Lecture Notes in Physics

Springer
Berlin
Heidelberg
New York
Barcelona
Hong Kong
London
Milan
Paris
Singapore
Tokyo

The Editorial Policy for Proceedings

The series Lecture Notes in Physics reports new developments in physical research and teaching – quickly, informally, and at a high level. The proceedings to be considered for publication in this series should be limited to only a few areas of research, and these should be closely related to each other. The contributions should be of a high standard and should avoid lengthy redraftings of papers already published or about to be published elsewhere. As a whole, the proceedings should aim for a balanced presentation of the theme of the conference including a description of the techniques used and enough motivation for a broad readership. It should not be assumed that the published proceedings must reflect the conference in its entirety. (A listing or abstracts of papers presented at the meeting but not included in the proceedings could be added as an appendix.)

When applying for publication in the series Lecture Notes in Physics the volume's editor(s) should submit sufficient material to enable the series editors and their referees to make a fairly accurate evaluation (e.g. a complete list of speakers and titles of papers to be presented and abstracts). If, based on this information, the proceedings are (tentatively) accepted, the volume's editor(s), whose name(s) will appear on the title pages, should select the papers suitable for publication and have them refereed (as for a journal) when appropriate. As a rule discussions will not be accepted. The series editors and Springer-Verlag will normally not interfere with the detailed editing except in fairly obvious cases or on technical matters.

Final acceptance is expressed by the series editor in charge, in consultation with Springer-Verlag only after receiving the complete manuscript. It might help to send a copy of the authors' manuscripts in advance to the editor in charge to discuss possible revisions with him. As a general rule, the series editor will confirm his tentative acceptance if the final manuscript corresponds to the original concept discussed, if the quality of the contribution meets the requirements of the series, and if the final size of the manuscript does not greatly exceed the number of pages originally agreed upon. The manuscript should be forwarded to Springer-Verlag shortly after the meeting. In cases of extreme delay (more than six months after the conference) the series editors will check once more the timeliness of the papers. Therefore, the volume's editor(s) should establish strict deadlines, or collect the articles during the conference and have them revised on the spot. If a delay is unavoidable, one should encourage the authors to update their contributions if appropriate. The editors of proceedings are strongly advised to inform contributors about these points at an early stage.

The final manuscript should contain a table of contents and an informative introduction accessible also to readers not particularly familiar with the topic of the conference. The contributions should be in English. The volume's editor(s) should check the contributions for the correct use of language. At Springer-Verlag only the prefaces will be checked by a copy-editor for language and style. Grave linguistic or technical shortcomings may lead to the rejection of contributions by the series editors. A conference report should not exceed a total of 500 pages. Keeping the size within this bound should be achieved by a stricter selection of articles and not by imposing an upper limit to the length of the individual papers. Editors receive jointly 30 complimentary copies of their book. They are entitled to purchase further copies of their book at a reduced rate. As a rule no reprints of individual contributions can be supplied. No royalty is paid on Lecture Notes in Physics volumes. Commitment to publish is made by letter of interest rather than by signing a formal contract. Springer-Verlag secures the copyright for each volume.

The Production Process

The books are hardbound, and the publisher will select quality paper appropriate to the needs of the author(s). Publication time is about ten weeks. More than twenty years of experience guarantee authors the best possible service. To reach the goal of rapid publication at a low price the technique of photographic reproduction from a camera-ready manuscript was chosen. This process shifts the main responsibility for the technical quality considerably from the publisher to the authors. We therefore urge all authors and editors of proceedings to observe very carefully the essentials for the preparation of camera-ready manuscripts, which we will supply on request. This applies especially to the quality of figures and halftones submitted for publication. In addition, it might be useful to look at some of the volumes already published. As a special service, we offer free of charge LaTeX and TeX macro packages to format the text according to Springer-Verlag's quality requirements. We strongly recommend that you make use of this offer, since the result will be a book of considerably improved technical quality. To avoid mistakes and time-consuming correspondence during the production period the conference editors should request special instructions from the publisher well before the beginning of the conference. Manuscripts not meeting the technical standard of the series will have to be returned for improvement.

For further information please contact Springer-Verlag, Physics Editorial Department II Tiergartenstrasse 17, D-69121 Heidelberg, Germany

Ingo Peschel Xiaoqun Wang
Matthias Kaulke Karen Hallberg (Eds.)

Density-Matrix Renormalization

A New Numerical Method in Physics

Lectures of a Seminar and Workshop Held at the
Max-Planck-Institut für Physik komplexer Systeme
Dresden, Germany, August 24th to September 18th, 1998

Springer

Editors

Prof. Dr. Ingo Peschel
Dr. Matthias Kaulke
FB Physik
Freie Universität Berlin
Arnimallee 14, D-14195 Berlin, Germany

Dr. Xiaoqun Wang
Institut Romand de Recherche Numérique en Physique des Matériaux
PPH 333-EPFL, CH-1015 Lausanne, Switzerland

Dr. Karen Hallberg
Centro Atomico Bariloche
8400 Bariloche, Argentina

Library of Congress Cataloging-in-Publication Data.

Die Deutsche Bibliothek - CIP-Einheitsaufnahme

Density matrix renormalization : a new numerical method in physics ; lectures of a seminar and workshop, held at the Max-Planck-Institut für Physik Komplexer Systeme, Dresden, Germany, August 24th to September 18th, 1998 / Ingo Peschel ... (ed.). - Berlin ; Heidelberg ; New York ; Barcelona ; Hong Kong ; London ; Milan ; Paris ; Singapore ; Tokyo : Springer, 1999
(Lecture notes in physics ; Vol. 528)
ISBN 3-540-66129-8

ISSN 0075-8450
ISBN 3-540-66129-8 Springer-Verlag Berlin Heidelberg New York

Typesetting: Camera-ready by the authors/editors
Cover design: *design & production*, Heidelberg

SPIN: 10731988 57/3144 - 5 4 3 2 1 0 – Printed on acid-free paper

Preface

This book deals with a method which is still not widely known, although it caused a revolution in the numerical treatment of low-dimensional quantum systems. How this started about ten years ago, is described in detail in a separate contribution. The reason for the impact it had, on the other hand, is easy to give. Density-matrix renormalization has two features which normally do not come together. With it, one can treat large systems containing, for example, several hundred spins and, at the same time, reach spectacular accuracies such as ten decimal places in ground-state energies. Thus the method combines the advantages of Monte Carlo calculations and of exact diagonalisations and it is not surprising that it was applied soon after its invention to a variety of problems, both old and new, and mostly connected with quantum chains. Parallel to that, it was extended in other directions, for example to finite temperatures, which increased the area of applications further. The number of groups using it grew also and in 1997 about sixty articles appeared in which it played an essential role.

This seemed a good time to bring the experts in the field together. On the one hand to summarize the status and to discuss open questions as well as future directions as, for example, the extension of the method to higher dimensions. On the other hand to share their experience with younger researchers interested in learning and applying the technique, including practical work on the computer. This was the concept of a four-week seminar and workshop at the Max-Planck-Institut für Physik komplexer Systeme in Dresden in the fall of 1998. It was the first meeting on density-matrix renormalization, and among its about 50 participants from all over the world were the leaders in the field. The workshop was viewed as very successful and the proposal to collect the contributions in the form of lecture notes was strongly supported from all sides, even though this had not been planned initially. This has led to the book which is presented here.

The volume is divided into two parts of roughly equal size which are closely related. The first one contains a series of seven longer lectures which present the method from various angles. This serves as a general introduction on the level of an advanced textbook. A central chapter is the second one which explains the basic principles and also contains, in line with the aims of the workshop, a computer program for a simple example. Other chapters deal with more advanced aspects, like the application to time-dependent problems or to finite temperatures. Two-dimensional systems, both classsical and quantum-mechanical, are also discussed. Finally, to put things into a broader perspective, there are contributions on Wilson's original renormalization method as well as on variational approaches.

The second part deals with the application of the technique to various physical problems, arranged in five different groups. The main themes of

the first part appear again, but also some additional aspects. However, the contributions are shorter and the focus is somewhat different. The physical questions and properties stand in the center and the method is in general only briefly discussed, except in those cases where new aspects come in. In this way, the second part is also a review of actual one-dimensional problems, interesting questions and their present status. Of course, it reflects the research topics of the participants, but it covers a large portion of the applications and thus gives a very good overview even though the additional posters are not included.

Throughout the book considerable effort has been made to obtain a clear, structured and self-contained presentation of the material, but also as much coherence as possible. Due to the structure, a certain amount of duplication in the references was inevitable, but we think that it can be accepted. We thank all authors for their, sometimes enthusiastic, cooperation in the project. We are particularly glad that Steven White agreed to write down his personal recollections on how it all began.

Of course, the whole undertaking would have been impossible without the Max-Planck-Institut in Dresden and its outstanding facilities. We thank its director, Peter Fulde, and its staff for their constant support, and also Springer-Verlag which agreed to publish the book in this well-known series. We hope that, besides being a source for everyone interested in the topic, it will also stimulate new research and thereby contribute to the further development of this field.

Berlin, April 1999

Ingo Peschel
Xiaoqun Wang
Matthias Kaulke
Karen Hallberg

Contents

Preface v

How It All Began: A Personal Account
S. White vii

Part I Introductory Lectures

1 Wilson's Numerical Renormalization Group
T. Costi 3

2 The Density Matrix Renormalization Group
R. Noack and S. White 27

3 Thermodynamic Limit and Matrix-Product States
S. Rommer and S. Östlund 67

4 A Recurrent Variational Approach
M. Martín-Delgado and G. Sierra 91

5 Transfer-Matrix Approach to Classical Systems
T. Nishino, K. Okunishi, Y. Hieida
T. Hikihara and H. Takasaki 127

6 Quantum Transfer-Matrix and Momentum-Space DMRG
T. Xiang and X. Wang 149

7 Calculation of Dynamical Properties
X. Wang, K. Hallberg and F. Naef 173

Part II Physical Applications

1 Chains and Ladders

1.1 Properties of the Hubbard Chain
R. Noack, S. Daul and S. Kneer 197

1.2 Soliton Bound-States in Dimerized Spin Chains
E. Sørensen, I. Affleck, D. Augier and D. Poilblanc 211

1.3 Haldane Phase, Impurity Effects and Spin Ladders
X. Wang 221

1.4 Spin-Chain Properties
K. Hallberg 231

2 Molecules and Polymers

2.1 Electronic Structure using DMRG
Steven R. White 237

2.2 Symmetrized DMRG Method for Conjugated Polymers
S. Ramasesha and K. Tandon 247

2.3 Conjugated One-Dimensional Semiconductors
W. Barford and R. Bursill 261

2.4 Strongly Correlated Complex Systems
S. Qin, J. Lou, Z. Su and L. Yu 271

3 Classical Statistical Physics

3.1 Non-Hermitian Problems and Some Other Aspects
I. Peschel and M. Kaulke 279

3.2 Walls, Wetting and Surface Criticality
E. Carlon 287

3.3 Critical Two-Dimensional Ising Films with Fields
A. Drzewiński 295

4 Thermodynamic Properties

4.1 One-Dimensional Kondo Lattices
N. Shibata 303

4.2 Impurities in Spin Chains
S. Rommer and S. Eggert 311

4.3 Thermodynamics of Ferrimagnets
U. Schollwöck 321

4.4 Thermodynamics of Metallic Kondo Lattices
S. Moukouri and L. Caron 329

5 Phonons and Disorder

5.1 Methods for Electron-Phonon Systems
E. Jeckelmann, C. Zhang and S. White 337

5.2 Disordered One-Dimensional Fermi Systems
P. Schmitteckert 345

How It All Began: A Personal Account

Steven R. White

Department of Physics and Astronomy, University of California
Irvine, CA 92697-4575, USA

In this chapter I'd like to take the opportunity to relate some of the history leading up to the development of DMRG. I think it is always interesting to look back, from a perspective where we know what works and what doesn't, and see the sometimes tortured path that got us here. The history I present here is a personal one: the work I was involved in, and the development of my ideas, which eventually led me to develop DMRG. I am not attempting to give proper credit to others who may have had similar ideas earlier, which an ordinary review should do – for that I refer to other chapters in this book. I will include many incidental details which one would not find in a review. Some of the events that happened along the way I found quite amusing, and I hope you will too.

Much of the development of DMRG traces back to my years as a graduate student at Cornell, from 1982 to 1987. I had first wanted to work for Michael Fisher, who worked on statistical mechanics and phase transitions, but during the first year that I would be working on my thesis, he was going to be on sabbatical at Caltech and so he wasn't taking any new students.

During the fall of 1983, the start of my second year at Cornell, Ken Wilson announced a set of lectures on "Chemistry". In these lectures, Wilson described an approach to solving the electronic structure of atoms and molecules using renormalization group and other ideas borrowed from particle physics and statistical mechanics. None of Wilson's approach had been carried out beyond the planning stages, and it is a testament to Wilson's prestige at the time that he could announce a set of lectures on what he hoped to do on a very difficult problem, and have everyone come. Wilson was strongly influenced by his father, E. Bright Wilson, a noted chemist at Harvard, who, among other things, wrote one of the first quantum mechanics books with a chemistry orientation in collaboration with Linus Pauling. This influence led Wilson to have as a long term goal the development of new electronic structure techniques, and Wilson's only publication during his first several years as an assistant professor at Cornell was on "Model Atomic Hamiltonians" [1], in which a lattice model was introduced for first and second row atoms.

I had worked for a chemist for three years as an undergraduate at UC San Diego, doing molecular dynamics simulations. (Coincidentally, this chemist's name is Kent Wilson. Kent, like Ken, is an unsual and remarkable person.) I thought Wilson's plan sounded like a good thing to work on, and I approached him about being his student. I remember one of the first things he said: "You

know there will be some computer work involved?" I assured him that that was right up my alley. However, he told me that he was only going to have shared students, not students of his own, so I asked John Wilkins, who worked on a variety of topics in solid state theory, if he would be my other thesis advisor. He agreed, and so I was a shared student with Wilson and Wilkins, and the eventual title of my thesis was "New methods for electronic structure calculations."

The main ideas of Wilson's plan were: 1) One can use RG language to describe very weak bound states of model "atoms". 2) With Grassmann algebra, one can integrate out fermions in an imaginary time path integral, and thus apply renormalization group ideas to electronic structure. This involved setting up a fine real-space lattice around a molecule, and then applying block-spin RG methods, using Grassmann integration, to "decimate" the lattice until the lattice spacing was comparable to an atomic radius. At that point, the problem would become nonperturbative, and decimation would stop. 3) The final part of the problem would be to apply the Langevin equation as a simulation tool to finish the problem. The Langevin approach had been developed by Klauder and others as a sort of early quantum Monte Carlo method. The effective action from the blocking procedure would be used as input to the Langevin equation.

When I started, I really didn't understand the big picture of what we were doing, but I was willing to dive in right away and learn as I went along. I spent a year working on a toy model which tested the block-spin approach with Grassmann variables, and then I spent a year working on the Langevin approach. This second year was actually spent at UC Santa Barbara – Wilkins had taken six students with him to spend a year there. At the end of this time, however, we realized the entire project was a failure. We ran into two serious, seemingly insurmountable problems: first, we weren't able to devise an effective method for integrating out core electrons in the Grassmann RG approach; and second, we found that the Langevin approach became numerically unstable and also gave the wrong answer, due to something similar to the fermion minus sign problem in quantum Monte Carlo.

I spent my last year at Cornell trying out some other approaches to electronic structure. Wilson didn't seem especially interested in these, and so I mostly talked to Wilkins about them. One of these was a variation on the configuration interaction method used in quantum chemistry. This approach is interesting in retrospect because a little of the flavor of DMRG is there: the wavefunction was expanded in an optimal way using the largest eigenvalues and eigenvectors of a matrix. I also worked on a variation of quantum Monte Carlo in the canonical ensemble and in applying the finite element method to electronic structure. Wilson continued to be interested in electronic structure methods in general, and he attended a regular group meeting of mostly Wilkins people in which this was discussed.

In the fall of my last year at Cornell, Wilson gave an interesting talk on the application of his numerical RG approach, which he developed for the Kondo impurity problem, to 1D lattice systems. This approach used a Hamiltonian, as opposed to an Lagrangian, and there was no extra time dimension. Another student of Wilkins at that time was Barbara Jones, who was applying this approach to two Kondo impurities. I had talked with Barbara about this method and thought it was very interesting. After Wilson had applied it to impurity problems, others applied it to 1D lattice systems, where it was called "real space RG". Wilson did not think very highly of real space RG, and in this talk Wilson used a toy model – a discretized particle in a 1D box – to analyze why it failed. Wilson showed how the truncation of the interactions at the edge of a block was unjustified, and led to nonsensical results. In pictorial terms, ignoring the interactions between blocks means that the retained states vanish at the edge of the blocks, and any subsequent states at later iterations always have kinks where the two blocks were joined. How would one fix this problem? Wilson suggested correcting for the neglected terms using a complicated form of perturbation theory. However, he concluded that this would be very difficult to carry out even in the 1D noninteracting case.

Perhaps Wilson was hoping someone would try out his ideas for fixing real space RG, but it was to be five years before this happened.

I had gotten to know Doug Scalapino, Bob Sugar, and their students quite well during our year at UCSB, and in September of 1987 I went back to UCSB for a post doc with Scalapino. There I focused on quantum Monte Carlo (QMC), Hubbard models, and in general the field of strongly correlated electrons and high temperature superconductivity, which I didn't know very much about at the start. We made good progress in improving the Monte Carlo methods, and produced some influential papers on the Hubbard model. For example, we found some of the first indications that d-wave pairing, rather than s-wave pairing, was prevalent. After two years as a post doc, I went to UC Irvine as an Assistant Professor.

While still at UCSB and for my first year or two at UCI I worked on methods for extracting dynamics from Monte Carlo. Some of our early results using a method I developed prompted Richard Silver and Jim Gubernatis to apply the maximum entropy method, which turned out to be superior. I switched to using maximum entropy coupled with QMC, and studied some of the dynamical properties of the Hubbard model. However, I also wanted to become more familiar with exact diagonalization methods, and a student and I developed a Lanczos program to study dynamics on 4×4 Hubbard systems.

During this period, I would occasionally try out some new idea to solve the fermion minus sign problem, the main bottleneck in the QMC method for fermions. Each of these attempts failed. (I would also occasionally hear about attempts by others to fix the minus sign problem, with at best only partial success.) For example, my student Marco Vekić and I tried a variation on the

world-line QMC method in which the basic unit was a block of sites rather than a single site. We found that this actually made the minus sign problem much worse – Marco found that there was a new type of "internal" minus sign which isn't there when you work with single sites! I began to conclude that the minus sign problem was really quite fundamental, and not likely to allow any easy solutions. I was also getting discouraged by the limitations of QMC on strongly-coupled systems, such as very slow evolution through phase space, large statistical errors, and poor scaling with system size, even in cases when there was no minus sign problem. This led me to once again think about numerical RG methods. (Since then, there has been more progress in dealing with the minus sign problem, but it is still a fundamental difficulty.)

I was not tempted to return to the Grassmann imaginary time formulation I had used as a graduate student. My work with quantum Monte Carlo had led me to conclude that it was very hard, and not very natural, to reach zero temperature by making the time direction of the lattice very long. Furthermore, I was very impressed with how the Lanczos method in exact diagonalization could pick out the ground state even with a very small gap to the first excited state. So, I began thinking back to Wilson's Hamiltonian-based numerical RG. Besides working at zero temperature directly, this approach allowed one to deal directly with composite particles or states: for example, suppose all of the electrons in a particular system (say, one with an attractive on-site interaction) were tightly bound in pairs. In the Hamiltonian approach, most of your states describing the Hilbert space would consist of pairs, with little trace of the original electrons. In the Grassmann approach, you would have to work with the original electrons, which seemed to me to be severe drawback.

However, because of the problems with real space RG, I thought that it might be promising to try to solve a finite Hubbard lattice using the numerical RG method in momentum space. In other words, one sets up a "lattice" where each site represents a particular allowed momentum, and the states of the site indicate whether a particle with that momentum is present. Another reason for trying out the momentum space RG was previous experience: my Lanczos work with a student on Hubbard systems had been in momentum space, in order to implement momentum conservation in a simple way. I carried out this approach on a 4×4 Hubbard system, and wrote a paper on it. I concluded that the results were pretty reasonable for energy differences, although total energies were poor. I wanted to know what Wilson thought of this work, and I sent him some email and a copy of the paper [2].

Wilson did not seem overly impressed. He stated emphatically that the particle-in-a-box problem of real space RG needed to be solved first before trying out many particle systems. He also suggested the perturbation approach to fix it, which he had mentioned in his talk at Cornell. He said I should talk to Wilkins and one of his post docs, who had also asked him recently about the particle-in-a-box problem again.

I took Wilson's opinions very seriously. I contacted Wilkins, who referred me to his post doc Kevin Ingersent. I proposed to Kevin, who had some additional notes on Wilson's perturbation approach, that we try out Wilson's ideas together.

Kevin and I tried Wilson's perturbation theory and many other variations, as many as we could think of. This was during the early spring of 1991. All of these approaches failed – in fact, the results were almost always worse than not doing the perturbative corrections at all. We ran out of ideas, concluding it was hopeless, and gave up. In retrospect, I know that the starting point for the perturbation theory was just too poor.

When the summer came, I couldn't resist thinking again about the particle-in-a-box problem, and thought more about boundary conditions(BCs). I knew that simply changing the BCs didn't fix the problem, although it changed what the errors looked like: for example, with fixed BCs, you had problems with slopes at the edges of a block, while with free BCs you got discontinuities. Trying a single BC which was in between fixed and free was possible, but it didn't work any better. Finally I got the idea of trying two different BCs at the same time – getting some states from one BC, some from another. I was still thinking in terms of fixed and free BCs, and it seemed that based on what the wavefunctions for each boundary condition looked like, this might work much better–you could combine the different states to get rid of the various discontinuities. I immediately tried out the "fixed-free" approach numerically – I always try things out numerically very soon after I get an idea, since I enjoy programming and trying out the idea more than trying to work out the details on paper. The test consisted of comparing energies of low lying states after ten RG iterations with exact results.

When I saw the results from the first fixed-free test, I was astonished! Previously, the results from all my numerical tests were garbage, orders of magnitude off from the exact solution. Not only had the fixed-free method worked, the results now seemed exact! The results agreed to at least ten digits, keeping only eight states, and I didn't know whether the miniscule differences were simply the results of round off error. (Some time later, I carried out the calculations again in quadruple precision, and found that the results were good only to ten digits, no more.)

I played around with this for just a short while more, and then I returned to thinking about interacting systems. I felt that this had indeed given me the key to understanding the many particle problem as well as the single particle one. I first tried out the fixed free technique on Heisenberg spin chains. I ended up trying several variations of this approach, including the antiperiodic/periodic combination of boundary conditions, without success. However, this led me to the conclusion that I needed extra boundary sites, which were not part of the block, in order to induce the right boundary condtions. This led to the idea of solving a "superblock" system, and then projecting the superblock state onto the block. I devised a projection method, which was

conceptually similar to the optimal configuration interaction approach from my thesis. The status of this work, as of September 1991, was written up in a paper for a conference in Osaka [3]. Already I was becoming confident that this was going to be a very promising approach, and I said so at the conference.

In September, 1991 Reinhard Noack came to work for me as a post doc. Reinhard had been a student of Scalapino, where he worked on quantum Monte Carlo calculations of a two chain Hubbard model. Reinhard had had a lot of trouble in studying the two chain system because of the minus sign problem. I suggested to him that he take over the particle-in-a-box work and turn it into a paper. He got going very quickly on it and the paper was written by December [4]. Subsequently, Reinhard worked on applying these single particle RG methods to problems in Anderson localization. (Eventually, Reinhard returned to studying the two chain Hubbard model, this time using DMRG and with much more success.)

In the late fall or early winter of 1992 I returned to the interacting problem and realized that my projection idea of the superblock onto a block was actually equivalent to a singular value decomposition:

$$\psi_{ij} = U_{i\alpha} D_{\alpha\alpha} V_{\alpha j} \tag{1}$$

where i denotes states of the block, and j denotes states of the remainder of the superblock. I had taught graduate statistical mechanics a few times since coming to UCI, for which I had read parts of Feynman's Lectures on Statistical Mechanics [5]. One of my favorite parts of the book was his introduction to density matrices. I soon realized that performing the singular value decomposition was equivalent to diagonalizing a density matrix:

$$\rho_{ii'} = \psi_{ij}\psi_{i'j} = U_{i\alpha} D^2_{\alpha\alpha} U_{i'\alpha}. \tag{2}$$

This made me very happy: now the technique was becoming quite elegant.

I then began numerical tests and more extensive program development. One early test was to diagonalize a finite Hubbard chain, split it in half, and look at the density matrix eigenvalues for the two sides. This behaved quite nicely. I then began writing a program to do the infinite-system DMRG method for the Heisenberg spin 1/2 chain, for which there is the exact Bethe ansatz solution. I was getting odd-even bond dimerization, so it didn't look like it was working well. However, I remember checking the average energy over two adjacent bonds and being very surprised at how close that was to the exact result – about 5 or 6 digits were correct! It was at that point that I realized things could work very well with this method even with interacting systems.

At that point I had a good understanding of all the pieces of the puzzle. I figured out how the finite system method should work. When I got that program working, and found it worked extremely well, I remember being most concerned about how I would explain this method to others – it was

completely unlike any other numerical method I had heard of. I felt the finite system method would look very strange and ad hoc, and I dreaded trying to write a paper to explain the algorithm and explain why, for example, there were two sites in the middle in the standard superblock configuration. It was not that I couldn't explain why, it was just that the explanation would be complicated, as would the description of the algorithm in general. I tried out periodic boundary conditions, found that they didn't work as as open BCs, and also developed an intuitive understanding of why that was.

I wanted a good problem to demonstrate the technique on and I settled on the spin-1 Heisenberg chain, where I got some nice results. I wanted to publicize the method a little. I had a family trip arranged to the East coast in May, and so I contacted friends at Bell Labs and IBM Yorktown Heights, telling them I had some results from an exciting new method and I wanted to give a talk. (I remember Andy Millis at Bell Labs introducing me, saying something like "This is Steve White who has some new results that *he* is very excited about...") The reception I got at Bell was very enthusiastic, and I started a collaboration with David Huse to study the spin-1 Heisenberg chain in more detail [6]. (At IBM, however, no one seemed particularly interested – they weren't working on those kinds of problems.)

I'd like to finish this chapter with some stories about the first DMRG-related papers and some interactions with the referees. For the particle-in-a-box paper [4], with Reinhard Noack, we felt that the editors would have a hard time finding someone to referee the paper, since this was not an active field. We suggested in our submittal letter to Physical Review Letters several people as referees, including Ken Wilson and Patrick Lee, who had worked in numerical RGs in the past. After some time we got a very sensible referee report back, pointing out that while this was very interesting, it was still just for a single particle, and might not generalize to many particle systems. Therefore, the referee recommended that it appear in Physical Review B, Rapid Communications. I thought this was completely reasonable and we told the editors to put it in Rapid Communications.

Very soon after I got a very surprising letter from the editors of PRL. It said that because of a late referee's report, they were now going to accept it for PRL. (We could also still send it to Rapid Communications if we wanted.) This didn't make any sense to me – if you get one good and one bad report, you always have to resubmit, and then maybe you get the paper in because the third referee likes it. So what happened is very unusual – I call it *Spontaneous Unrejection.* Then I read the new referee's report, and I realized why. The report was incredibly insightful. After saying that we had solved an important (toy) problem, and saying that the paper should be accepted, it went on to speculate on the prospects for applying the methods to many particle systems. It said that the fixed-free method probably wouldn't work for interacting systems, since the boundary conditions would apply to all particles identically, whereas it would need to apply in different ways to

different particles. It said that the superblock method might work, but that putting three or more blocks together would be very hard to diagonalize. Now, I had already come to these conclusions (or very similar ones) after months of further work. I realized that this report had to be from Wilson – only he had this level of insight about this problem – and that this explained why the editor would now accept the paper: Wilson was the final word in RG methods.

A few months after this exchange I submitted to PRL the original DMRG paper [7]. I got back one positive and one negative report. Both reports were critical of the presentation, which I was sympathetic with – I found it very hard to explain the method in a modest number of words. I rewrote it, taking out a description of the finite system method, which was too brief to make sense, and resubmitted. I got back a third report, which said, "I agree with Referee B. This paper is not appropriate for publication in Physical Review Letters. The reason is as follows. This paper is making a calculation on the Heisenberg linear chain problem. In my opinion, the method is not very new and the above problem has been widely worked in connection with Haldane problem. Hence this paper is inappropriate for publication in PRL..."

I have never appealed a PRL decision before or since, but in this case I did. I asked it be sent to a divisional editor, and I believe they sent it to Peter Young. The divisional editor accepted it at once.

It took me quite a while to write the longer paper describing the algorithms in detail [8]. I also had a hard time getting started because it seemed like too much work and I enjoyed applying DMRG to problems more than I liked writing. However, the long paper did finally get written, and shortly thereafter DMRG began to be used by a number of other groups.

I have been absolutely delighted by the marvelous work done by many other groups using DMRG since then. One of the biggest compliments to a scientist is to have his work used by others, and seeing all the uses, improvements, and extensions to DMRG, as discussed in the rest of this book, is a source of great pleasure to me.

References

1. K.R. Piech and K.G. Wilson, J. Chem. Phys. **48**, 3740 (1968)
2. S.R. White, Phys. Rev. B **45**, 5752 (1992).
3. S.R. White, in Computational Approaches in Condensed-Matter Physics, edited by S. Miyashita, M. Imada, and H. Takayama, Springer, p 97 (1992)
4. S.R. White and R.M. Noack, Phys. Rev. Lett. **68**, 3487 (1992)
5. R.P. Feynman, Statistical Mechanics: A Set of Lectures, Benjamin (1972)
6. S.R. White and D.A. Huse, Phys. Rev. B**48**, 3844 (1993)
7. S.R. White, Phys. Rev. Lett. **69**, 2863 (1992)
8. S.R. White, Phys. Rev. B**48**, 10345 (1993)