function, see Fig. 12.6. A difference in behaviour is clear and the task now is to check wether the differences scale similarly as in two dimensions, where the disorder renormalization is stated to be [5]:

$$\frac{1}{l_p^*} = \frac{1}{l_p} + \frac{1}{l_p^D},$$

with  $l_p^*$  the renormalized persistence length,  $l_p$  the persistence length given as simulation parameter and  $l_p^D$  the measured disorder persistence length.

- [1] O. Otto et al.: Nat. Commun. 4, 1780 (2013)
- [2] S. Schöbl et al.: Phys. Rev. E 84, 051805 (2011)
- [3] T. Garel, H. Orland: J. Phys. A: Math. Gen. 23, L621 (1999)
- [4] S. Schöbl et al.: J. Phys. A: Math. Theor. 45, 475002 (2012)
- [5] S. Schöbl et al.: Phys. Rev. Lett. 113, 238302 (2014)

## **12.5** From particle condensation to polymer aggregation

J. Zierenberg<sup>\*</sup>, P. Schierz, W. Janke



**Figure 12.7:** (a) Illustration of the free-energy landscape  $\beta \hat{F}(E_p, N_D)$  (color map) as a function of potential energy  $E_p$  and droplet size  $N_D$  for N = 512 Lennard-Jones particles. The minimal free-energy path (black solid line) connects a droplet ( $E_p \approx E_p^-$ ) and a gaseous ( $E_p \approx E_p^+$ ) phase, visualized by the snapshots at  $E_p^{\pm}$ . The projection onto the reaction-coordinate  $E_p$  yields the canonical potential-energy probability distribution  $\hat{P}_{\beta}(E_p)$ , where the free-energy barrier  $\beta \Delta \hat{F}$  is encoded in the ratio between maximum and minimum at  $\hat{\beta}_{eqh}$ . (c) Equivalently,  $\beta \Delta \hat{F}$  is the (equal) area size enclosed between the microcanonical inverse temperature  $\hat{\beta}(E_p)$  and the accordingly defined transition temperature  $\hat{\beta}_{eqa}$ , where  $\hat{\beta}_{eqa} = \hat{\beta}_{eqh} = 1.72099(3)$ .

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A common approach to study nucleation rates is the estimation of free-energy barriers. This usually requires knowledge about the shape of the forming droplet, a task that becomes notoriously difficult in macromolecular setups starting with a proper definition of the cluster boundary or a proper ensemble choice. Here, we demonstrate that a shape-free determination of temperature-driven cluster formation is directly accessible in the canonical ensemble for particle as well as polymer systems. Combined with rigorous results on canonical equilibrium droplet formation, this allows for a well-defined finite-size scaling analysis of the effective interfacial free energy at fixed density as illustrated in Fig. 12.7. We first verified the theoretical predictions for the formation of a liquid droplet in a supersaturated particle gas by (parallelized) generalized-ensemble Monte Carlo simulations [1–3] of a Lennard-Jones system [4, 5]. Going one step further, we then generalized this approach to the aggregation process in a dilute polymer solution [5], cf. Fig. 12.8. Our results suggest an analogy between particle condensation and polymer aggregation, when the macromolecules are interpreted as extended particles.

Because the standard approach in Monte Carlo simulations is to work in the conformational ensemble governed by potential energy only, we show that excluding the



**Figure 12.8:** Illustration of an aggregate of polymers in a dilute solution (N = 64 bead-spring polymers with 13 monomers each; monomer density  $\rho = 10^{-2}$ ). The snapshot stems from the droplet phase ( $E_p \approx E_p^-$ ).

kinetic energy from the partition function leads to finite-size differences in the free energy compared to the full ensemble [6–9] but retains intensive parameters in the thermodynamic limit [5]. Our study of nucleation rates at fixed density corresponds to a heating-cooling framework where simulation and experiment may meet at the nanometer scale.

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## 12.6 Droplet condensation of 2D Lennard-Jones particles

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**Figure 12.9:** Sketch of the transition between the pure gas phase and the mixed phase of a liquid droplet surrounded by vapour. Below the critical point, the black infinite-size transition line can be crossed in either one of two orthogonal directions: The blue horizontal arrow depicts the fixed-temperature approach in which density serves as the control parameter, where  $\rho_g(T_{sim})$  is the infinite-size transition density. Alternatively, the red vertical arrow depicts the fixed-density approach in which temperature serves as the control parameter and  $T_g(\rho_{sim})$  is the infinite-size transition temperature.

The formation and dissolution of a droplet is an important mechanism related to various nucleation phenomena [1, 2]. Here, we address the droplet formation-dissolution transition in a two-dimensional Lennard-Jones gas to demonstrate a consistent finitesize scaling approach from two perspectives using orthogonal control parameters [3, 4], see Fig. 12.9. For the canonical ensemble, this means that we fix the temperature while varying the density and vice versa. An example for the resulting grand canonical probability distribution  $P(\rho)$  iat fixed temperature is shown in Fig. 12.10. Using specialised parallel multicanonical methods for both cases, we confirm analytical predictions at fixed temperature (rigorously only proven for lattice systems [5–8]) and corresponding scaling predictions from expansions at fixed density [3]. Importantly, our methodological approach provides us with reference quantities from the grand canonical ensemble that enter the analytical predictions [9]. Our orthogonal finite-size scaling setup can be exploited for theoretical and experimental investigations of general nucleation phenomena - if one identifies the corresponding reference ensemble and adapts the theory accordingly [4]. In this case, our numerical approach can be readily translated to the corresponding ensembles and thereby proves very useful for numerical studies of equilibrium cluster formation, in general.

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**Figure 12.10:** Grand canonical probability distribution  $P(\rho)$  for a system of linear size L = 30 at temperature T = 0.4 and equal-height chemical potential  $\mu \approx -1.6518$ .  $P(\rho)$  shows peaks at the densities corresponding to the gas ( $\rho_g$ ) and the liquid ( $\rho_l$ ) phase. In between a suppressed plateau developed around the density where a stripe occurs ( $\rho_s$ ). On the top representative snapshots are shown for the whole density region over which the gas-liquid transition takes place.

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# 12.7 Effect of temperature on the scaling laws governing the kinetics of collapse of a homopolymer

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The collapse transition of a polymer upon transfer from a good solvent (high temperature) to a poor solvent (low temperature) bears significant connection to the folding process of a proteins and other biomolecules. Thus understanding the kinetics of a homopolymer in that respect may provide useful primary information on the underlying



**Figure 12.11:** (a) Snapshots [1] showing the sequence of events occurring during the collapse of a polymer upon being quenched from an expanded state (at high temperature) into the globular phase (at low temperatures). (b) Universal finite-size scaling function  $Y(y_p)$  with a non-universal metric factor  $f_s$  in the scaling variable  $y_p$  describing the scaling in the cluster growth during the collapse [2]. (c) Temperature-independent scaling plot for the aging and related dynamical scaling, probed by the behavior of a suitable density-density autocorrelation function  $C(t, t_w)$  against  $x_c = C_s(t)/C_s(t_w)$ , the ratio of cluster sizes  $C_s(t)$  at the observation time t and the waiting time  $t_w$  [2].

mechanism of more realistic problems [1, 2]. On the other hand, if one considers the usual "pear-necklace" like picture of the collpase [3] as shown in Fig. 12.11(a), it also resembles coarsening phenomena popular in spin and particle systems [4]. Over the last two years we have been exploiting this connection to understand the kinetics of collapse of a homopolymer [5, 6].

In this work, from the state of the art Monte Carlo simulations of an off-lattice polymer model, we understand the effect of the quench temperature ( $T_q$ ) on the various scaling laws related to the collapse viz., scaling of the cluster growth and the dynamical scaling related to the aging. Our results in conjunction with the nonequilibrium finite-size scaling analysis [7] show that the cluster growth is rather universal in nature and can be described by a universal finite-size scaling function with a non-universal metric factor that depends on the amplitudes of the growth [2], see Fig. 12.11(b). This observation has recently been confirmed in a related lattice model for the polymer [8]. For a direct comparison of the lattice and off-lattice formulations, see Ref. [9]. Furthermore, the scaling related to the aging (which is probed by a suitable two-time density-density autocorrelation function) is also found to be independent of the quench temperature  $T_q$ , shown in Fig. 12.11(c).

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## 12.8 Coarsening and aging of lattice polymers: Influence of bond fluctuations

H. Christiansen, S. Majumder, W. Janke



**Figure 12.12:** (a) The two-time correlation function  $C(t, t_w)$  against the ratio of length-scales  $x_C = \ell(t)/\ell(t_w)$  for the model with fixed bonds and different quench-temperatures  $T_q$ . In (b) the growth of the length-scales for the model with flexible bonds is shown for different  $T_q$ . Here the growth is independent of  $T_q$  and follows a power law with exponent  $\alpha = 0.62(5)$ .

The nonequilibrium properties of homopolymer collapse were investigated using Monte Carlo simulations of the interacting self-avoiding walk on a simple cubic lattice (with lattice-spacing 1) using fixed bond lengths 1 and flexible bond lengths; 1,  $\sqrt{2}$ , and  $\sqrt{3}$  [1]. The phenomenological picture of pearl necklace polymer collapse [2] was observed, in which a polymer, when transferred from a good solvent ( $T_h > T_{\theta}$ ) to a bad solvent ( $T_a < T_{\theta}$ ), undergoes a collapse transition from an expanded coil by forming clusters at locally higher densities which then subsequently coalesce with each other until only a single globular cluster is left. The aging exponent  $\lambda \approx 1.25$  was found to be independent of the bond conditions and the same as in the off-lattice exponent [3] [see Fig. 12.12(a) for the model with fixed bonds at different quench temperatures  $T_a$ ]. For the model with flexible bonds, the power-law growth exponent of the clusters of monomers was likewise observed to be independent of temperature  $\alpha = 0.62(5)$  [see Fig. 12.12(b)], while the same exponent was found to be dependent on the temperature in the fixed bond model. In the off-lattice model on the other hand,  $\alpha = 1$  was found [4]. The discrepency in the exponent  $\alpha$  is attributed to the constraints introduced by the lattice structure. For a recent review, see Ref. [5].

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## 12.9 Scaling laws during collapse of a homopolymer: Lattice versus off-lattice

S. Majumder, H. Christiansen, W. Janke



**Figure 12.13:** (a) Time evolution snapshots of the collapse of a homopolymer, after being quenched from an extended coil phase to a temperature,  $T_q = 1$  for OLM, and  $T_q = 2.5$  for LM, in the globular phase.(b) Plots of the average cluster size  $C_s(t)/N$  as function of time for the two models. To make both the data visible on the same plot, we divide the time axis by a factor m to obtain  $t_p = t/m$ , where  $m = 1 \times 10^6$  and  $3.5 \times 10^6$ , respectively, for OLM and LM. The solid lines there are fits to the form  $C_s(t) = C_0 + At^{\alpha_c}$  with  $\alpha_c = 0.98$  for OLM and  $\alpha_c = 0.62$  for LM. (c) Plot showing that universal aging scaling at different  $T_q$  for the two models can be described by a single master-curve behavior. The solid line here also corresponds to  $C(t, t_w) = A_C x_c^{-\lambda_C}$  with  $\lambda_C = 1.25$ . Note that  $C(t, t_w)$  is multiplied by a factor f to make them collapse onto the same curve. For OLM  $t_w = 10^4$  whereas for LM  $t_w = 10^3$ .

The pathways of collapse of a homopolymer, upon a transfer from a good to a poor solvent, bears resemblance to coarsening processes. Simulation results in this context can be explained by the phenomenonlogical "pearl-necklace" picture of Halperin and Goldbart (HG) [1]. Recently we have shown via Monte Carlo simulations of both a lattice model (LM) and an off-lattice model (OLM) polymer that this nonequilibrium evolution dynamics is also a scaling phenomenon [2]. In this work we compared the results obtained from the LM and OLM, in particular the scaling of the cluster growth [3] and the aging scaling [4] probed by the two-time density-density autocorrelation function.

For the OLM, we opt for the bead-spring model of a flexible homopolymer in d = 3 dimensions where bonds between successive monomers are maintained via the standard finitely extensible non-linear elastic (FENE) potential

$$E_{\text{FENE}}(r_{ii+1}) = -\frac{KR^2}{2} \ln\left[1 - \left(\frac{r_{ii+1} - r_0}{R}\right)^2\right],\tag{12.1}$$

with K = 40,  $r_0 = 0.7$  and R = 0.3. The nonbonded interaction energy is modeled by  $E_{nb}(r_{ij}) = E_{LJ}(\min(r_{ij}, r_c)) - E_{LJ}(r_c)$ , where

$$E_{\rm LJ}(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$
(12.2)

is the standard Lennard-Jones (LJ) potential with  $\sigma = r_0/2^{1/6}$  as the diameter of the monomers,  $\epsilon$  (= 1) as the interaction strength and  $r_c = 2.5\sigma$  as the cut-off radius.

For LM, we consider [5] a variant of the interactive self-avoiding walk on a simplecubic lattice, where each lattice site can be occupied by a single monomer. The energy is given by

$$E_{\rm LM} = -\frac{1}{2} \sum_{i \neq j, j \pm 1} w(r_{ij}), \text{ where } w(r_{ij}) = \begin{cases} J & r_{ij} = 1\\ 0 & \text{else} \end{cases}.$$
 (12.3)

In Eq. (12.3),  $r_{ij}$  is the Euclidean distance between two nonbonded monomers *i* and *j*,  $w(r_{ij})$  is an interaction parameter that considers only nearest neighbors, and J(= 1) is the interaction strength. We allow a fluctuation in the bond length by considering diagonal bonds, i.e., the possible bond lengths are 1,  $\sqrt{2}$ , and  $\sqrt{3}$ .

Phenomenonlogically both LM and OLM show intermediate structures consistent with the "pear-necklace" picture of HG [Fig. 12.13(a)]. However, the cluster-growth scaling in LM and OLM are different. While the OLM yields a linear growth ( $\alpha_c \approx 1$ ), in the LM the growth is slower ( $\alpha_c \approx 0.62$ ) [Fig. 12.13(b)], which could be attributed to the topological constraints one experiences in a lattice model. On the other hand, surprisingly, both the models show evidence of simple aging scaling having the same autocorrelation exponent  $\lambda_C \approx 1.25$  [Fig. 12.13(c)], thus implying that the aging scaling is rather universal. This allowed us to demonstrate that scaling of the autocorrelation functions for the two models can be described by a single master curve. For a more detailed discussion, see the recent review in Ref. [6]

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# 12.10 Dynamics of collapse of a flexible polymer with Vicsek-like active beads

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A polymer undergoes a collapse transition when it is quenched from a high-temperature extended coil state (or in good solvent) to a temperature lower (or in poor solvent) than its  $\theta$ -transition value, for which the equilibrium phase is a globular one. Though various aspects of equilibrium and nonequilibrium dynamics of such transition for the case of a passive polymer is reasonably well understood [1, 2], studies with active polymers are relatively new [3, 4]. Studying the motion of a single flexible polymer in



**Figure 12.14:** (a) Time evolution snapshots of the events occurring during the collapse transition of a polymer with  $N_b = 512$  beads when quenched from an extended coil state into the globular phase at low temperature.  $f_A = 0$  stands for the passive case, while  $f_A = 1$  and 5 corresponds to the case of the active polymer. (b) Average size of clusters as a function of time for the three cases.

presence of controlled active forces is necessary in case of drug delivery, directed self assembly, etc. Experimental realizations of such a system are given by linking artificially synthesized colloidal particles that show controlled motion and enhanced diffusion [5]. Here we have modeled each bead as an active element for which we applied Vicsek-like alignment interaction rules [6]. Our main aim is to look at the nonequilibrium dynamics, such as, relaxation time of collapse, cluster growth, etc. by tuning the activity and to compare them with the case of a passive polymer.

Here we consider a flexible bead-spring model of a polymer chain with  $N_b$  beads, determining the degree of polymerization [1]. The equation of motion of each bead is solved via molecular dynamics simulation using the Langevin equation, in which the quenching temperature has been chosen as T = 0.5. The interaction potentials acting among the beads consist of two terms. The non-bonded interaction is the standard LJ potential and the bonded interaction between two monomers is the FENE potential. As we have applied Vicsek-like alignment interaction rule [6], the velocity of each bead gets modified by the average direction of its neighbors present within a cut-off distance  $r_c$ , for which we choose  $r_c = 2.5\sigma$ , where  $\sigma$  is the diameter of each bead. Following Ref. [7], the active force  $\vec{f_i}$  for the *i*'th bead can be written as,

$$\vec{f_i} = f_A \vec{D}_n , \qquad (12.4)$$

where  $f_A$  determines the strength of the active force and  $D_n$  is the average direction determined by the neighbors.

In Fig. 12.14(a) we present comparative snapshots for a chain with  $N_b$  = 512 beads during the collapse of the polymer for the passive case as well for two different values of the active force. Whereas the intermediate snapshots look quite different in the higher

activity case ( $f_A = 5$ ) than in the passive or  $f_A = 1$  case, the final state is in all cases a globular phase. However, for  $f_A = 0, 1$  the polymer evolves to a rather compact spherical globule, while for  $f_A = 5$  it remains in a slightly elongated or sausage-like globular phase. And the time scale required to reach the final state is much higher for  $f_A = 5$  than in the other two cases. The run time for  $f_A = 5$  is up to  $t = 10^4$  measured in units of LJ time scale. Though the preferred final phase is a globular one because of the presence of an attractive potential among the beads, a few realizations still remain in a dumbbell phase for  $f_A = 5$ . The persistance of this dumbbell phase for  $f_A = 5$  increases with the value of  $N_b$  as well. To make a quantitative comparison, here in Fig. 12.14(b) we plot the average cluster size  $C_s(t)$  of the clusters as a function of time for all the three cases. We see that for the active cases, though initially the growth amplitude is higher than in the passive case suggesting a faster initialization of the coarsening process, at later time  $C_s(t)$  crosses over to a lower amplitude as well as a smaller exponent for the growth. This lowering of the exponent for the active case compared to the passive one is more prominent for  $f_A = 5$ . We will investigate these issues in more detail.

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## 12.11 Explicit solvent model for polymer dynamics using Lowe-Andersen approach

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Dynamics of a polymer chain in a dilute solution, although being extensively studied, is still a topic of utmost importance. In particular, this topic serves as a benchmark for establishing a coarse-grained or mesoscopic approach to understand more realistic problems on larger time and length scales. The dynamics of a single chain, generally, is characterized by the self-diffusion coefficient *D* which scales with chain length *N* as  $D \sim N^{-x}$ . In absence of hydrodynamic effects, one has x = 1, whereas in presence of hydrodynamic effects, one expects x = 3/5. The former is referred to as Rouse scaling [1] and the latter as Zimm scaling [2].

In this work [3] we construct an explicit solvent model for a polymer by considering a bead-spring model of a flexible homopolymer in three spatial dimensions. The bonds between successive monomers are maintained via the standard finitely extensible nonlinear elastic (FENE) potential

$$E_{\text{FENE}}(r_{ii+1}) = -\frac{K}{2}R^2 \ln\left[1 - \left(\frac{r_{ii+1} - r_0}{R}\right)^2\right], \qquad (12.5)$$


**Figure 12.15:** Left panel: The trajectory of the center of mass of a polymer of length N = 512, over a time period of  $200\tau$  in equilibrium at T = 1.0. Right panel: Dependence of the self-diffusion coefficient *D* on the chain length *N* of a polymer for different solvents with a collision frequency  $\Gamma$  as indicated. The solid and dashed lines represent the Zimm ( $D \sim N^{-3/5}$ ) and Rouse scaling ( $D \sim N^{-1}$ ), respectively.

with K = 40,  $r_0 = 0.7$  and R = 0.3. The monomers and the solvent molecules both are considered to be spherical beads of mass m = 1 and diameter  $\sigma$ . All nonbonded interactions are modeled by

$$E_{\rm nb}(r_{ij}) = E_{\rm LJ}\left[\min(r_{ij}, r_c)\right] - E_{\rm LJ}(r_c) , \qquad (12.6)$$

where  $E_{LJ}(r)$  is the standard Lennard-Jones (LJ) potential given as

$$E_{\rm LJ}(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$
(12.7)

with  $\sigma = r_0/2^{1/6}$  as the diameter of the beads,  $\epsilon$ (= 1) as the interaction strength and  $r_c = 2^{1/6}\sigma$  as cut-off radius that ensures a purely repulsive interaction.

We simulate our system via molecular dynamics (MD) simulations at constant temperature using the Lowe-Andersen (LA) thermostat [?]. In this approach, one updates the position  $\vec{r_i}$  and velocity  $\vec{v_i}$  of the *i*-th bead using Newton's equations as follows,

$$\frac{d\vec{r}_i}{dt} = \vec{v}_i, \quad \frac{d\vec{v}_i}{dt} = \vec{f}_i, \qquad (12.8)$$

where  $f_i$  is the conservative force (originating from the bonded and nonbonded interactions) acting on the bead. For controlling the temperature with the LA thermostat, one considers a pair of particles within a certain distance  $R_T$  [4]. Then, with a probability  $\Delta t\Gamma$ , a bath collision is executed, after which the pair gets a new relative velocity from the Maxwellian distribution. Here,  $\Delta t$  is the width of the time step chosen for the updates in Eq. (12.8) and  $\Gamma$  determines the collision frequency. By varying  $R_T$  and  $\Gamma$ , one can effectively control the frictional drag or in other words the solvent viscosity. The exchange of relative velocities with the bath is only done on its component parallel to the line joining the centers of the pair of particles, thus conserving the angular momentum. Additionally, the new velocities are distributed to the chosen pair in such a way that the linear momentum is also conserved.

Via the scaling of the radius of gyration  $R_g$  with the chain length N as  $R_g \sim N^{3/5}$  we confirm that our approach yields the known static critical exponent. The method conserves both the linear and angular momenta locally, thereby preserving the hydrodynamics. Thus the scaling of the self-diffusion coefficient D with chain length N (shown in the right panel of Fig. 12.15) indicates a much faster dynamics than the Rouse dynamics, and in fact is pretty consistent with Zimm scaling  $D \sim N^{-3/5}$  valid in the presence of hydrodynamic effects.

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#### 12.12 Kinetics of the collapse of polyglycine in water

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**Figure 12.16:** Left panel: Snapshots showing the sequence of events during the collapse of polyglycine with 200 residues. Below each snapshot the corresponding contact maps are also shown revealing the pearl-necklace formation more clearly. Right panel: The upper plot shows the scaling of the collapse time  $\tau_c$  with respect to the chain length. The solid line demonstrates the consistency of the data with power-law scaling with an exponent z = 0.5. The lower plot shows the scaling associated with the cluster coarsening from pearl-necklace to globule.

The collapse of homopolymers was first described by de Gennes' seminal "sausage" model [1], but today the phenomenological "pearl-necklace" picture by Halperin and

Goldbart [2] is more commonly used, both for flexible and semiflexible polymer models. In this picture the collapse begins with nucleation of small local clusters (of monomers) leading to formation of an interconnected chain of (pseudo-)stable clusters, i.e., the "pearl-necklace" intermediate. These clusters grow by eating up the un-clustered monomers from the chain and subsequently coalesce, leading eventually to a single cluster. Finally, monomers within this final cluster rearrange to form a compact globule.

Of central interest in this context is the scaling of the collapse time  $\tau_c$  with the degree of polymerization *N* (the number of monomers). While scaling of the form

$$\tau_c \sim N^z, \tag{12.9}$$

where *z* is the dynamic exponent, has been firmly established, there is no consensus on the value of *z*. Molecular dynamics (MD) simulations provide much smaller values  $(z \approx 1)$  than Monte Carlo (MC) simulations  $(z \approx 2)$ . This difference is often explained with the presence of hydrodynamics in the MD simulations, but a value  $z \approx 1$  has been reported recently also for MC simulations [3]. The "pearl-necklace" stage or the cluster-growth kinetics can be understood by monitoring the time (*t*) dependence of the mean cluster size  $C_s(t)$ , the relevant length scale. By drawing analogy with coarsening ferromagnets, it has been shown that scaling of the form

 $C_s(t) \sim t^{\alpha_c} \tag{12.10}$ 

with growth exponent  $\alpha_c \approx 1$  holds for flexible homopolymers [3, 4].

In this work [5] we investigated the nonequilibrium pathways by which the biological homopolymer polyglycine  $[(Gly)_N]$  collapses in water with the aim of exploring the above mentioned scaling laws. For short chains, the pathway has few noticeable features and is driven by the competition between the hydration of the peptide, opposing the collapse, and the intra-peptide attractions, favoring the collapse [6]. For chains with N > 20, the importance of hydration effects decreases, and the kinetics of hydrogen bonds indicates that van der Waals interactions of the backbone dominate [6] and drive the collapse. The nonequilibrium intermediates seen during the collapse exhibit local ordering or clustering that is analogous to the phenomenological "pearl-necklace" picture [cf. Fig. 12.16 (left)], known to be valid for the earlier studied coarse-grained homopolymer models [2]. Using the contact probability of the C $\alpha$ -atoms in the backbone, we extract a relevant dynamic length scale, i.e., cluster size, that as in simple homopolymer models grows linearly with time [3].

Especially intriguing is that the scaling of the collapse time with length of the chain indicates a faster dynamics, with a critical exponent z = 0.5 [cf. Fig. 12.16 (upper right)] instead of z = 1 that was seen in earlier homopolymer collapse studies which considered simplified models describing non-hydrogen-bonded polymers such as polyethylene and polystyrene. The smaller exponent found in this study may be connected with a mechanism that allows in amino acid based polymers a more rapid collapse than seen in non-biological homopolymers such as poly(N-isoporpylacrylamide) and polystyrene, where collapse times of  $\approx 300$  ms up to  $\approx 350$  s have been reported. We conjecture that the smaller exponent z is characteristic for collapse transitions in amino acid based polymers where the presence of intra-chain hydrogen bonding immediately seeds (transient) local ordering, while in non-hydrogen-bonded polymers such local ordering only happens as a consequence of diffusive motion.

The scaling of the cluster growth during the collapse is shown in Fig. 12.16 (lower right). The solid and the dashed lines represent power-law behavior,  $C_s(t) \sim t^{\alpha_c}$ , with  $\alpha_c = 1$  and 2/3, respectively. In the inset, two different choices for a crossover time  $t_0$  are taken into account by plotting  $C_s^p(t) \equiv C_s(t) - C_s(t)_0$  vs.  $t_p = t - t_0$ . Here the solid line indicates a power-law behavior with exponent  $\alpha_c = 1$ .

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# 12.13 Universal finite-size scaling for kinetics of phase separation in multicomponent mixtures

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**Figure 12.17:** Left panel: Typical snapshots at two different times demonstrating the domain growth during phase separation in the *q*-state Potts model, for two different *q*. Results were obtained via Monte Carlo simulations mimiking diffusive dynamics. Right panel: The main frame illustrates the universality of the finite-size scaling function  $Y(y_q)$  with a nonuniversal metric factor  $f_q$  in the scaling variable  $y_q$ , for different *q*. The inset shows the dependence of the metric factor  $f_q$  on *q*.

In this work [1] we have presented results for the kinetics of phase separation in multicomponent solid mixtures in space dimension d = 2, via Monte Carlo simulations

of the *q*-state conserved Potts model that has the Hamiltonian [2]

$$H = -J \sum_{\langle ij \rangle} \delta_{\sigma_i,\sigma_j}; \quad \sigma_i = 1, 2, \dots, q; \quad J > 0 .$$
(12.11)

The primary interest in our work was to quantify the domain-growth kinetics. We achieve this via the application of appropriate finite-size scaling analyses [3–5]. Like in critical phenomena [6], this technique allows one to obtain a precise estimation of the growth exponent  $\alpha$ , without using very large systems. We observe that finite-size effects are weak, as in the Ising model [3, 4]. By considering an initial domain length [3] in the scaling ansatz, we show that one obtains the Lifshitz-Slyozov growth, for all q, from rather early time, like in the Ising case.

Intriguingly, we find that the growth for different q can be described by a universal finite-size scaling function  $Y(y_q)$ , with a nonuniversal q-dependent metric factor  $f_q$  in the scaling variable  $y_q$ , arising from the amplitude of growth. This is illustrated in the main frame of the right panel of Fig. 12.17. Similarly, for a range of quench depth, viz.  $T \in [0.5T_c, 0.8T_c]$ , we show that the growth follows Lifshitz-Slyozov law, irrespective of the temperature, for all q. This also can be described by a similar common finite-size scaling function. Another important fact we observed is the crossover in the behaviour of  $f_q$  as a function of q [7]. Surprisingly, this crossover happens at q = 5 where the nature of phase transition changes from second order to first order [2].

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#### 12.14 Phase-ordering kinetics of the long-range Ising model

H. Christiansen, S. Majumder, W. Janke

The nonequilibrium properties of the long-range Ising model with Hamiltonian

$$\mathcal{H} = -\sum_{i} \sum_{j < i} J(r_{ij}) s_i s_j, \text{ with } J(r_{ij}) = \frac{1}{r_{ij}^{d+\sigma}}$$
(12.12)

are investigated. We vary the exponent  $\sigma$ , which controls the decay of the potential  $J(r_{ij})$  between spins  $s_i$  and  $s_j$  at distance  $r_{ij}$ . In Fig. 12.18(a) we show snapshots of this system for some of those  $\sigma$  and for two different times. The ordering of structured regions is clearly visible, where obviously the amplitude of growth depends on  $\sigma$ . However, this does not tell us something about the underlying law of growth. To quantify this, we investigate the characteristic length  $\ell(t)$ , which we extract from the decay of the



**Figure 12.18:** (a) Snapshots of the coarsening in the two-dimensional Ising model with longrange interactions with different  $\sigma = 0.6$ , 1.0, and 1.5 for the two times t = 100 and 400. Only spins pointing up are marked blue. (b) Length scale  $\ell(t)$  for different  $\sigma$ , where the solid lines correspond to the prediction (12.13). The inset shows the influence of a finite cut-off on the growth of length scale.

equal-time two-point spin-spin autocorrelation function. For this model, there exists a prediction [3], reading

$$\ell(t) \propto t^{\alpha} = \begin{cases} t^{\frac{1}{1+\sigma}} & \sigma < 1\\ (t\ln t)^{\frac{1}{2}} & \sigma = 1\\ t^{\frac{1}{2}} & \sigma > 1 \end{cases}$$
(12.13)

A previous publication observed  $\ell(t) \propto t^{1/2}$  independent of  $\sigma$ , however, using a cut-off in the potential  $J(r_{i,j})$  [4]. In the inset of Fig. 12.18(b) we show the influence of the cut-off for  $\ell(t)$  with  $\sigma = 0.6$  and observe that one indeed finds the exponent 1/2 for small cut-offs, whereas prediction (12.13) is confirmed for a sufficiently large cut-off. In the main plot of Fig. 12.18(b) we demonstrate for the first time that indeed (12.13) holds for all  $\sigma$  investigated when no cut-off is used.

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## 12.15 Percolation on square lattices with long-range correlated defects

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**Figure 12.19:** Correlated continuous variables on a  $2^{11} \times 2^{11}$  lattice for (a) correlation strength a = 0.5 and (b) corresponding discrete lattice at the percolation threshold with defects shown in black.

Structural obstacles (impurities) play an important role for a wide range of physical processes as most substrates and surfaces in nature are rough and inhomogeneous [1]. For example, the properties of magnetic crystals are often altered by the presence of extended defects in the form of linear dislocations or regions of different phases. Another important class of such disordered media are porous materials, which often exhibit large spatial inhomogeneities of a fractal nature. Such fractal disorder affects a medium's conductivity, and diffusive transport can become anomalous [2] This aspect is relevant, for instance, for the recovery of oil through porous rocks [3], for the dynamics of fluids in disordered media [4], or for our understanding of transport processes in biological cells [5].

In nature, inhomogeneities are often not distributed completely at random but tend to be correlated over large distances. To understand the impact of this, it is useful to consider the limiting case where correlations asymptotically decay by a power law rather than exponentially with distance:

$$C(r) \sim |r|^{-a}$$
 (12.14)

where *a* is the correlation parameter. If *a* is smaller than the spatial dimension *D*, the correlations are considered long-range or "infinite." An illustration of such power-law correlations for continuous and discrete site variables on a square lattice is shown in Fig. 12.19.

In this project we studied long-range power-law correlated disorder on square and cubic lattices [6, 7]. In particular, we obtained high-precision results for the percolation thresholds and the fractal dimension of the largest clusters as a function of correlation parameter *a*. The correlations are generated using a discrete version of the Fourier filtering method [8]. We consider two different metrics to set the length scales over which the correlations decay, showing that the percolation thresholds are highly sensitive to such system details. By contrast, we verify that the fractal dimension  $d_f$  is a universal

quantity and unaffected by the choice of metric. We also show that for weak correlations, its value coincides with that for the uncorrelated system. In two dimensions we observe a clear increase of the fractal dimension with increasing correlation strength, approaching  $d_f \rightarrow 2$ . The onset of this change, however, does not seem to be determined by the extended Harris criterion.

As a follow-up project that heavily relies on these results, we are currently studying the site-disordered Ising model on three-dimensional lattices with long-range correlated defects [9].

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## 12.16 Monte Carlo study of the Ising model in three dimensions with long-range correlated disorder

S. Kazmin, W. Janke



**Figure 12.20:** Slices of a three-dimensional Ising model with linear lattice extension L = 128 at critical temperatures for different defect concentrations and correlation exponents. White dots represent the defects  $\eta = 0$ , blue and red the spin states  $s = \pm 1$ .

The aim of this work is to study the critical behaviour of the Ising model with longrange correlated disorder on the lattice with Monte Carlo simulation techniques. In nature the disorder often does come with a certain structure and not at random. We want to mimic this by introducing spatially correlated defects on the lattice. We use the



**Figure 12.21:** Universality classes of the three-dimensional Ising model for different disorder concentrations  $p_d$  and correlation exponents *a*. The curve  $\hat{p}_d(a) = 1 - \hat{p}(a)$  is the percolation threshold below which the system has the probability 1 to have an infinite cluster of spins for  $L \rightarrow \infty$  and therefore the Ising model is well defined. As can be seen qualitatively and was studied in [2] one can add more defects without destroying the infinite cluster when the defects are correlated.

Fourier method for the generation of the correlation between the defects as introduced by Makse et al. [1] and modified by Zierenberg et al. [2]. The main goal is to obtain the critical exponents in dependence of the disorder concentration and correlation strength as well as to analyze other aspects of the phase transition from paramagnetic to ferromagnetic state.

The Ising model with site disorder on a lattice is described by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle xy \rangle} \eta_x \eta_y s_x s_y - h \sum_x \eta_x s_x , \qquad (12.15)$$

where *J* is the coupling constant,  $s_x = \pm 1$  is a spin at site x,  $\langle \cdot \rangle$  stands for next-neighbour indices, *h* is the external magnetic field and  $\eta_x = 1$  when the site is occupied by a spin or  $\eta_x = 0$  if it is a defect (vacant site). We can recover the pure Ising model by setting  $\eta_x = 1$  for each site *x* on the lattice. In one disorder realization the defects can be placed randomly and uniformly in which case we speak about the uncorrelated disorder. In the case of correlated disorder we place them randomly but in such a way that they obey the spatial correlation decay of the form

$$\langle \eta_x \eta_y \rangle \propto \frac{1}{d(x,y)^a}$$
, (12.16)

where *d* is the distance between two sites and *a* is the so-called correlation decay exponent. Formally,  $a = \infty$  corresponds to the uncorrelated case. Finally, the mean concentration of the defects over a number of realizations is denoted by  $p_d$ . In Fig. 12.20 one can see the influence of the disorder correlation.

The universality class of the three-dimensional Ising model is expected to be different for the pure system, the uncorrelated disorder system according to the Harris criterion [3] and the correlated disorder system for  $a \le d = 3$  (strong correlation) according to the extended Harris criterion [4]. The situation is sketched in Fig. 12.21.

Before dealing with the critical exponents we must determine the critical temperatures at which the transition happens for various disorder concentrations  $p_d$  and various



**Figure 12.22:** Critical temperatures  $T_c$  of the three-dimensional Ising model with disorder for different disorder concentrations  $p_d$  and different correlation exponents a. The value for the pure Ising model is taken from [6].

correlation exponents *a*. We performed Monte Carlo Simulations on lattices with maximal linear extent of L = 64 at different temperatures and obtained the critical temperatures from the intersections of the Binder cumulant observables  $U_2 = 1 - \langle |m|^2 \rangle / (3\langle m \rangle^2)$  for different *L*. This method is commonly used and is explained in, e. g., Ref. [5]. Results are shown in Fig. 12.22, where the precise critical temperature is taken from Ref. [6]. The critical temperature decays with larger defect concentration and is expected to go to zero as  $p_d$  approaches the percolation threshold. On the other hand for stronger correlation of the defects (smaller *a*) the temperature increases at each concentration  $p_d$ .

The simulation at critical temperatures and the observation of the critical exponents is ongoing research. In particular, we want to apply the histogram reweighting technique [7] to the observables of interest. While the overall program is clear, there are various subtle aspects like different competing length scales which render the problem less trivial than may be thought at first glance.

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# 12.17 Distribution of local minima for the Edwards-Anderson spin-glass model

S. Schnabel, W. Janke

In statistical physics the term "complex behavior" is usually used to characterize systems that posses a rough free-energy landscape with many metastable states. This can be the result of competing interactions on different scales like in the case of protein folding or it may arise from quenched disorder as for spin glasses. A conceptually simple model for such a system is the Edwards-Anderson spin-glass model [1], whose Hamiltonian is given by

$$\mathcal{H} = \sum_{\langle ij\rangle} J_{ij} S_i S_j,$$

where the spins sit on the sites of a cubic lattice, can take two values  $S_i \in \{-1, 1\}$ , and adjacent spins interact via normally distributed random couplings  $J_{ij}$ . Since these interactions can be either ferromagnetic (positive) or antiferromagnetic (negative), there is no trivial order established at low temperatures. Instead, many very different pure states might coexist, each one of them corresponding to a minimum in free energy.

Albeit not identical, minima of the energy, i.e. spin configurations that are stable against single spin flips are closely related to these pure states. It is thought that minima in energy form the end-points of hierarchical tree-like structures with branches corresponding to different pure states. Understanding their properties might, therefore, improve our understanding of the behavior of the system. However, they have proven to be a very demanding subject of inquiry.

We have developed an advanced Monte Carlo method that in its basic form allows to sample the local energy minima with uniform distribution, i.e., each minimum configuration is occupied with equal probability. This is achieved by establishing within the simulation the combination of a spin configuration together with a random minimization thereof. I.e., the repeated flipping of spins with positive energy until a local minimum is reached. If one now alters the spin configuration and the parameters of the minimization in a suitable way it is possible to ensure that all local minima are equally likely found this way. This corresponds to 'simple sampling' in the space of local minima. It is also possible to perform 'importance sampling' by including suitable weight functions. We can for instance sample a canonical distribution of local minima in energy by including the Boltzmann weight.

A basic application of this method is the measurement of the distribution of the energy minima. Since existing algorithms are unable to perform such a task, there is no numerical data for comparison. However, we can use our results to test analytical approximations [2] that are based on the expansion of meanfield solutions. We found that there are considerable deviations (Fig. 12.23) [3]. In fact, the distributions much more closely – although not entirely – resemble Gaussian distributions.

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#### **12.18** Spin glasses with variable frustration

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**Figure 12.23:** The distribution of local minima for different system sizes and the analytical approximation.

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Together with randomness, frustration is believed to be a crucial prerequisite for the occurrence of glassy behaviour in spin systems. The degree of frustration is normally the result of a chosen distribution of exchange couplings in combination with the structure of the lattice under consideration. Here, however, we discuss a process for tuning the frustration content of the Edwards-Anderson model on arbitrary lattices. With the help of extensive parallel-tempering Monte Carlo simulations we study such systems on the square lattice and compare the outcomes to the predictions of a recent study employing the Migdal-Kadanoff real-space renormalization procedure [1]. We use a cluster algorithm proposed in [2] in order to reduce the equilibration time. The phase transition studies are done by looking at the divergence of the correlation length, see Fig. 12.24. The results are benchmarked by comparing to the stochastic case described in [3]. We also study the freezing temperature of such a system and observe a different behaviour compared to the stochastically frustrated case. Studies on larger system sizes are very crucial to confirm these differences.

We find that the divergence of the correlation length occurs at non-zero finite temperature for the 2D Ising spin glass. This gives hints of a phase transition, but such transitions have to be studied carefully in order to fully understand the phases [4].

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**Figure 12.24:** Correlation length as a function of temperature for (a) stochastically frustrated system, (b) a system with 46% frustration, and (c) a system with 20% frustration.

# 12.19 Random field *q*-state Potts model: Ground states and low-energy excitations

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**Figure 12.25:** Overlap between the lowest states found by graph-cut methods (GCM) and the putative ground state (a) as a function of the number of Potts states *q* and (b) as a function of system size *L*.

While the ground-state (GS) problem for the random-field Ising model is polynomial and can be solved by using a number of well-known algorithms for maximum flow [1–4], the analogue random-field *q*-state Potts model with  $q \ge 3$  corresponds to a multi-terminal flow problem that is known to be NP hard. Hence an efficient exact algorithm is extremely unlikely to exist [5]. Still, it is possible to employ an embedding of binary

degrees of freedom into the Potts spins to use graph-cut methods (GCMs) to solve the corresponding ground-state problem approximately with polynomial methods. It is shown in this project [6] that this works relatively well. We compare results produced by this heuristic algorithm to energy minima found by an appropriately tuned parallel tempering method that is configured to find ground states for the considered system sizes with high probability. The method based on graph cuts finds the same states in a fraction of the time. The new method is used for a first exploratory study of the random-field Potts model in d = 2, 3.

We observe that the probability of finding a ground state decreases exponentially with *q* for GCM, but for parallel tempering this decay is linear [Fig. 12.25(a)]. Hence, GCM is more suitable for lower *q* studies. We also find that the lower energies found by GCM are very close to the ground state and the excess energy is very small. The probability of finding the ground state falls exponentially with the system size, whereas for GCM it falls linearly [Fig. 12.25(b)]. Therefore, GCM is better suited for studying larger system sizes. This is one very good feature of GCM as for the smaller system sizes we have larger finite-size effects. The overlap between the states found by GCM and the ground state is observed to be very large. Hence, we conclude that GCM produces the approximate GS which can be treated as an exact GS for sufficiently small *q* (*q* = 3, 4) for studying the critical behaviour and ground-state morphologies.

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## 12.20 Effects of the low-temperature phase degeneracy of the fcc Ising antiferromagnet on its finite-size scaling behavior

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The ordering of the Ising antiferromagnet on a face-centered cubic (fcc) lattice presents a long-standing problem which has received extensive attention since the 1930s. An important motivation for research on this model is the interest in frustrated magnetism in general which mainly prompted the later publications on this model. The model is well known to exhibit a macroscopic (exponential in the system size *L*) ground-state degeneracy. With increasing temperature, this degeneracy is expected to be lifted and the model undergoes a first-order phase transition. For a model with an exponential degeneracy in the *whole* low-temperature phase, it was recently found that the finite-size scaling behaviour is governed by leading correction terms ~  $L^{-2}$  instead of ~  $L^{-3}$  as usual [1, 2]. To test the conjecture that such a transmuted behaviour may effectively persist also for the fcc antiferromagnet up to some crossover system size, we have performed multicanonical Monte Carlo simulations [3, 4] in a parallelized implementation



**Figure 12.26:** Quality of fit parameter  $Q \in [0, 1]$  for the fits of  $\beta_{eqw}(L)$  with the different fit functions. Here, the lattice size range  $[L_{min,fit}, L_{max,fit}]$ , over which the fit is performed, is varied. The color-value-key of Q is shown above.

[5] for lattices of linear size  $L \le 18$  with periodic boundary conditions and determined various inverse pseudo phase-transition temperatures, as well as the extremal values of the specific heat and the energetic Binder parameter.

Via least-squares fits [6], the regarded inverse pseudo phase-transition temperatures were fitted with the fit functions

$$f_{n}^{(o)}(L) = k_{0} + \frac{k_{1}}{L^{2}} + \frac{k_{2}}{L^{3}} + \frac{k_{3}}{L^{4}}, \qquad (12.17)$$

$$f_{\rm s}^{(o)}(L) = k_0 + \frac{k_1}{L^3} + \frac{k_2}{L^6} + \frac{k_3}{L^9}, \qquad (12.18)$$

where  $f_n^{(o)}$  corresponds to the non-standard scaling and  $f_s^{(o)}$  represents the standard ansatz, and o = 1, 2, 3 denotes the order of the fit function. We also compared with the ansatz

$$f_{\rm BR}^{(1)}(L) = \left(k_0 + \frac{k_1}{L}\right)^{-1}$$
(12.19)

which Beath and Ryan [7] employed, however, without a theoretical justification.

The results for the fits of  $\beta_{eqw}(L)$  are shown in Fig. 12.26 by means of the quality of fit parameter Q. The corresponding heat maps for  $\beta_{c_{max}}(L)$ ,  $\beta_{B_{min}}(L)$  and  $\beta_{eqh}(L)$  look very similar and hence are not depicted here. One can see that up to the first order, the ansatz  $f_{BR}^{(1)}$  of Beath and Ryan [7] is slightly better than the standard ansatz  $f_s^{(1)}$  but clearly not as good as the non-standard ansatz  $f_n^{(1)}$ . Taking into account also the second order, the non-standard ansatz  $f_n^{(2)}$  yields good fits for all ranges [ $L_{min,fit}$ ,  $L_{max,fit}$ ] of fitted lattice

sizes *L*. Of course, also the results of the standard ansatz  $f_s^{(o)}$  improve with increasing order *o*, but they stay behind the non-standard ansatz  $f_n^{(o)}$  in any case. This leads to the conclusion that up to the largest simulated lattice size L = 18, the non-standard ansatz fits best [8]. A crossover between the different ansatzes is not observable in the range of the simulated lattice sizes. However, it cannot be excluded that such a crossover might occur for larger lattice sizes L > 18.

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# 12.21 The two-dimensional Blume-Capel model: Scaling and universality

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The Blume-Capel model [1, 2] is a perfect test model for studies of phase transitions. We consider this spin-one Ising model in a crystal field on a square lattice in two dimension (2D), described by the Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j + \Delta \sum_i \sigma_i^2 = E_J + \Delta E_\Delta , \qquad (12.20)$$

where the spin variables  $\sigma_x \in \{-1, 0, +1\}$  and the couplings are  $J_{ij} \equiv J$  in the pure model or drawn randomly from a bimodal distribution

$$\mathcal{P}(J_{xy}) = \frac{1}{2} \left[ \delta(J_{xy} - J_1) + \delta(J_{xy} - J_2) \right]$$
(12.21)

in the disordered model, where we choose  $J_1 + J_2 = 2$  and  $J_1 > J_2 > 0$ , so that  $r = J_2/J_1$  defines the disorder strength (for r = 1 one recovers the pure model). We investigated the behaviour in the vicinity of the first-order and second-order regimes of the ferromagnet-paramagnet phase boundary, respectively [3], see the phase diagram for the pure model in Fig. 12.27. To achieve high-precision results, we utilized a combination of (i) a parallel version of the multicanonical algorithm and (ii) a hybrid updating



**Figure 12.27:** Phase diagram of the pure two-dimensional Blume-Capel model, showing the ferromagnetic (F) and paramagnetic (P) phases that are separated by a continuous transition for small (solid line) and a first-order transition for large (dotted line). The line segments meet at a tricritical point, as indicated by the black diamond. The horizontal arrows indicate the paths of crossing the phase boundary implemented in the simulations of the present work.

scheme combining Metropolis and generalized Wolff cluster moves. These techniques are combined to study for the first time the correlation length  $\xi$  of the model, using its scaling with system size *L* in the regime of second-order transitions to illustrate universality through the observed identity of the limiting value of  $\xi/L$  with the exactly known result for the Ising universality class.

In contrast to most previous work, we focused on crossing the phase boundary at constant temperature by varying the crystal field  $\Delta$  [4]. Employing a multicanonical scheme in  $\Delta$  allowed us to get results as continuous functions of  $\Delta$  and to overcome the free-energy barrier in the first-order regime of the transitions. A finite-size scaling analysis based on a specific-heat-like quantity and the magnetic susceptibility provided us with precise estimates for the transition points in both regimes of the phase diagram that compare very well to the most accurate estimates of the current literature. In the first-order regime, we found a somewhat surprising 1/L correction in the scaling of the conventionally defined magnetic susceptibility  $\chi$ . As it turns out, this is due to the explicit symmetry breaking by using the absolute value of the magnetisation (i.e., |M| instead of M) in the definition of  $\chi$ . For a modified symmetry breaking prescription that leaves the disordered peak invariant, this correction disappears. It would be interesting to see whether similar corrections are found in other systems with first-order transitions, such as the Potts model.

More recently we extended this study by considering the effect of the quenched disorder in the exchange couplings  $J_{ij}$  [5]. We find that the first-order transition for large crystal-field coupling is softened to become continuous, with a divergent correlation length. An analysis of the scaling of the correlation length as well as the susceptibility and specific heat reveals that this transition belongs to the Ising universality class with additional logarithmic corrections which are also observed for the Ising model itself if coupled to weak disorder. While the leading scaling behavior of the disordered system

is thus identical in the second-order and first-order segments of the phase diagram of the pure model, the finite-size scaling in the ex-first-order regime turns out to be strongly affected by transient effects with a crossover length scale  $L^* \approx 32$  for the chosen parameters [5].

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## 12.22 Simulation of self-avoiding walks and polymers in continuum by means of binary trees

#### S. Schnabel, W. Janke

A few years ago Nathan Clisby has introduced a novel technique [1] for the simulation of self-avoiding walks on lattice geometries. These systems serve as simple models for polymers with excluded-volume interaction and allow for the investigation of the related scaling behaviour. With the new method walks are stored as binary trees where the leaves correspond to individual occupied lattice sites and any internal node contains collective geometric information of the subtree to which it is root in form of a box (in case of a simple-cubic lattice) that contains all derived monomers. This allows one to test for non-intersection of large parts of the walk very efficiently using nodes high up in the tree which represent many occupied lattice sites. Lower nodes representing few sites in more detail are only accessed if necessary. It was possible to determine the 3d Flory exponent with great accuracy,  $\nu = 0.5875970(4)$  [2], with the new method.

Our first goal is to apply this method to the slightly more realistic hard-sphere polymer model, also known as continuum self-avoiding walks. A set of monomers  $\mathbf{x}_i$  that are connected by bonds of fixed length  $|\mathbf{x}_i - \mathbf{x}_{i+1}| = 1$  and represent hard spheres of diameter D:  $|\mathbf{x}_i - \mathbf{x}_j| \ge D$ . Otherwise the chain is fully flexible. The adaptation of the binary-tree method to the latter system is straightforward. The boxes are replaced by spheres and transformations are generalized. Now it is easily possible to simulate systems with many million monomers. In Fig. 12.28 we show the dependence of the end-to-end distance as a function of the polymer length divided by the asymptotic scaling law. The crossover from a behaviour akin to a random walk (where  $\nu = 1/2$ ) for small chains and small diameters to the self-avoiding walk (horizontal in Fig. 12.28) can be observed. It becomes apparent that for  $D \approx 0.45$  the corrections to scaling become very small and asymptotic behaviour is already realized for comparatively short chains.

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**Figure 12.28:** Rescaled quadratic end-to-end distance  $r_{ee}$  of the hard-sphere polymer as a function of length *L* for different sphere diameters *D*. The crossover from the random walk (D = 0) to the self-avoiding walk is apparent.

### 12.23 Non-flat histogram techniques for spin glasses

F. Müller, S. Schnabel, W. Janke



**Figure 12.29:** Histograms of the simulation with the different methods together with the prescribed power-law shape  $P_{SH}(E)$ .

We took into consideration the three-dimensional bimodal Edwards-Anderson (EA) spin-glass model [1]. Spin glasses are difficult to simulate with conventional simulation methods and their investigation requires calculating disorder averages over a sufficiently large set of samples. Each sample has its own characteristics and it is known that finding the ground state of hard samples, i.e., solving the underlying optimization problem of that sample, is NP-hard.

There are existing methods such as the multicanonical (MUCA) method [2, 3], the 1/*k* ensemble [4] and parallel tempering (PT) [5] which have already been applied to the

	flat MUCA		parallel tempering	
L	r <sub>pop</sub>	$r_{\epsilon=10^{-4}}$	r <sub>pop</sub>	$r_{\epsilon=10^{-4}}$
3	$1.16^{+0.02}_{-0.02}$	$1.17^{+0.04}_{-0.04}$	$1.64^{+0.03}_{-0.03}$	$1.64^{+0.04}_{-0.04}$
4	$1.62^{+0.05}_{-0.05}$	$1.66^{+0.09}_{-0.08}$	$1.17^{+0.04}_{-0.04}$	$1.22^{+0.07}_{-0.07}$
5	$2.3^{+0.2}_{-0.2}$	$2.34_{-0.3}^{+0.3}$	$1.14^{+0.05}_{-0.05}$	$1.14^{+0.1}_{-0.09}$
6	$3.8^{+0.6}_{-0.5}$	$3.5^{+0.7}_{-0.6}$	$2.8^{+0.4}_{-0.4}$	$3.3^{+0.8}_{-0.6}$
8	$13^{+12}_{-7}$	$15^{+25}_{100}$	$3^{+3}_{2}$	$3^{+6}_{2}$

**Table 12.1:** Ratios of the population mean and the quantile mean of round-trip times of the flat MUCA and parallel-tempering methods with respect to the power-law MUCA method.

three-dimensional EA model. Especially also their performance in terms of the ability to solve the underlying optimization problem has been investigated. We looked at the round-trip times in energy which are defined as the average time which a simulation takes to reach the ground state and travel back to high energies. The ability of finding the ground state strongly influences the round-trip times of the respective method.

In addition to the above mentioned methods we modified the MUCA approach from sampling a flat distribution in energy to sampling a power-law shaped distribution in energy with a parametric form of the distribution of the form

$$P_{\rm SH}(E,\Delta E,\alpha) = \left(\frac{E}{\Delta E - E_g} + 1\right)^{\alpha}, \qquad (12.22)$$

where  $\Delta E = 96$  is the position of the pole of the power law relative to the ground-state energy  $E_g$  and  $\alpha = -3.6$  is the exponent [6]. In Fig. 12.29 the outcoming histograms of one sample with linear lattice size L = 8 are plotted. The figure shows clearly that the effort of the simulation is concentrated towards the ground-state region for all methods but the traditional MUCA. The power-law MUCA and PT have similar distributions of sampled states which increase drastically towards the ground-state energy.

Table 1 shows the comparison of the mean round-trip times for the three different methods. The mean round-trip times of the power-law MUCA improve significantly compared to the traditional MUCA and also compared to the other methods.

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### 12.24 Population annealing: A massively parallel computer simulation scheme

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**Figure 12.30:** Schematic illustration of the population annealing method: *R* replica of the system are cooled down in discrete temperature steps. At each temperature *T* the current configurations at the next higher temperature are resampled according to their Boltzmann weights. This amounts to deleting some of them (e.g., the red one in the upper row) and replicating others one, two or more times (e.g., the dark green one in the second row). This new population is then further evolved in "time" *t* by any valid update procedure at this temperature.

The generic technique for Monte Carlo simulations in statistical physics is importance sampling via a suitably constructed Markov chain [1]. While such approaches are quite successful, they are not particularly well suited for parallelization as the chain dynamics is sequential, and if replicated chains are used to increase statistics each of them relaxes into equilibrium with an intrinsic time constant that cannot be reduced by parallel work. Population annealing is a sequential Monte Carlo method that simulates an ensemble of system replica under a cooling protocol as sketched in Fig. 12.30. This method was first suggested in 2001 by Iba [2] and later on discussed in more detail by Hukushima and Iba [3] as a method to tackle potentially difficult sampling problems, but with no particular view to a parallel implementation. More recently, Machta [4] used a variant that avoids the recording of weight functions through population control in every step. This is the variant we adapted in our own implementation.

The population element makes this method naturally well suited for massively parallel simulations, and both the bias in estimated quantities and the statistical errors can be systematically reduced by increasing the population size. To demonstrate this, we developed an implementation of population annealing on graphics processing units (GPUs) [5] and benchmarked its behaviour for different systems undergoing continuous and first-order phase transitions [6, 7]. For a recent overview, see Ref. [8].

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# 12.25 Accelerating molecular dynamics with population annealing

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**Figure 12.31:** (a) Energy histogram for Met-enkephalin at the lowest temperature (T = 200 K) considered for the different methods. (b) Speedup  $S_p$  and, in the inset, efficiency  $S_p/p$  for different number of CPU cores p.

Systems having a rugged free-energy landscape cannot be simulated using naive canonical (NVT) simulations, because they get trapped in local minima. Therefore, one uses so-called generalized ensemble methods to overcome those barriers. In Molecular Dynamics, one mostly uses Parallel Tempering [1], which is easy to parallelize. However, this method can only effectively use a limited number of CPU cores. In this work, we adapt Population Annealing [2, 3] to Molecular Dynamics simulations. This method has the advantage that it scales to effectively "arbitrary" number of CPU cores while having comparable performance to Parallel Tempering when using the same computational resources. For a broad range of systems, this opens the door to the world of highly efficient computer simulations on petaflop supercomputers of the present and the exaflop machines of the future. To demonstrate this advantage, we have investigated the penta-peptide Met-enkephalin [4, 5], a system commonly used to probe the performance of novel simulation methods. In Fig. 12.31(a) we show the energy histogram for the lowest temperature considered at T = 200 K, where the free-energy barriers are most prominent. Both Population Annealing (PA) and Parallel Tempering (PT) produce energy histograms that are compatible with each other, whereas a single canonical simulation leads to a shifted histogram. Here "anneal" corresponds to an ensemble of independent Simulated Annealing runs. The excellent scaling with the number of CPU cores *p* is presented in Fig. 12.31(b), where we show the speedup  $S_p$  for up to p = 500 CPU cores. In the inset, the efficiency  $S_p/p$  is shown, indicating a parallel performance of clearly above 80% in this case.

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### **12.26** Framework for programming Monte Carlo simulations (βMC)

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Monte Carlo (MC) computer simulations are a very powerful tool for investigating and understanding the thermodynamic behavior of a wide variety of physical systems. These systems range from such simple ones like the Ising or Blume-Capel spin models to complex ones like semiflexible polymers confined in a sphere or proteins interacting with surfaces. In contrast to Molecular Dynamics (MD) simulations, the other important class of algorithm to simulate microscopic systems, MC simulations are not suitable to investigate dynamical properties. On the other hand, the ability of modern MC methods to explore effectively the phase space of physical systems, especially those with a phase transition, makes them a very powerful and indispensable tool.

Another difference to MD simulations is the lack of a widely used program package for generic MC simulations. One reason for this lack is the versatility of modern MC algorithms – there are various different algorithm and many different possibilities to adjust a MC simulation to a specific problem. This was the starting point for the development of our framework for advanced MC algorithms. The aim of the framework is to enable the programmer to implement specific simulations in an easy and efficient way, without the need to implement all the tricky details for every new problem. The framework is implemented in the C++ programming language and is designed such



Figure 12.32: The 5 basic building blocks.



**Figure 12.33:** Scaling properties of the parallel multicanonical algorithm as a function of the number of processors *p*.

that it separates basics parts of a MC algorithm in separate building blocks. These building blocks can be used by the programmer to implement a specific simulation.

There are 5 basic building blocks as illustrated in Fig. 12.32: The first one is the "system", which defines the Hamiltonian and the structure of the physical system. This means that the "system" building block encapsulates the energy calculation and the structure of the considered physical problem. For off-lattice system this block contains a smaller subpart, the "atom" block, which encodes the geometry of the system (e.g., boundary conditions). As systems we have implemented so far different kinds of coarse-grained homopolymers, the Lennard-Jones gas, the TIP4P water model, lattice polymers and the Potts model in different dimensions. On top of the "system" are the last two other building blocks, the "move" and the "MC technique". A "move" defines a single update proposal, propagating the system from the current state to the next one. Additionally a "constraint" can be added to every "move" in order to simulate efficiently systems with geometrical confinements. The "MC technique" implements the Monte Carlo algorithm itself. At the moment we have implemented various algorithms such as Metropolis MC, parallel tempering, multicanonical MC, multimagnetic MC and the Wang-Landau MC algorithm. One of the most advanced MC algorithms we have implemented is a parallel version of the multicanonical algorithm [1, 2], see Fig. 12.33.

The boundaries between these blocks are well defined, so that one can easily exchange one of them. For example one can use two different algorithm to simulate a specific system without implementing a completely new program. The framework is already in practical use for different studies, for example the investigation of the influence of bending stiffness on a coarse-grained homopolymer, the influence of a spherical confinement to pseudo-phase transitions of homopolymers, and the study of polymer aggregation of several polymers for a large set of parameters (temperature, bending stiffness). Thus, the framework is very useful and has led already to several publications [3–9].

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## 12.28 Organizational Duties

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- Principal Investigator of "Profillinie" Mathematical and Computational Sciences, Universität Leipzig
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- Permanent Member of the International Advisory Board for the Annual Conference of the Middle European Cooperation in Statistical Physics (MECO)
- Organizer of the Workshop CompPhys18 19th International NTZ Workshop on New Developments in Computational Physics, ITP, Universität Leipzig, 29. November – 01. December 2018
- Organizer (with M. Weigel, Coventry University, UK) of the CECAM Workshop New Methods in Monte Carlo Simulations: Parallel, Adaptive, Irreversible, CECAM-HQ-EPFL, Lausanne, Switzerland, 02.–04. September 2019
- Organizer of the Workshop CompPhys19 20th International NTZ Workshop on New Developments in Computational Physics, ITP, Universität Leipzig, 28.–30. November 2019
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- Member of Editorial Board, Condens. Matter Phys., Lviv, Ukraine
- External Reviewer for Deutsche Forschungsgemeinschaft (DFG); Humboldt-Stiftung (AvH); Studienstiftung des deutschen Volkes; Fond zur Förderung der wissenschaftlichen Forschung (FWF), Österreich; The Royal Society, UK; The Engineering and Physical Sciences Research Council (EPSRC), UK; Israel Science Foundation, Israel; National Science Foundation (NSF), USA; Natural Sciences and Engineering Research Council of Canada (NSERC), Canada; The Jeffress Memorial Trust, Bank of America, Virginia, USA; Universität Mainz, Germany; The University of Warwick, England, UK; Coventry University, England, UK; CECAM, Lausanne, Switzerland

• Referee for Physical Review Letters, Physical Review B, Physical Review E, Journal of Chemical Physics, Europhysics Letters, Physics Letters A, Physics Letters B, The European Physical Journal B, Physica A, Proceedings of the Royal Physical Society, Journal of Physics A, Computer Physics Communications, JSTAT, Canadian Journal of Physics, Condens. Matter Phys., PLOS ONE, New Journal of Physics, International Journal of Modern Physics C

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- CERN (PH-SFT), Geneva, Switzerland Dr. Sandro Wenzel
- Department of Engineering of Physics, Ankara University, Ankara, Turkey Prof. Dr. Handan Arkın-Olgar, Mustafa Bilsel, Dogukan Hazar Özbey, Buket Taşdizen
- Dept. of Physics, Hacettepe University, Ankara, Turkey Prof. Dr. Tarik Çelik, Gökhan Gökoğlu
- Dept. of Physics Engineering, Hacettepe University, Ankara, Turkey Prof. Dr. Fatih Yaşar
- Institute for Condensed Matter Physics, National Academy of Sciences, Lviv, Ukraine Dr. Viktoria Blavatska, Prof. Dr. Yurij Holovatch
- Yerevan Physics Institute, Yerevan, Armenia Prof. Dr. David B. Saakian
- Alikhanyan National Science Laboratory, Yerevan, Armenia Prof. Dr. Nerses Ananikyan, Dr. Nikolay Izmailyan
- Landau Institute for Theoretical Physics, Chernogolovka, Russia Dr. Lev Yu. Barash, Prof. Dr. Lev N. Shchur
- National Research University Higher School of Economics, Moscow, Russia Prof. Dr. Evgeni Burovski, Maria Guskova
- Center for Simulational Physics, The University of Georgia, Athens, USA Prof. Dr. Michael Bachmann, Prof. Dr. David P. Landau

- Dept. of Physics, Florida State University, Tallahassee, USA Prof. Dr. Bernd A. Berg
- Dept. of Chemistry and Biochemistry, University of Oklahoma, Norman, USA Prof. Dr. Ulrich H.E. Hansmann
- Los Alamos National Laboratory, Los Alamos, USA Dr. Christoph Junghans
- Dept. of Physics and Astronomy, Texas A&M, College Station, USA Prof. Dr. Helmut G. Katzgraber
- Dept. of Physics, Virginia Tech, Blacksburg, USA Prof. Dr. Michel Pleimling, Prof. Dr. Royce K.P. Zia
- Physics Department, Carnegie Mellon University, Pittsburgh, USA Prof. Dr. Robert H. Swendsen
- University of North Georgia, Dahlonega, USA Dr. Thomas Vogel
- Banaras Hindu University, Varanasi, India Prof. Dr. Sanjay Kumar
- Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur, India Prof. Dr. Subir K. Das
- School of Physical Sciences, Jawaharlal Nehru University, New Delhi, India Manoj Kumar, Prof. Dr. Sanjay Puri
- Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi, India Prof. Dr. Varsha Banerjee
- Computational Chemistry Unit Cell (CCUC), Department of Chemistry, Chulalongkorn University, Bangkok, Thailand Prof. Dr. Supot Hannongbua, Dr. Oraphan Saengsawang
- Metallurgy and Materials Science Research Institute (MMRI), Chulalongkorn University, Bangkok, Thailand Prof. Dr. Rungroj Chanajaree
- Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok, Thailand Dr. Tatiya Chokbunpiam
- Faculty of Applied Science and Engineering, Khon Kaen University, Nong Khai Campus, Nong Khai, Thailand Prof. Dr. Tawun Remsungnen
- Laboratory of Statistical and Computational Physics, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan Prof. Dr. Chin-Kun Hu
- Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, P.R. China Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng
- The University of Tokyo, Tokyo, Japan Prof. Dr. Nobuyasu Ito

• Nagoya University, Nagoya, Japan Dr. Tetsuro Nagai, Prof. Dr. Yuko Okamoto

## 12.30 Publications

#### Journals

K.S. Austin, M. Marenz, W. Janke: *Efficiencies of Joint Non-Local Update Moves in Monte Carlo Simulations of Coarse-Grained Polymers*, Comput. Phys. Commun. **224**, 222–229 (2018)

N.G. Fytas, J. Zierenberg, P.E. Theodorakis, M. Weigel, W. Janke, A. Malakis: *Universality from Disorder in the Random-Bond Blume-Capel Model*, Phys. Rev. E **97**, 040102(R)-1–6 (2018)

J. Gross, J. Zierenberg, M. Weigel, W. Janke: *Massively Parallel Multicanonical Simulations*, Comput. Phys. Commun. **224**, 387–395 (2018)

W. Janke: *Generalized Ensemble Computer Simulations of Macromolecules*, invited Ising Lecture Notes 2016, in *Order, Disorder and Criticality: Advanced Problems of Phase Transition Theory*, Vol. 5, ed. Y. Holovatch (World Scientific, Singapore, 2018), pp. 173–225

W. Janke, J. Zierenberg: *From Particle Condensation to Polymer Aggregation*, invited Plenary Talk, International Conference *Computer Simulations in Physics and beyond (CSP2017)*, 09.–12. October 2017, Moscow, Russia, J. Phys.: Conf. Ser. **955**, 012003-1–10 (2018)

M. Kumar, R. Kumar, M. Weigel, V. Banerjee, W. Janke, S. Puri: *Approximate Ground States of the Random-Field Potts Model from Graph Cuts*, Phys. Rev. E **97**, 053307-1–10 (2018)

S. Majumder, H. Christiansen, W. Janke: *Scaling Laws During Collapse of a Homopolymer: Lattice Versus Off-Lattice*, J. Phys.: Conf. Ser. **955**, 012008-1–6 (2018)

S. Majumder, S.K. Das, W. Janke: Universal Finite-Size Scaling Function for Kinetics of *Phase Separation in Mixtures with Varying Number of Components*, Phys. Rev. E **98**, 042142-1–13 (2018)

N. Oberthür, J. Groß, W. Janke: *Two-Dimensional Monte Carlo Simulations of Coarse-Grained Poly(3-hexylthiophene) (P3HT) Adsorbed on Striped Substrates*, J. Chem. Phys. **149**, 144903-1–12 (2018)

S. Schnabel, W. Janke: *Distribution of Metastable States of Ising Spin Glasses*, Phys. Rev. B **97**, 174204-1–10 (2018)

F.P. Spitzner, J. Zierenberg, W. Janke: *The Droplet Formation-Dissolution Transition in Different Ensembles: Finite-Size Scaling from Two Perspectives*, SciPost Phys. **5**, 062-1–24 (2018)

R. Stübel, W. Janke: Finite-Size Scaling of Monte Carlo Simulations for the FCC Ising Antiferromagnet: Effects of the Low-Temperature Phase Degeneracy, Phys. Rev. B **98**, 174413-1–8 (2018)

#### in press

L. Shchur, L. Barash, M. Weigel, W. Janke: *Population Annealing and Large Scale Simulations in Statistical Mechanics*, Communications in Computer and Information Science (CCIS) **965**, 354–366 (2019)

H. Christiansen, S. Majumder, W. Janke: *Phase Ordering Kinetics of the Long-Range Ising Model*, Phys. Rev. E **99**, 011301(R)-1–5 (2019)

H. Christiansen, M. Weigel, W. Janke: Accelerating Molecular Dynamics Simulations with Population Annealing, Phys. Rev. Lett. **122**, 060602-1–5 (2019)

S. Majumder, H. Christiansen, W. Janke: *Dissipative Dynamics of a Single Polymer in Solution: A Lowe-Andersen Approach*, J. Phys.: Conf. Ser. **1163**, 012072-1–6 (2019)

W. Janke, H. Christiansen, S. Majumder: *Coarsening in the Long-Range Ising Model: Metropolis versus Glauber Criterion*, invited Plenary Talk at the International Conference on *Computer Simulation in Physics and beyond (CSP2018)*, 24.–27. September 2018, Moscow, Russia, J. Phys.: Conf. Ser. **1163**, 012002-1–10 (2019)

H. Christiansen, M. Weigel, W. Janke: *Population Annealing Molecular Dynamics with Adaptive Temperature Steps*, J. Phys.: Conf. Ser. **1163**, 012074-1–6 (2019)

S. Schnabel, W. Janke: *Distribution of Metastable States of Spin Glasses*, in *Computer Simulation Studies in Condensed-Matter Physics XXXI*, eds. D.P. Landau, M. Bachmann, S.P. Lewis, H.-B. Schüttler, J. Phys.: Conf. Ser. **1252**, 012001-1–6 (2019)

S. Majumder, U.H.E. Hansmann, W. Janke: *Pearl-Necklace-Like Local Ordering Drives Polypeptide Collapse*, Macromolecules **52**, 5491–5498 (2019)

#### Talks

H. Christiansen, S. Majumder, W. Janke: *Efficient Method of Simulating with Long-Range Interactions: The Case of Coarsening in the Ising Model*, DPG Frühjahrstagung 2018, TU Berlin, Germany, 12.–16. March 2018

H. Christiansen, M. Weigel, W. Janke: *Application of Population Annealing to Molecular Dynamics Simulations for Protein Folding*, Annual BuildMoNa Conference 2018, Universität Leipzig, Germany, 20. March 2018

H. Christiansen, M. Weigel, W. Janke: *Population Annealing for Molecular Dynamics Simulations of Protein Folding*, Soft Matter Day 2018, Universität Leipzig, Germany, 06. July 2018

H. Christiansen, S. Majumder, W. Janke: *Coarsening and Ageing in the Long-Range Ising Model*, Statistical Physics Seminar, Université de Lorraine Nancy, France, 15. November 2018

H. Christiansen, M. Weigel, W. Janke: Accelerating Molecular Dynamics Simulations with Population Annealing, 19th International NTZ-Workshop on New Developments in Computational Physics – CompPhys18, Universität Leipzig, Germany, 29. November – 01. December 2018

W. Janke: Stochastic Approximation Monte Carlo vs Wang-Landau Algorithm, 31st Annual CSP Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, The University of Georgia, Athens, Georgia, USA, 19.–23. February 2018

W. Janke: Thermodynamically Stable Phases for Semiflexible Polymers Characterized by Knots of Specific Topologies, APS March Meeting, Los Angeles, California, USA, 05.–09. March 2018

W. Janke: Scaling Behavior of Self-Avoiding Walks on Critical Percolation Clusters in Two to Seven Dimensions from Exact Enumeration, DPG Frühjahrstagung 2018, TU Berlin, Germany, 11.–16. March 2018

W. Janke: From Particle Condensation to Polymer Aggregation, 2nd Changchun and Halle-Leipzig Discussion Seminar on Polymer Science, Universität Halle, Germany, 11. April 2018

W. Janke: Long-Range Power-Law Correlated Percolation in Two and Three Dimensions, Conference of the Middle European Cooperation in Statistical Physics – MECO43, Krakow, Poland, 01.–04. May 2018

W. Janke: *Coarsening Dynamics of the Long-Range Ising Model*, invited plenary talk, 3rd International Conference on *Computer Simulations in Physics and beyond* (*CSP2018*), National Research University Higher School of Economics, Moscow, Russia, 24.–27. September 2018

R. Kumar: *Computer Simulation Studies of Frustrated Spin Systems*, PhD thesis defence, Coventry University, Coventry, UK, 07. December 2018

S. Majumder, H. Christiansen, W. Janke: *Dissipative Dynamics of a Single Polymer in Solution: A Lowe-Andersen Approach*, 3rd International Conference on *Computer Simulations in Physics and beyond (CSP2018)*, National Research University Higher School of Economics, Moscow, Russia, 24.–27. September 2018

S. Majumder, H. Christiansen, W. Janke: *Dissipative Dynamics of a Single Polymer in Solution: A Lowe-Andersen Approach*, 19th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys18*, Universität Leipzig, Germany, 29. November – 01. December 2018

M. Marenz: Morphologies of Semiflexible Polymers in Bulk and Spherical Confinement, PhD thesis defence, Universität Leipzig, Germany, 13. June 2018

M. Mueller: Nonstandard Finite-Size Effects at Discontinuous Phase Transitions – Degenerate Low-Temperature States and Boundary Conditions, PhD thesis defence, Universität Leipzig, Germany, 01. February 2018 S. Paul, S.K. Das: Dimension Dependence of Clustering Dynamics in Models of Ballistic Aggregation and Freely Cooling Granular Gas, 19th International NTZ-Workshop on New Developments in Computational Physics – CompPhys18, Universität Leipzig, Germany, 29. November – 01. December 2018

S. Schnabel, W. Janke: Distribution of Metastable States of Spin Glasses, 31st Annual CSP Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, The University of Georgia, Athens, USA, 19.–23. February 2018

S. Schnabel, W. Janke: Simulation of a Large Polymer with Untruncated Interaction Near the Collapse, 19th International NTZ-Workshop on New Developments in Computational Physics – CompPhys18, Universität Leipzig, Germany, 29. November – 01. December 2018

#### Posters

H. Christiansen, S. Majumder, W. Janke: *Coarsening in the Long-Range Interacting Ising Model*, Conference of the Middle European Cooperation in Statistical Physics – MECO43, Krakow, Poland, 01.–04. May 2018

J. Gross, J. Zierenberg, M. Weigel, W. Janke: *Massively Parallel Multicanonical Simulations*, DPG Frühjahrstagung 2018, TU Berlin, Germany, 12.–16. March 2018

S. Kazmin, W. Janke: Critical Exponent v of the Ising Model in Three Dimensions with Long-Range Correlated Disorder, 19th International NTZ-Workshop on New Developments in Computational Physics – CompPhys18, Universität Leipzig, Germany, 29. November – 01. December 2018

F. Müller, S. Schnabel, W. Janke: *Non-Flat Histogram Techniques for Spin Glasses*, DPG Frühjahrstagung 2018, TU Berlin, Germany, 12.–16. March 2018

F. Müller, M. Ivanov, N. Oberthür, J. Gross, W. Janke: *Nanopatterns of Macromolecules*, 19th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys18*, Universität Leipzig, Germany, 29. November – 01. December 2018

F. Müller, M. Ivanov, N. Oberthür, J. Gross, W. Janke: *Nanopatterns of Macromolecules*, SFB-Transregio 102, 6th Miniworkshop, Universität Halle, Germany, 09. July 2018

F.P. Spitzner, J. Zierenberg, W. Janke: *Two Perspectives on the Droplet Condensation-Evaporation Transition*, DPG Frühjahrstagung 2018, TU Berlin, Germany, 12.–16. March 2018

J. Zierenberg, W. Janke: *Parallel Multicanonical Simulations and their Application*, APS March Meeting, Los Angeles, California, USA, 05.–09. March 2018

## 12.31 Graduations

Doctorate

• Marco Müller

Nonstandard Finite-Size Effects at Discontinuous Phase Transitions – Degenerate Low-Temperature States and Boundary Conditions 01. February 2018

- Martin Marenz Morphologies of Semiflexible Polymers in Bulk and Spherical Confinement 13. June 2018
- Ravinder Kumar Computer Simulation Studies of Frustrated Spin Systems 07. December 2018

#### Diploma

 Hans-Joachim Lange Kollaps von Homopolymeren auf zweidimensionalen Gittern 29. March 2018

#### Master

- Simon Schneider The 3D Gonihedric Ising Model and its Phase Diagram for κ ≠ 0 11. January 2018
- David Nicolai Oberthür Two-Dimensional Monte Carlo Simulations of Coarse-Grained Poly(3-Hexylthiophene) Polymers on Striped Substrates
   18. January 2018
- Ronja Stübel Finite-Size Scaling of Monte Carlo Simulations for the FCC Ising Antiferromagnet: Effects of the Low-Temperature Phase Degeneracy 27. February 2018
- Lisa Fiedler HP Polymers under Investigation – A Coarse-Grained Approach to Study Protein Folding 07. June 2018
- Dimitrij Tschodu *Machine Learning the q-State Potts Model* 12. July 2018

#### Bachelor

- Adrian Häußler Exact Enumeration of a Lattice Polymer in Confinement
- Jakob Bürgermeister Finite-Size Scaling of the Three-Dimensional Lennard-Jones Gas 28. June 2018

 Michel Michalkow *Applications of the Bond-Propagation Algorithm* 05. October 2018

### 12.32 Guests

- Kseniia Shapovalova
   Far Eastern Federal University, Vladivostok, Russia
   DAAD Michail-Lomonosov-Programm
   01. October 2017 31. March 2018
- Dr. Fabian Senf Leibniz-Institut für Troposphärenforschung e.V., AG Satellitenfernerkundung NTZ/DFH-UFA Seminar (25. January 2018) Statistical Physics Approaches for Deep Convection in the Tropical Atmosphere 25. January 2018
- Prof. Dr. Ulrich H.E. Hansmann University of Oklahoma, Norman, USA 24.–25. April 2018
- Prof. Dr. Jaroslav Ilnytskyi ICMP, National Academy of Sciences of Ukraine, Lviv, Ukraine NTZ/DFH-UFA Colloquium (16. May 2018) Patchy Ligand Shell Nanoparticles: Modelling and Micronetwork Formation 16. May 2018
- Dr. Martin Weigel Coventry University, England, UK 18.–20. June 2018
- Franz Paul Spitzner Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany 21.–22. June 2018
- Dr. Johannes Zierenberg Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany NTZ/DFH-UFA Seminar (21. June 2018) Homeostatic Plasticity and External Input Shape Neural Network Dynamics 21.–22. June 2018
- Dogukan Hazar Özbey Faculty of Engineering, Ankara University, Turkey ERASMUS internship 01. July – 01. September 2018
- Prof. Dr. Subir K. Das Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India 07.–09. October 2018
- Prof. Dr. Peter Grassberger FZ Jülich, Germany

NTZ/DFH-UFA Colloquium (18. October 2018) Self-Repelling Biased Walks on Arbitrary Graphs and YAMMI (Yet Another Montecarlo Method for dummIes 18.-19. October 2018

- Dr. Elmar Bittner
   Universität Heidelberg, Germany
   29. November 01. December 2018
- Dr. Nikolaos Fytas Coventry University, England, UK An Overview of Recent Numerical Results on the Random-Field Ising Model 29. November – 01. December 2018
- Prof. Dr. Peter Grassberger
   FZ Jülich, Germany
   Does KPZ Describe Pushed Interfaces with Quenched Disorder?
   29. November 01. December 2018
- Prof. Dr. Ulrich H.E. Hansmann University of Oklahoma, Norman, OK, USA Conformational Transitions in Prions and Amyloids 29. November – 01. December 2018
- Prof. Dr. Alexander Hartmann Universität Oldenburg, Germany Phase Transition in Detecting Causal Relationships from Obervational and Interventional Data
   29. November – 01. December 2018
- Prof. Dr. Malte Henkel Université de Lorraine Nancy, France Axiomatic Construction of Quantum Langevin Equations 29. November – 01. December 2018
- Dr. Hsiao-Ping Hsu MPI Polymer Research, Mainz, Germany Indication of Chain Retraction in Highly Entangled Polymer Melts after a Large Step Deformation
   29. November – 01. December 2018
- Dr. Fred Hucht Universität Duisburg-Essen, Germany A Multiplicative Monte Carlo Rate for Nonequilibrium Dynamics 29. November – 01. December 2018
- Prof. Dr. Ferenc Igloi
   Wigner Research Centre, Budapest, Hungary
   Quantum Relaxation and Metastability of Lattice Bosons with Cavity-Induced Long-Range Interactions
   29. November – 01. December 2018
- Prof. Dr. Nobuyasu Ito The University of Tokyo, Japan
Simulation of Quantum Computer 29. November – 01. December 2018

- Dr. Nikolay Izmailyan Alikhanyan National Science Laboratory, Yerevan, Armenia Specific Heat and Partition Function Zeros for the Dimer Model on the Checkerboard B Lattice: Finite-Size Effects
   29. November – 01. December 2018
- Prof. Dr. Desmond A. Johnston Heriot-Watt University, Edinburgh, Scotland, UK *Fractons* 29. November – 01. December 2018
- Prof. Dr. Werner Krauth Ecole Normale Supérieur, Paris, France *Irreversible, Totally Asymmetric Markov Chains in Statistical Physics* 29. November – 01. December 2018
- Dr. Eunsang Lee Martin-Luther Universität Halle, Germany *Thermodynamics of Supramolecular Polymers with Hydrogen Bonding Ends* 29. November – 01. December 2018
- Prof. Dr. Jutta Luettmer-Strathmann University of Akron, Ohio, USA Steady State of a Protein-Ligand System in a Temperature Gradient 29. November – 01. December 2018
- Prof. Dr. Arnulf Möbius IFW Dresden, Germany
  29. November – 01. December 2018
- Dr. Gergö Roósz TU Dresden, Germany Quench Dynamics of the Disordered Quantum Ising Chain 29. November – 01. December 2018
- Dr. Timur Shakirov Martin-Luther Universität Halle, Germany Aggregation of Short Polyethylene Chains 29. November – 01. December 2018
- Paul Spitzner Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany Inferring Dynamical Properties of Subsampled Networks
   29. November – 01. December 2018
- Prof. Dr. Mark P. Taylor Dept. of Physics, Hiram College, USA Entropy Reduction and Entropy Driven Folding for Confined Polymers 29. November – 01. December 2018
- Dr. Martin Weigel Coventry University, England, UK

Approximate Ground States of the Random-Field Potts Model from Graph Cuts 29. November – 01. December 2018

 Dr. Johannes Zierenberg Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany *Extending the Dynamic Range by an Ensemble of Neural Networks* 29. November – 01. December 2018

# 13

# Molecular Dynamics / Computer Simulation

### 13.1 Introduction

Introductory text ...

Group Leader

### 13.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 †Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

Table 13.1: Test table – example of column alignment types.

left	right	center	page (width 60 mm)
icit	11511	center	puge (whath oo min)
abc	abc	abc	The quick brown fox jumps over
			the lazy dog.
de	de	de	Six big devils from Japan quickly
			forgot how to waltz.
fghi	fghi	fghi	Oh, welch Zynismus, quiekte
			Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

## 13.3 Contribution 2

#### J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 13.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

- [1] Akiyoshi's illusion pages, www.ritsumei.ac.jp/ akitaoka/index-e.html
- [2] Reference 2

## 13.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

## 13.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

## **13.6** External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

## 13.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

#### Posters

Poster 1

Poster 2

## 13.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## 13.9 Guests

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

# **Quantum Field Theory and Gravity**

### 14.1 Introduction

Introductory text ...

Group Leader

### 14.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor $^*$ , A. Uthor $^{\dagger}$ , A.U.T. Hor $^*$ 

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

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fghi	fghi	fghi	Oh, welch Zynismus, quiekte
5	5	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

### 14.3 Contribution 2

J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 14.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

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- [2] Reference 2

## 14.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

## 14.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

## 14.6 External Cooperations

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

## 14.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

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Reference 3

Reference 4

#### Talks

Talk 1

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#### Doctorate

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- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## 14.9 Guests

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

# 15

# **Statistical Physics**

### 15.1 Introduction

Introductory text ...

Group Leader

### 15.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

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**Table 15.1:** Test table – example of column alignment types.

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[1] Reference 1

[2] Reference 2

### 15.3 Contribution 2

J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 15.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

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- [2] Reference 2

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Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

## **15.5** Organizational Duties

Person 1

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

## **15.6 External Cooperations**

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

### 15.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

#### Posters

Poster 1

Poster 2

## 15.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
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#### Diploma

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- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## 15.9 Guests

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

# 16

# **Theory of Condensed Matter**

### 16.1 Introduction

Introductory text ...

Group Leader

### 16.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

Table 16.1: Test table – example of column alignment types.

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5	5	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

### 16.3 Contribution 2

J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 16.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

- [1] Akiyoshi's illusion pages, www.ritsumei.ac.jp/ akitaoka/index-e.html
- [2] Reference 2

## 16.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

## 16.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

## **16.6 External Cooperations**

#### Academic

- Institution 1 Collaborator(s)
- Institution 2 Collaborator(s)
- Institution 3 Collaborator(s)

#### Industry

- Company 1 Collaborator(s)
- Company 2 Collaborator(s)
- Company 3 Collaborator(s)

### 16.7 Publications

#### Journals

Reference 1

Reference 2

#### Books

Book 1

Book 2

#### in press

Reference 3

Reference 4

#### Talks

Talk 1

Talk 2

#### Posters

Poster 1

Poster 2

## 16.8 Graduations

#### Doctorate

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Diploma

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Master

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## 16.9 Guests

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

# 17

# **Theory of Elementary Particles**

### 17.1 Introduction

Introductory text ...

Group Leader

### 17.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor<sup>\*</sup>, A. Uthor<sup>†</sup>, A.U.T. Hor<sup>\*</sup>

\*Institution 1 <sup>†</sup>Institution 2

Text of the contribution, including an example table (Tab. 17.1) ...

Table 17.1: Test table – example of column alignment types.

left	right	center	page (width 60 mm)
abc	abc	abc	The quick brown fox jumps over
			the lazy dog.
de	de	de	Six big devils from Japan quickly
			forgot how to waltz.
fghi	fghi	fghi	Oh, welch Zynismus, quiekte
5	5	2	Xavers jadegrüne Bratpfanne.

[1] Reference 1

[2] Reference 2

### 17.3 Contribution 2

J. Doe, M. Mustermann

Text of the contribution, in this case accompanied by an example figure (Fig. 17.1) ...



Figure 17.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

- [1] Akiyoshi's illusion pages, www.ritsumei.ac.jp/ akitaoka/index-e.html
- [2] Reference 2

## 17.4 Funding

Project Name 1 Awardees Project Code

Project Name 2 Awardees Project Code

## 17.5 Organizational Duties

Person 1

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

## **17.6** External Cooperations

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- Institution 2 Collaborator(s)
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- Name 2 *Thesis Title* Graduation Date

#### Bachelor

- Name 1 *Thesis Title* Graduation Date
- Name 2 *Thesis Title* Graduation Date

## 17.9 Guests

- Name 1 Institution 1 Time
- Name 2 Institution 2 Time

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## UNIVERSITÄT LEIPZIG