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2012

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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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Preface

Leipzig,
Month 2010

Director 1
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Structure and Staff of the Institutes

1.1 Institute for Experimental Physics I

1.1.1 Office of the Director

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Simon Schneider
Franz Paul Spitzner
Ronja StÃ¼bel
Dimitrij Tschodu
Tobias Weiss
Chris Allen
Jakob Bürgermeister
Adrian Häußler
Michel Michalkow

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PD Dr. S. Fritzsche

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PhD candidates

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Students

1.3.5 Statistical Physics, Statistische Physik [STP]

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Students

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

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

Prof. Dr. Klaus Sibold

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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*, A. Uthor†, A.U.T. Hor*

*Institution 1
†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 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) ...

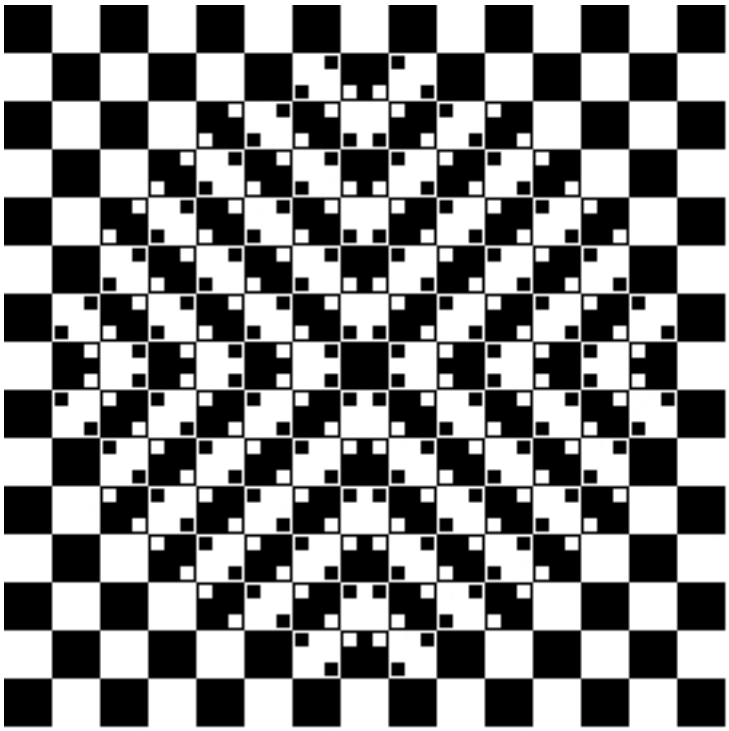

Figure 2.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

[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*, A. Uthor†, A.U.T. Hor*

*Institution 1
†Institution 2

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J. Doe, M. Mustermann

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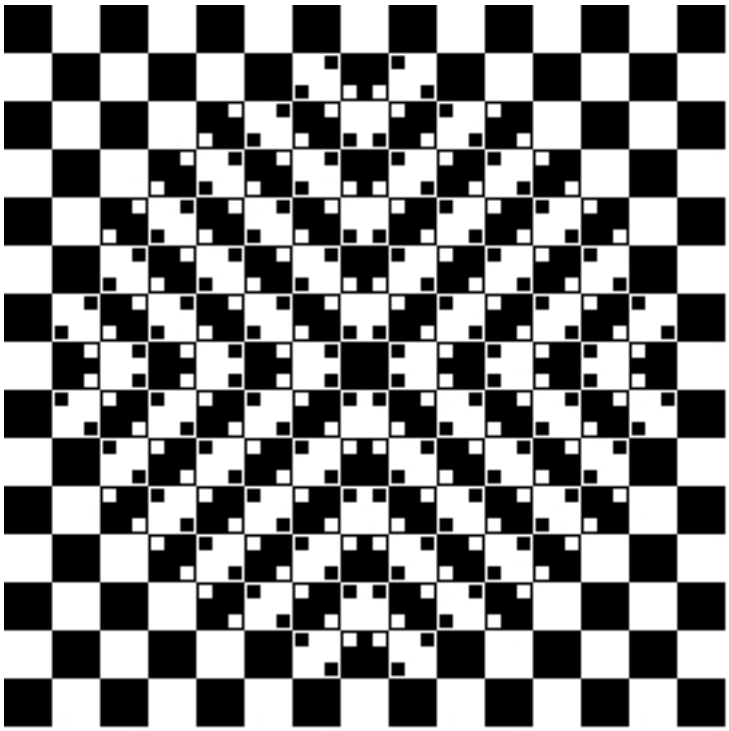

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Person 2

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- Duty 2

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3.9 Guests

- 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*, A. Uthor†, A.U.T. Hor*

*Institution 1
†Institution 2

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

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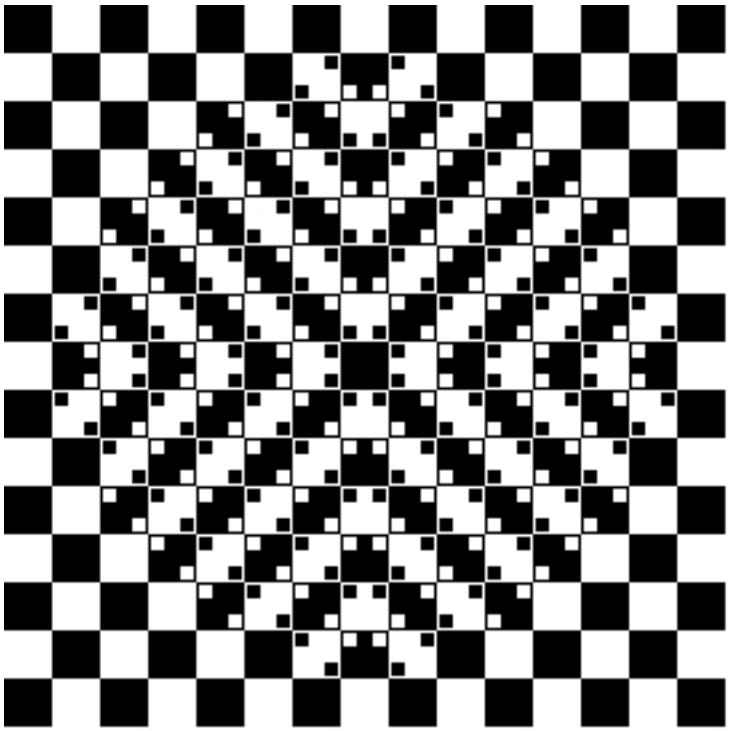

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- Name 2
  Thesis Title
  Graduation Date

Bachelor

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

4.9 Guests

- 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*, A. Uthor†, A.U.T. Hor*

*Institution 1
†Institution 2

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J. Doe, M. Mustermann

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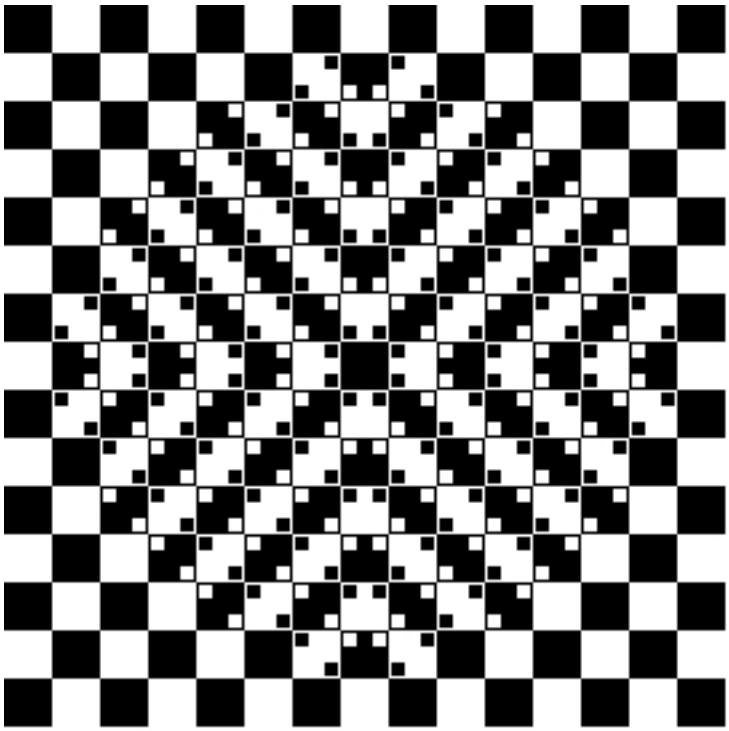

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Awardees
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Awardees
Project Code

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Person 1

- Duty 1
- Duty 2

Person 2

- Duty 1
- Duty 2

5.6 External Cooperations

Academic

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

Industry

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

5.7 Publications

Journals

Reference 1

Reference 2

Books

Book 1

Book 2

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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

5.9 Guests

- 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*, A. Uthor†, A.U.T. Hor*

*Institution 1
†Institution 2

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

Table 6.1: 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 Xavers jadegrüne Bratpfanne.

[1] Reference 1
[2] Reference 2

6.3 Contribution 2

J. Doe, M. Mustermann

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

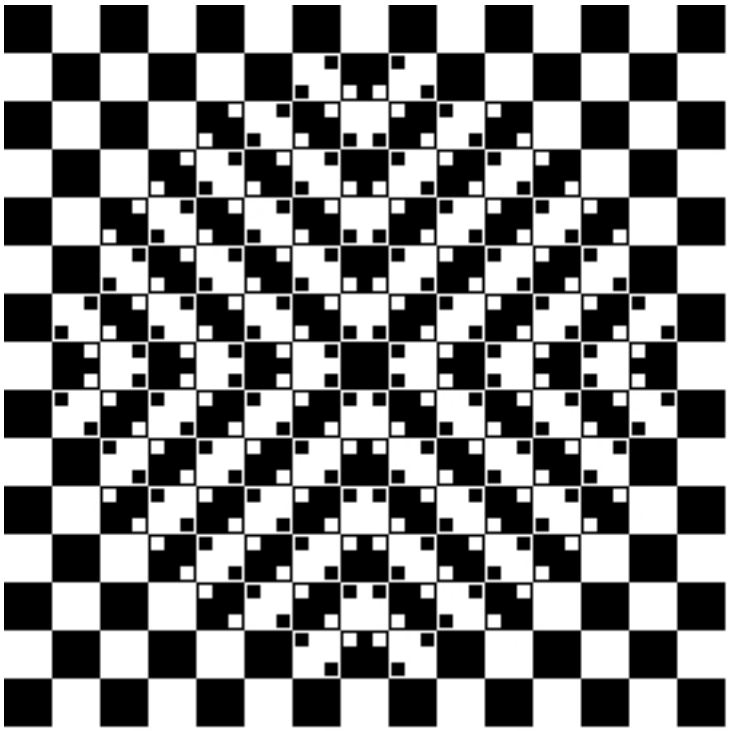

Figure 6.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

[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

Person 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

6.9 Guests

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

II

Institute for Experimental Physics II

7

Magnetic Resonance of Complex Quantum Solids

7.1 Introduction

Introductory text ...

Group Leader

7.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor*, A. Uthor†, A.U.T. Hor*

*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 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) ...

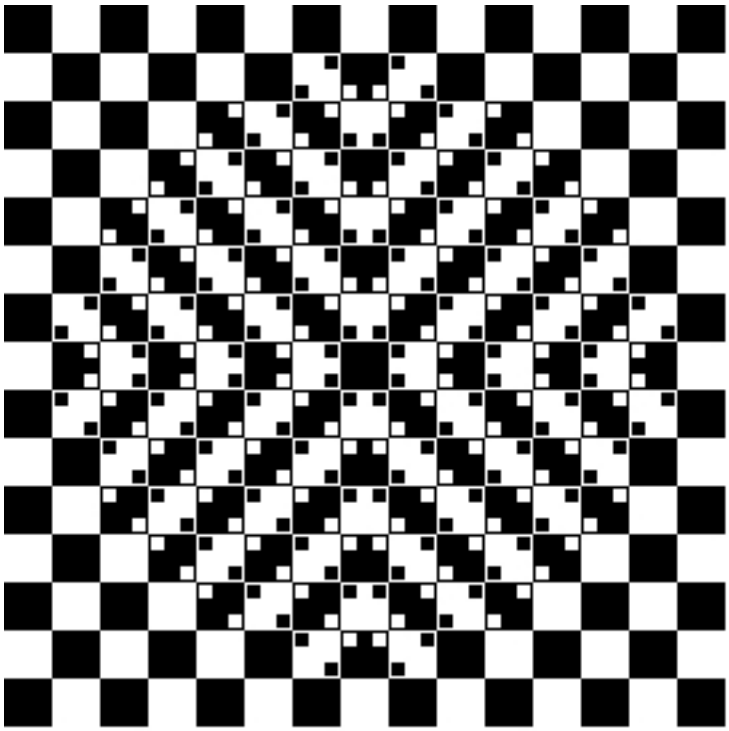

Figure 7.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

[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

Person 1
- 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

7.9 Guests

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

8

Nuclear Solid State Physics

8.1 Introduction

Introductory text ...

Group Leader

8.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor*, A. Uthor†, A.U.T. Hor*

*Institution 1
†Institution 2

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

Table 8.1: 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 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) ...

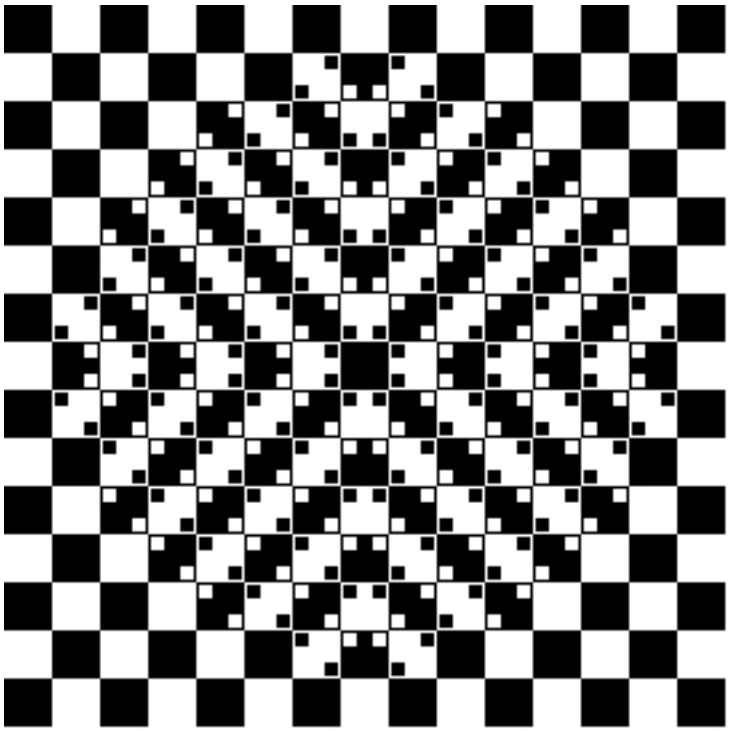

Figure 8.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

[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

Person 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
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  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

8.9 Guests

- 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*, A. Uthor†, A.U.T. Hor*

*Institution 1
†Institution 2

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

Table 9.1: 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 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) ...

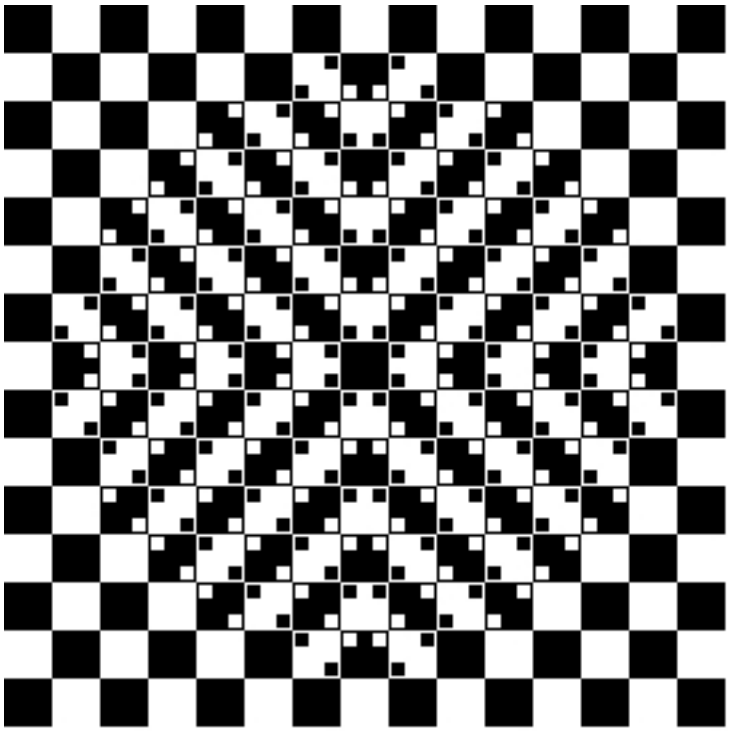

Figure 9.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

[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

Person 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

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Reference 2

Books

Book 1

Book 2

in press

Reference 3

Reference 4

Talks

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Talk 2

Posters

Poster 1

Poster 2

9.8 Graduations

Doctorate

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

Diploma

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- Name 2
  Thesis Title
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Master

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- 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

10

Solid State Optics and Acoustics

10.1 Introduction

Introductory text ...

Group Leader

10.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor*, A. Uthor†, A.U.T. Hor*

*Institution 1
†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)
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

10.3 Contribution 2

J. Doe, M. Mustermann

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

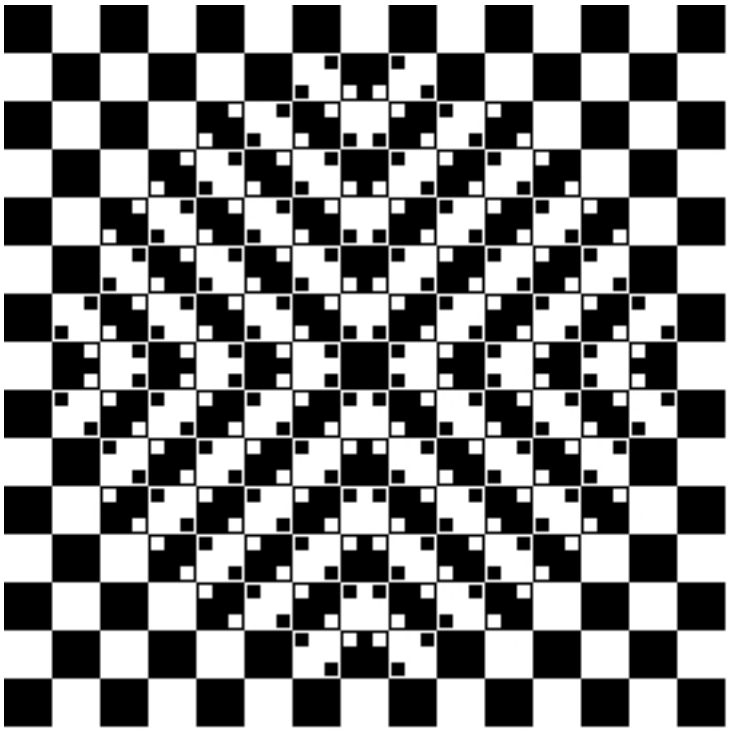

Figure 10.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

[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

Journals

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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
- Name 2
  Thesis Title
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Diploma

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Master

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  Graduation Date

Bachelor

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

10.9 Guests

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

11

Superconductivity and Magnetism

11.1 Introduction

Introductory text ...

Group Leader

11.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor*, A. Uthor†, A.U.T. Hor*

*Institution 1
†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)
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

11.3 Contribution 2

J. Doe, M. Mustermann

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

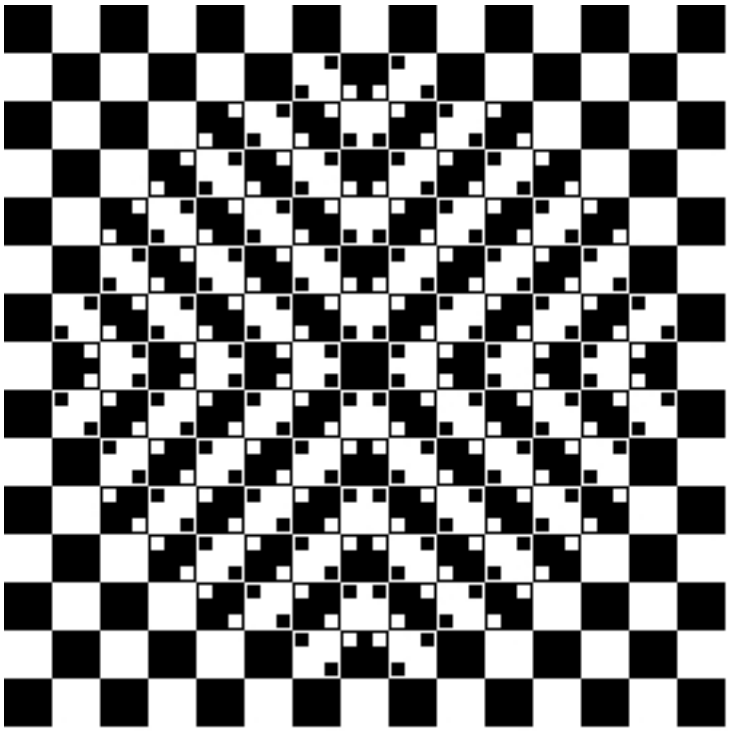

Figure 11.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

[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

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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

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  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

III

Institute for Theoretical Physics

12

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 "BuildMoNa": Leipzig School of Natural Sciences – *Building with Molecules and Nano-*

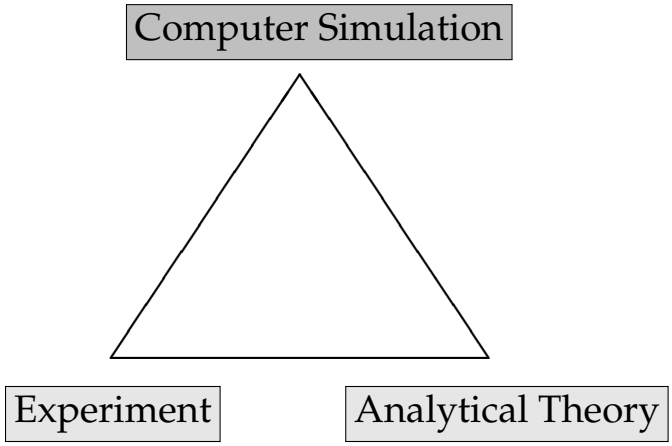


Figure 12.1: Sketch of the "triangular" relationship between experiment, analytical theory and computer simulation.

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 another 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 "$\mathbb{L}^4$" 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.

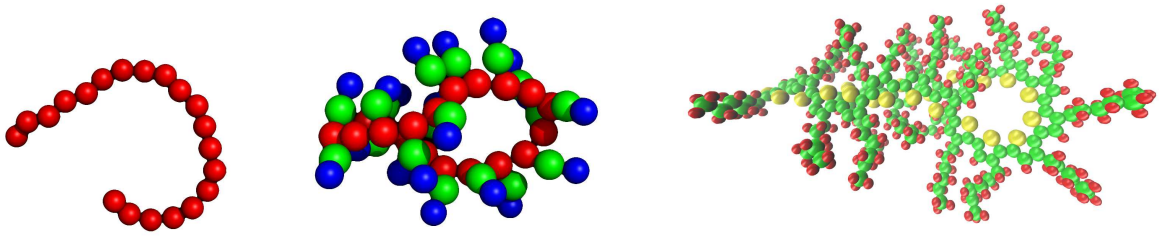
On an international scale, our research projects are carried out in a wide net of collaborations which are currently mainly funded by the Alexander von Humboldt Foundation through an Institute Partnership with the National Academy of Sciences in Lviv, Ukraine, on *Polymers in Porous Environments and on Disordered Substrates* 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, which commenced work in 2014. 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, W. Janke



(a) (b) (c)

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 coarse-grained 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 also to the fully adsorbed (two-dimensional) case [9].

[1] 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.: *Two-dimensional Monte Carlo simulations of coarse-grained poly(3-hexylthiophene) (P3HT) adsorbed on striped substrates*, Leipzig preprint (2018), submitted to J. Chem. Phys. (under revision)

12.3 Polymer knots as a topological order parameter

M. Marenz, W. Janke

For the investigation of the generic behaviour of polymers and proteins with computer simulations, it is common to use minimalistic, coarse-grained models since this is the only possibility to investigate large time scales, length scales or parameter ranges. In this study we used a bead-stick model for a semiflexible polymer defined by the Hamiltonian

$$H = E_{\mathrm{LJ}} + \kappa E_{\mathrm{Bend}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} \left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}} \right) + \kappa \sum_{i} (1 - \cos\theta_i) \ , \tag{12.1}$$

where r_{ij} is the distance between non-adjacent monomers, and θ_i is the angle of two adjacent bonds. The parameter κ allows to vary the bending stiffness of the polymer from flexible over semiflexible to stiff [1, 2].

To simulate the system in the complete (T, κ)-plane we used two advanced Monte Carlo algorithms. A parallel multicanonical algorithm [3] combined with a one-dimensional replica exchange in the κ direction and a two-dimensional replica-exchange method, which simulates the system in parallel in the T and κ direction. Employing

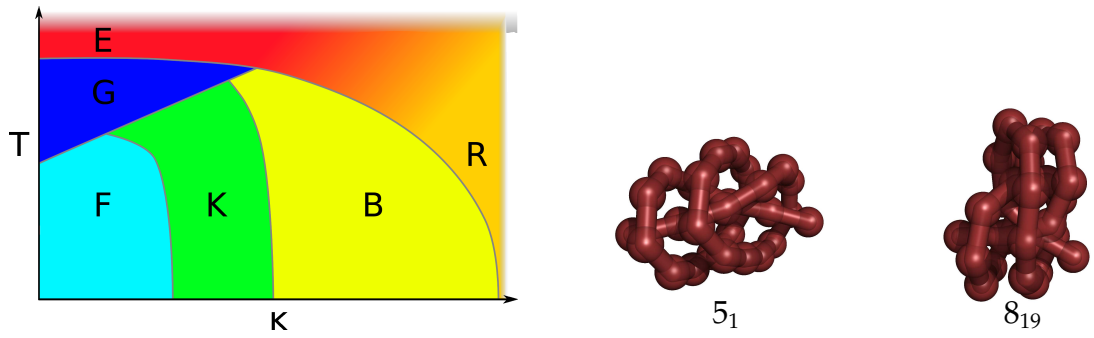


Figure 12.3: Sketch of the phase diagram for a semiflexible bead-stick model exhibiting several phases: E – elongated, R – rod-like, G – globular, F – frozen, K – knotted, B – bent. Next to the phase diagram two typical knots of types 5_1 and 8_{19} for a 28mer are shown.

both algorithms, we calculated surface plots of various observables (energy, end-to-end distance, radius of gyration, eigenvalues of gyration tensor) to construct the full pseudo-phase diagram for several polymer lengths ($N = 14, 28, 42$) [4, 5].

Despite the simplicity of the model, the phase diagram sketched in Fig. 12.3 is remarkably rich. Compared to former work simulating similar coarse-grained models [6], we observed a novel type of phases labeled by "K", which are characterized by thermodynamically stable knots [7], which may be considered as topological order parameters. The transitions into these knot phases exhibit some intriguing characteristics. Although we observed clear signals of a first-order transition between the knotted and unknotted phases, the transition apparently shows no latent heat [4, 5]. Instead the two sub-energies, the Lennard-Jones energy and the bending energy, are transformed into each other while the polymer knots itself, see Fig. 12.4.

[1] J. Zierenberg et al.: Polymers **8**, 333 (2016)
[2] W. Janke et al.: Lobachevskii J. Math. **38**, 978 (2017)
[3] J. Zierenberg et al.: Comput. Phys. Commun. **184**, 1155 (2013)
[4] M. Marenz, W. Janke: Phys. Rev. Lett. **116**, 128301 (2016)
[5] M. Marenz, W. Janke: In *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. **750**, 012006 (2016)
[6] D.T. Seaton et al.: Phys. Rev. Lett. **110**, 028103 (2013)
[7] L.H. Kauffman: *Knots and Physics*, 2nd ed. (World Scientific, Singapore, 1991)

12.4 Polymer adsorption to a nano-sphere

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The interaction of macromolecules with differently shaped substrates is particularly important for interdisciplinary research and nano-technological applications including, e.g., the fabrication of biosensors and peptide adhesion to metals or semiconductors.

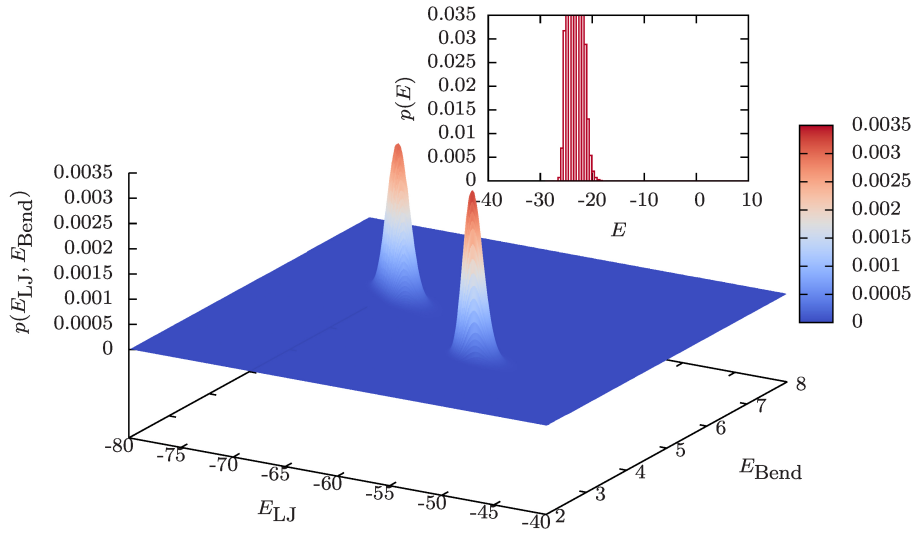

Figure 12.4: Two-dimensional energy histogram $p(E_{\mathrm{LJ}}, E_{\mathrm{Bend}})$ of a 28mer at the transition into the knot phase signaling clear phase coexistence. The inset shows the one-dimensional energy histogram $p(E)$ of the total energy $E = E_{\mathrm{LJ}} + \kappa E_{\mathrm{Bend}}$, which corresponds to a projection along the diagonal of the two-dimensional histogram. In this projection, the two peaks fall on top of each other, so only a single peak is visible in $p(E)$.

The knowledge of structure formation for a variety of interfaces has therefore been a challenging subject of numerous experimental and computational studies.

Recently we have investigated the purely steric confinement effect of a spherical cage enclosing a simple flexible polymer chain to determine its influence on the location of the collapse and freezing transitions [1]. Another hybrid system under consideration was a polymer chain inside an attractive spherical cage for which we have constructed the finite-temperature phase diagram depending on the attraction strength of the sphere inner wall and the temperature [2, 3] and investigated the ground-state properties [4]. We have also compared the results with the attractive flat surface [5, 6]. These systems exhibit a rich phase behaviour ranging from highly ordered, compact to extended, random coil structures.

Here, we consider the opposite situation: A nano-sphere whose attractive outer spherical surface is the target for the adsorbing polymer. This problem could have practical implications for a broad variety of applications ranging from protein-ligand binding, designing smart sensors to molecular pattern recognition and for the discovery of new drugs that bind to specific receptors. Therefore it is interesting to study the adsorption of macromolecules on different types of substrates and identify the conformational changes that a polymer can experience at the interface.

In this project we investigate a simple coarse-grained polymer model interacting with a spherical surface of varying radius (and consequently curvature) by means of extensive generalized-ensemble Monte Carlo computer simulations [7]. The employed multicanonical method enables us to describe the different phases of the finite chain over a wide range of sphere radius and temperature. In a comparative study, we determined how the structural phase diagram changes with the sphere radius and

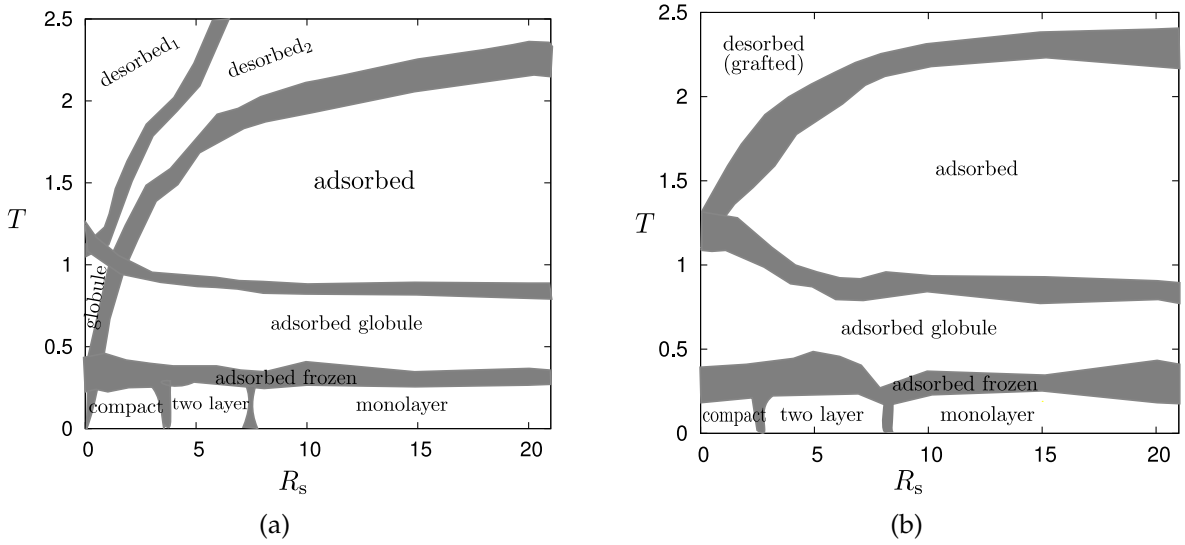

Figure 12.5: The phase diagram of a homopolymer interacting with an attractive spherical surface of radius R_s for (a) a non-grafted and (b) an end-grafted 20mer.

temperature, both for non-grafted and end-grafted polymer chains. The band widths of the boundaries separating the individual conformational phases in Fig. 12.5 indicate the variation of the peak locations of temperature derivatives of different structural observables which we have analyzed simultaneously [7]. Typical conformation for the case of a non-grafted polymer are shown in Fig. 12.6.

[1] M. Marenz et al.: Condens. Matter Phys. **15**, 43008 (2012)
[2] H. Arkın, W. Janke: Phys. Rev. E **85**, 051802 (2012)
[3] H. Arkın, W. Janke: J. Chem. Phys. **138**, 054904 (2013)
[4] H. Arkın, W. Janke: J. Phys. Chem. B **116**, 10379 (2012)
[5] M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009); Phys. Chem. Chem. Phys. **12**, 11548 (2010); Macromolecules **44**, 9013 (2011)
[6] H. Arkın, W. Janke: Eur. Phys. J. – Special Topics **216**, 181 (2013)
[7] H. Arkın, W. Janke: Phys. Rev. E **96**, 062504 (2017)

12.5 Adsorption of semiflexible polymers

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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

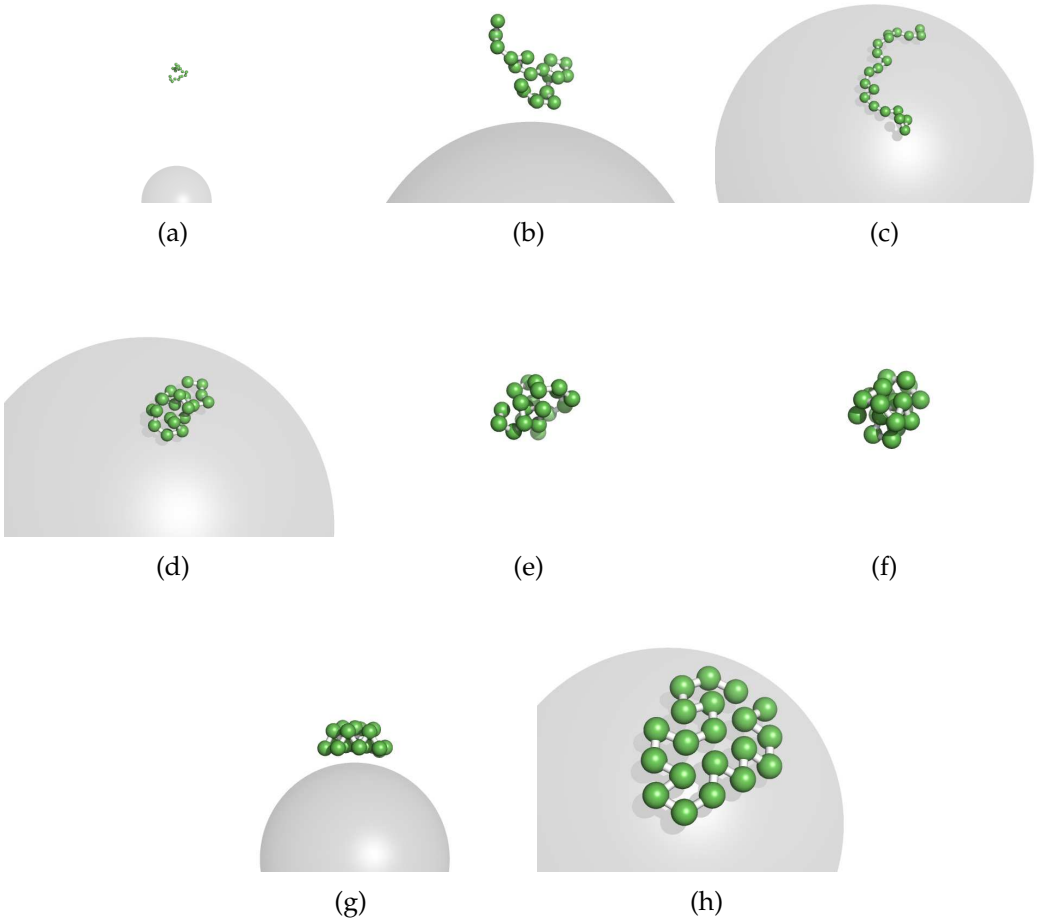

Figure 12.6: Typical conformations for the regions (a) desorbed$_1$, (b) desorbed$_2$, (c) adsorbed, (d) adsorbed globule, (e) globule, (f) compact, (g) two layer, and (h) monolayer in the phase diagram of a non-grafted polymer.

solvent conditions with purely *repulsive* monomer-monomer interactions [1, 2]. Finite-size 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, 4]. Similar observations were made for the adsorption of specific lattice proteins [5]. If the surface shows complex attractive motifs, one observes in addition pattern recognition effects [5, 6].

Semiflexible, *self-attractive* polymers undergoing a collapse transition exhibit a rich variety of structural phases already in the case of an isolated chain [7, 8]. These include collapsed, toroidal, hairpin, and knotted conformations, partially depending on the

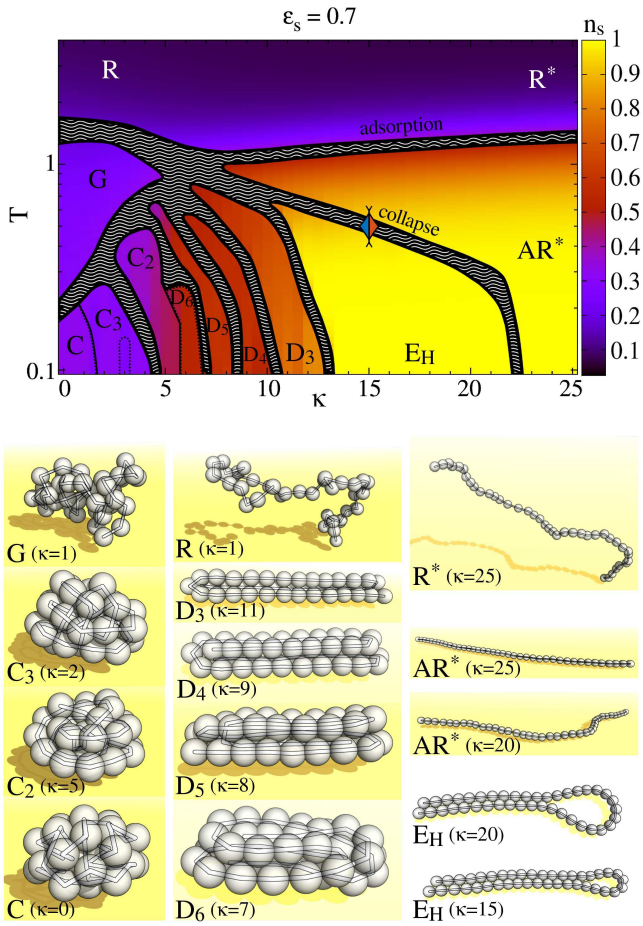

Figure 12.7: Structural phase diagram for a semiflexible polymer of length $N = 40$ grafted to a weakly attractive surface ($\epsilon_s = 0.7$). The background color encodes the average fraction of surface contacts $n_s = N_s/N$. Dotted lines indicate that signals are found only in a small subset of 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.

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. [9] we intended to fill this gap.

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 en-

ergy terms: bond-vibrational energy, non-neighboring 12-6 Lennard-Jones interactions, bending energy parametrized by the bending stifness κ, and 9-3 Lennard-Jones surface interaction parametrized by the interaction strength ε_s. As a typical example of our results, Fig. 12.7 shows the κ-T phase diagram for a weakly attractive surface with $\varepsilon_s = 0.7$.

[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)
[4] M. Möddel et al.: Phys. Chem. Chem. Phys. **12**, 11548 (2010)
[5] A.D. Swetnam, M.P. Allen: Phys. Chem. Chem. Phys. **11**, 2046 (2009); Phys. Rev. E **85**, 062901 (2012)
[6] M. Möddel et al.: Phys. Rev. Lett. **112**, 148303 (2014)
[7] D.T. Seaton et al.: Phys. Rev. Lett. **110**, 028103 (2013)
[8] M. Marenz, W. Janke: Phys. Rev. Lett. **116**, 128301 (2016)
[9] K.S. Austin et al.: Macromolecules **50**, 4054 (2017)

12.6 Binding transition of two grafted polymers

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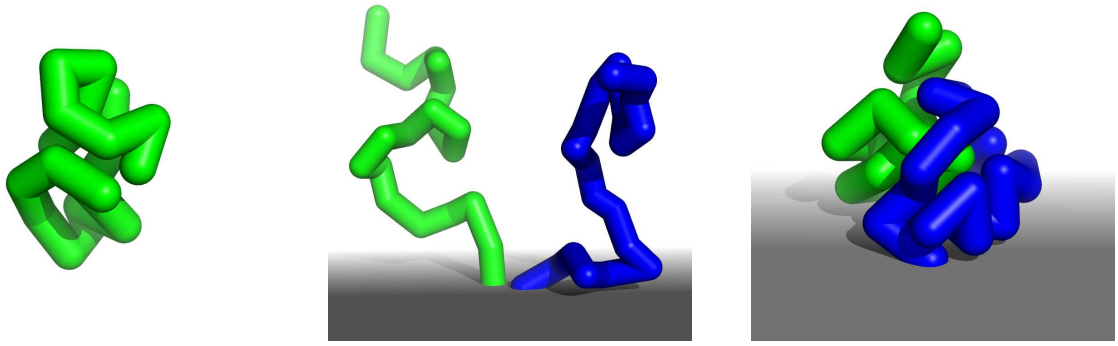
In this project we studied the binding of two flexible polymers grafted closeby to a steric surface. More specifically, we fixed one of their end points to a steric surface covering the $x - y$ plane at $z = 0$. No monomer was allowed to cross this geometric constraint, i.e., monomer coordinates with $z_i < 0$ were forbidden. No further interactions with the (inert) surface are assumed. The end points are grafted with distance $d = r_0$ (the equilibrium bond length of a FENE spring connecting the monomers) and are immobilized. If the polymers are not grafted, we enclose them in a cubic box of side length L with steric walls. For an illustration see Fig. 12.8.

As "binding" we refer to the process where two polymers attach to each other, in our case flexible polymers. If specific inter-polymer interactions are considered this may quickly lead to effects also characterized as zipping. Even more interesting is the equivalence between two-polymer binding of directed polymers and adsorption [1]. This should qualitatively remain valid also for flexible polymers, especially if one imagines the crossover scenario of a flexible polymer adsorbed to a nanowire, equivalent to the stiff limit of a polymer chain [2, 3], or a flexible polymer adsorbing to a flexible surface [4]. In fact, it was shown that grafting alters the first-order-like adsorption transition to a second-order-like transition [5].

From our Monte Carlo simulation data we conclude [6] that when grafting two polymers to a steric surface at a close distance an analogous scenario holds true, i.e., we observe a second-order-like binding transition, which is in contrast to the first-order-like finite-size binding transition for free polymers in a steric box. This is relevant for an experimental study of polymer binding, where in vitro polymers would be



(a) (b) (c)

Figure 12.8: Snapshots of (a) a single polymer of length $N = 20$ in the globular phase below the collapse transition ($T = 0.7$) and two polymers of length $N = 20$ grafted to a steric surface (b) above (T = 4) and (c) below ($T = 0.7$) the binding transition.

commonly grafted. In this case, one will neither observe a latent heat nor hysteresis effects associated with first-order-like transitions, which would be expected to occur in vivo. Still, grafted polymers may be studied with respect to aggregate properties and their dynamics which are expected to sufficiently coincide for observables which are not directly influenced by the geometric constraint. One exception is the average end-to-end distance and subsequently (no longer isotropic) geometric properties. Interesting effects may be anticipated for interacting surfaces, where the binding of polymers would compete with the surface attraction. Connecting to experimental setups, the surfaces may be considered both flat or curved, e.g., when grafting polymers to nanoparticles.

[1] J. Kierfeld, R. Lipowsky: Europhys. Lett. **62**, 285 (2003)
[2] T. Vogel et al.: J. Chem. Phys. **142**, 104901 (2015)
[3] J. Gross et al.: Phys. Chem. Chem. Phys. **17**, 30702 (2015)
[4] S. Karalus et al.: Phys. Rev. E **84**, 031803 (2011)
[5] M. Möddel et al.: Macromolecules **44**, 9013 (2011)
[6] J. Zierenberg et al.: Eur. Phys. J. – Special Topics **226**, 683 (2017)

12.7 Polymer versus particle condensation

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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

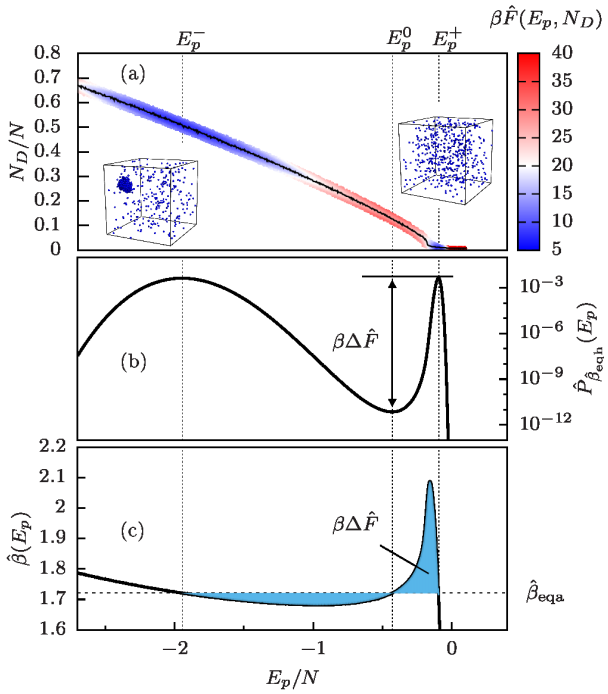


Figure 12.9: (a) Illustration of the free-energy landscape $\beta\hat{F}(E_p, N_D)$ (color map) as a function of potential energy E_p and droplet size N_D for $N = 512$ Lennard-Jones particles. The minimal free-energy path (black solid line) connects a droplet ($E_p \approx E_p^-$) and a gaseous ($E_p \approx E_p^+$) 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 $\hat{\beta}_{\rm eqh}$. (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 $\hat{\beta}_{\rm eqa}$, where $\hat{\beta}_{\rm eqa} = \hat{\beta}_{\rm eqh} = 1.72099(3)$.

finite-size scaling analysis of the effective interfacial free energy at fixed density as illustrated in Fig. 12.9. 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 [4–6]. Going one step further, we then generalized this approach to the aggregation process in a dilute polymer solution [6], cf. Fig. 12.10. 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 kinetic energy from the partition function leads to finite-size differences in the free energy compared to the full ensemble [7, 8] but retains intensive parameters in the thermodynamic limit [6]. Our study of nucleation rates at fixed density corresponds to a heating-cooling framework where simulation and experiment may meet at the nanometer scale.

[1] B.A. Berg, T. Neuhaus: Phys. Lett. B **267**, 249 (1991); Phys. Rev. Lett. **68**, 9 (1992)
[2] W. Janke: Int. J. Mod. Phys. C **03**, 1137 (1992); Physica A **254**, 164 (1998)
[3] J. Zierenberg et al.: Comput. Phys. Commun. **184**, 1155 (2013)

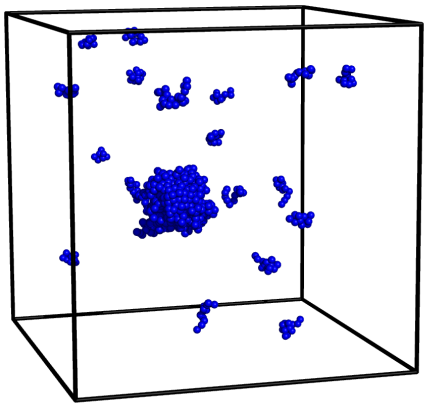


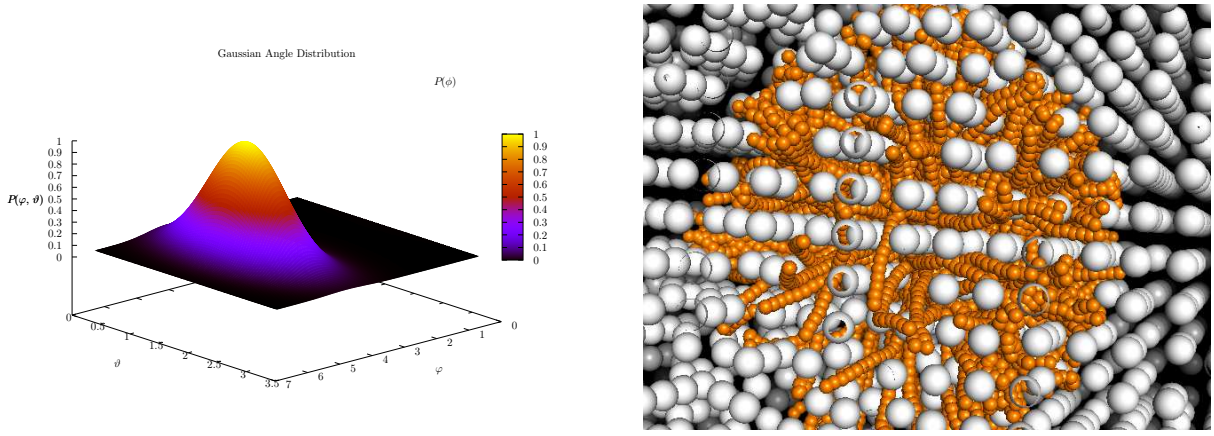
Figure 12.10: Illustration of an aggregate of polymers in a dilute solution ($N = 64$ bead-spring polymers with 13 monomers each; monomer density $\rho = 10^{-2}$). The snapshot stems from the droplet phase ($E_p \approx E_p^-$).

[4] J. Zierenberg, W. Janke: Phys. Rev. E **92**, 012134 (2015)
[5] J. Zierenberg, W. Janke: in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. **750**, 012017 (2016)
[6] J. Zierenberg et al.: Nat. Commun. **8**, 14546 (2017)
[7] P. Schierz et al.: Phys. Rev. E **94**, 021301(R) (2016)
[8] W. Janke et al.: in *Computer Simulation Studies in Condensed-Matter Physics XXX*, eds. D.P. Landau, M. Bachmann, S.P. Lewis, and H.-B. Schüttler, J. Phys.: Conf. Ser. **921**, 012018 (2017)

12.8 Computer simulations of semiflexible polymers in disordered environments

J. Bock, W. Janke

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 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



(a) Weighting histogram (b) Semiflexible polymer in 3D disorder

Figure 12.11: (a) Histogram used for the guiding field in 3D and (b) an examplary configuration of a polymer with $N = 30$ and $\xi = 1$.

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. 12.11. 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. 12.12. 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]:

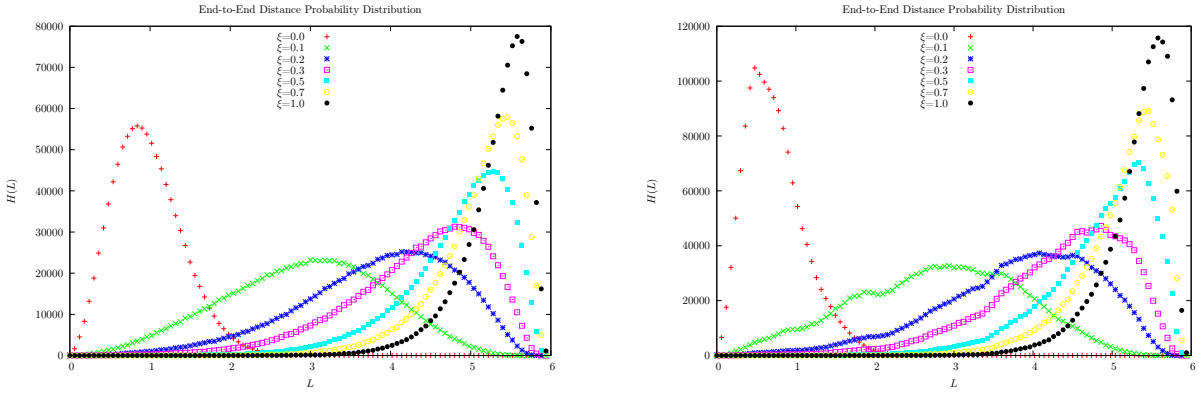
$$\frac{1}{l_p^*} = \frac{1}{l_p} + \frac{1}{l_p^D},$$

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)

12.9 Periodically driven DNA: A comparative study of Langevin and Brownian dynamics

R. Kumar, S. Kumar*, W. Janke



(a) Free polymers (b) Polymers in disorder

Figure 12.12: End-to-end distance distributions for (a) free polymers and (b) polymers in gaseous disorder, both in 3D.

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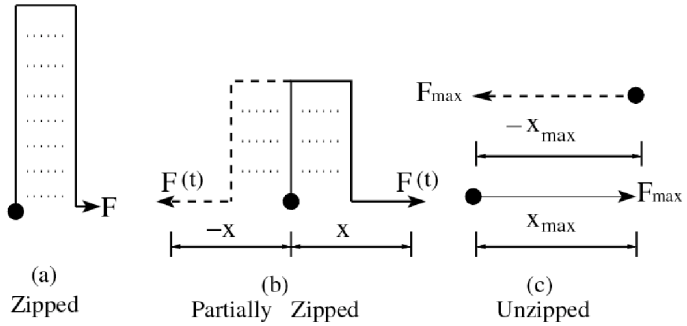
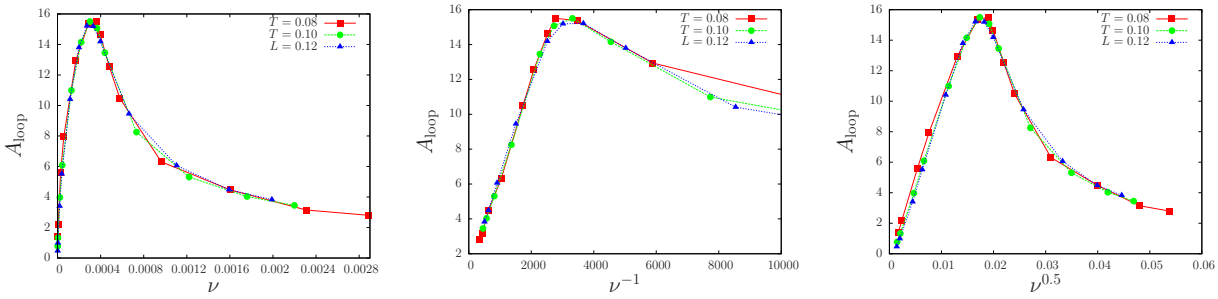


Figure 12.13: Schematic representations of DNA: (a) zipped, (b) partially zipped, and (c) unzipped state. One end is kept fixed (indicated by solid circles), while the other end may move.

DNA replication is one of the most important biological processes in living organisms. Under the influence of special enzymes, two strands of the DNA double helix can separate themselves like a zip. The first step in the process of DNA replication is to unzip the double-helix structure of the DNA molecule. Therefore, it is very important to study the unzipping of DNA. There has been some experimental studies at a constant force or loading rate used in SMFS experiments to unzip the DNA *in vitro*. In these experiments one end of the DNA was fixed and a constant force was applied on its other end. However, such processes are driven by different types of molecular motors *in vivo* [1].

A constant force or loading rate used in SMFS experiments provides a limited picture of these processes *in vitro*. Hence, the picture provided by constant force unzipping is not complete. This has been highlighted in recent studies, where it was suggested that by varying the frequency and amplitude of the applied force new aspects of a force-driven transition can be introduced [2–5], which otherwise would not be possible in the case of a steady force. The considered situation is sketched in Fig. 12.13.

This model was further simplified in [6, 7] by reducing the degrees of freedom



(a) (b) (c)

Figure 12.14: Effect of temperature on the area of the hysteresis loop for the model with parameters $L = 32$, $F = 1.0$, and $\gamma = 0.4$ for (a) A_{loop} vs. ν, (b) area vs. ν^{-1} in the higher frequency regime, and (c) area vs. $\nu^{0.5}$ in the lower frequency regime. Here the x-axis is rescaled in order to show the data collapse for all temperatures.

and studying the overdamped limit using Brownian dynamics. This simplified model was investigated only at zero temperature. Therefore, it became crucial to further investigate how the temperature effects the dynamics of such system using the detailed model described in [3]. Emphasis was placed on the effect of different temperatures on the scaling properties. Moreover, we compared results of the Langevin dynamics for the detailed model and Brownian dynamics for the simplified model. We observed that the temperature and over-damped limit does not effect the scaling exponentsi, cf. Fig. 12.14. Hence, the model proposed by us is good enough to study the scaling properties and provides a possibility of analytic studies within certain limits. Moreover, currently we are trying to understand the effect of the over-damped limit in the detailed model proposed in [3].

[1] B. Alberts et al.: *Molecular Biology of the Cell* (Garland Publishing, New York, 1994)
[2] S. Kumar, M. S. Li: Phys. Rep. **486**, 1 (2010)
[3] S. Kumar, G. Mishra: Phys. Rev. Lett. **110**, 258102 (2013)
[4] G. Mishra et al.: Phys. Rev. E **87**, 022718 (2013)
[5] R.K. Mishra et al.: J. Chem. Phys. **138**, 244905 (2013)
[6] S. Kumar et al.: Phys. Rev. E **93**, 010402(R) (2016)
[7] R. Kumar et al.: *Comparative study of Brownian and Langevin dynamics for periodically driven DNA*, Leipzig/Varanasi preprint (2017), to be published

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

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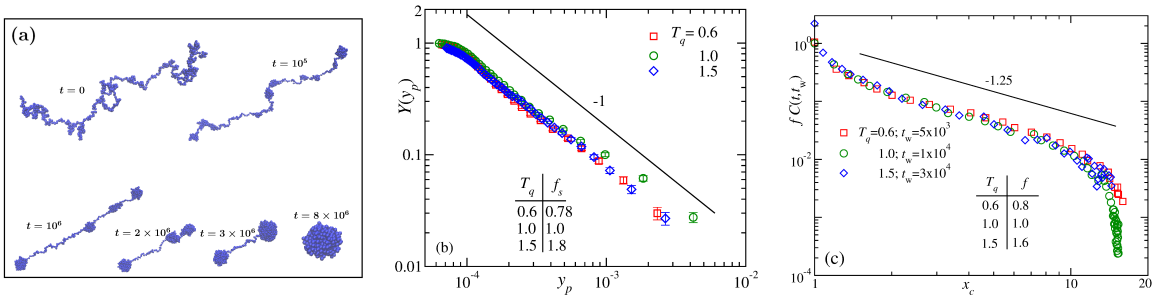

Figure 12.15: (a) Snapshots [1] showing the sequence of events occurring during the collapse of a polymer upon being quenched from an expanded state (at high temperature) into the globular phase (at low temperatures). (b) Universal finite-size scaling function $Y(y_p)$ with a non-universal metric factor (f_p) 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].

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 mechanism of more realistic problems [1, 2]. On the other hand, if one considers the usual "pear-necklace" like picture of the collpase [1] as shown in Fig. 12.15(a), it also resembles coarsening phenomena popular in spin and particle systems [6]. Over the last two years we have been exploiting this connection to understand the kinetics of collapse of a homopolymer [7, 8].

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 [9] 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. 12.15(b). This observation has recently been confirmed in a related lattice model for the polymer [3]. For a direct comparison of the lattice and off-lattice formulations, see Ref. [4]. 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. 12.15(c).

[1] S. Majumder, W. Janke: J. Phys.: Conf. Ser. **750**, 012020 (2016)
[2] S. Majumder et al.: Soft Matter **13**, 1276 (2017)
[3] H. Christiansen et al.: J. Chem. Phys. **147**, 094902 (2017)
[4] S. Majumder et al.: J. Phys.: Conf. Ser. **955**, 012008 (2018)
[5] A. Halperin, P. Goldbart: Phys. Rev. E **61**, 565 (2000)
[6] A.J. Bray: Adv. Phys. **51**, 481 (2002)
[7] S. Majumder, W. Janke: Europhys. Lett. **110**, 58001 (2015)
[8] S. Majumder, W. Janke: Phys. Rev. E **93**, 032506 (2016)

[9] S. Majumder, S.K. Das: Phys. Rev. E **81**, 050102(R) (2010); Phys. Rev. E **84**, 021110 (2011)

12.11 Coarsening and aging of lattice polymers: Influence of bond fluctuations

H. Christiansen, S. Majumder, W. Janke

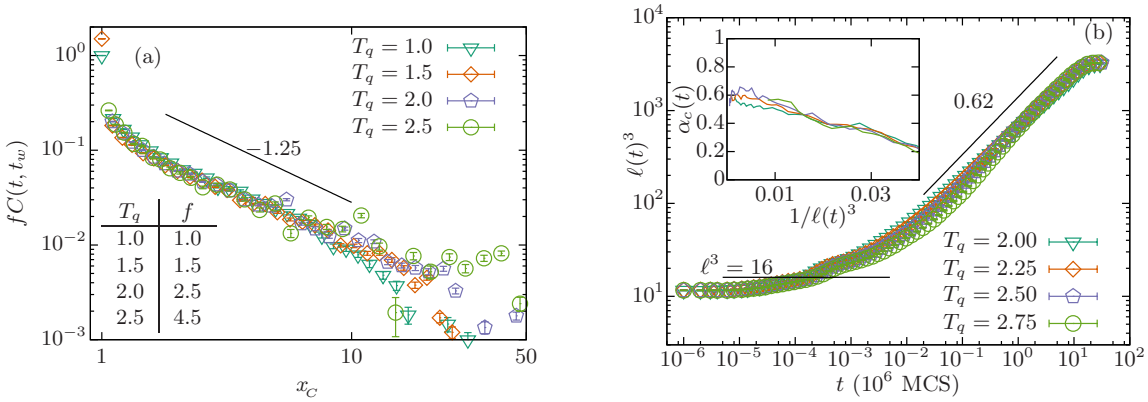

Figure 12.16: (a) The two-time correlation function $C(t, t_w)$ against the ratio of length-scales $x_C = \ell(t)/\ell(t_w)$ for the model with fixed bonds and different quench-temperatures T_q. In (b) the growth of the length-scales for the model with flexible bonds is shown for different T_q. Here 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 ($T_q < T_\theta$), 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 [4] (see Fig. 12.16(a) for the model with fixed bonds at different quench temperatures T_q). 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. 12.16(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 [3]. The discrepency in the exponent α is attributed to the constraints introduced by the lattice structure.

[1] H. Christiansen et al.: J. Chem. Phys. **147**, 094902 (2017)
[2] A. Halperin, P. M. Goldbart: Phys. Rev. E **61**, 565 (2000)
[3] S. Majumder, W. Janke: Phys. Rev. E **93**, 032506 (2016)
[4] S. Majumder, W. Janke: Europhys. Lett. **110**, 58001 (2015)

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

S. Majumder, H. Christiansen, W. Janke

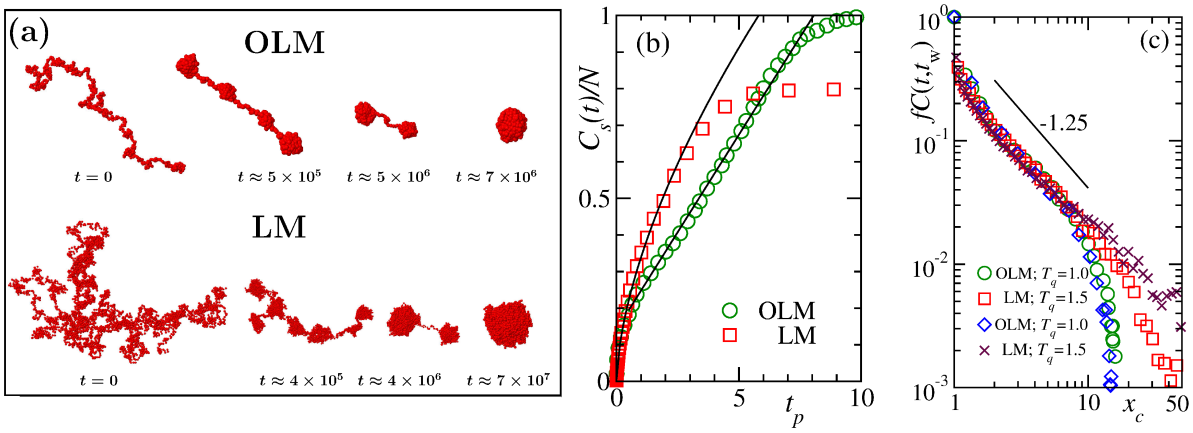

Figure 12.17: (a) Time evolution snapshots of the collapse of a homopolymer, after being quenched from an extended coil phase to a temperature, $T_q = 1$ for OLM, and $T_q = 2.5$ for LM, in the globular phase.(b) Plots of the average cluster size $C_s(t)/N$ as function of time for the two models. To 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 3.5×10^6, 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

$$E_{\mathrm{FENE}}(r_{ii+1}) = -\frac{KR^2}{2} \ln\left[1 - \left(\frac{r_{ii+1} - r_0}{R}\right)^2\right], \tag{12.2}$$

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

$$E_{\mathrm{LJ}}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{12.3}$$

is the standard Lennard-Jones (LJ) potential with $\sigma = r_0/2^{1/6}$ as the diameter of the monomers, ϵ (= 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 simple-cubic lattice, where each lattice site can be occupied by a single monomer. The energy is given by

$$E_{\mathrm{LM}} = -\frac{1}{2}\sum_{i\neq j,j\pm 1} w(r_{ij}), \quad \text{where} \quad w(r_{ij}) = \begin{cases} J & r_{ij} = 1 \\ 0 & \text{else} \end{cases}. \tag{12.4}$$

In Eq. (12.4), 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. 12.17(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. 12.17(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. 12.17(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.

[1] A. Halperin, P. M. Goldbart: Phys. Rev. E **61**, 565 (2000)
[2] S. Majumder et al.: J. Phys.: Conf. Ser. **955**, 012008 (2018)
[3] S. Majumder, W. Janke: Europhys. Lett. **110**, 58001 (2015)
[4] S. Majumder, W. Janke: Phys. Rev. E **93**, 032506 (2016)
[5] H. Christiansen et al.: J. Chem. Phys. **147**, 094902 (2017)

12.13 Universal finite-size scaling for kinetics of phase separation in mixtures with varying number of components

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In this work [1] we have presented results for the kinetics of phase separation in multicomponent solid mixtures, from Monte Carlo simulations of the q-state conserved Potts model, in space dimension $d = 2$, for $2 \leq q \leq 10$. Evolution snapshots for $q = 4$ are shown in Fig. 12.18 (left). In agreement with previous reports [2], we also find that, even though for a fixed q various morphology-characterizing functions obey the expected scaling relations, there exists no common scaling function for different q. The primary interest in our work was to quantify the domain-growth kinetics, cf. Fig. 12.18 (middle).

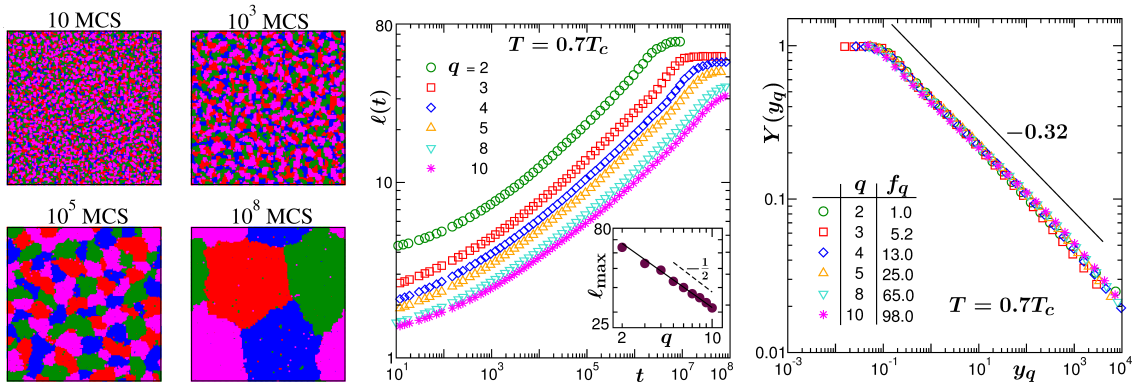

Figure 12.18: (left) Evolution snapshots from different times for 4-state Potts model, obtained from the MC simulations following a quench from the high-temperature homogeneous phase to $T = 0.7\,T_c$, that lies inside the miscibility gap. The used system size is $L = 128$. Different colors correspond to different states. (middle) Double-log plots of the average domain length, $\ell(t)$, versus time. Data for few different q-component mixtures are presented, all from $T = 0.7\,T_c$, using $L = 128$. Inset: Plot showing the dependence of the saturated domain length, $\ell_{\rm max}$, on q. The solid line is a fit to the form $\ell_{\rm max} = Kq^{\eta}$, that yields $\eta = -0.45$. The dashed line shows the expected power-law decay with an exponent $-1/2$, corresponding to the behavior $\ell_{\rm max} \sim q^{-1/d}$. (right) Demonstration of the fact that the finite-size scaling curves in domain growth for different q can be collapsed onto a single master curve, such that there exists a universal finite-size scaling function $Y(y_q)$, when plotted against the modified scaling variable y_q. The values of the metric factor f_q, used to obtain the optimum collapse of data, are tabulated inside the figure. The results correspond to $L = 128$ and $T = 0.7\,T_c$. The solid line represents the behavior $Y(y_q) \sim y_q^{-\alpha}$, with $\alpha = 0.32$.

This we achieve via the application of appropriate finite-size scaling analysis [3, 4]. Like in critical phenomena [5], this technique allows one to obtain a precise estimation of the growth exponent α, 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. This was previously confirmed [2] to be true in the asymptotic limit, via the application of a renormalization group method of analysis to the Monte Carlo results.

Furthermore, we show that the growth for different q could be described by a universal finite-size scaling function, with a nonuniversal, q-dependent, metric factor [6], arising from the amplitude of growth (that varies with q), see Fig. 12.18 (right). In a similar way, 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. We have also shown the equivalence between the evolution of a equi-proportion q-component mixture and an off-critical binary mixture with composition of the minority species $m_c = 1/q$.

[1] S. Majumder et al.: Leipzig/Bangalore preprint (2018), submitted to Phys. Rev. E
[2] S.K. Das, S. Puri: Phys. Rev. E **65**, 026141 (2002)
[3] S. Majumder, S.K. Das: Phys. Rev. E **81**, 050102(R) (2010)
[4] S.K. Das et al.: Europhys. Lett. **97**, 66006 (2012).
[5] M.E. Fisher: *The theory of critical point singularities*, in *Critical Phenomena*, Proc.

51st Enrico Fermi Summer School, Varenna, Italy, edited by M.S. Green (Academic Press, London, 1971), p. 1
[6] S. Majumder et al.: Soft Matter **13**, 1276 (2017)

12.14 Adsorption and diffusion of H_2/CH_4 gas mixture in ZIF-90

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‡Peter-Debye-Institut für Physik der weichen Materie, Universität Leipzig, Germany
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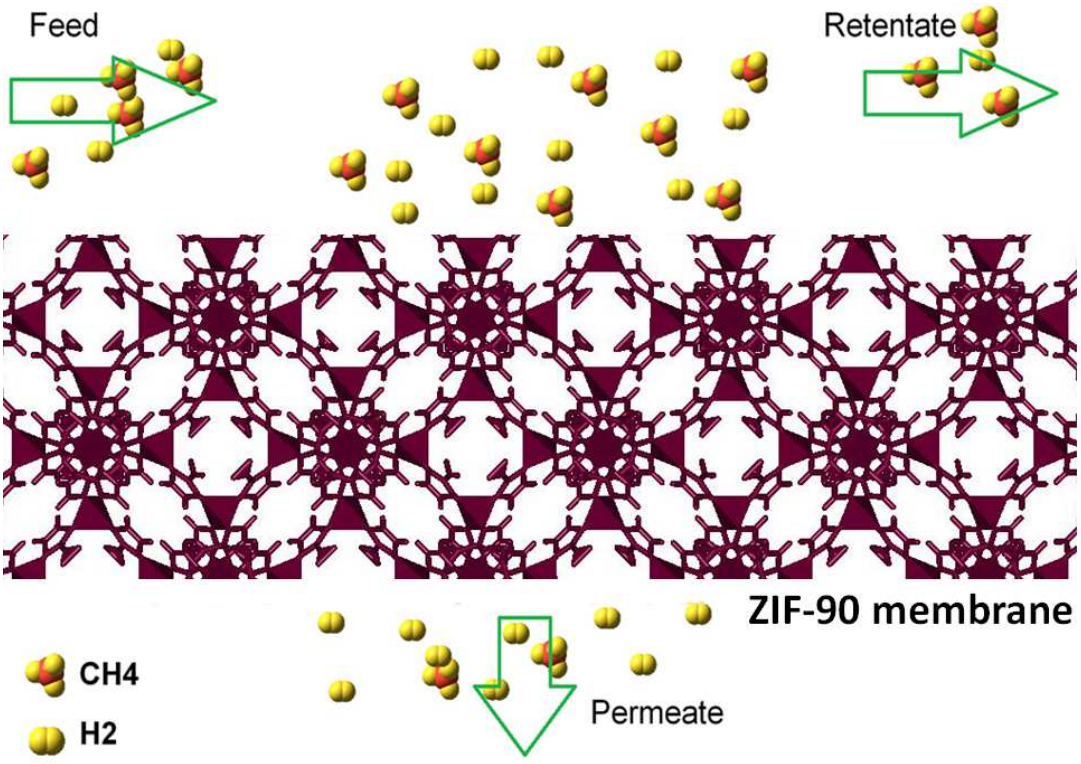

Figure 12.19: Illustration of the considered experimental setup based on a ZIF-90 membrane.

Adsorption and diffusion of the gas mixture H_2/CH_4 in the metal-organic framework (MOF) of structure type zeolitic imidazolate framework-90 (ZIF-90) [1, 2] are revisited in this project [3]. The considered setup is sketched in Fig. 12.19. While the adsorption can successfully be examined in Gibbs ensemble Monte Carlo (GEMC) simulations using the common approximation of a rigid lattice, the dynamics of methane in ZIF-90 is remarkably influenced by the lattice flexibility [4]. Molecular dynamics (MD)

simulations not only show a strong influence of the lattice flexibility on the diffusion of methane but even find a slight structural phase transition of the lattice. This structural change appeared at higher temperatures and was not caused by the content of guest molecules like in most former discoveries of gate opening. For prediction of mixed gas ZIF-90 membrane selectivity, the adsorption and diffusion results show that the high CH_4 adsorption selectivity is overcompensated by the high H_2 mobility. The comparison of our results for the H_2/CH_4 membrane selectivity with experimental findings from mixed gas permeation through supported ZIF-90 membranes shows better agreement than other simulations that use a rigid lattice for MD [3]. Also, the increase of the membrane selectivity by increased temperature could be found.

[1] W. Morris et al.: J. Am. Chem. Soc. **130**, 12626 (2008)
[2] A. Huang et al.: J. Am. Chem. Soc. **132**, 15562 (2010)
[3] T. Chokbunpiam et al.: J. Phys. Chem. C **121**, 10455 (2017)
[4] V.T. Phuong et al.: Microporous Mesoporous Mater. **235**, 69 (2016)

12.15 Self-avoiding walks on critical percolation clusters in 2 – 7 dimensions

N. Fricke, W. Janke

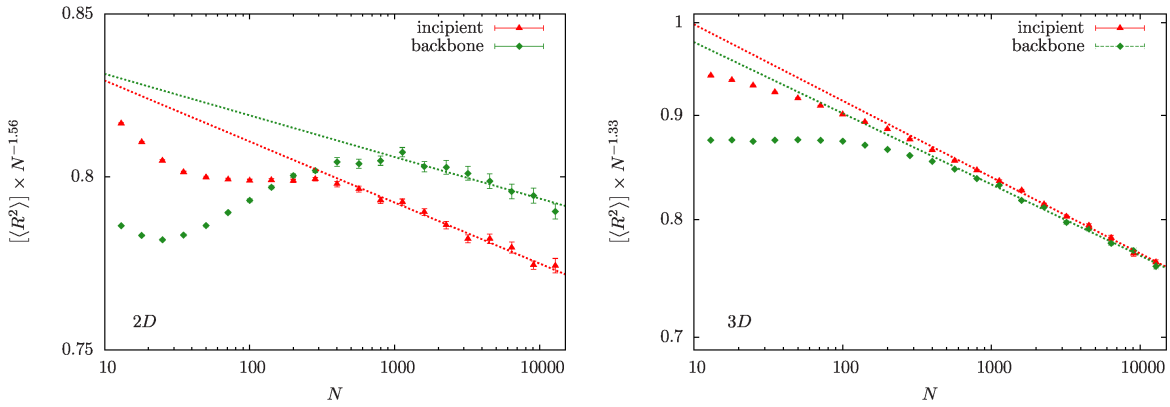

Figure 12.20: Scaled disorder averages of the mean squared end-to-end distance as a function of the number of SAW steps on critical clusters and cluster backbones in (a) 2D and (b) 3D on a double-logarithmic scale. The values have been divided by $\approx N^{2\nu_{pc}}$ for better visibility. Straight lines show least-squares power-law fits to the data in the range $N = 800 - 12\,800$ for 2D and 3D incipient clusters and $N = 1131 - 12\,800$ for 3D backbones.

Self-avoiding walks (SAWs) on critical percolation clusters are a simple model for polymers in highly disordered environments such as porous rocks or a biological cell [1, 2]. The system is also appealing from a theoretical perspective as it combines two of the most ubiquitous models from statistical physics. It has therefore been studied

intensely in the past both analytically and numerically. However, despite its conceptual simplicity, the problem proved extremely challenging. Few reliable predictions exist for the SAWs' scaling exponents, and our qualitative understanding of the model is also still limited. In particular, it is unclear how the disorder and the medium's fractal structure, characterized by its various fractal dimensions, impacts the SAWs' asymptotic scaling behavior. This understanding is crucial when we want to generalize from the results and make predictions for real-world systems.

The main difficulty for numerical investigation of the problem can be overcome by making use of the self-similar geometry of critical percolation clusters to factorize the problem, in an approach that we called scale-free enumeration (SFE) [3, 4]. In two preceding studies, we had used this method to investigate SAWs on critical percolation clusters in 2D [5] and 3D [6]. Recently we have expanded this perspective and looked at systems in up to 7D [7], above the supposed upper critical dimension of $D_{\mathrm{uc}} = 6$.

We mainly focused on the scaling of the increase of the mean squared end-to-end distance with the number of steps,

$$[\langle R^2 \rangle] \sim N^{2\nu} \tag{12.5}$$

where ν is a universal scaling exponent. The reduced time complexity of our recently introduced SFE method allows us to exactly enumerate SAWs of over $N = 10^4$ steps, easily amounting to 10^{2000} conformations. Previously, only up to $N = 45$ steps on 2D clusters and 40 steps on 3D clusters could be handled by the standard "brute-force" enumeration method.

In 2D and 3D we studied walk lengths increasing in multiplicative steps of $\sqrt{2}$ from $N = 13$ up to $N = 12\,800$ ($= 100 \times 2^7$). For each length we took independent samples of at least 5×10^4 randomly generated percolating clusters and backbones. The results for the mean squared end-to-end distance as a function of N and least-squares fits of Eq. (12.5) to the data are shown in Fig. 12.20 on a double-logarithmic scale. The y-axes have been rescaled by $\approx N^{-2\nu_{pc}}$, so that the slopes are close to zero and more details are visible. Note that while the conformational averages are evaluated exactly, we still have statistical fluctuations of the disorder averages reflected by the error bars.

Repeating this procedure in 4D – 7D, we finally arrive at Fig. 12.21, where we have also included a comparison with analytical predictions from various sources.

[1] D. Ben-Avraham, S. Havlin: *Diffusion and Reactions in Fractals and Disordered Systems* (Cambridge University Press, Cambridge, 2000)
[2] B.K. Chakrabarti (ed.): *Statistics of Linear Polymers in Disordered Media* (Elsevier, Amsterdam, 2005)
[3] N. Fricke, W. Janke: Eur. Phys. J. – Special Topics **216**, 175 (2013)
[4] N. Fricke, W. Janke: *How to enumerate* 10^{1000} *self-avoiding walk conformations on a critical percolation cluster*, Leipzig preprint (2017), to be published
[5] N. Fricke, W. Janke: Europhys. Lett. **99**, 56005 (2012)
[6] N. Fricke, W. Janke: Phys. Rev. Lett. **113**, 255701 (2014); Phys. Rev. Lett. **115**, 149902 (Erratum)
[7] N. Fricke, W. Janke: J. Phys. A: Math. Theor. **50**, 264002 (2017)
[8] C. von Ferber et al.: Phys. Rev. E **70**, 035104 (2004)
[9] H.K. Janssen, O. Stenull: Phys. Rev. E **75**, 020801 (2007); Phys. Rev. E **85**, 051126 (2012)

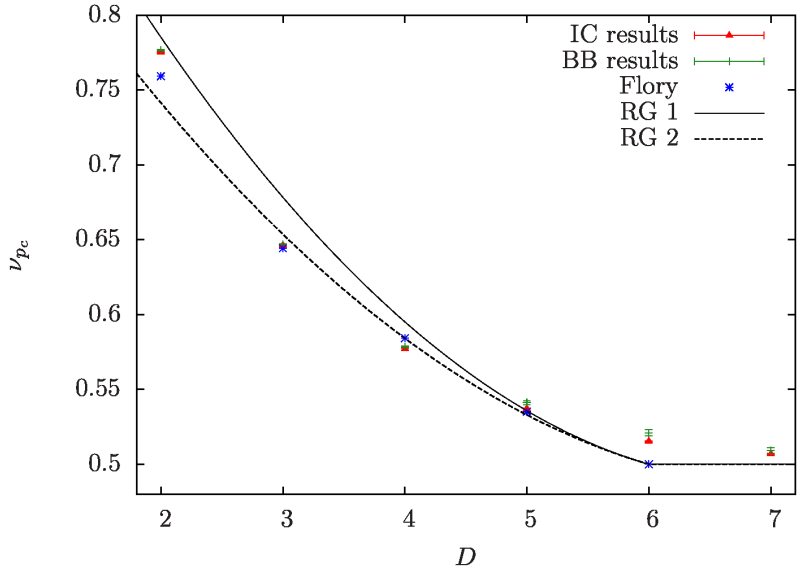

Figure 12.21: Results for ν_{p_c} on incipient clusters (IC, red) and backbones (BB, green) as a function of dimension compared to various analytical predictions. The blue asterisks correspond to Flory estimates [7]. The lines represent the field-theory estimates from [8] (RG1, solid) and [9] (RG2, dashed).

12.16 Percolation on square lattices with long-range correlated defects

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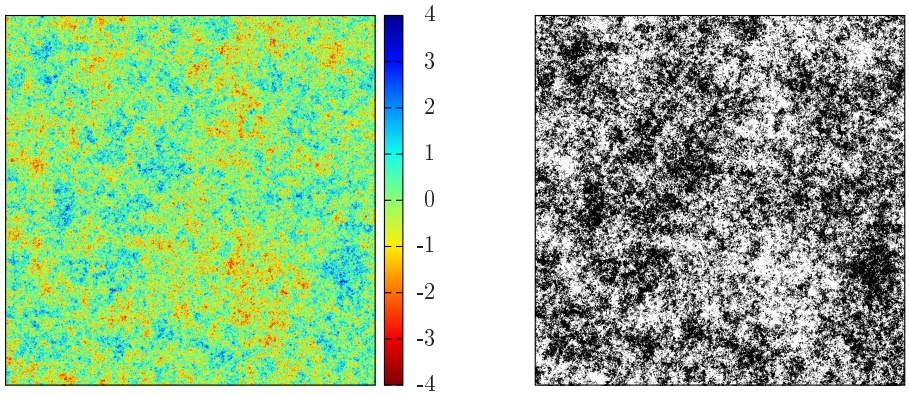
Structural obstacles (impurities) play an important role for a wide range of physical processes as most substrates and surfaces in nature are rough and inhomogeneous [1]. For example, the properties of magnetic crystals are often altered by the presence of extended defects in the form of linear dislocations 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, 3]. This aspect is relevant, for instance, for the recovery of oil through porous rocks [4], for the dynamics of fluids in disordered media [5], or for our understanding of transport processes in biological cells [6].

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:

$$C(r) \sim |r|^{-a} \tag{12.6}$$



(a) (b)

Figure 12.22: 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.

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. 12.22.

In this project we studied long-range power-law correlated disorder on square and cubic lattices [7, 8]. 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 [9]. 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 $d_f \to 2$. The onset of this change, however, does not seem to be determined by the extended Harris criterion.

[1] D. Avnir et al.: Nature (London) **308**, 261 (1984)
[2] J.-P. Bouchaud, A. Georges: Phys. Rep. **195**, 127 (1990)
[3] I. Goychuk et al.: Phys. Rev. E **96**, 052134 (2017)
[4] M. Sahimi: *Flow and Transport in Porous Media and Fractured Rock* (VCH, Weinheim, 1995)
[5] M. Spanner et al.: Phys. Rev. Lett. **116**, 060601 (2016)
[6] F. Höfling, T. Franosch: Rep. Prog. Phys. **76**, 046602 (2013)
[7] N. Fricke et al.: Condens. Matter Phys. **20**, 13004 (2017)
[8] J. Zierenberg et al.: Phys. Rev. E **96**, 062125 (2017)
[9] H.A. Makse et al.: Phys. Rev. E **53**, 5445 (1996)

12.17 Dynamical greedy algorithm for the Edwards-Anderson model

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One of the most intuitive and natural approaches to optimization problems is realized by so-called greedy algorithms. These methods create trajectories in the space of possible solution by always choosing the next step such that the energy is maximally reduced (or a fitness function maximally increased). Naturally, this will usually not find the global optimum, just as starting at a random spot and always walking uphill will usually not lead a wanderer to the summit of Mt. Everest. Therefore, in practice many attempts with randomly created starting points are made and if the problem is not too difficult the global optimum may be found this way.

On the other hand, there is practically no chance of success if the energy landscape is as complicated and possesses as many local minima as in the case of 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 can take two values $S_i \in \{-1, 1\}$ and adjacent spins interact via normally distributed random couplings J_{ij}. If such a model on a three-dimensional cubic lattice of 1000 spins is considered, about 10^{30} attempts would be necessary in order to find the ground state this way.

However, the greedy algorithm can still be a very helpful tool, since it is a comparatively simple and reliable method to reach states of low energy. We devised a method to efficiently update the greedy algorithm, i.e., to reuse the data created during a minimization from a configuration $\mathbf{S}$ to the configuration $\mathbf{S}_{\min}$ to obtain the result $\mathbf{S}'_{\min}$ of the minimization from a configuration $\mathbf{S}'$ which differs from $\mathbf{S}$ only in the values of one or very few spins [2]. If furthermore, both, the terminal configuration, delivered by the greedy algorithm, and its energy are understood as attributes of the starting configuration, it is possible to use the energy of the minimized configurations $\mathbf{S}_{\min,t}$ to steer a path in the space of starting configurations $\mathbf{S}_t$.

A simple application is to apply the greedy algorithm again: It is tested which alteration (e.g., which single spin flip) of the starting configuration will reduce the energy of the *minimized* configuration by the largest amount and this locally optimal step is performed. Repeating this simple procedure as long as viable as a "second order greedy algorithm" will lead to much lower energies albeit not the ground state.

Alternatively, the energy of the minimized configuration can be used as argument for the occupation probability for a generalized ensemble [3]:

$$P(\mathbf{S}) = P(\mathbf{S}_{\min}),$$

which can then be sampled using Monte Carlo techniques. All states in the same "valley" in the energy landscape, i.e., all configuration which minimize to the same local energy minimum, now occur with the same probability and the barriers of high energy which greatly hamper standard Monte Carlo simulations simply vanish. In consequence, the configuration space is sampled much more easily and the performance of ground-state search is greatly improved.

[1] S.F. Edwards, P.W. Anderson: J. Phys. F **5**, 965 (1975)
[2] S. Schnabel, W. Janke: Comput. Phys. Commun. **220**, 74 (2017)
[3] D.J. Wales: J. Phys. Chem. A **101**, 5111 (1997)

12.18 Distribution of local minima for the Edwards-Anderson 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 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.

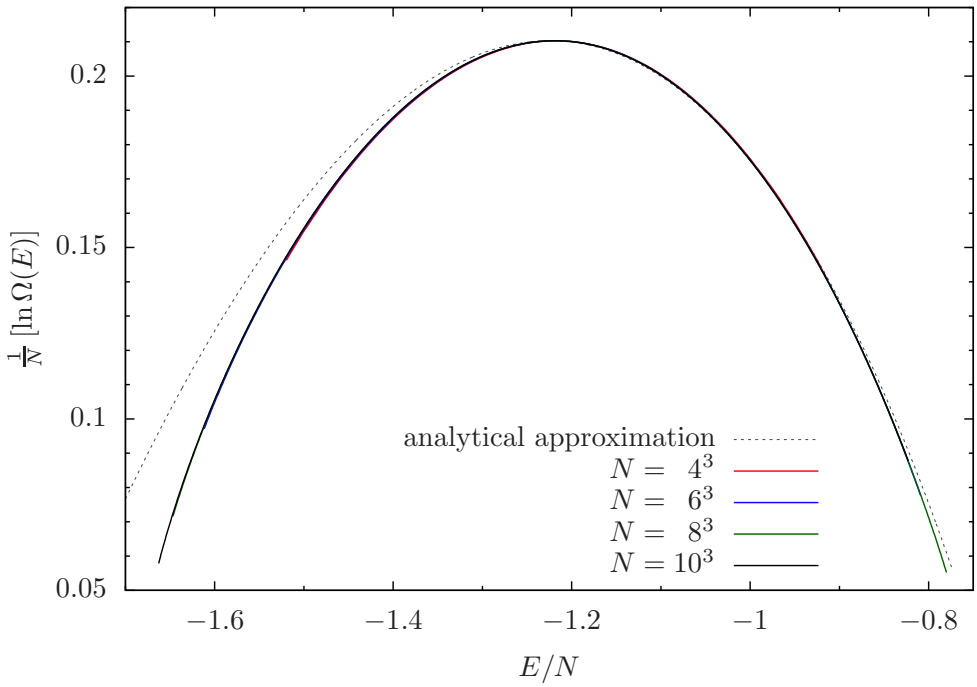

Figure 12.23: The distribution of local minima for different system sizes and the analytical approximation.

[1] S.F. Edwards, P.W. Anderson: J. Phys. F **5**, 965 (1975)
[2] A.J. Bray, M.A. Moore: J. Phys. C **14**, 1313 (1981)
[3] S. Schnabel, W. Janke: Phys. Rev. B **97**, 174204 (2018)

12.19 Spin glasses with variable frustration

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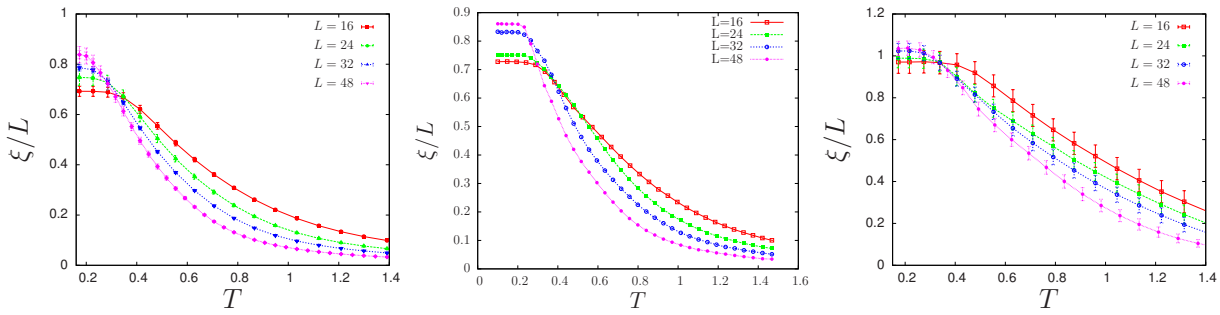

(a) (b) (c)

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.

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].

[1] E. Ilker, A.N. Berker: Phys. Rev. E **89**, 042139 (2014)
[2] J. Houdayer: Eur. Phys. J. B **22**, 479 (2001)
[3] H.G. Katzgraber, L.W. Lee: Phys. Rev. B **71**, 134404 (2005)
[4] A. Hartmann: Phys. Rev. B **67**, 214404 (2003)

12.20 Random field q-state Potts model: Ground states and low-energy excitations

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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 $q \geq 3$ 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

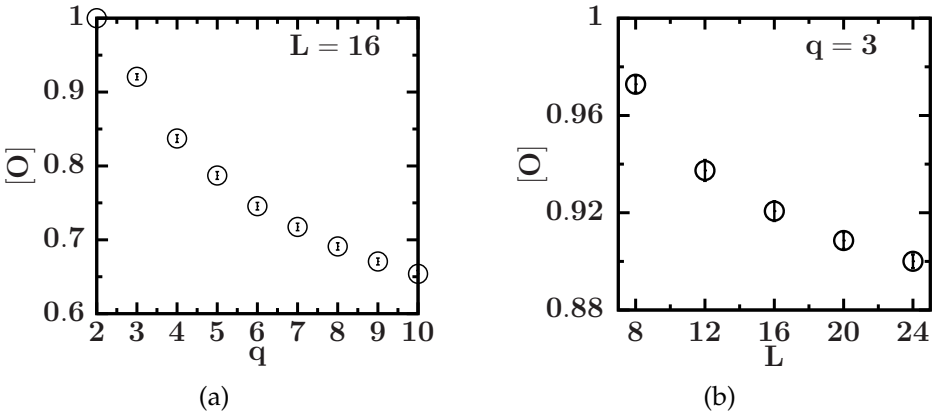

Figure 12.25: Overlap between the lowest states found by graph-cut methods (GCM) and the putative ground state (a) as a function of the number of Potts states q and (b) as a function of system size L.

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.

[1] G.P. Shrivastav et al.: Europhys. Lett. **96**, 36003 (2011)
[2] G.P. Shrivastav et al.: Phys. Rev. E **90**, 032140 (2014)
[3] G.P. Shrivastav et al.: Eur. Phys. J. E **37**, 98 (2014)
[4] V. Banerjee et al.: Ind. J. Phys. **88**, 1005 (2014)
[5] J.C. Angles d'Auriac et al.: J. Physique Lett. **46**, L173 (1985)
[6] M. Kumar at al.: Phys. Rev. E **97**, 053307 (2018)

12.21 Gonihedric plaquette models of Fuki-Nuke type: Boundary conditions and non-local constraints

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An anisotropic limit of the $3d$ plaquette Ising model, in which the plaquette couplings in one direction were set to zero, was solved for free boundary conditions by Suzuki [1],

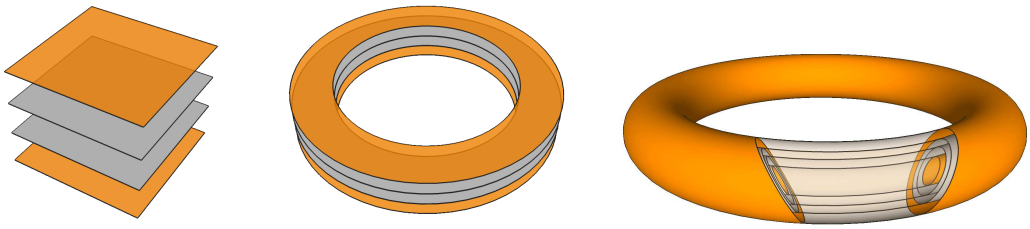

Figure 12.26: Fuki-Nuke models with free boundary conditions in one direction permit different topology of the lattice. We sketch the layers of independent layers of spins: (a) free boundary conditions in *all* directions, (b) periodic boundary conditions are set in one, and only one direction, and (c) periodic boundary conditions are set in both other directions.

who later dubbed it the fuki-nuke, or "no-ceiling", model. Defining new spin variables as the product of nearest-neighbour spins transforms the Hamiltonian into that of a stack of (standard) $2d$ Ising models and reveals the planar nature of the magnetic order, which is also present in the fully isotropic $3d$ plaquette model [2]. More recently, the solution of the fuki-nuke model was discussed for periodic boundary conditions applied to the spin lattice, which require a slightly different approach to defining the product spin transformation, by Castelnovo et al. [3].

We find that the essential features of the differences between free and periodic boundary conditions when using a product spin transformation are already present in the $1d$ Ising model [4], which thus provides an illuminating test case for its use in solving plaquette spin models and an alternative method for solving the $1d$ Ising model with periodic boundary conditions.

We clarify the exact relation between partition functions expressed in terms of the original and product spin variables for the $1d$ Ising model, $2d$ plaquette and $3d$ fuki-nuke models with free and periodic boundary conditions. Representing graphically the combinatorial factors that contribute to the partition function, we are able to solve the $2d$ plaquette model with free, periodic and helical boundary conditions and various combination of these in x- and y-directions, see Fig. 12.26. The various exactly solved examples illustrate how correlations can be induced in finite systems as a consequence of the choice of boundary conditions.

For the three-dimensional fuki-nuke model the exact finite-size partition function may be written as a product of $2d$ Ising partition functions in the case of free boundary conditions using the product variable transformation. A similar decoupling is not manifest with periodic boundary conditions, where all n-point $2d$ Ising spin-spin correlations also contribute to the expression for the $3d$ fuki-nuke partition function. As illustrated in Fig. 12.27, this can be most easily understood in a pictorial way by employing the high-temperature expansion/dimer approach. It is perhaps worth remarking that the discussion of the fuki-nuke model in [3] conflates the discussion of free and periodic boundary conditions, although the overall picture of a $2d$ Ising-like transition in the thermodynamic limit of the $3d$ fuki-nuke model remains, of course, correct in both cases.

A further consequence of the planar flip symmetry is found in a Hamiltonian related to the quantum dual of the plaquette model. This fits into the general framework developed in [5, 6] in which novel fracton topological phases are constructed by gauging

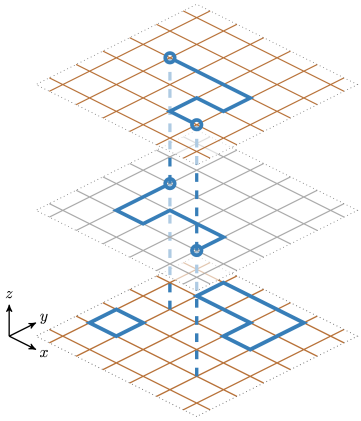

Figure 12.27: A dimer configuration of the Fuki-Nuke model with $L_z = 3$ that can contribute to the partition function, although the mid and top layer have dangling ends (symbolised by open circles). These are connected through the constraints (dashed vertical lines) and contribute to the two-point function in each of the two upper layers. Notice that additional, standard $2d$ Ising loops may appear, as those shown in the bottom layer, which are the standard contributions to the partition function of each layer.

symmetries acting on subsystems of dimension $2 \leq d_s < d$. Since the spin-flip symmetry in the $3d$ plaquette model acts on $2d$ planes it has precisely this property. The procedure for constructing the fracton Hamiltonian follows closely that of the Kitaev toric code, giving commuting electric and magnetic operators. We outline the role played by the spin-flip symmetry in enabling the appearance of fracton topological defects in a Hamiltonian related to the dual of the quantum version of the model [7].

[1] M. Suzuki: Phys. Rev. Lett. **28**, 507 (1972)
[2] M. Mueller et al.: Nucl. Phys. B **894**, 1 (2015); D.A. Johnston et al.: Mod. Phys. Lett. **B29**, 1550109 (2015)
[3] C. Castelnovo et al.: Phys. Rev. B **81**, 184303 (2010)
[4] M. Mueller et al.: Nucl. Phys. B **914**, 388 (2017)
[5] S. Vijay et al.: Phys. Rev. B **94**, 235157 (2016)
[6] D.J. Williamson: Phys. Rev. B **94**, 155128 (2016)
[7] D.A. Johnston et al.: Eur. Phys. J. – Special Topics **226**, 749 (2017)

12.22 The two-dimensional Blume-Capel model: Scaling and universality

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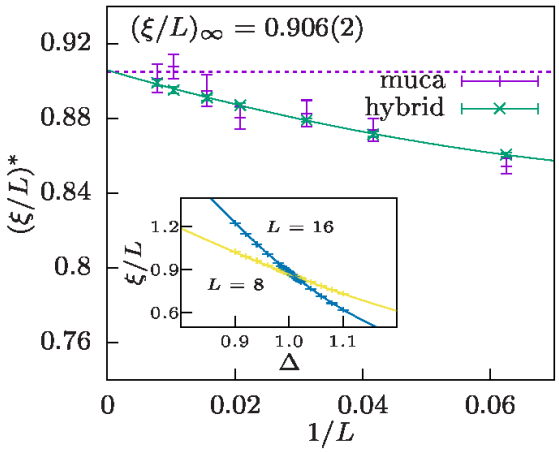

Figure 12.28: Finite-size scaling at $T = 1.398$ of the correlation length crossings $(\xi/L)^*$. The dashed horizontal shows the asymptotic value for the square-lattice Ising model with periodic boundaries. Compared are data from the multicanonical ("muca") and hybrid methods. The line shows a quadratic fit in $1/L$ to the data from the hybrid method. The inset demonstrates the crossing point of $L = 8$ and $L = 16$ obtained from both the muca (lines) and hybrid (data points) method.

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

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j + \Delta \sum_i \sigma_i^2 = E_J + \Delta E_\Delta \,. \tag{12.7}$$

We investigate the behaviour in the vicinity of the first-order and second-order regimes of the ferromagnet-paramagnet phase boundary, respectively [3]. To achieve high-precision results, we utilize a combination of (i) a parallel version of the multicanonical algorithm and (ii) a hybrid updating scheme combining Metropolis and generalized Wolff cluster moves. These techniques are combined to study for the first time the correlation length ξ 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 ξ/L with the exactly known result for the Ising universality class, see Fig. 12.28.

In contrast to most previous work, we focused on crossing the phase boundary at constant temperature by varying the crystal field Δ [4]. Employing a multicanonical scheme in Δ allowed us to get results as continuous functions of Δ 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 χ. 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 χ. 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.

[1] M. Blume: Phys. Rev. **141**, 517 (1966)
[2] H.W. Capel: Physica (Utr.) **32**, 966 (1966)
[3] J. Zierenberg et al.: Eur. Phys. J. – Special Topics **226**, 789 (2017)
[4] J. Zierenberg et al.: Phys. Rev. E **91**, 032126 (2015)

12.23 Finite-size scaling properties of the real microcanonical ensemble

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The definition of the microcanonical ensemble can be found in any standard text book on statistical physics. Usually this ensemble is quickly dismissed in favor of the canonical ensemble since it is quite unrealistic for most physical systems in a laboratory. In the literature on phase transitions, however, this ensemble gained some interest also due to the development of the generalized ensemble methods MUCA [1, 2] and Wang-Landau [3]. Here, however, one refers to the microcanonical ensemble at constant *potential* energy while the "real" microcanonical ensemble was originally defined at constant *total* energy.

We previously investigated the behaviour of molecular dynamics and Monte Carlo simulations within this ensemble and made the interesting observation that a Monte Carlo simulation in this ensemble sampled the first-order aggregation transition in a very efficient way [4]. Such a behaviour behaviour was previously described by Martin-Mayor [5] for the temperature-driven first-order phase transition in the Potts lattice model. We further investigated this simulation technique in the real microcanonical ensemble for a continuous Lennard-Jones system and found the same sampling advantage [7]. We reached the same amount of particles with these simulations as with the sophisticated MUCA simulation technique.

In Ref. [6] we were able to develop a framework based on the generalization of the equal-area rule which allowed us to explain the obtained simulation behaviour of the real microcanonical ensemble. For comparison we introduced the transition barrier of an ensemble as

$$B = \ln\left[P^{\mathrm{eqh}}\left(E_p^{\pm}\right)/P^{\mathrm{eqh}}\left(E_p^{0}\right)\right], \tag{12.8}$$

where $P^{\mathrm{eqh}}\left(E_p^{\pm}/E_p^{0}\right)$ denotes the equal-height histogram emerging due to phase coexistence, $E_p^{\pm}$ the positions of the two maxima and E_p^{0} the position of the minimum in between, cf. Fig. 12.29(a). This quantity hence allows one to evaluate how "hard" the first-order transition between two phases is within an ensemble. This framework leads to the conclusion that the barrier in the canonical ensemble is always larger than in the microcanonical ensemble, $B_{\mathrm{NVT}} > B_{\mathrm{NVE}}$. In the microcanonical ensemble the transition

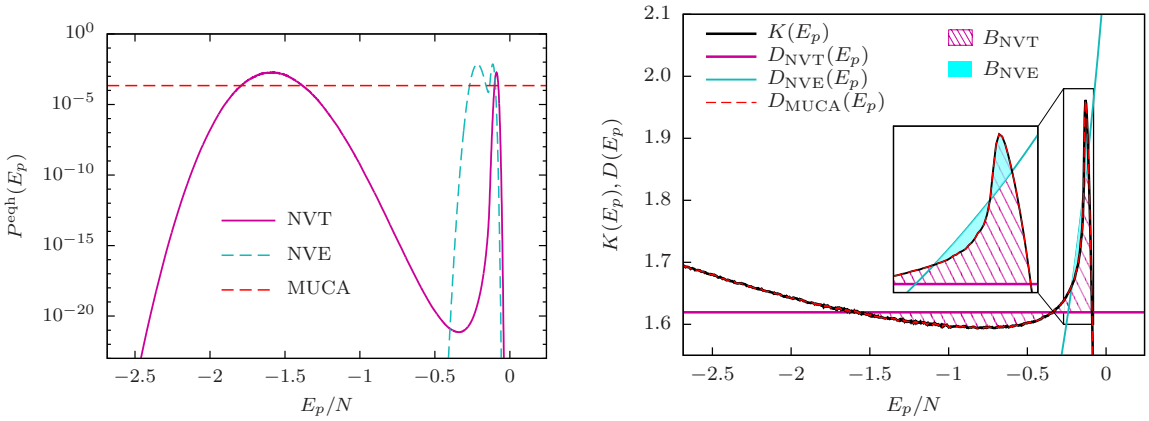

Figure 12.29: (a) The potential-energy histogram at equal height for three different ensembles for the $N = 2048$ Lennard-Jones system [6]. (b) The system dependent quantity $K(E_p)$ and the ensemble dependent $D(E_p)$ for the considered ensembles as defined in [6].

barrier can even vanish as it was observed in [4, 8] for polymer aggregation and by reproducing the data from Ref. [5]. For the example of the Lennard-Jones system with $N = 2048$ particles we discovered that the sampling with the microcanonical ensemble is of the order of $\exp\left(B_{\rm NVT} - B_{\rm NVE}\right) \approx 10^{16}$ more efficient than simulations in the canonical ensemble due to the difference of the barriers. The underlying mechanism is discussed in Ref. [6] and sketched in Fig. 12.29(b).

[1] B.A. Berg, T. Neuhaus: Phys. Lett. B **267**, 249 (1991); Phys. Rev. Lett. **68**, 9 (1992)
[2] W. Janke: Int. J. Mod. Phys. C **03**, 1137 (1992); Physica A **254**, 164 (1998)
[3] F. Wang, D.P. Landau: Phys. Rev. Lett. **86**, 2050 (2001); Phys. Rev. E **64**, 056101 (2001)
[4] P. Schierz et al.: J. Chem. Phys. **143**, 134114 (2015)
[5] V. Martin-Mayor: Phys. Rev. Lett. **98**, 137207 (2007)
[6] P. Schierz et al.: Phys. Rev. E **94**, 021301(R) (2016)
[7] J. Zierenberg et al.: Nat. Commun. **8**, 14546 (2017)
[8] W. Janke et al.: in *Computer Simulation Studies in Condensed-Matter Physics XXX*, eds. D.P. Landau, M. Bachmann, S.P. Lewis, and H.-B. Schüttler, J. Phys.: Conf. Ser. **921**, 012018 (2017)

12.24 Stochastic Approximation Monte Carlo versus modified Wang-Landau algorithms: Convergence tests for the Ising model

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The Wang-Landau algorithm [1] has proven to be a very efficient tool for determining the density of states (DOS) of statistical systems near phase transitions where traditional local importance sampling algorithms like the Metropolis algorithm are likely to run into critical slowing down or become trapped in local free-energy minima [2]. It has,

however, been pointed out that the error of the estimator for the DOS obtained by the Wang-Landau algorithm cannot be made arbitrarily small just by using longer simulations [3], the (systematic) error saturates at some (small) value. To overcome this, it has been suggested to change the behaviour of the refinement parameter in the $1/t$ modification ($1/t$-WL) of the Wang-Landau algorithm in order to circumvent the error saturation [4].

Another approach is the Stochastic Approximation Monte Carlo (SAMC) algorithm [5], which works similar to the modified Wang-Landau algorithm regarding the choice of refinement scheme. While the $1/t$ algorithm has been tested for the Ising model, the calculation of multidimensional integrals, and in applications to lattice polymer models, the SAMC algorithm has only been tested for an artificial, non-physical model with a very small number of states [5] and for a special off-lattice polymer model [6]. The standard test case, the Ising model, however, was still missing and we closed this gap [7].

The $1/t$-method inherits the problem of needing to know the range of admissible energies for the considered model from the Wang-Landau algorithm. In SAMC, this needs not to be known beforehand, since histogram checking is not necessary in principle. The SAMC algorithm, on the other hand, sometimes failed to converge in our examined run times. This is caused by the simulation failing to explore the low-energy states. Therefore no flat histogram can be produced, see Fig. 12.30. Since both variants of the Wang-Landau algorithm regularly check the histogram for adequate flatness, it is ensured that all energies are visited at least once. While the SAMC algorithm should converge to the desired distribution if all conditions are met, it is necessary to check if the histogram measured during the simulation was really flat at the end. This dampens the advantage of a predictable run time, since it is possible that a complete run of the algorithm turns out to be unusable due to an inappropriate choice of t_0. Monitoring the flatness of the histogram during the run is no help, because this would introduce a stochastic quantity into the algorithm, making the run time unpredictable and require the same *a-priori* knowledge of the admissible energy range as the Wang-Landau algorithm and its modifications. The rule of thumb for the choice of t_0 given by Liang et al. [5] is violated even by the 128×128 Ising model, showing that finding an appropriate t_0 can be a quite cumbersome task. The $1/t$-WL algorithm suffers from a similar restriction in this regard: While we could not find anything comparable in the Ising model, other studies suggest that the overall convergence behaviour can also be sensitive to the details of the $1/t$-refining scheme for more complicated models [4, 8]. Regarding the common features of the SAMC and $1/t$-WL algorithms, it seems reasonable to assume that the proof of convergence for SAMC also extends to the $1/t$-WL algorithm as well, since their long-time behaviour is the same. Therefore the choice of algorithm to apply to a certain problem is a practical one. With the various refinements allowing it to adapt to *a-priori* unknown energy ranges and to determine the right time for the onset of the $1/t$-refinement, the $1/t$-WL algorithm might be able to overcome its drawback for complicated systems with unknown ground states. SAMC still has the advantage of allowing to generate weights not only according to the density of states, but also according to other distributions [5], which can improve estimators and might prove useful for complex systems like spin glasses or polymers, because sampling with distributions other than the inverse density of states can speed up round trip times significantly [9].

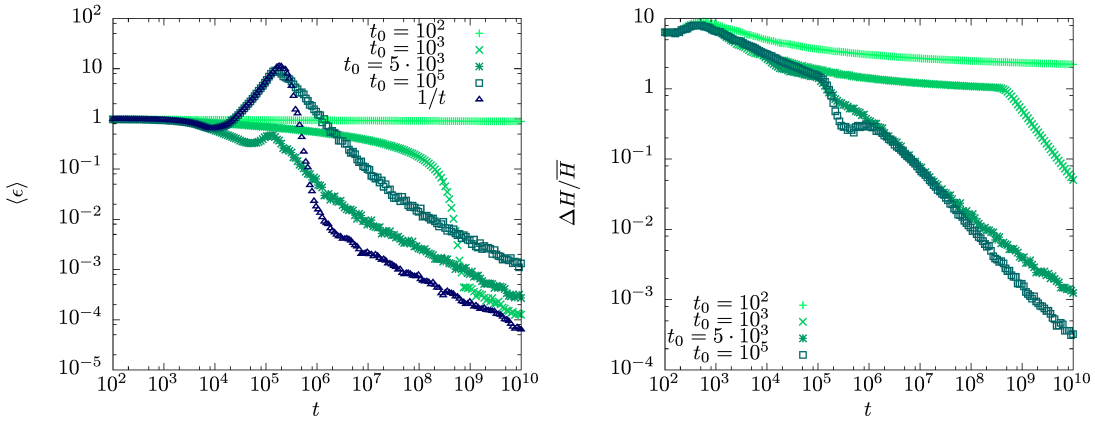

Figure 12.30: (a) The behaviour of the average deviation from the exact solution $\langle \epsilon(t) \rangle_E$ over MC time t for SAMC for different t_0 and $1/t$-WL simulations of the 16×16 Ising model. Obviously, tweaking the free parameter t_0 is essential for practical convergence. (b) The flatness of the histogram over MC time t for different choices of t_0. All data was obtained by averaging over 40 independent runs of the algorithm to reduce statistical noise.

[1] F. Wang, D.P. Landau: Phys. Rev. Lett. **86**, 2050 (2001); Phys. Rev. E **64**, 056101 (2001)
[2] W. Janke, W. Paul: Soft Matter **12**, 642 (2016)
[3] Q. Yan, J.J. de Pablo: Phys. Rev. Lett. **90**, 035701 (2003)
[4] R.E. Belardinelli, V.D. Pereyra: J. Chem. Phys. **127**, 184105 (2007); Phys. Rev. E **75**, 046701 (2007); C. Zhou, J. Su: Phys. Rev. E **78**, 046705 (2008)
[5] F. Liang: J. Stat. Phys. **122**, 511 (2006); J. Amer. Statist. Assoc. **102**, 305 (2007)
[6] B. Werlich et al.: Comput. Phys. Commun. **186**, 65 (2015)
[7] S. Schneider et al.: Comput. Phys. Commun. **216**, 1 (2017)
[8] A. D. Swetnam, M. P. Allen: J. Comput. Chem. **32**, 816 (2011); T. Wüst, D.P. Landau: Phys. Rev. Lett. **102**, 178101 (2009)
[9] B. Hesselbo, R.B. Stinchcombe: Phys. Rev. Lett. **74**, 2151 (1995); S. Trebst et al.: Phys. Rev. E **70**, 046701 (2004)

12.25 Population annealing: A massively parallel simulation scheme

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The canonical 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. 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 bias 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].

[1] D.P. Landau, K. Binder: *A Guide to Monte Carlo Simulations in Statistical Physics*, 4th ed. (Cambridge University Press, Cambridge, 2015)
[2] Y. Iba: Trans. Jpn. Soc. Artif. Intell. **16**, 279 (2001)
[3] K. Hukushima, Y. Iba: AIP Conf. Proc. **690**, 200 (2003)
[4] J. Machta: Phys. Rev. E **82**, 026704 (2010)
[5] L.Yu. Barash et al.: Comput. Phys. Commun. **220**, 341 (2017)
[6] L.Yu. Barash et al.: Eur. Phys. J. – Special Topics **226**, 595 (2017)
[7] M. Weigel et al.: in *Computer Simulation Studies in Condensed-Matter Physics XXX*, eds. D.P. Landau, M. Bachmann, S.P. Lewis, and H.-B. Schüttler, Phys.: Conf. Ser. **921**, 012017 (2017)

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 behaviour of a wide variety of physical systems. These systems range from such simple ones like the Ising spin model to complex ones like the adsorption properties of proteins on 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

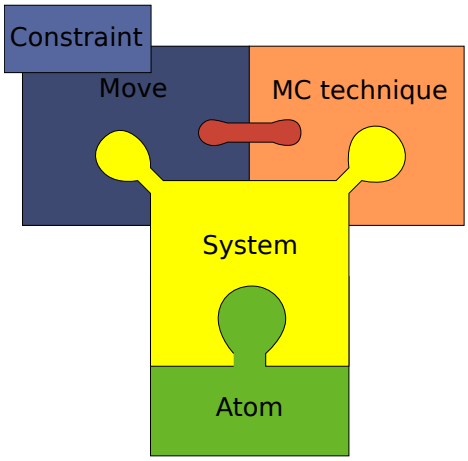

Figure 12.31: The 5 basic building blocks.

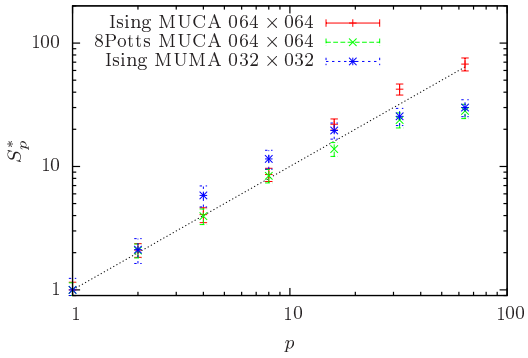

Figure 12.32: Scaling properties of the parallel multicanonical algorithm as a function of the number of processors p.

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 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. 12.31: 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. 12.32.

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].

[1] J. Zierenberg et al.: Comput. Phys. Commun. **184**, 1155 (2013)
[2] J. Gross et al.: Comput. Phys. Commun. **224**, 387 (2018)
[3] J. Zierenberg et al.: J. Chem. Phys. **141**, 114908 (2014)
[4] J. Zierenberg, W. Janke: Europhys. Lett. **109**, 28002 (2015)
[5] J. Zierenberg at al: Phys. Rev. E **91**, 032126 (2015)
[6] M. Marenz, W. Janke: Phys. Rev. Lett. **116**, 128301 (2016)
[7] J. Zierenberg et al: Polymers **8**, 333 (2016)
[8] J. Zierenberg et al.: Nat. Commun. **8**, 14546 (2017)
[9] N.G. Fytas et al.: Phys. Rev. E **97**, 040102(R) (2018)

12.27 Funding

Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility*
W. Janke (Principal Investigator, project B04)
Deutsche Forschungsgemeinschaft (DFG)

Free-Energy Landscapes of Semiflexible Theta-Polymer Aggregation with and without External Force
W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/31-1

Stable Knotted Phases in Semiflexible Polymers
W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/33-1

Institute Partnership with the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine, *Polymers in Porous Environments and on Disordered Substrates*
W. Janke (with V. Blavatska, Lviv)
Alexander von Humboldt Foundation (AvH)

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W. Janke (Principal Investigator, Head of Leipzig node)
European Union (EU), Contract No. PIRSES-GA-2013-612707

Doctoral College *Statistical Physics of Complex Systems* ($\mathbb{L}^4$)
W. Janke (with B. Berche, Nancy)
Deutsch-Französisches Doktorandenkollegium (DFDK) with "Co-tutelle de Thèse", jointly with Université de Lorraine, Nancy, France, and Coventry University, UK, and National Academy of Sciences of Ukraine, Lviv, Ukraine, as associated partners
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Graduate School *"BuildMoNa": Leipzig School of Natural Sciences – Building with Molecules and Nano-objects*
W. Janke (Principal Investigator)

International Max Planck Research School (IMPRS) *Mathematics in the Sciences*
W. Janke (Scientific Member)
Max Planck Society and Klaus Tschira Foundation

Free-Energy Landscapes of Semiflexible Polymer Aggregation
W. Janke, J. Zierenberg
NIC Jülich (computer time grant for "JURECA"), Grant No. HLZ24

12.28 Organizational Duties

Wolfhard Janke

- *Adjunct Professor* of The University of Georgia, Athens, Georgia, USA
- *International Visiting Professor* of Coventry University, England, UK
- Director, Institute for Theoretical Physics (ITP), Universität Leipzig
- Director, Naturwissenschaftlich-Theoretisches Zentrum (NTZ), Universität Leipzig
- Member of Department Council ("Fakultätsrat"), Faculty for Physics and Earth Sciences, Universität Leipzig
- Member of the Steering Committee ("Direktorium") of the Graduate Centre *Mathematics/Computer Science and Natural Sciences*, Research Academy Leipzig
- Principal Investigator of the Graduate School "BuildMoNa"
- Scientific Member of the International Max Planck Research School (IMPRS) *Mathematics in the Sciences*
- Principal Investigator of the DFG Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility*
- Principal Investigator of "Profillinie" *Complex Matter*, Universität Leipzig
- Principal Investigator of "Profillinie" *Mathematical and Computational Sciences*, Universität Leipzig
- Spokesperson of the German-French Graduate College *Statistical Physics of Complex Systems* with Nancy (France), and associated partners in Coventry (England, UK) and Lviv (Ukraine), of the Deutsch-Französische Hochschule (DFH-UFA)
- Spokesperson of the German-Ukrainian Institute Partnership Leipzig-Lviv of the Alexander von Humboldt Foundation (AvH)
- External Member of the Jagiellonian University Graduate School *International Ph.D. Studies in Physics of Complex Systems*, Krakow, Poland
- Permanent Member of the International Advisory Board for the Annual *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Organizer (with W. Paul, Universität Halle) of the *1st Discussion Meeting HalLei17*, ITP, Universität Leipzig, 19. July 2017
- Organizer of the Workshop *CompPhys17* – 18th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 30. November – 02. December 2017
- Organizer of the Workshop *CompPhys18* – 19th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 29. November –01. December 2018

- Editor "Computational Physics", Central European Journal of Physics, Krakow, Poland
- 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, Lyon, France
- 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, Condens. Matter Phys., PLOS ONE, New Journal of Physics, International Journal of Modern Physics C

12.29 External Cooperations

Academic

- Institute of Physics, Jagiellonian University, Kraków, Poland
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  Dr. Richard A. Blythe, Prof. Dr. Martin R. Evans, Dr. Bartłomiej Wacław
- P.J. Šafárik University, Košice, Slovak Republic
  Dr. Michal Borovský
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- IAC-1, Universität Stuttgart, Germany
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  Prof. Dr. Ramon Villanova
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  Prof. Dr. Sanjay Kumar
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  Prof. Dr. Nobuyasu Ito
- Nagoya University, Nagoya, Japan
  Dr. Tetsuro Nagai, Prof. Dr. Yuko Okamoto

12.30 Publications

Journals

H. Arkın, W. Janke: *Polymer Adsorption on Curved Surfaces*, Phys. Rev. E **96**, 062504-1–14 (2017)

K.S. Austin, J. Zierenberg, W. Janke: *Interplay of Adsorption and Semiflexibility: Structural Behavior of Grafted Polymers under Poor Solvent Conditions*, Macromolecules **50**, 4054–4063 (2017)

L.Yu. Barash, M. Weigel, M. Borovský, W. Janke, L.N. Shchur: *GPU Accelerated Population Annealing Algorithm*, Comput. Phys. Commun. **220**, 341–350 (2017)

L. Yu. Barash, M. Weigel, L.N. Shchur, W. Janke: *Exploring First-Order Phase Transitions with Population Annealing*, Eur. Phys. J. – Special Topics **226**, 595–604 (2017)

T. Chokbunpiam, S. Fritzsche, J. Caro, C. Chmelik, W. Janke, S. Hannongbua: *Importance of ZIF-90 Lattice Flexibility on Diffusion, Permeation, and Lattice Structure for an adsorbed H_2/CH_4 Gas Mixture: A Re-Examination by Gibbs Ensemble Monte Carlo and Molecular Dynamics Simulations*, J. Phys. Chem. C **121**, 10455–10462 (2017)

H. Christiansen, S. Majumder, W. Janke: *Coarsening and Aging of Lattice Polymers: Influence of Bond Fluctuations*, J. Chem. Phys. **147**, 094902-1–12 (2017)

N. Fricke, W. Janke: *Exact Enumeration of Self-Avoiding Walks on Critical Percolation Clusters in 2–7 Dimensions*, J. Phys. A **50**, 264002-1–17 (2017)

N. Fricke, J. Zierenberg, M. Marenz, F. P. Spitzner, V. Blavatska, W. Janke: *Scaling Laws for Random Walks in Long-Range Correlated Disordered Media*, Condens. Matter Phys. **20**, 13004-1–11 (2017)

J. Gross, M. Ivanov, W. Janke: *Single-Chain Behavior of Poly(3-hexyl-thiophene)*, Eur. Phys. J. – Special Topics **226**, 667–681 (2017)

W. Janke, M. Marenz, J. Zierenberg: *Generalized Ensemble Computer Simulations for Structure Formation of Semiflexible Polymers*, Lobachevskii J. Math. **38**, 978–985 (2017)

W. Janke, P. Schierz, J. Zierenberg: *Transition Barrier at a First-Order Phase Transition in the Canonical and Microcanonical Ensemble*, in *Computer Simulation Studies in Condensed-Matter Physics XXX*, eds. D.P. Landau, M. Bachmann, S.P. Lewis, H.-B. Schüttler, J. Phys.: Conf. Ser. **921**, 012018-1–5 (2017)

D.A. Johnston, M. Mueller, W. Janke: *Plaquette Ising Models, Degeneracy and Scaling*, Eur. Phys. J. – Special Topics **226**, 749–764 (2017)

S. Majumder, J. Zierenberg, W. Janke: *Kinetics of Polymer Collapse: Effect of Temperature on Cluster Growth and Aging*, Soft Matter **13**, 1276–1290 (2017)

S. Mascotto, W. Janke, R. Valiullin: *Ice Nucleation in Periodic Arrays of Spherical Nanocages*, J. Phys. Chem. C **121**, 23788–23792 (2017)

M. Mueller, D.A. Johnston, W. Janke: *Exact Solutions to Plaquette Ising Models with Free and Periodic Boundaries*, Nucl. Phys. B **914**, 388–404 (2017)

S. Schnabel, W. Janke: *Dynamic Greedy Algorithms for the Edwards-Anderson Model*, Comput. Phys. Commun. **220**, 74–80 (2017)

S. Schneider, M. Mueller, W. Janke: *Convergence of Stochastic Approximation Monte Carlo and Modified Wang-Landau Algorithms: Tests for the Ising Model*, Comput. Phys. Commun. **216**, 1–7 (2017)

M. Weigel, L.Yu. Barash, M. Borovský, W. Janke, L.N. Shchur: *Population Annealing: Massively Parallel Simulations in Statistical Physics*, in *Computer Simulation Studies in Condensed-Matter Physics XXX*, eds. D.P. Landau, M. Bachmann, S.P. Lewis, H.-B. Schüttler, J. Phys.: Conf. Ser. **921**, 012017-1–10 (2017)

J. Zierenberg, N. Fricke, M. Marenz, F.P. Spitzner, V. Blavatska, W. Janke: *Percolation Thresholds and Fractal Dimensions for Square and Cubic Lattices with Long-Range Correlated Defects*, Phys. Rev. E **96**, 062125-1–11 (2017)

J. Zierenberg, N.G. Fytas, M. Weigel, W. Janke, A. Malakis: *Scaling and Universality in the Phase Diagram of the 2D Blume-Capel Model*, Eur. Phys. J. – Special Topics **226**, 789–804 (2017)

J. Zierenberg, P. Schierz, W. Janke: *Canonical Free-Energy Barrier of Particle and Polymer Cluster Formation*, Nat. Commun. **8**, 14546-1–7 (2017)

J. Zierenberg, K. Tholen, W. Janke: *Effect of Grafting on the Binding Transition of Two Flexible Polymers*, Eur. Phys. J. – Special Topics **226**, 683–692 (2017)

in press

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

S. Schnabel, W. Janke: *Distribution of Metastable States of Spin Glasses*, to appear 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. (2018), in print

Talks

H. Christiansen, S. Majumder, W. Janke: *The Influence of Bond Fluctuations on the Coarsening and Aging of Lattice Polymers*, Joint Steering Committee Meeting of the IRSES Projects DIONICOS and STREVCOMS, Lviv, Ukraine, 14. June 2017

H. Christiansen, S. Majumder, W. Janke: *Efficient Method of Simulating with Long-Range Interactions: The Case of Coarsening in the Ising Model*, 18th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys17*, Universität Leipzig, Germany, 30. November – 02. December 2017

J. Gross, M. Ivanov, W. Janke: *Poly(3-hexylthiophene) Interacting with Gold and "other" Striped Substrates*, 1st Discussion Meeting HalLei17, Universität Leipzig, Germany, 19. July 2017

W. Janke: *Canonical Free-Energy Barrier of Particle and Polymer Cluster Formation*, Conference of the Middle European Cooperation in Statistical Physics – MECO42, Lyon, France, 08.–10. February 2017

W. Janke: *The Real Microcanonical Ensemble: Free-Energy Barriers for Particle and Polymer Aggregation*, 30th Annual CSP Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, USA, 20.–24. February 2017

W. Janke: *Knots as Stable Topological Order Parameter for Semiflexible Polymers*, invited talk ("Hauptvortrag"), Focus Session *Topological Problems in the Physics of Polymers, Biopolymers and Fibers* within DPG Frühjahrstagung 2017, TU Dresden, Germany, 23.–24. March 2017

W. Janke: *Knots as Stable Topological Order Parameter for a Semiflexible Polymer*, Workshop on *Polymer Physics and Chemistry*, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, China, 27.–30. March 2017

W. Janke: *Exact Enumeration of Self-Avoiding Walks on Critical Percolation Clusters in Two to Seven Dimensions*, ICMP Workshop, Lviv, Ukraine, 14.–16. June 2017

W. Janke: *Exact Enumeration of Self-Avoiding Walks on Critical Percolation Clusters in Two to Seven Dimensions*, International Workshop and Young Scientist School on *Critical Phenomena and Phase Transitions CPPT17*, A.I. Alikhanyan National Science Laboratory, Yerevan, Armenia, 20.–24. September 2017

W. Janke: *From Particle Condensation in the Ising Lattice Gas to Polymer Aggregation: Computer Simulation Studies*, invited talk, Workshop on *Stochastic Spin Systems: models, theory, simulation and real world applications*, ZIF Bielefeld, Germany, 28.–30. September 2017

W. Janke: *From Particle Condensation to Polymer Aggregation*, invited plenary talk, International Conference on *Computer Simulation in Physics and beyond*, National Research University Higher School of Economics, Moscow, Russia, 09.–12. October 2017

M. Kumar, R. Kumar, V. Banerjee, S. Puri, M. Weigel, W. Janke: *Approximate Ground States of the Random-Field Potts Model from Graph Cuts and Parallel Tempering*, DPG Frühjahrstagung 2017, TU Dresden, Germany, 19.–24. March 2017

S. Majumder, H. Christiansen, W. Janke: *Universal Scaling for Coarsening and Aging During Collapse of a Polymer*, 1st Discussion Meeting HalLei17, Universität Leipzig, Germany, 19. July 2017

S. Majumder, W. Janke: *Scaling laws in Kinetics of Collapse of a Polymer*, International Conference on *Computer Simulation in Physics and beyond*, Moscow, Russia, 09.–12. October 2017

S. Schnabel, W. Janke: *Coarse-Graining the State Space of a Spin Glass*, 18th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys17*, Universität Leipzig, Germany, 30. November – 02. December 2017

M. Weigel, L.Yu. Barash, L.N. Shchur, W. Janke: *Understanding Population Monte Carlo Simulations*, DPG Frühjahrstagung 2017, TU Dresden, Germany, 19.–24. March 2017

Posters

H. Christiansen, S. Majumder, W. Janke: *The Influence of Bond Fluctuations on the Coarsening and Aging of Lattice Polymers*, Soft Matter Day, Universität Leipzig, Germany, 23. June 2017

J. Gross, W. Janke: *Monte Carlo Studies of Polymer Aggregation*, International Discussion Meeting on *Polymer Crystallization 2017 – From Classical Systems to Functional Materials and Biopolymers*, Wittenberg, Germany, 17.–20. September 2017

J. Gross, M. Ivanov, D.N. Oberthür, W. Janke: *Monte Carlo Studies of P3HT Aggregation*, 18th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys17*, Universität Leipzig, Germany, 30. November – 02. December 2017

S. Kazmin, W. Janke: *Site-Diluted Ising Model in Two Dimensions – Towards Long-Range Correlated Defects* 18th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys17*, Universität Leipzig, Germany, 30. November – 02. December 2017

S. Majumder, W. Janke: *Universal Scaling of Cluster growth and Aging During Collapse of a Polymer*, DPG Frühjahrstagung 2017, TU Dresden, Germany, 19.–24. March 2017

F. Müller, S. Schnabel, W. Janke: *Non-Flat Histogram Methods for Spin Glasses*, 18th International NTZ-Workshop on *New Developments in Computational Physics – Comp Phys17*, Universität Leipzig, Germany, 30. November – 02. December 2017

F.P. Spitzner, J. Zierenberg, W. Janke: *Two Perspectives on the Condensation-Evaporation Transition*, 18th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys17*, Universität Leipzig, Germany, 30. November – 02. December 2017

12.31 Graduations

Doctorate

- Philipp Schierz
  Liquid-Gas-Like Phase Transitions in Various Ensembles: A Computational Study of Liquid-Gas-Like Phase Transitions with Various Simulation Techniques and a Focus on Polymer Aggregation
  11. January 2017

Master

- Franz Paul Spitzner
  Two Perspectives on the Condensation-Evaporation Transition of the Lennard-Jones Gas in 2D
  06. July 2017
- Fabio Müller
  Non-Flat Histogram Methods for Spin Glasses
  12. September 2017

Bachelor

- Christopher Allen
  Microcanonical Simulations of Phase Transitions in the Potts Model
  04. October 2017

12.32 Guests

- Prof. Dr. George Savvidy
  Demokritos Nat. Res. Center, Athens, Greece

NTZ/DFH-UFA Colloquium (03. November 2016)
The Gonihedric Ising Model
01. November 2016 – 31. January 2017

- Prof. Dr. Subir K. Das
Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India
18.–21. May 2017

- Prof. Dr. Ulrich H.E. Hansmann
University of Oklahoma, Norman, USA
Sabbatical, NTZ/DFH-UFA Seminar (12. September 2017)
Direct Coupling Analysis
01. June – 31. December 2017

- Dr. Lev Yu. Barash
Landau Institute, Chernogolovka, Russia
NTZ/DFH-UFA and EU IRSES Network DIONICOS Colloquium (08. June 2017)
Applying Population Annealing to First- and Second-Order Phase Transitions
02.–12. June 2017

- Prof. Dr. Lev Shchur
Landau Institute, Chernogolovka, Russia
04.–10. June 2017

- Prof. Dr. Handan Arkın-Olgar
Ankara University, Turkey
Alexander-von-Humboldt Fellowship for Experienced Researchers
15. June – 15. September 2017

- Marina Fadeeva
Landau Institute, Chernogolovka, and Higher School of Economics, Moscow, Russia
NTZ/DFH-UFA and EU IRSES Network DIONICOS Colloquium (20. July 2017)
Control of Accuracy in the Wang-Landau Algorithm
27. June – 28. July 2017

- Dr. Johannes Zierenberg
Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany
NTZ/DFH-UFA Seminar (07. July 2017)
Homeostatic Plasticity in Neural Networks Induces a Diverse Range of Dynamic States
06.–08. July 2017

- Prof. Dr. Jutta Luettmer-Strathmann
University of Akron, Ohio, USA
1st Discussion Meeting HalLei17 (19. July 2017)
Sexithiophene Phase Diagram from Simulations of a Gay-Berne Type Model
19. July 2017

- Prof. Dr. Mark P. Taylor
Dept. of Physics, Hiram College, USA
1st Discussion Meeting HalLei17 (19. July 2017)
Polymer Collapse and Folding in a Crowded Environment
19. July 2017

- Kseniia Shapovalova
  Far Eastern Federal University, Vladivostok, Russia
  DAAD Michail-Lomonosov-Programm
  NTZ/DFH-UFA Seminar (09. November 2017)
  High-Performance Algorithms for the Research of Frustrated Systems of Spin Ice and Spin Glass
  01. October 2017 – 31. March 2018

- Dr. Khristine Haydukivska
  ICMP, National Academy of Sciences of Ukraine, Lviv, Ukraine
  22. November – 09. December 2017

- Dr. Viktoria Blavatska
  ICMP, National Academy of Sciences of Ukraine, Lviv, Ukraine
  01. – 31. December 2017

- Dr. Elmar Bittner
  Universität Heidelberg, Germany
  On the Interface Tension of the Ising Model
  29. November – 02. December 2017

- Dr. Nathan Clisby
  Swinburne University of Technology, Hawthorn, Victoria, Australia
  Efficient Implementation of Connectivity Changing Moves for Dense Polymers
  29. November – 02. December 2017

- Dr. Eren Metin Elçi
  Monash University, Clayton, Victoria, Australia
  On Critical Speeding-up in an Irreversible Worm Dynamics for High-Dimensional Ising Models
  29. November – 02. December 2017

- Dr. Nikolaos Fytas
  Coventry University, England, UK
  On the Effect of Disorder on First-Order Phase Transitions: The Case of the 2D Random-Bond Blume-Capel Model
  29. November – 02. December 2017

- Dr. Antonio Gordillo
  Universidad de Extremadura, Badajoz, Spain
  Crumpling Transition and Low-Temperatures Properties of Crystalline Membranes with Perforation Patterns
  29. November – 02. December 2017

- Prof. Dr. Ulrich H.E. Hansmann
  University of Oklahoma, Norman, OK, USA
  Enhanced Sampling Simulations of Folding and Aggregation
  29. November – 02. December 2017

- Prof. Dr. Alexander Hartmann
  Universität Oldenburg, Germany
  High-Precision Simulation of Height Distribution for Directed Polymers in Random

Media
29. November – 02. December 2017

- Priv.-Doz. Dr. Martin Hasenbusch
Humboldt Universität zu Berlin, Germany
Interface Tension and the Cluster Exchange Algorithm
29. November – 02. December 2017

- Dr. Hsiao-Ping Hsu
MPI Polymer Research, Mainz, Germany
Non-Linear Viscoelasticity of Highly Strained Polymer Melts: Primitive Path Analysis
29. November – 02. December 2017

- Dr. Fred Hucht
Universität Duisburg-Essen, Germany
Analytic Finite-Size Scaling Functions in the Anisotropic Ising Rectangle
29. November – 02. December 2017

- Prof. Dr. Ferenc Igloi
Wigner Research Centre, Budapest, Hungary
Contact Process in Inhomogeneous Environment
29. November – 02. December 2017

- Prof. Dr. Viktor Ivanov
Moscow State University, Russia
29. November – 02. December 2017

- Prof. Dr. Desmond A. Johnston
Heriot-Watt University, Edinburgh, Scotland, UK
Spin Chain SUSY
29. November – 02. December 2017

- Prof. Dr. David P. Landau
The University of Georgia, Athens, GA, USA
Complexity and Optimization: Physical Science Meets Biological Science via Computer Simulations
29. November – 02. December 2017

- Daria Maltseva
Moscow State University, Russia
29. November – 02. December 2017

- Prof. Dr. Arnulf Möbius
IFW Dresden, Germany
Simulated Annealing, Effective but Inefficient? A Case Study for the 3D136 Instance of the HP Model of Protein Folding
29. November – 02. December 2017

- Prof. Dr. Juan J. Ruiz-Lorenzo
Universidad de Extremadura, Badajoz, Spain
Numerical Construction of the Aizenman-Wehr Metastate
29. November – 02. December 2017

- Prof. Dr. Lev N. Shchur
  Landau Institute and Science Center, Chernogolovka, Moscow Region, Russia
  Control of Accuracy in the Wang-Landau Algorithm
  29. November – 02. December 2017
- Dr. Francesco Parisen Toldin
  Universität Würzburg, Germany
  Finite-Size Effects in Canonical and Grand-Canonical Quantum Monte Carlo Simulations for Fermions
  29. November – 02. December 2017
- Dr. Erol Vatansever
  Dokuz Eylul University, Izmir, Turkey
  Dynamically Order-Disorder Transition in Triangular Lattice Driven by a Time Dependent Magnetic Field
  29. November – 02. December 2017
- Dr. Zeynep Demir Vatansever
  Dokuz Eylul University, Izmir, Turkey
  Monte Carlo Study of Hysteresis Features of a Cylindrical Nanowire under Quenched Disorder
  29. November – 02. December 2017
- Dr. Dimitris Voliotis
  University of Sao Paulo, Brazil
  Critical Behavior of the Quantum Potts Chain with Aperiodic Perturbation
  29. November – 02. December 2017
- Dr. Johannes Zierenberg
  Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany
  Diversity of Dynamic States in Neural Networks induced by Homeostatic Plasticity
  29. November – 02. December 2017

13

Molecular Dynamics / Computer Simulation

13.1 Introduction

Introductory text ...

Group Leader

13.2 Contribution 1

J. Doe, M. Mustermann, A.U. Thor*, A. Uthor†, A.U.T. Hor*

*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)
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) ...

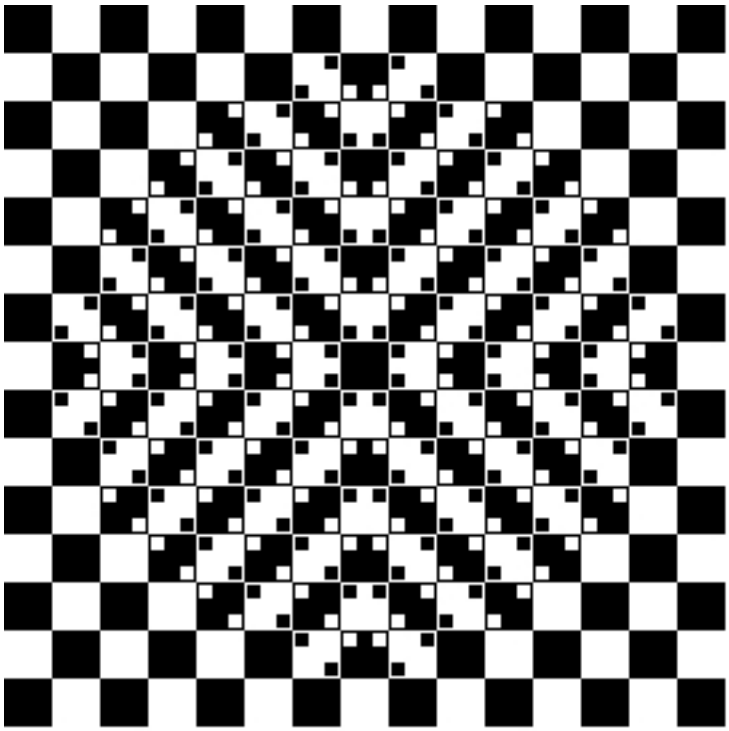

Figure 13.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

[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

14

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†, A.U.T. Hor*

*Institution 1
†Institution 2

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

Table 14.1: 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 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) ...

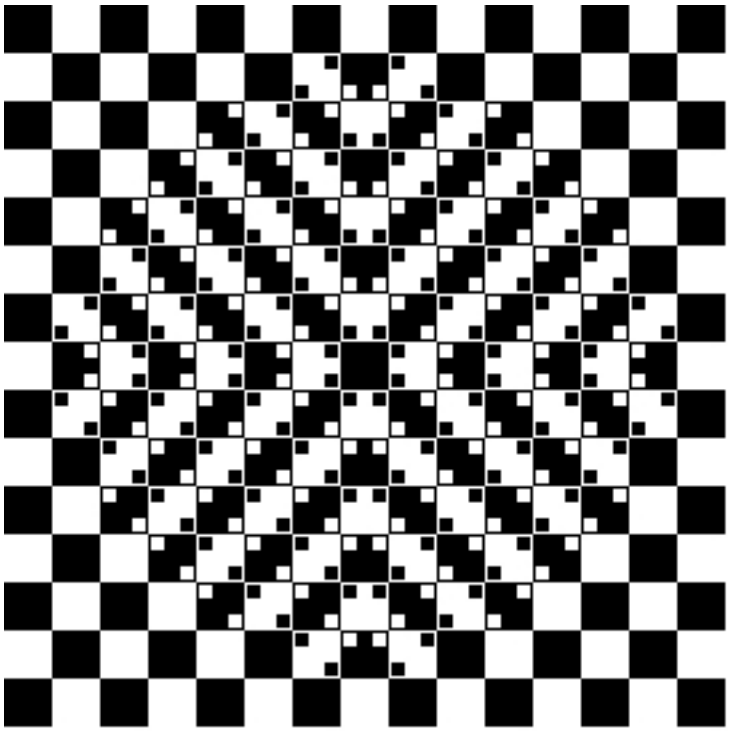

Figure 14.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

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

in press

Reference 3

Reference 4

Talks

Talk 1

Talk 2

Posters

Poster 1

Poster 2

14.8 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

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*, A. Uthor†, A.U.T. Hor*

*Institution 1
†Institution 2

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

Table 15.1: 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.
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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) ...

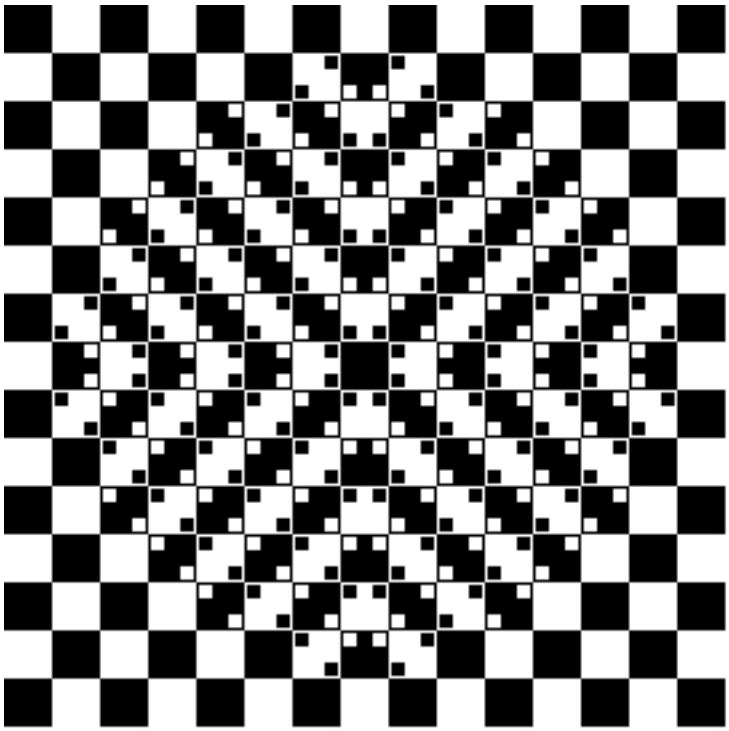

Figure 15.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

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

15.4 Funding

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
- Name 2
  Thesis Title
  Graduation Date

Diploma

- Name 1
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  Thesis Title
  Graduation Date

Master

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  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*, A. Uthor†, A.U.T. Hor*

*Institution 1
†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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[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) ...

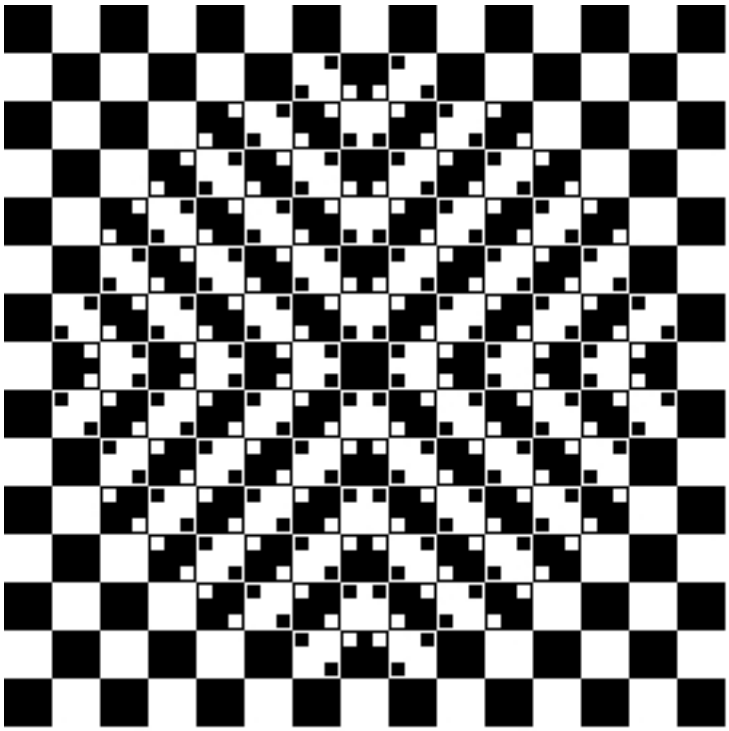

Figure 16.1: Test figure (©Akiyoshi Kitaoka – see [1] for more information).

[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

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  Thesis Title
  Graduation Date
- Name 2
  Thesis Title
  Graduation Date

Diploma

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  Graduation Date
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  Graduation Date

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  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*, A. Uthor†, A.U.T. Hor*

*Institution 1
†Institution 2

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

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

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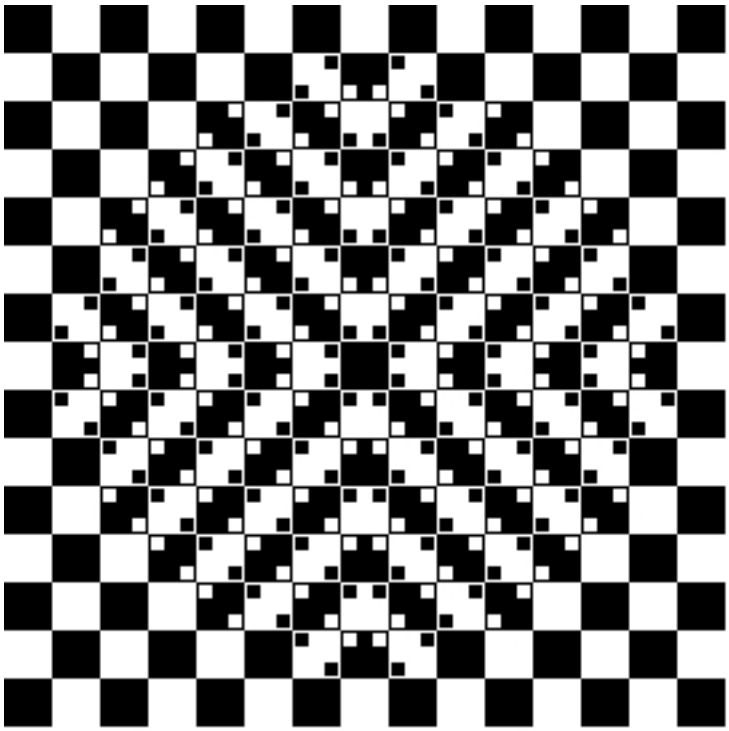
[2] Reference 2

17.3 Contribution 2

J. Doe, M. Mustermann

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



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

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17.5 Organizational Duties

Person 1

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- Duty 2

Person 2

- Duty 1
- Duty 2

17.6 External Cooperations

Academic

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  Collaborator(s)
- Institution 3
  Collaborator(s)

Industry

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

17.7 Publications

Journals

Reference 1

Reference 2

Books

Book 1

Book 2

in press

Reference 3

Reference 4

Talks

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Talk 2

Posters

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Poster 2

17.8 Graduations

Doctorate

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  Graduation Date
- 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