

Cambridge University Press

0521842425 - Series Expansion Methods for Strongly Interacting Lattice Models

Jaan Oitmaa, Chris Hamer and Weihong Zheng

Frontmatter

[More information](#)

SERIES EXPANSION METHODS FOR STRONGLY INTERACTING LATTICE MODELS

Perturbation series expansion methods are sophisticated numerical tools used to provide quantitative calculations in many areas of theoretical physics. This book gives a comprehensive guide to the use of series expansion methods for investigating phase transitions and critical phenomena, and lattice models of quantum magnetism, strongly correlated electron systems and elementary particles.

Early chapters cover the classical treatment of critical phenomena through high-temperature expansions, and introduce graph theoretical and combinatorial algorithms. The book then discusses high-order, linked cluster perturbation expansions for quantum lattice models, finite temperature expansions, and lattice gauge models. Numerous detailed examples and case studies are also included, and an accompanying resources website, www.cambridge.org/9780521842426, contains programs for implementing these powerful numerical techniques.

A valuable resource for graduate students and postdoctoral researchers working in condensed matter and particle physics, this book will also be useful as a reference for specialized graduate courses on series expansion methods.

JAAN OITMAA was born in Tallinn, Estonia in 1943. After the war his family migrated to Australia, where he has spent most of his life. He received his undergraduate and graduate education at the University of New South Wales, in Sydney, obtaining his Ph.D. in 1968. His early postdoctoral work was in lattice dynamics at the University of California, Irvine. During his second postdoctoral position, at the University of Alberta, he became interested in the field of critical phenomena, and learnt the techniques of series expansions from Donald Betts' group. On returning to Australia he held a Queen Elizabeth II Research Fellowship at Monash University and then rejoined his *alma mater* as a lecturer in Physics, in 1972. He was promoted to full Professor in 1991, and upon his retirement in 2003 was accorded the title of Professor Emeritus. Throughout his long career he has been an enthusiastic teacher at all levels, supervised many Ph.D. students, published over 170 research papers in top international journals, and served as Head of School for 6 years (1993–1998) and President of the Australian Institute of Physics for 2 years (1997–1998). He is a Fellow of both the Australian Institute of Physics and the American Physical Society.

Cambridge University Press

0521842425 - Series Expansion Methods for Strongly Interacting Lattice Models

Jaan Oitmaa, Chris Hamer and Weihong Zheng

Frontmatter

[More information](#)

CHRIS HAMER received a B.Sc. and M.Sc. from the University of Melbourne, and a Ph.D. from the California Institute of Technology in 1972. He began his research career in elementary particle physics, and studied series expansions in lattice gauge theory. His later interests moved towards statistical mechanics and condensed matter physics, including the theory of finite-size scaling, and linked cluster methods for series expansions. He held research positions at the Brookhaven National Laboratory, the Universities of Cambridge, Liverpool and Melbourne, and was a Senior Research Fellow at the Australian National University for 8 years from 1979, before taking up a position as Senior Lecturer at the University of New South Wales (UNSW) in 1987. He is now a Visiting Associate Professor at UNSW. He has authored about 150 research publications. He is a Fellow of the Australian Institute of Physics, and was editor of the AIP journal, *The Physicist*, for 5 years from 1998–2002.

WEIHONG ZHENG was born in Guangdong, China. He obtained a B.Sc. in 1984 and then a Ph.D. in 1989 at Zhongshan University in Guangdong, studying Hamiltonian lattice gauge theory. He was subsequently appointed as a lecturer at Zhongshan University. He moved to the University of New South Wales in 1990, where he began a long and productive collaboration with Jaan Oitmaa and Chris Hamer, working on linked cluster series expansion methods. He is presently a Senior Research Associate at UNSW, and has built up a worldwide reputation as an acknowledged expert in the techniques of perturbative series expansions. His early work was in the field of particle physics, but more recently he has concentrated on the theory of condensed matter systems. He has written around 100 research publications.

Cambridge University Press

0521842425 - Series Expansion Methods for Strongly Interacting Lattice Models

Jaan Oitmaa, Chris Hamer and Weihong Zheng

Frontmatter

[More information](#)

SERIES EXPANSION METHODS FOR STRONGLY INTERACTING LATTICE MODELS

JAAN OITMAA, CHRIS HAMER AND
WEIHONG ZHENG

School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia.



CAMBRIDGE
UNIVERSITY PRESS

Cambridge University Press

0521842425 - Series Expansion Methods for Strongly Interacting Lattice Models

Jaan Oitmaa, Chris Hamer and Weihong Zheng

Frontmatter

[More information](#)

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore, São Paulo

Cambridge University Press
The Edinburgh Building, Cambridge CB2 2RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9780521842426

© J. Oitmaa, C. Hamer and W. Zheng 2006

This publication is in copyright. Subject to statutory exception
and to the provisions of relevant collective licensing agreements,
no reproduction of any part may take place without
the written permission of Cambridge University Press.

First published 2006

Printed in the United Kingdom at the University Press, Cambridge

A catalogue record for this publication is available from the British Library

ISBN-13 978-0-521-84242-6 hardback
ISBN-10 0-521-84242-5 hardback

Cambridge University Press has no responsibility for the persistence or accuracy of URLs for
external or third-party internet websites referred to in this publication, and does not guarantee that
any content on such websites is, or will remain, accurate or appropriate.

Contents

	<i>Preface</i>	<i>page viii</i>
1	Introduction	1
1.1	Lattice models in theoretical physics	1
1.2	Examples and applications	1
1.3	The important questions	10
1.4	Series expansion methods	14
1.5	Analysis of series	19
2	High- and low-temperature expansions for the Ising model	26
2.1	Introduction	26
2.2	Graph generation and computation of lattice constants	30
2.3	A case study: high-temperature susceptibility for the Ising model on the simple cubic lattice	36
2.4	Low-temperature expansion	39
2.5	Reducing the number of graphs	42
2.6	More on Ising models	47
3	Models with continuous symmetry and the free graph expansion	53
3.1	Introduction	53
3.2	The free graph expansion	55
3.3	The plane rotator ($N = 2$) model	66
3.4	Analysis of the $N = 2$ susceptibility	69
3.5	Discussion	72
4	Quantum spin models at $T = 0$	74
4.1	Introduction	74
4.2	Linked cluster expansions	74
4.3	An example: the transverse field Ising model in one dimension	78
4.4	Magnetization and susceptibility	82
4.5	One-particle excitations	84
4.6	The transverse field Ising model in two and three dimensions	92

vi	<i>Contents</i>	
5	Quantum antiferromagnets at $T = 0$	99
5.1	Introduction: simple antiferromagnets	99
5.2	Dimerized systems and quantum phase transitions	106
5.3	The J_1 – J_2 square lattice antiferromagnet	112
5.4	Other systems	118
5.5	Open questions	122
6	Correlators, dynamical structure factors and multi-particle excitations	124
6.1	Introduction	124
6.2	Two-spin correlators for the Heisenberg antiferromagnet	125
6.3	Dynamical and static structure factors	126
6.4	Two-particle and multi-particle excitations	134
6.5	Two-particle structure factors	145
6.6	Summary and further work	147
7	Quantum spin models at finite temperature	150
7.1	Introduction	150
7.2	Derivation of high-temperature series	151
7.3	The cubic (SC and BCC) lattices	165
7.4	Generalizations	168
7.5	Perturbation expansions at finite T	169
7.6	Further applications	175
7.7	Fitting to experimental data	176
8	Electronic models	179
8.1	Introduction	179
8.2	The Hubbard model	180
8.3	The t – J model	197
8.4	Further topics and possibilities	209
9	Review of lattice gauge theory	211
9.1	Quantum chromodynamics	211
9.2	The path integral approach to field theory	214
9.3	Euclidean lattice gauge theory	217
9.4	Confinement and phase structure on the lattice	219
9.5	Renormalization theory and the continuum limit	221
9.6	Monte Carlo simulations	222
9.7	Including fermions on the lattice	225
9.8	The Hamiltonian lattice formulation	227
9.9	Conclusions	228
10	Series expansions for lattice gauge models	230
10.1	Strong coupling expansions for Euclidean lattice Yang–Mills theory	230

Cambridge University Press

0521842425 - Series Expansion Methods for Strongly Interacting Lattice Models

Jaan Oitmaa, Chris Hamer and Weihong Zheng

Frontmatter

[More information](#)

<i>Contents</i>		vii
10.2	Strong coupling expansions in Hamiltonian Yang–Mills theory	244
10.3	Models with dynamical fermions	251
10.4	The t -expansion	259
10.5	Conclusions	263
11	Additional topics	265
11.1	Disordered systems	265
11.2	Other series expansion methods	274
	Appendix 1: some graph theory ideas	283
	Appendix 2: the ‘pegs in holes’ algorithm	286
	Appendix 3: free graph expansion technicalities	288
	Appendix 4: matrix perturbation theory	291
	Appendix 5: matrix block diagonalization	294
	Appendix 6: the moment–cumulant expansion	297
	Appendix 7: integral equation approach to the two-particle Schrödinger equation	299
	Appendix 8: correspondences between field theory and statistical mechanics	304
	Appendix 9: computer programs	307
	<i>Bibliography</i>	311
	<i>Index</i>	324

Preface

The past 50 years have seen much progress in our understanding of the behaviour of complex physical systems, made up of large numbers of strongly interacting particles. This includes a rather detailed, if not complete, understanding of such phenomena as phase transitions of various kinds, macroscopic quantum phenomena such as magnetic order and superconductivity, and the response of such systems to external probes, vital for the interpretation of experimental results. Such unifying concepts as scaling and universality, long-range order (including off-diagonal, long-range order), and spontaneous symmetry breaking have led to a unified understanding of diverse and complex phenomena.

Central to this endeavour has been the detailed and systematic study of lattice models of various genera; models which are precisely defined mathematically, which are believed to embody the *essential physics* of interest, and which are, to a greater or lesser extent, mathematically tractable. Exact analytic treatment of these models is rarely possible. Series expansion techniques, the subject of this book, provide one of the main systematic and powerful approximate methods to treat such lattice models.

Our decision to write this book arose from a request from a journal editor to write a review of our group's work over the last decade on series studies of quantum lattice models. On reflection, we came to the view that it would be more useful to write a book covering the entire field, at a level which would be accessible to graduate students and other researchers wishing to learn about these methods. We were also strongly influenced by the appearance of another book, *A Guide to Monte Carlo Simulations in Statistical Physics* by Landau and Binder (Cambridge University Press, 2000), which provides an excellent introduction to Monte Carlo methods. We felt there was a need for a book, with the same general approach, for the series expansion field. The response of the physics community will show whether we were justified in this belief.

Our archetypal reader, then, is a graduate student or young researcher who wishes to use series expansion methods for some particular project and who is not overly familiar with the subject and does not have access to a local expert. As with any technical area, there are many skills to learn and pitfalls to be avoided. Many of the computational algorithms needed are heavily combinatorial in nature and wise or unwise programming can make orders of magnitude difference in both time and memory demands. In this book we provide examples of efficient computer programs to do the most commonly needed tasks – there is no need for every worker in the field to reinvent these things from scratch.

Our approach is to demonstrate results, wherever possible, by means of specific calculations for simple models, which are worked out in some detail. We hope that these will provide useful examples and checks for researchers building their own programs in these areas. We do not attempt to give formal proofs of results, although an outline proof is sketched in a few basic cases: in general, the reader must consult the listed references if a more rigorous approach is required.

The choice of content is, as in any book, partly a reflection of our interests. The later chapters, in particular, are influenced by our own work, over the last 10–15 years, on series studies of quantum spin models and electronic models. However we wish to explain rather than to expound and the early chapters, in particular, are intended to be largely pedagogical. While much of this material is well known (to those who know it well) and well documented in volume 3 of the Domb and Green series (Domb, 1974) and in a number of books (e.g. Baker, 1990), it has not, to our knowledge, been presented in a unified *hands-on* way with supporting computer programs.

Inevitably some interesting and important topics have had to be curtailed: for example the large field of series analysis, where other good sources exist, and the area of disordered systems, which is treated very briefly. Very little has been included on those lattice models which are primarily of interest in mathematical physics, such as Potts models, random walks, and lattice polygons. We have concentrated primarily on models with more direct physical applications.

The chapters are relatively self contained and some may be skipped at first reading. In particular Chapter 3 (the free graph method) and Chapter 5 (quantum antiferromagnets at $T = 0$) are not prerequisites for chapters which come after them. A comment on referencing is appropriate. While we have tried to be true to history, and to acknowledge the pioneers on particular topics by name, we have not attempted to cite every source. It seemed appropriate to cite in the book only those sources which, in our view, readers may benefit from following up, or more recent articles, which give references to earlier work. We can only apologize to any of our fellow workers whose work has not been fully referenced.

Cambridge University Press

0521842425 - Series Expansion Methods for Strongly Interacting Lattice Models

Jaan Oitmaa, Chris Hamer and Weihong Zheng

Frontmatter

[More information](#)

x

Preface

Our knowledge of this field has been acquired over many years and through interactions with colleagues too numerous to mention individually. We thank all of them, but particularly George Baker, Michael Barber, Donald Betts, Conrad Burden, Chuck Elliott, Shuohong Guo, Tony Guttmann, Hong-Xing He, Alan Irving, and Rajiv Singh. We also gratefully acknowledge support, over many years, from the Australian Research Council.

We are grateful for permission to reproduce the following figures: Fig. 11, T.M.R. Byrnes *et al.*, *Phys. Rev. D* 69, 074509 (2004); Fig. 1, M. Creutz, *Phys. Rev. Letts.* 43, 553 (1979); Fig. 4, M. Creutz and K.J.M. Moriarty, *Phys. Rev. D* 26, 2166 (1982); Figs. 3, 5, C.J. Hamer *et al.*, *Phys. Rev. D* 56, 55 (1997); Figs. 3, 15, C.J. Hamer *et al.*, *Phys. Rev. B* 68, 214408 (2003); Fig. 2, D. Horn and G. Lana, *Phys. Rev. D* 44, 2864 (1991); Figs. 4, 5, D. Horn and D. Schreiber, *Phys. Rev. D* 47, 2081 (1993); Fig. 2, J. Oitmaa and W. Zheng, *Phys. Rev. B* 54, 3022 (1996); Fig. 3, J.D. Stack, *Phys. Rev. D* 29, 1213 (1984); Figs. 3, 5, O.P. Sushkov *et al.*, *Phys. Rev. B* 63, 104420 (2001); Fig. 4, S. Trebst *et al.*, *Phys. Rev. Letts.* 85, 4373 (2000); Fig. 4, C.P. Van en Doel and D. Horn, *Phys. Rev. D* 33, 3011 (1986); Figs. 1, 6, W-H. Zheng, *Phys. Rev. B* 55, 12267 (1997); Figs. 2, 3, W-H. Zheng *et al.*, *Phys. Rev. Letts.* 91, 037206 (2003); Figs. 1, 2, 5, W-H. Zheng *et al.*, *Phys. Rev. B* 63, 144411 (2001); Fig. 2, W-H. Zheng and J. Oitmaa, *Phys. Rev. B* 63, 064425 (2001); Figs. 3, 4, W-H. Zheng *et al.*, *Phys. Rev. B* 58, 14147 (1998); Fig. 6, W-H. Zheng *et al.*, *Phys. Rev. B* 65, 014408 (2001); all copyright by the American Physical Society; Fig. 2, G.T. Rado, *Solid State Commun.*, 8, 1349 (1970); Fig. 1, C.J. Hamer, *Phys. Letts.* B224, 339 (1989); Fig. 12, C.J. Hamer and A.C. Irving, *Nucl. Phys.* B230, 336 (1984); Figs. 2, 5, J. Smit, *Nucl. Phys.* B206, 309 (1982); copyright by Elsevier; and Fig. 3, G. Aeppli *et al.*, *Physics World* 10, 33 (December 1997), copyright by Institute of Physics (UK).