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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 with a round-a-face interaction.

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 size m in order to make numerical manipulation possible. This finite *bond dimension* m 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 methods for simulating many-body systems that grew out of White’s breakthrough, known as *tensor network algorithms*.

1.1 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 showed, 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, 21] for two-dimensional quantum systems.

1.3 Structure of this thesis

It is in the mostly quantum-oriented context sketched above that the research for this thesis was carried out. 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).

Chapter four introduces the concepts of critical behaviour and finite-size scaling and chapter five

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