UNIVERSITY OF AMSTERDAM

MSc Physics

Track: Theoretical Physics

MASTER THESIS

Finite bond dimension scaling with the corner transfer matrix renormalization group method

Geert Kapteijns

10275037

July 2017

60 ECTS

Supervisor:
Dr. Philippe Corboz

Examiner:
Prof. dr. Bernard Nienhuis

Institute for Theoretical Physics

Abstract

Lorem ipsum dolor sit amet, consectetur adipisicing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Contents

Acknowledgements

hallo

1
Introduction

This thesis investigates a numerical approximation method put forth by Baxter in 1978 [1–3] based on the corner transfer matrix formulation of the partition function for two-dimensional classical lattice models.

The method rose to prominence in 1996, under the name *corner transfer matrix renormalization group* (CTMRG), when Nishino showed [4] that in the thermodynamic limit, it is equivalent to the hugely successful density matrix renormalization group (DMRG) method for one-dimensional quantum systems [5], discovered a few years earlier by White.

The error in the CTMRG method comes from the fact that the corner transfer matrices, whose dimension diverges exponentially in the lattice size, have to be truncated at a maximum dimension m in order to make numerical manipulation possible. This finite *bond dimension* m (also denoted by χ or D in the literature) introduces finite-size effects, comparable to those observed for systems that are finite in one or more spatial dimensions. This was already realized by Nishino [6].

The main objective of this thesis is to study how *finite bond dimension scaling* may be performed with the CTMRG method.

Before the structure of this thesis is laid out, I will first make some general remarks on statistical mechanics and phase transitions, and on how the CTMRG method relates to the class of newer methods for simulating many-body systems that grew out of White's breakthrough, known as *tensor network algorithms*.

1.1 Statistical mechanics and phase transitions

Statistical mechanics is concerned with describing the average properties of systems consisting of many particles. Examples of such systems are the atoms

making up a bar magnet, the water molecules in a glass of water, or virtually any other instance of matter around us.

Matter can arrange itself in various structures with fundamentally different properties. We call these distinct states of matter *phases*. When matter changes from one phase to another, we say it undergoes a phase transition.

Physics has made great strides in understanding these transitions. The complete history of the field is beyond the scope of this introduction and this thesis, but the reader may wish to consult [7, 8] to get an idea.

Only as late as 1936, the occurrence of a phase transition within the framework of statistical physics was established by R. Peierls [9]. He showed that the two-dimensional Ising model has a non-zero magnetization for sufficiently low temperatures. Since for high enough temperatures the Ising model loses its magnetization, it follows that there must be phase transition in between.

The effort to understand the Ising model culminated with Onsager's exact solution in 1944 [10], which rigorously established a sharp transition point in the thermodynamic limit.

One may question the relevance of studying very simple models such as the Ising model. As it turns out, systems that are at first sight vastly different may show qualitatively similar behaviour near a phase transition. For example, exponents that characterize the divergence of quantities near a transition are conjectured to be independent on microscopic details of the interactions between particles, but instead fall into distinct *universality classes* [11, 12]. Thus, studying the very simplest model may yield universal results.

1.2 Baxter's method as a precursor to tensor network methods

Baxter showed that the optimal truncation of corner transfer matrices corresponds, in the thermodynamic limit, to a variational optimization of the row-to-row transfer matrix within a certain subspace, now known as the subspace of *matrix product states* (MPSs) [2, 13].

After the success of White's DMRG, which, as Nishino pointed out, is equivalent to Baxter's method, the underlying matrix-product structure was rediscovered in the context of one-dimensional quantum systems by Östlund and Rommer [14, 15].

It is historically significant but little known that Nightingale, in a footnote of a 1986 paper [16], already made the remark that "The generalization [of Baxter's method] to quantum mechanical systems is straightforward."

After Östlund and Rommer, it was realized that reformulating White's algorithm directly in terms of matrix product states provided the explanation of the algorithm's shortcomings around phase transitions. An MPS-ansatz fundamentally limits the entropy of the ground state approximation and since the entropy diverges at a conformally invariant critical point [17], DMRG gives inaccurate results.

This gave rise to other ansätze, formulated in the language of tensor networks [18], specifically designed to represent states with a certain amount of entropy. Examples are multi-scale entanglement renormalization ansatz (MERA) for critical one-dimensional quantum systems [19] and projected entangled-pair states (PEPS) [20] for two-dimensional quantum systems.

Other tensor network algorithms, such as infinite time-evolving block decimation [21] in one dimension and iPEPS (infinite PEPS) [22] in two dimensions made it possible to directly approximate quantum systems in the thermodynamic limit.

iTEBD was used to study finite bond dimension scaling (under the slightly different name of *finite-entropy scaling*) [23]. Some theoretical predictions were later made in [24].

The goal of this thesis is twofold: (i) investigate how finite bond dimension scaling works in the CTMRG algorithm for classical systems, where we can directly compare it with finite-size scaling, and (ii) investigate how it compares to different numerical approaches, such as iTEBD or Monte Carlo.

For (i), I have studied the Ising model, for which all results may be checked against the exact solution. For (ii), I have studied the clock model with $q = \{5, 6\}$ states, which is regarded as difficult numerically and subject to some controverse.

1.3 Structure of this thesis

It is in the mostly quantum-oriented research field sketched above that the work for this thesis was done. Therefore, I have chosen to begin by introducing White's algorithm in its original description (chapter two), before making the connection to two-dimensional classical lattices and properly introducing the corner transfer matrix formulation (chapter three).

In chapter four, the concepts of critical behaviour and finite-size scaling are introduced and in chapter five these concepts are connected to the work already done on finite bond dimension (or finite-entropy) scaling.

Technical details and convergence behaviour of the CTMRG algorithm are reported in chapter six. It is found that the values of observables may be accurately extrapolated in the chosen convergence criterion of the algoritm.

Results for the Ising model are presented and analyzed in chapter seven. With finite-m simulations, it is much easier to reach large system sizes, but thermodynamic quantities do not grow smoothly as a function of the bond dimension, as a result of the underlying spectrum of the corner transfer matrix.

Quantities calculated with finite-size simulations do not suffer this unsmooth behaviour. Results for both methods are comparable, but it is plausible that finite-size data turns out to be more accurate when corrections to scaling are included.

A numerical analysis of the clock model with $q = \{5, 6\}$ states is given in chapter eight. The model has a low-temperature ordered phase, a massless phase and a high-temperature disordered phase. We locate the transition temperatures T_1 and T_2 by extrapolating the positions of pseudocritical temperatures, assuming the transitions are of the Kosterlitz-Thouless type. We find slightly contradictory results, based on exact results in a related formulation of the model, but we argue it is plausible that this is due to finite-size effects.

Bibliography

[1] R. J. Baxter, "Variational approximations for square lattice models in statistical mechanics", Journal of Statistical Physics **19**, 461–478 (1978).

[2] R. J. Baxter, *Exactly solved models in statistical mechanics* (Elsevier, 1982) Chap. 13.

[3] S. K. Tsang, "Square lattice variational approximations applied to the Ising model", Journal of Statistical Physics **20**, 95–114 (1979).

[4] T. Nishino, and K. Okunishi, "Corner transfer matrix renormalization group method", Journal of the Physical Society of Japan **65**, 891–894 (1996).

[5] S. R. White, "Density matrix formulation for quantum renormalization groups", Physical Review Letters **69**, 2863 (1992).

[6] T. Nishino, K. Okunishi, and M. Kikuchi, "Numerical renormalization group at criticality", Physics Letters A **213**, 69–72 (1996).

[7] L. P. Kadanoff, "More is the same; phase transitions and mean field theories", Journal of Statistical Physics **137**, 777 (2009).

[8] C. Domb, *The critical point: a historical introduction to the modern theory of critical phenomena* (CRC Press, 1996).

[9] R. Peierls, "On Ising's model of ferromagnetism", Mathematical Proceedings of the Cambridge Philosophical Society **32**, 477–481 (1936).

[10] L. Onsager, "Crystal statistics. I. a two-dimensional model with an order-disorder transition", Phys. Rev. **65**, 117–149 (1944).

[11] R. B. Griffiths, "Dependence of critical indices on a parameter", Physical Review Letters **24**, 1479–1482 (1970).

[12] M. E. Fisher, "Quantum corrections to critical-point behavior", Physical Review Letters **16**, 11–14 (1966).

[13] R. J. Baxter, "Dimers on a rectangular lattice", Journal of Mathematical Physics **9**, 650–654 (1968).

[14] S. Östlund, and S. Rommer, "Thermodynamic limit of density matrix renormalization", Physical Review Letters **75**, 3537 (1995).

[15] S. Rommer, and S. Östlund, "Class of ansatz wave functions for one-dimensional spin systems and their relation to the density matrix renormalization group", Physical Review B **55**, 2164 (1997).

[16] M. P. Nightingale, and H. W. J. Blöte, "Gap of the linear spin-1 Heisenberg antiferromagnet: a Monte Carlo calculation", Physical Review B **33**, 659–661 (1986).

[17] P. Calabrese, and J. Cardy, "Entanglement entropy and quantum field theory", Journal of Statistical Mechanics: Theory and Experiment **2004**, P06002 (2004).

[18] R. Orús, "A practical introduction to tensor networks: matrix product states and projected entangled pair states", Annals of Physics **349**, 117–158 (2014).

[19] G. Vidal, "Entanglement renormalization", Physical Review Letters **99**, 220405 (2007).

[20] F. Verstraete, and J. I. Cirac, "Renormalization algorithms for quantum-many body systems in two and higher dimensions", arXiv cond-mat/0407066 (2004).

[21] G. Vidal, "Classical simulation of infinite-size quantum lattice systems in one spatial dimension", Physical Review Letters **98**, 070201 (2007).

[22] J. Jordan, R. Orús, G. Vidal, F. Verstraete, and J. I. Cirac, "Classical simulation of infinite-size quantum lattice systems in two spatial dimensions", Physical Review Letters **101**, 250602 (2008).

[23] L. Tagliacozzo, T. R. De Oliveira, S. Iblisdir, and J. I. Latorre, "Scaling of entanglement support for matrix product states", Physical Review B **78**, 024410 (2008).

[24] F. Pollmann, S. Mukerjee, A. M. Turner, and J. E. Moore, "Theory of finite-entanglement scaling at one-dimensional quantum critical points", Physical Review Letters **102**, 255701 (2009).