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Curriculum vitae

10 February 1944	I was born in Korneuburg, Austria to Eduard Binder, technical engineer and Anna Binder, née Eppel
1950 – 1962	Public schools of Vienna, Austria
1962 – 1969	Studies in Technical Physics at the Technical University of Vienna, Austria
9 March 1965 2 June 1967	I State board examination II State board examination (Diploma in Physics)
1967 – 1969	Doctoral thesis at the Austrian Institute of Atomic Physics, Vienna: "Berechnung der Spinkorrela- tionsfunktionen von Ferromagnetika" (Calculation of the spin correlation functions in ferromagnets)
21 March 1969	PhD in "Technical Sciences"
1969	Karoline & Guido Krafft-Medal, Techn. Univ. Vienna, Austria
1 February 1969 - 15 September 1969	Assistant to Prof. Dr. G. Ortner at the Austrian Academic Institute of Atomic Physics, Vienna
15 September 1969 - 30 September 1974	Scientific assistant in Physics Dept. E 14 at the Technical University of Munich, Germany (Prof. Dr. H. Maier-Leibnitz and Prof. Dr. H. Vonach)
1 April 1972 - 31 March 1973	IBM postdoctoral fellow at IBM Zürich Research Laboratory, 8803 Rüschlikon, Switzerland
13 November 1973	Professorship offered for Theoretical Physics of Condensed Matter at the Free University of Berlin, Germany (which I declined)
20 December 1973	Qualification as university professor of physics ("Habilitation") at the Technical University of Munich, Germany
1 April 1974 - 30 September 1974	Research consultant at Bell Laboratories in Murray Hill, NJ, USA (as guest of Dr. P. C. Hohenberg)
1 October 1974 - 30 September 1977	Professor of Theoretical Physics at the University of Saarland in Saarbrücken, Germany
15 July 1977	Marriage with Marlies Ecker (born 12 December 1948 in St. Wendel/Saar)

1 October 1977 - 30 September 1983	Full Professor at the University of Cologne, Germany in joint appointment at the Kernforschungsanlage (KFA) Jülich, with leave of absence to direct the Institute of Theory II at the Institute of Solid State Research (IFF), Jülich
5 June 1978	Birth of my son Martin
30 April 1981	Birth of my son Stefan
since October 1983	Full Professor for Theoretical Physics at the Johannes Gutenberg-University in Mainz, Germany
2 December 1986 – December 1992	Appointment to the Technology Advisory Board for the German federal state Rhineland-Palatinate
1985	The chair offered to me at Florida State University, Tallahassee, with a research group lead at SCRI, Super-computer Computations Research, I also declined
May 1986 – Jan 1996	Chairman of the Coordination Committee of the Materials Research Center (MWFZ) at the University of Mainz
since Feb. 1987	"adjunct professor" at the Center for Simulational Physics, Univ. of Georgia, USA
July 1987 – Dec. 2001	Speaker for Special Research Program SFB 262, funded by the German National Research Foundation DFG for research on "The glass state and glass transition of non-metallic amorphous materials"
July 1987 – July 1995	Appointment to the "Scientific Advisory Board" at HLRZ high-performance computing center in Jülich, Germany
1988 – 1990 and 1996 – 1999	Member of the IUPAP Commission C3 "Thermodynamics and Statistical Physics" as well as the DNK (German national committee for IUPAP)
29 November 1988	Position offered as Director of the Max Planck Institute for Polymer Research (Mainz), which I refused
20 June 1989	Appointment as External Member of the Max Planck Society
12 May 1992	Appointment as Corresponding Member of the Austrian Academy of Sciences, Vienna
24 March 1993	Receipt of the Max Planck Medal awarded by the German Physical Society (DPG)
1999 – 2002	Chairman of the IUPAP C3 Commission and Member of the IUPAP Executive Council
2001	Distinguished as "Highly Cited Researcher" by ISI, Philadelphia ("Top 100" List in Science Citation Index 1981-1999)
2001 (Sept. 6th)	Berni J. Alder CECAM Prize (for Computational Physics) of the EPS

2003 (Jan. 15th) – 2005 (April 30th)	Elected for 2 years as the Chairman of the Physics Department
2003 (Jan. 24th)	The Staudinger-Durrer-Prize (for outstanding contributions to Monte Carlo Simulations) of the ETH Zürich
2003 (Feb. 21th)	Appointment as Member of the Academy of Sciences and Literature, Mainz
since 2006	Honorary Member of the British Institute of Physics (IOP)
2003 (Oct.) - 2006 (Sept.)	Member of the University Council of the University of Stuttgart
2005 (Nov. 2nd)	Appointment as External Member of the Bulgarian Academy of Sciences, Sofia, Bulgaria
2007 (Jan. 24th)	Honorary Ph.D. in Chemistry, Maria Curie-Sklodowska Univ. Lublin, Poland
2007 (July 11th)	Receipt of the Boltzmann Medal of IUPAP
2007 (Oct. 2007)	Receipt of the Gutenberg Fellowship of the Johannes Gutenberg University Mainz
2008 - 2013	Scientific Advisory Board of the Max Planck Institute for Colloid- and Interface Research, Potsdam
since 2009	Member of the "Rat für Technology, Rheinland-Pfalz"
2009 (Sept. 23rd)	Receipt of the Lennard-Jones Medal by the Royal Society of Chemistry, London.
2010 – 2012	Member of the Scientific Steering Committee of the Partnership for Advanced Computing in Europe (PRACE)
2011	Deputy Chair of the Scientific Council of the John von Neumann Institute for Computing (NIC), Jülich
April 2011	Appointment as member of the German Academy of Sciences Leopoldina/Halle/Germany
2012 - 2017	Chair of the Scientific Council of the john von Neumann Institute for Computing (NIC) Jülich
2012 - 2017	Vice-chair of the Steering Committee of the Gauss Center for Supercomptuing
since April 1st, 2012	retired from active service as Professor emeritus
Sept. 19th, 2012	Honorary Medal "Marin Drinov" of the Bulgarian Academy of Sciences

Jan. 30th, 2013	Honorary PhD by the Mathematical & Natural Science Department/Faculty of the Heinrich-Heine University Duesseldorf for outstanding contributions to the special research field "TR6" "Physics of colloidal dispersions in external fields"
since Jan 1st, 2018	Deputy chairman of the John von Neumann Institute for Computing (NIC) Jülich

Supervision of Ph.D. theses/Betreuung von Doktorarbeiten

Prior to the "Habilitation" (1973), only an "inofficial" Ph.D. advisor status was possible for the following two cases:

(i) Volker Wildpaner "Berechnung der Magnetisierung um Gitterfehler in einem Heisenberg Ferromagneten" Technische Hochschule Wien, 1972

(ii) Heiner-Müller-Krumbhaar "Bestimmung kritischer Exponenten am Heisenberg-Ferromagneten mit einem selbstkonsistenten Monte-Carlo Verfahren" Physik-Department, Technische Hochschule München, 1972

A) Universität des Saarlandes, Saarbrücken

1. Artur Baumgärtner "Die verallgemeinerte kinetische Ising-Kette: Ein Modell für die Dynamik von Biopolymeren" 1977

2. Claudia Billotet "Nichtlineare Relaxation bei Phaseübergängen: Eine Ginzburg-Landau Theorie mit Fluktuationen" 1979

3. Rüdiger Kretschmer "Kritisches Verhalten und Oberflächeneffekte von Systemen mit lang- und kurzreichweitigen Wechselwirkungen: Phänomenologische Theorie und Monte Carlo Simulation" 1979

4. Ingo Morgenstern "Ising Systeme mit eingefrorener Unordnung in zwei Dimensionen" 1980

B) Universität zu Köln

5. Kurt Kremer "Untersuchungen zur statistischen Mechanik von linearen Polymeren unter verschiedenen Bedingungen" 1983

6. Jozsef Reger "Untersuchungen zur statistischen Mechanik von Spingläsern" 1985

C) Johannes Gutenberg Universität

7. Ingeborg Schmidt "Oberflächenanreichung und Wettingphasenübergänge in Polymermischungen" 1986

8. Jannis Batoulis "Monte Carlo Simulation von Sternpolymeren" 1987

9. Hans-Otto Carmesin "Modellierung von Orientierungsgläsern" 1988

10. Wolfgang Paul "Theoretische Untersuchungen zur Kinetik von Phasenübergängen erster Ordnung" 1989

11. Manfred Scheucher “Phasenverhalten und Grundzustandseigenschaften kurzreichweitiger Pottsgläser” 1990

12. Hans-Peter Wittmann “Monte Carlo Simulationen des Glasübergangs von Polymerschmelzen im Rahmen des Bondfluktuationsalgorithmus” 1991

13. Burkhard Dünweg “Molekulardynamik-Untersuchungen zur Dynamik von Polymerketten in verdünnter Lösung” 1991

14. Friederike Schmid “Volumen-Grenzflächeneigenschaften von Modellen kubisch-raumzentrierter binärer Legierungen: Untersuchung mittels Monte Carlo Simulation” 1991

15. Hans-Peter Deutsch “Computer-Simulation von Polymer-Mischungen ” 1991

16. Werner Helbing “Quanten Monte Carlo Simulation eines Rotatormoleküls” 1992

17. Dominik Marx “Entwicklung von Pfadintegral Monte Carlo Methoden für adsorbierte Moleküle mit inneren Quantenfreiheitsgraden” 1992

18. Gernot Schreider “Hochtemperaturreihenentwicklungen zum geordneten und ungeordneten Potts-Modell” 1993

19. Jörg Baschnagel “Monte Carlo Simulationen des Glasübergangs und Glaszustandes von dichten dreidimensionalen Polymerschmelzen” 1993

20. Marco d’Onorio de Meo “Monte Carlo Methoden zur Untersuchung reiner und verdünnter Ferromagnete mit kontinuierlichen Spins” 1993

21. Marcus Müller “Monte Carlo Simulation zur Thermodynamik und Struktur von Polymer-Mischungen” 1994

22. Klaus Eichhorn “Pottsmodelle zu Zufallsfeldern” 1995

23. Frank M. Haas “Monolagen steifer Kettenmoleküle auf Oberflächen. Eine Monte Carlo Simulationsuntersuchung” 1995

24. Matthias Wolfgardt “Monte Carlo Simulation zur Zustandsgleichung glasartiger Polymerschmelzen” 1995

25. Martin H. Müser “Klassische und quantenmechanische Computer Simulationen zur Orientierungsgläsern und Kristallen” 1995

26. Stefan Kappler “Oberflächenspannung und Korrelationslängen im Pottsmodell” 1995

27. Felix S. Schneider “Quanten-Monte-Carlo-Computersimulationsstudie der Dynamik des inneren, quantenmechanischen Freiheitsgrades eines Modell-Fluids in reeller Zeit” 1995

28. Katharina Vollmayr “Abkühlungsabhängigkeiten von strukturellen Gläsern: Eine Computersimulation” 1995

29. Volker Tries “Monte Carlo Simulationen realistischer Polymerschmelzen mit einem vergröberten Modell” 1996

30. Martina Kreer “Quantenmechanische Anomalien bei Phasenübergängen in 2D: Eine Pfadintegral-Monte-Carlo Studie zu H_2 und O_2 physisorbiert auf Graphit” 1996

31. Bernhard Lobe “Stargraph-Entwicklungen zum geordneten und ungeordneten Potts-Modell und deren Analysen” 1997

32. Stefan Kämmerer “Orientierungsdynamik in einer unterkühlten Flüssigkeit: eine MD-Simulation” 1997

33. Henning Weber “Monte Carlo-Simulationen der Gasdiffusion in Polymermatrizen” 1997

34. Rüdiger Sprengard “Raman-spectroscopyin $Li_2O \cdot Al_2O_3 \cdot SiO_3$- glass ceramics: Simulation and crystal spectra and experimental investigations on the Ceramization "1998

35. Frank F. Haas “Oberflächeninduzierte Unordnung in binären bcc Legierungen” 1998

36. Jürgen Horbach “Molekulardynamiksimulationen zum Glasübergang von Silikatschmelzen” 1998

37. Matthias Presber “Pfadintegral-Monte Carlo Untersuchungen zu Phasenübergängen in molekularen Festkörpern” 1998

38. Christoph Stadler “Monte Carlo Simulation in Langmuir Monolagen” 1998

39. Andres Werner “Untersuchung von Polymer-Grenzflächen mittels Monte Carlo Simulationen” 1998

40. Christoph Bennemann “Untersuchung des thermischen Glasübergangs von Polymer-schmelzen mittels Molekular-Dynamik Simulationen” 1999

41. Tobias Gleim “Relaxation einer unterkühlten Lennard-Jones Flüssigkeit” 1999

42. Fathollah Varnik “Molekulardynamik-Simulationen zum Glasübergang in Makromolekularen Filmen” 2000

43. Dirk Olaf Löding “Quantensimulationen physisorbierter Molekülschichten auf Graphit: Phasenübergänge, Quanteneffekte, und Glaseigenschaften” 2000

44. Alexandra Roder “Molekulardynamik-Simulationen zu Oberflächeneigenschaften” von Siliziumdioxidschmelzen“ 2000

45. Oliver Dillmann “Monte Carlo Simulationen des kritischen Verhaltens von dünnen” Ising Filmen” 2000

46. Harald Lange “Oberflächengebundene flüssigkristalline Polymere in nematischer Lösung: eine Monte Carlo Untersuchung” 2001

47. Peter Scheidler “Dynamik unterkühlter Flüssigkeiten in Filmen und Röhren” 2001

48. Claudio Brangian “Monte Carlo Simulation of Potts-Glasses” 2002

49. Torsten Kreer “Molekulardynamik-Simulation zur Reibung zwischen polymerbeschichten Oberflächen” 2002

50. Stefan Krushev “Computersimulationen zur Dynamik und Statistik von Polybutatien-schmelzen” 2002

51. Susanne Metzger “Monte Carlo Simulationen zum Adsorptionsverhalten von Homo-Copolymeren” 2002

52. Claus Mischler “Molekulardynamik-Simulation zur Struktur von SiO_2-Oberflächen mit adsorbiertem Wasser” 2002

53. Ellen Reister “Zusammenhang zwischen der Einzelkettendynamik und der Dynamik von Konzentrationsfluktuationen in mehrkomponentigen Polymersystemen: dynamische Mean-Field Theorie und Computersimulation” 2002

54. Anke Winkler “Molekulardynamik-Untersuchungen zur atomistischen Struktur und Dynamik von binären Mischgläsern Na_2O_2 und (Al_2O_3) $(2SiO_2)$” 2002

55. Martin Aichele “Simulation Studies of Correlation Functions and Relaxation in Polymeric Systems” 2003

56. Peter M. Virnau “Monte Carlo Simulationen zum Phasen-und Keimbildungsverhalten von Polymerlösungen” 2003

57. Daniel Herzbach “Comparison of Model Potentials for Molecular Dynamics Simulation of Crystallline Silica” 2004

58. Hans R. Knoth “Molekular-Dynamik-Simulation zur Untersuchung des Mischalkali-Effekts in silikatischen Gläsern” 2004

59. Florian Krajewski “New path integral simulation algorithms and their application to creep in the quantum sine-Gordon chain” 2004

60. Ben Jesko Schulz “Monte Carlo Simulation of Interface Transitions in Thin Film with Competing Walls” 2004

61. Torsten Stühn “Molekular-Dynamik Computersimulation einer amorph-kristallinen SiO_2 Grenzschicht” 2004

62. Ludger Wenning “Computersimulation zum Phasenverhalten binärer Polymerbürsten ” 2004

63. Juan Guillermo Diaz Ochoa “Theoretical investigation of the interaction of a polymer film with a nanoparticle” 2005

64. Federica Rampf “Computer Simulationen zur Strukturbildung von einzelnen Polymerketten” 2005

65. Michael Hawlitzky “Klassische und ab initio Molekulardynamik-Untersuchungen zu Germaniumdioxidschmelzen” 2006

66. Andrea Ricci “Computer Simulations of two-dimensional colloidal crystals in confinement” 2006

67. Antione Carré “Development of emperical potentials for liquid silica” 2007

68. Swetlana Jungblut “Mixtures of colloidal rods and spheres in bulk and in confinement” 2008

69. Yulia Trukhina “Monte Carlo Simulation of Hard Spherocylinders under confinement” 2009

70. Leonid Spirin “Molecular Dynamics Simulations of sheared brush-like systems” 2010

71. Daniel Reith “Computersimulationen zum Einfluß topologischer Beschränkungen auf Polymere” 2011

72. Alexander Winkler “Computer simulations of colloidal fluids in confinement” 2012

73. David Winter “Computer simulations of slowly relaxing systems in external fields” 2012

74. Dorothea Wilms “Computer simulations of two-dimensional colloidal crystals under confinement and shear” 2013

75. Benjamin Block “Nucleation Studies on Graphics Processing Units” 2014

76. Fabian Schmitz “Computer Simulation Methods to study Interfacial Tensions: From the Ising Model to Colloidal Crystals” 2014

77. Antonia Statt “Monte Carlo Simulations of Nucleation of Colloidal Crystals” 2015

78. Peter Koss “Computer Simulations on Homogeneous Nucleation ion Crystalline Systems” 2018

Main Research Interests

1. Monte Carlo simulation as a tool of computational statistical mechanics to study phase transitions

A main research goal has been to develop Monte Carlo techniques for the numerical study of classical interacting many body systems, with an emphasis on phase transitions in condensed matter [33,41,76,153,189,205,244,321,491,551,630,970,1132, number refer to the list of publications, see:publication list Binder.] A central obstacle to overcome are finite size effects: Ising and classical Heisenberg ferromagnets [5] exhibit the “finite size tail” in the root mean square magnetization, which is strongly enhanced near the critical point (due to the divergence of correlation length and susceptibility in the thermodynamic limit), leading to finite size rounding and shifting of the transition [16,29]. Combining this starting point with the finite size scaling theory developed by M.E. Fisher at about the same time, numerous promising first studies of phase transitions were given [33,41,75,76,92,103] but the main breakthrough came from a study of the order parameter probability distribution and its fourth order cumulant [135]. For different system sizes the cumulants (studied as function of the proper control parameter, e.g. temperature) intersect at criticality at an (almost) universal value, and this allows an easy and unbiased estimation of the critical point location. This method has helped to study phase transitions and phase diagrams of many model systems and now is widely used by many research groups. A recent extension of this finite-size scaling analysis of phase transitions [1179] has considered the case of first order transitions. While for the case of the order-disorder transition of the q-state Potts model the q-fold degeneracy of the ordered phase leads to a finite-size shift of the transition temperature, proportional to ln(q), it had been unclear what the analogy of the degeneracy number q is when a continuous symmetry is broken. In [1179] it is argued that $q=\pi$, in the case where a XY-like order parameter occurs. It was also shown that the first and second moments of the order parameter distribution also exhibit unique (universal) intersection points, in addition to the cumulant intersection. Thus, 50 years after the first formulation of finite-size scaling concepts still gaps in the description needed to be filled. Lattice models for adsorbed monolayers at crystal surfaces have been studied to clarify corresponding experiments (e.g. H on Pd (100) [127], H on Fe (100) [145,154] or CO and N_2 on graphite [398,411]. Lattice models for solid alloys have been used to understand the ordering in Cu-Au alloys [16,124,210,215], of Fe-Al alloys [355,380], and of magnetic ordering of EuS diluted with SrS [86,103,105]. Recently finite size scaling methods have also been used to study off-lattice models for the $\alpha - \beta$ phase transition in SiO_2 [676] and the vapor-liquid phase transitions of CO_2 [916] and various liquid mixtures [943] and good agreement with

experiment was found. The technique could also be extended to very asymmetric systems, such as the Asakura-Oosawa model for colloid-polymer mixtures [823] and rod-sphere mixtures [910].

Since finite size scaling in its standard formulation needs "hyperscaling" relations between critical exponents to hold (see e.g. [135]), nontrivial generalizations needed to be developed for cases where hyperscaling does not hold, such as model systems in more than 4 space dimensions [184,195,596] and Ising-type systems with quenched random fields (such as colloid-polymer mixtures inside a randomly-branched gel) [883,939,1016]. Other generalizations concern anisotropic critical phenomena [261], e.g. critical wetting transitions [1061,1068,1095], and crossover from one universality class to another [369,524,593], e.g. when the effective interaction range increases the system criticality changes to become mean-field like (an application being binary polymer blends when the chain length of the macromolecules increases [414]). An important task in the study of phase transitions by simulations is the distinction of second order phase transitions from first-order ones, a problem studied in collaboration with David Landau since also the latter are rounded (and possibly shifted) by finite size (e.g. [182,212,262,375,1066]). Some of the "recipes" developed to study phase transitions by simulations using Monte Carlo methods are reviewed in [201,375,656,912]; we also note that finite size scaling concepts are also useful for Molecular Dynamics methods, and then allow also the study of dynamic critical behavior of fluids [801,868,873].

2. Monte Carlo simulation as a tool to study dynamical behavior in condensed matter systems

One can give the Monte Carlo sampling process a dynamic interpretation in terms of a Markovian master equation [24]; on the one hand, one can thus give statistical errors an appropriate interpretation in terms of dynamic correlation functions of the appropriate stochastic model, and understand what the slowest relaxing variables are: e.g., for a fluid these are long wavelength Fourier components of the density, when the fluid is simulated in the canonical ensemble. This "hydrodynamic slowing down" [33,76] was not recognized in the early literature on Monte Carlo simulations of fluids, where the relaxation of the internal energy was advocated to judge the approach to equilibrium. In this way, it also becomes possible to understand that the so-called "statistical inefficiency" of the Monte Carlo algorithm near second-order phase transitions simply reflects critical slowing down, and it is possible to study the latter systematically by Monte Carlo e.g. for finite kinetic Ising models [26,1132], although even with the computer power available in the 21st century this is a demanding task, and thus the early work [26] could not reach a meaningful accuracy. A subtle aspect (that still does not seem to be widely recognized) is the fact that critical slowing down leads to a systematic bias (due to finite time averaging) in the sampling of susceptibilities using fluctuation relations [298]. One also needs to be aware that the latter suffer from a lack of self-averaging [214]. At first-order transitions, rather than critical slowing down one may encounter metastability and hysteresis [33,76], but on the other hand, the decay of metastable states (via nucleation and growth) is an interesting problem, both from the point of view of analytical theory [25], phenomenological theories based on the dynamical evolution of the "droplet" size distribution [53] and via attempts to directly study nucleation kinetic by simulation [27,30]. However, these early studies of nucleation phenomena in kinetic Ising models encountered two basic difficulties: (i) due to by far insufficient computer resources, only nucleation barriers of a few times the thermal energy were accessible. (ii) ambiguities in the definition of "clusters" [51]. Both difficulties could only recently be overcome [1090], showing that only the use of the Swendsen-Wang definition of "physical clusters" allows a consistent description of nucleation phenomena in the Ising model, and then the classical theory of nucleation is compatible with the observations of the kinetics [1153].

The dynamic interpretation of Monte Carlo sampling is the basis for a broad range of kinetic Monte Carlo studies of stochastic processes, such as diffusion in concentrated (and possibly interacting) lattice gases [126,146,163], surface diffusion [161] and kinetics of domain growth [168,179], and last but not least interdiffusion in alloys [263] and spinodal decomposition of alloys using the vacancy mechanism [297,301,319]. Other groups have taken the subject of kinetic Monte Carlo and developed it to become a powerful tool of computational materials science.

3. Spinodal decomposition and the non-existence of spinodal curves

While generalized nonlinear Cahn-Hilliard type equations for phase separation kinetics could be derived from kinetic Ising models [37], it was emphasized that the critical singularities that result from the linearization of the Cahn-Hilliard equation are a mean-field artefact, and rather one has a gradual and smooth transition between nonlinear spinodal decomposition and nucleation [52,53,68,80,87]. To show this, a phenomenological description of spinodal decomposition in terms of the dynamics of many growing clusters was developed [68,70,80], which also allowed to understand the diffusive growth law for spinodal decomposition in liquid binary mixtures [43], and provided a dynamic scaling concept for the structure factor of phase separating systems [61,68,80]. It was numerically demonstrated by Monte Carlo estimations of small subsystem free energies that the spinodal has a well defined meaning for subsystems with a linear dimension L that is small in comparison with the correlation length [162,181], since the order parameter in such small subsystems always is essentially homogeneous. For large L the distance of the "spinodal" from the coexistence curve decays with the minus 4^{th} power of L (in d=3 dimensions). Later this observation was explained via the phenomenological theory for the "droplet evaporation/condensation transition" [750]. The latter has been studied via simulations [966].

It needs to be emphasized that the above results apply for systems with short-range interactions. When the interaction range R diverges, nucleation gets more and more suppressed (since the interfacial free energy is proportional to R), and metastable states still have a large life time rather close to the mean field spindoal [169,219,221]. Similarly, for large R the linearized Cahn theory of spinodal decomposition is predicted to hold in the initial stages, and this has been verified for phase separation of symmetrical polymer mixtures, as reviewed in [288,702]. These Ginzburg criteria [169,219,221] explain why the spinodal is useful for mean field systems but not beyond [1074].

4. Surface critical phenomena, interfaces, and wetting

At the critical point of a ferro- or antiferromagnet critical correlations at a free surface show an anisotropic power law decay, and the critical exponents describing this decay differ from the bulk [19,31,42,48,151,270]. A phenomenological scaling theory for surface critical phenomena could be derived [19,31] in collaboration with Pierre Hohenberg, including scaling laws relating the new critical exponents to each other and to bulk ones, and numerical evidence from both systematic high temperature expansions and simulations was obtained to support this theoretical description. The Monte Carlo simulation method uses periodic boundary conditions throughout to describe bulk systems, but free boundary conditions in one direction (and periodic in the other) are used to study thin magnetic films [29]. Also small (super paramagnetic) particles can be studies [8], where a combination of surface and size effects matters (see also [1082]). In ferroelectrics and dipolar magnets even on the mean field level the description gets more complicated [91,137], due to the fact that depolarizing fields cannot be neglected. For short-range systems, on the other hand, estimations of the critical exponents associated with the "surface-bulk multicritical point" have remained a longstanding challenge [178,276,283,294]. An interesting extension also is needed for surface criticality if the bulk system exhibits a Lifshitz point [590,637], since then the system exhibits anisotropic critical behavior in the bulk. This problem was treated by deriving an appropriate Landau theory from the lattice mean field theory of a semi-infinite ANNNI model. A similar concept was used to describe the dynamics of surface enrichment, deriving the proper boundary conditions at a surface for a Cahn-Hilliard type description from a lattice formulation [325], which also is the starting point to study surface-directed spinodal decomposition [333,348,427,495,559,565,605,668,748,963]. Finally, critical surface induced ordering or disordering at bulk first-order transitions was studied [302,500,618]. Qualitatively, such transitions are understood in terms of the gradual unbinding of an interface between the ordered and disordered phase of the system from a surface, reminiscent of wetting phenomena.

In fact, the understanding of interfaces between coexisting phases has been one of the longstanding research interests as well. It was already realized soon [140] that sampling the size-dependence of the minimum of the distribution of the order parameter that describes the two coexisting phases yields

information on the "surface tension" (i.e., the interfacial excess free energy). Originally developed for the Ising model [140] and then for lattice models of polymer mixtures [472], this method has become one of the widely used standard methods to estimate surface tensions at gas-liquid transitions (e.g. [823,916,943], but only recently could the subtle finite size corrections to this method be clarified [1119,1127].

An interesting property of interfaces is the order parameter profile across the interface [391,392]. In d=3 dimensions lattice models can show a roughening transition [260,391], where in the thermodynamic limit the interfacial width diverges. The interfacial width then scales logarithmically with the interfacial area [392,611,669,673,833,968,999], and the mean field (van der Waals, Cahn-Hilliard, etc) concept of an "intrinsic interfacial profile" becomes doubtful. While this logarithmic broadening of the interfacial profile could also be established for solid-fluid interfaces [968,999], in solid-solid interfaces elastic interactions may suppress this broadening [819], yielding a well-defined intrinsic profile again. Particularly interesting are interfaces confined between walls in thin film geometry [555,587,588]; the resulting anomalous dependence of the interfacial width on the film thickness could also be proven to occur in thin films of unmixed polymer blends through appropriate experiments [513,578].

Interfaces confined between parallel walls can also undergo an interface location/delocalization transition [272,442,468,503,571,638,653,659,681,820]. This transition is the analog of the interface unbinding from a surface of a semi-infinite system, i.e. wetting transition, which is a difficult critical phenomenon in the case of short-range forces [206,222,233,277,295,313,353,572,1024,1061,1092]. Interesting interface unbinding transitions were also found in wedges [764,767] and bi-pyramide confinement [815,835], giving rise to unconventional new types of critical phenomena. Also interesting first-order transitions such a capillary condensation [344,356,677] can be studied for systems confined in strips, cylindrical or slit-like pores [275,834,874,1006,1008]. Then also phenomena such as heterogeneous nucleation at walls [967,974,1062] come into play; however, this problem is difficult since it requires consideration of both curvature effects on the interfacial free energy [966,1011,1045,1047,1051] and possible effects due to the line tension [1021,1131]. First steps of a methodology to deal with all these problems via simulations were developed [966,968, 1011,1021,1029,1045,1047,1051,1057,1062,1131]. Particularly challenging is the treatment of crystal nucleation from fluid phases, since in general the interface free energy depends on the interface orientation relative to the lattice axes [1135,1137,1138]. A methodology to circumvent this problem was invented [1133,1135], analyzing the equilibrium between a crystal nucleus and surrounding fluid in a finite simulation box, using a new method to sample the fluid chemical potential.

5. Spin glasses and glass-forming fluids

The "standard model" for spin glasses is the Edwards-Anderson model, i.e. an Ising Hamiltonian where the exchange coupling is a random quenched variable, either drawn from a Gaussian distribution or chosen as +/- J. First Monte Carlo simulations of this model in d=2 dimensions [60,66] showed a cusp-like susceptibility peak similar to experiment; however, now it is known that this peak simply is an effect of the finite (short) observation time, and spin glass-like freezing in d=2 occurs at zero temperature only [104,106]. Recursive transfer matrix calculations [104,106] showed that at T=0 spin-glass-type correlations exhibit a power law decay with distance in the +/-J model. The spin-glass correlation length and associated susceptibility diverge with power laws of 1/T as the temperature T tends to zero [106]. Also a more realistic site disorder model for the insulating spin glasses EuS diluted with SrS was developed, and good agreement with experiment was found [86,105], and critical magnetic fields in spin glasses were discussed [164,171]. Also some aspects of random field Ising models [159,174,421] and random field Potts models [479,521] were considered. Together with Peter Young a comprehensive review on spin glasses was written, encompassing experiments, theory, and simulation; this highly cited paper still is the standard review of the field.

Considering Edwards-Anderson models where spins are replaced by quadrupole moments one obtains models for "quadrupolar glasses" [234,238,250,268,291,306,474,515,567,583,679,691,694,730,766], which can be realized experimentally by diluting molecular crystals with atoms which have no

quadrupole moment (e.g. N_2 diluted with Ar, or K(CN) diluted with K Cl [387]). An atomistic model for such a system was simulated in [540], and a detailed review is found in [387].

Also various contributions were made attempting to elucidate the "grand challenge problem" how a supercooled fluid freezes into a glass. First studies were devoted to develop a lattice model for the glass transition of polymers, introducing "frustration" in the bond fluctuation model via energetic preference for long bonds, which "waste" lattice sites for further occupation by monomers [334,374,388,400,405,417,423,433,435,476,493,496,506,528,549,696]. It was shown that much of the experimental phenomenology could be reproduced (stretched relaxation, time-temperature superposition principle, Vogel-Fulcher relation describing the increase of the structural relaxation time, and evidence in favor of the mode coupling theory as a description of the initial stages of slowing down). Many of these features could also be demonstrated by molecular dynamics simulations of a more realistic off-lattice bead spring model of macromolecules [577,598,600,617,628,708,709], including an analysis of the surface effects on the glass transition in thin polymer films [708,709]. However, a particular highlight of the bond fluctuation model studies was the evidence [493,506,528] that the Gibbs-DiMarzio description of the "entropy catastrophe" at the Kauzman temperature is an artefact of rather inaccurate approximations. Also attempts to map the lattice model to real polymers gave promising results [329,519]. Finally, also a rather realistic model for the glassy behavior of confined polybutadiene was addressed [11,22,1158].

Molecular dynamics simulations were also carried out for two other models of glassforming fluids, the Kob-Anderson binary Lennard-Jones mixture [510,568,684,690,738] and a model for SiO_2 and its mixtures with other oxides [531,535,568,569,597,632,649,672,685] in particular; the logarithmic dependence of the apparent glass transition temperature on the cooling rate [510,535], evidence for the Goetze mode coupling theory [586], evidence for growing dynamic length scales extracted from surface effects [690,738,756,781], and percolative sodium transport in sodium disilicate melts [736] deserve to be mentioned. However, none of these studies gave insight whether or not the structural relaxation time truly diverges at nonzero temperatures, and what a proper "order parameter" distinguishing the glass from the supercooled fluid is. The current state of the art is summarized in a textbook (written with W. Kob) [1035]

6. Studies of macromolecular systems

While a formulation of a Monte Carlo Renormalization Group scheme [121 aimed at a better understanding of the critical exponents describing the self-avoiding walk problem, the first simulation of a dense melt of short chains [128] was motivated by experimental work [130,150] that gave evidence for the Rouse-like motions of the monomers only, not for snakelike "reptation" of the chain in a tube formed by its environment. However, later simulations of much longer chains [307,339,379,418,666] succeeded to study the crossover from the Rouse model to reptation in detail.

A famous problem of polymer science is the adsorption transition of a long flexible macromolecule from a dilute solution (under good solvent conditions) at an attractive wall [149,745,763,1012,1034,1083,1084]. In early work [149], recognizing the analogy to the surface-bulk multicritical point of the phase transitions of semi-infinite n-vector models, the deGennes conjecture for the crossover exponent could be disproven, but the precise value of this exponent has remained controversial for decades, and only recent work [1083] applying the pruned-enriched Rosenbluth method to very long chain molecules and using a comparative study of various ranges of the adsorption potential could clarify the situation. However, open questions still remain concerning the adsorption of semiflexible chains [1084]. The latter show a complicated crossover behavior also in bulk solution, particularly when exposed to stretching forces, which could be elucidated only recently [1039,1052,1077]. The fact that the standard definition of the persistence length of semiflexible polymers holds only for Gaussian "phantom chains" [933] has hampered progress in this field, in particular when the extension to polymers with complex chemical architecture (such as "bottlebrush polymers" [877,904,985,1025,1055]) is considered.

A very interesting problem involving only the statistical mechanics of a single chain concerns confinement inside a tube [188,899,934,1000] or in between parallel plates [455,566,935], or the

competition between chain collapse in poor solvents [148,439,969,978] and adsorption [915,945,948,1129]. Related single chain phase transitions (which often show inequivalence between different ensembles of statistical mechanics due to the geometrical constraints that are present) concern the "escape transition" of compressed mushrooms [609,610] or compressed polymers [1107] or the "coil-bridge"-transition [1118]. Polymer collapse in poor solvents gives rise to a rich phase diagram, when bottle-brushes are considered, due to pearl necklace type structures [988,997,1010].

While for phase transition of single chains their connectivity provides unique features, phase transitions in many-chain systems often have analogs in small molecule systems, but show also characteristic differences due to the large size of a polymer coil. Nucleation and spinodal decomposition in polymer mixtures for very long chains behave almost mean-field like [166,169,399]; with respect to the critical point of unmixing, crossover from Ising to mean field behavior is observed with increasing distance from the critical point [390,399,414]. Nevertheless, the Flory-Huggins theory for polymer blends is fairly inaccurate [226], when one extracts Flory-Huggins parameter from scattering experiments via this theory a spurious concentration dependence results [240,264] and the chain linear dimensions depend on the thermodynamic state [251], particularly in semidilute solutions [446]. But early versions of integral equation theories of blends even performed worse [338]. In d=2 dimensions, however, the critical temperature scales sublinearly with chain length [744,828]. Particularly interesting is mesophase separation in block copolymer melts [315,318], where simulations revealed a pretransitional stretching (into a dumbbell-like conformation) of the chains, in agreement with experiments performed independently at the same time. Also the interplay of confinement in thin films and lamellar ordering produces a rich phase diagram, relevant for experiment [385,432,622,623], while block copolymers in selective solvent show micelle formation [585,602,654,664,878,930]. These simulations (for finite chain lengths) clearly reveal the shortcomings of the "selfconsistent field theory", which in theoretical polymer physics often is taken as something like the "gold standard". Also simulations of "polymer brushes" (chains grafted densely with one chain end on a planar or curved substrate) [336,365,381,434,461,697,750,771,790,837,847,869,906,944,1017,1043,1059,1067,1069 1073,1093,1116,1124] have revealed similar limitations of the standard theories. Thus, Monte Carlo simulation for polymeric systems has become a particularly fruitful method.

MEMBERSHIPS

- Deutsche Physikalische Gesellschaft (German Physical Society)
- Hochschulverband (union of the institutes of higher education in Germany)
- Institute of Physics, UK (Fellow)
- American Physical Society

Participation in Special Research Programs funded by DFG, German research foundation

SFB 130 "Ferroelectrics" 1976 – 1978 (heading a subdivision)
SFB 125 "Magnetic moments in metals" 1978 – 1983
SFB 41 "Macromolecules" 1984 – 1987 (heading a subdivision)
SFB 262 "The glass state and glass transition of non-metallic amorphous materials" (heading a subdivision 1987-2001)
SFB 625 "From single molecules to nanoscopic structural materials" (heading a subdivision 2002-2013)
SFB TR6 "Physics of Colloidal Dispersions in External Fields" (heading a subdivision 2002-2013)

Work on conference organization and program committees

1975 NATO Advanced Study Institute, Geilo, Norway
as of 1975 MECO (Middle European Cooperation on Statistical Physics)
1979 ICM (International Conference on Magnetism) Munich, Germany
1979 Jülicher Ferienkurs – The Physics of Alloys, Jülich, Germany
1980 IUPAP Conference on Statistical Physics, Edmonton, AL / Canada
1981 Les Houches "Winter School", Les Houches, France
1982 Jülicher Ferienkurs – The Physics of Polymers, Jülich, Germany
1983 IUPAP Conference on Statistical Physics, Edingburgh, Great Britain
1985 ICM (International Conference on Magnetism) San Francisco, CA, USA
1986 IUPAP Conference on Statistical Physics, Boston, MA. USA
1989 IUPAP Conference on Statistical Physics, Rio de Janeiro, Brazil

1992 IUPAP Conference on Statistical Physics, Berlin, Germany
1993 13th General Conference of the EPS Condensed Matter Division, Regensburg, Germany
1995 IUPAP Conference on Statistical Physics, Xiamen, China
1995 Director of Euroconference "Monte Carlo and Molecular Dynamics of Condensed Matter Systems" Como, Italy (with G. Ciccotti)
1996 EPS-APS Conference on Computational Physics, Cracow, Poland
1998 EPS-APS-IUPAP Conference on Computational Physics, Granada, Spain
2000 Co-Director of NATO ARW "Multiscale Simulations in Chemistry and Biology", Eilat, Israel (with A. Brandt and J. Bernholc)
2001 IUPAP Conference on Statistical Physics, Cancun, Mexico
2001 EPS-APS-IUPAP Conference on Computational Physics, CCP 2001, Aachen, Germany (Vice Chairman)
2002 EPS-APS-IUPAP Conference on Computational Physics, CCP2002, San Diego, USA
2004 IUPAP Conference on Statistical Physics, Bangalore, India
2004 EPS-APS-IUPAP Conference on Computational Physics, CCP2004, Genova, Italy
2005 Co-Director of Erice Summer School, Erice, Italy
2007 IUPAP Conference on Statistical Physics, Genova, Italy
2007 EPS-APS-IUPAP Conference on Computational Physics, CCP2007, Brussels, Belgium
since 2010 Steering Committee of the Granada Seminar on Computational and Statistical Physics
2010 IUPAP Conference on Statistical Physics, Cairns, Australia
2010 EPS-APS-IUPAP Conference on Computational Physics, CCP2010, Trondheim, Norway
2011 Liquid Matter Conference, Vienna, Austria
2013 IUPAP Conference on Statistical Physics, Seoul, Korea
2015 EPS-APS-IUPAP Conference on Computational Physics, CCP 2015, Guwahati, India
2016 IUPAP Conference on Statistical Physics, Lyon, France
2020 Liquid Matter Conference, Prague, Czech Republic

PUBLISHING WORK (AS AN EDITOR)

1979 Springer, Berlin *Monte Carlo Methods in Statistical Physics* (2nd Edition 1986)
1984 Springer, Berlin *Applications of the Monte Carlo Method in Statistical Physics* (2nd Edition)
1992 Springer, Berlin *The Monte Carlo Method in Condensed Matter Physics*

1995 Oxford University Press, New York *Monte Carlo and Molecular Dynamics Simulations in Polymer Science*
1996 Societa Italiana di Fisica, Bologna *Monte Carlo and Molecular Multiscale Computational Methods in Chemistry and Physics*
2001 IOS Press, Amsterdam *Multiscale Computational Methods in Chemistry and Physics*
2006 Springer, Berlin *Computer Simulations in Condensed Matter: From Materials to Chemical Biology I, II*
1979 – 1982, 1988 – 1990 Editorial board *Journal of Statistical Physics*
1984 – 1989 Editorial board *Journal of Computational Physics*
as of 1983 Editorial board *Ferroelectrics Letters*
as of 1987 Editorial board *Computer Physics Communications*
as of 1991 Editorial board *International Journal of Modern Physics C (Physics and Computers)*
as of 1992 Editorial board *Die Makromolekulare Chemie, Theory and Simulations*
1993 – 1996 Advisory board *Journal of Physics: Condensed Matter*
as of 1996 Advisory board *Physica A*
as of 1998 Editorial boards, *Monte Carlo Methods and Applications*
2000-2002 Editorial board, *European Journal of Physics*
2000-2002 Editorial board, *Journal of Statistical Physics*
2000-2003 Editorial board, *Europhysics Letters* Editorial board, *Journal of Statistical Physics*
2003-2005 Editorial board, *Current Opinion in Materials Science*
2003-2005 Editorial board, *Physical Chemistry and Chemical Physics*
as of 2010 Journal of Statistical Physics
2006-2011 Editorial board, *Journal of Physics A: Mathematics and General*
2011-2013 Advisory Board, *Journal of Chemical Physics*

REVIEWING

I provide expert reviews for the following institutions:

German National Research Foundation, DFG

Membership in SFB expert reviewal groups *(Bayreuth, Bochum-Düsseldorf-Essen, Bonn, Tübingen-Stuttgart, Aachen-Jülich-Köln, Berlin, Halle*) and expert opinions for DFG priority "Computer-Simulation in der Gitterreichtheorie", I was also serving as referee for individual reviews and the Heisenberg Program.

Volkswagen Foundation
Alexander von Humboldt Foundation
Austrian Fund to promote scientific research (Vienna)
National Science Foundation (Washington D.C.)
NATO Division for Scientific Affairs (Brussels)
Science Foundation of the Czech Republic, of Israel, the Netherlands, etc.
German Israeli Foundation (GIF)
BSF (Binational USA-Israel Science Foundation)
Leopoldina

Referee for numerous journals: *Phys. Rev. Lett., Phys. Rev. A, B, E, Physics Letters, Journal of Physics A, C, F, Europhysics Lett., Journal de Physique (Paris), Zeitschrift für Physik B, Journal of Chemical Physics, Solid State Comm., Physics Reports, Advances in Physics, Journal of Statistical Physics, Journal of Computational Physics, Physica status solidi, Canadian Journal of Physics, Surface Science, Computer Phys. Commun., Colloid & Polymer Sci., Die makromolekulare Chemie, Journal of Polymer Science, Macromolecules, Ferroelectrics, Journal of Noncrystalline Solids, Nuclear Physics B, Langmuir; Revs. Mod. Phys.; Eur. Phys. J. B, E; J. Phys. Chem. B, etc.*

FREE TIME

Once in a while I find time to be at home. I enjoy playing the piano and do work in our garden.

Mainz, December 16th, 2019 **Prof. Dr. Kurt Binder**