Computational approach to scaling and criticality in planar Ising models

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Declaration

This thesis is an account of research undertaken in the Department of Theoretical Physics within the Research School of Physics and Engineering at the Australian National University between June 2007 and July 2011 while I was enrolled for the Doctor of Philosophy degree.

I hereby declare that, unless specifically stated otherwise, the material presented within this thesis is my own. None of the work presented here has ever been submitted for any degree at this or any other institution of learning.

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Abstract

In this thesis, we study the critical behaviour of the two-dimensional Ising model on the regular lattices. Using the numerical solution of the model on the square, triangular and honeycomb lattices we compute the universal scaling function, which turns out to be identical on each of the lattices, in addition to being identical to the scaling function of the Ising Field Theory, computed previously by Fonseca and Zamolodchikov.

To cope with the lattice contributions we carefully examined series expansions of the lattice free energy derivatives. We included the non-scaling regular part of the free energy as well as non-linear Aharony-Fisher scaling fields, which all have non-universal expansions. Using as many of the previously known exact results as possible, we were able to fit the unknown coefficients of the scaling function expansion and obtain some non-universal coefficients. In contrast to the IFT approach of Fonseca and Zamolodchikov, all coefficients were obtained independently from separate datasets, without using dispersion relations.

These results show that the Scaling and Universality hypotheses, with the help of the Aharony-Fisher corrections, hold on the lattice to very high precision and so there should be no doubt of their validity.

For all numerical computations we used the Corner Transfer Matrix Renormalisation Group (CTMRG) algorithm, introduced by Nishino and Okunishi. The algorithm combines Baxter's variational approach (which gives Corner Transfer Matrix (CTM) equations), and White's Density Matrix Renormalisation Group (DMRG) method to solve the CTM equations efficiently. It was shown that given sufficient distance from the critical point, the algorithmic precision is exceptionally good and is unlikely to be exceeded with any other general algorithm using the same amount of numerical computations.

While performing tests we also confirmed several critical parameters of the three-state Ising and Blume-Capel models, although no extra precision was gained, compared to previous results from other methods. In addition to the results pre-

sented here, we produced an efficient and reusable implementation of the CTMRG algorithm, which after minor modifications could be used for a variety of lattice models, such as the Kashiwara-Miwa and the chiral Potts models.

Citations to previously published papers

Publications related to this thesis are as follows:

- V. V. Mangazeev, M. T. Batchelor, V. V. Bazhanov, and M. Yu. Dudalev. Variational approach to the scaling function of the 2D Ising mode in a magnetic field. *J. Phys. A*, **42** 042005. (2009)

- V. V. Mangazeev, M. Yu. Dudalev, V. V. Bazhanov, and M. T. Batchelor. Scaling and universality in the two-dimensional Ising model with a magnetic field. *Phys. Rev. E*, **81** 060105. (2010)

- M. Yu. Dudalev, V. V. Mangazeev, V. V. Bazhanov, and M. T. Batchelor. Scaling function of the honeycomb lattice Ising model. *In preparation.*

Contents

Introduction

Condensed matter physics is one of the most widely studied areas of physics. The well known public preprint Arxiv has an umbrella section "cond-mat" that has a larger number of publications per month than any other section. This seems to be quite natural, because this branch of physics enjoys considerable applicability in modern technology; one could say it is directly commercialisable. Just as quantum mechanics serves as a basis for all other quantum-related physics, statistical mechanics forms the foundation of condensed matter physics. The elementary laws governing small elements of the system multiplied by the huge number of those elements creates plausible explanations for the majority of the effects we see in experiments. Statistical mechanics also shows a deep interconnection with quantum field theory, both being mutual sources of inspiration and techniques during the last few decades.

One of the simplest models in statistical mechanics is the Ising model. It was originally introduced as a model of a phase transition in magnets, i.e. the Curie point. While viewing the magnet as just a combination of small magnets aligned along a single axis and interacting only with their nearest-neighbours could be viewed as an oversimplification, it has nevertheless revealed rather rich physics, and in fact can be seen as more correct model than a naive ensemble of magnets due to quantum effects. When it was originally proposed by Lenz [1] and solved for the 1D case by Ising [2], rich physics was not seen because for the 1D case there is no phase transition in the model, and the free energy is always a regular function except at zero temperature. Overgeneralisation of this result even led to the theories that still reside in some text books, namely Landau [3] theory, that most phase transitions are not represented by any singularities in the free energy, but are just some change of the internal arrangements or symmetry.

The above mentioned theory was clearly seen to be wrong when the 2D case was solved for zero external field by Lars Onsager in 1944 [4]. The solution clearly showed that the phase transition is an actual singularity and that the

specific heat becomes infinite at the critical point. Onsager's work is also credited with creating a branch inside statistical mechanics, devoted to the exactly solved models, which in turn catalysed development of many new areas of mathematics, such as quantum algebra.

But despite numerous attempts there is still no exact solution for the non-zero field 2D Ising Model. There is no exact solution for the three-dimensional Ising model as well, but in dimensions more then three the Ising model could be treated very well using a mean-field approximation, although no exact solution exists. There are a lot of other 2D models which have been solved exactly (like 6-vertex [5] and 8-vertex [6] models, the Kashiwara-Miwa [7, 8] model and many others). Naturally, all these models are exceptions, since general lattice models can not be solved exactly. It appears though that the most interesting things are happening in the vicinity of the critical point. One such thing is scale invariance, which also could help to get an approximate solution of the model near the point where it works. Scaling is an old and obvious concept, that is especially easy to understand in mechanics. The rescaled system has the same properties as the original system, and differs only by some scaling factor. Scale invariance means that some system's physics is unchanged by rescaling. Measured values, if they are not dimensionless, of course are also scaled, but the whole physics of the system, and dimensionless combinations of observable values stay the same. Sufficiently close to the critical point the correlation length becomes infinitely large and can not be a natural scale any more. Thus the free energy becomes a homogeneous function of the model parameters, or, in another words,a function only of the dimensionless combinations of the model parameters.

The first consistent application of scaling invariance (or strictly speaking a Renormalisation Group theory) came to quantum field theory with works of Gell-Mann and Low [9], and a little bit later was introduced to statistical mechanics by Fisher [10] in the form of critical exponents, i.e. dimensions of the model's parameters and observable values near the critical point. Fisher was one of the people who proposed the scaling and universality hypotheses. The first hypothesis states that around the critical point a singular part of the free energy is expressed via a scaling function which depends on the dimensionless combinations of the model parameters only. The universality hypothesis states that all models are split in equivalence classes depending on dimensionality and symmetry, and share the same scaling function. There is also a belief that there are a lot of interesting models that belong to the Ising universality class.

While there is a lot of evidence that these hypotheses are true, strictly speak-

ing there is no proof or precise demonstration even for the Ising model itself, because of the absence of a solution with sufficient precision (let alone an exact solution) for $H \neq 0$.

Nevertheless, the hypotheses were accepted, used and developed, e.g. by Kadanoff and Wilson. Works of the latter brought the statistical mechanics variant of scale invariance to quantum field theory. Generalisation of the scale invariance to the local scale transformation in 2D gave a brilliant and powerful theory called Conformal Field Theory [11], which found widespread use in many areas of theoretical physics. It also describes the critical limit of the lattice Ising Model allowing us to obtain its approximate solution around the critical point, and ultimately to verify the scaling and universality hypotheses.

Besides the family of exact solutions of the lattice statistical models, in the 70's a related field of research began to flourish. Starting from the quantum inverse scattering method [12, 13], a branch of quantum field theory dedicated to exact solutions started to develop. One of the key ingredients of the exactly solved QFT models is the Yang-Baxter equation. Nowadays there are also many exactly solved models related to string theory, AdS/CFT models and many others. Most of them use methods originally developed in statistical mechanics.

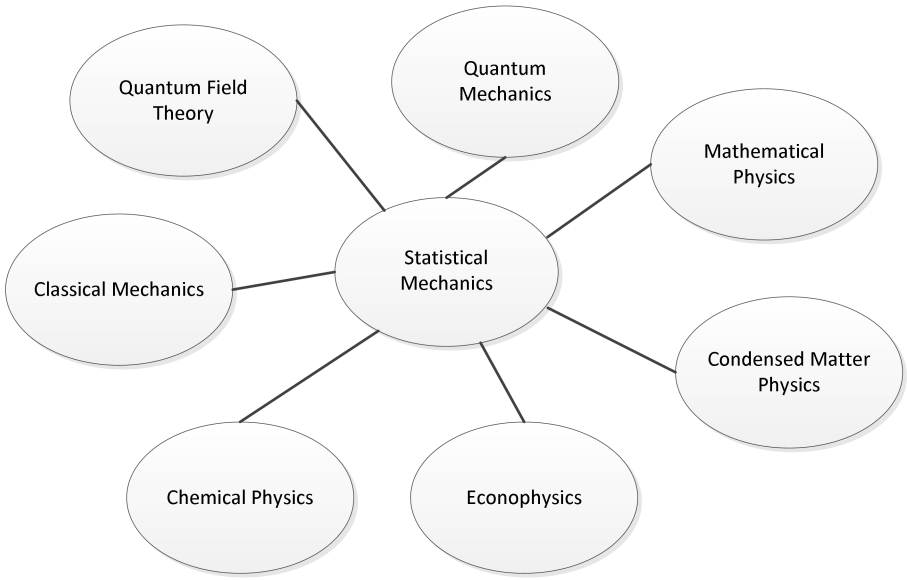

Figure 1: Relation of statistical mechanics to the other branches of physics.

The motivation of the present work was to convincingly demonstrate the validity of the scaling and universality hypotheses using high-precision numerical methods, which in turn, ironically, descend from the application of scaling invariance. A short description of the chapters now follows.

In the first part of the Chapter 1 we describe the 2D Ising model, its solution for the $H = 0$ case, and other exact results that are relevant to obtaining the scaling function, such as the series for the magnetic susceptibility. The second part is devoted to explaining what Baxter's variational approach is, and how very important objects called Corner Transfer Matrices emerge in this approach. The approach gives a system of matrix equations with infinite matrices. While it is not entirely rigorous, it is possible to show that the truncated form of the equations with finite matrices is a good approximation to the infinite case.

There are many ways to solve a system of non-linear equations, such as the Newton-Raphson algorithm; some of them are well-suited to the matrix system. But for Baxter's equation a special iterative method exists. It not only solves the equations, but gives them an extra physical sense; connecting them with White's Real Space Renormalisation Group [14], originally proposed to compute a density matrix in quantum models. Developed by Nishino and Okunishi [15, 16], the method seems to be the most optimal way of solving Baxter's equations. For instance, for the Ising model it always converges (that would be a miracle for any general iterative non-linear method). In Chapter 2 we first describe in detail the White and Nishino methods. Then various generalisations of the algorithm to the non-square lattices are made, such as regular triangular and honeycomb lattices, as well as for lattices with symmetry group less than the full group of symmetries for such a lattice, e.g. the rectangular lattice with different bond strengths for horizontal and vertical bonds.

We also provide practical details of the actual algorithm implementation, the number of iterative steps, and practical observations that helped the research. For example we noticed that the structure of the Corner Transfer Matrix for $H \neq 0$ bears only a superficial resemblance to the exact $H = 0$ matrix and essentially only follows the universal asymptotics, but does not have any degenerate levels that are believed to be a sign of integrability of the system.

Technical details of all computer codes plus a short user manual for them constitutes Appendix A. The actual program is a combination of small subprograms, that are written in Fortran (the performance-critical part) and Python (the control part). Most of the data flow between these subprograms is saved to disk, so it is very easy to do the computation on cluster machines using almost no parallelisation techniques, but with just a simple distribution of the points in parameter space among different nodes of the cluster.

Besides the above mentioned algorithms, at the beginning of our research we tried to use a couple of other algorithms without much success. At the end of

Chapter 2 we outline these algorithms together with possible reasons for their failure.

Without any additional knowledge of the scaling behaviour of the Ising model free energy it is impossible to reach high precision while computing the scaling function. While it is possible to use only numerical results to get the scaling function, it is much more useful to employ as many exact results as possible. Thus it is worth gathering as much additional information about the non-zero field Ising model as possible and then study carefully the scaling behaviour of the model. This is also motivated by the actual structure of the Ising Model scaling function, which has not just a power law singularity but has an additional logarithmic singularity, which requires special treatment to extract the scaling function. The zero-field solution is given in Chapter 1; there are also several notable results for the non-zero field case which are presented in Chapter 3. Some of them relate to not just the lattice Ising model, but also to the so called Ising Field Theory (IFT), a Conformal Field Theory with central charge $\frac{1}{2}$ perturbed by two operators with coupling constants corresponding to the temperature and magnetic fields. This theory was thoroughly examined by Fonseca and Zamolodchikov [17]. Zero coupling to the magnetic field operator gives the singular part of the Onsager solution, while zero coupling to the thermal operator gives Zamolodchikov's E_8 theory [18], an exact solution for the critical isotherm of the IFT. It is exact in the IFT only, nevertheless it gives two expansion coefficients of the scaling function exactly, and that helps greatly determining the next coefficients with increased precision. Finally, Vicari et al. [19] showed how to link all the pieces to the lattice theory and that it is possible to track so called irrelevant operators which essentially are higher-order deviations from the scaling theory on the lattice.

In Chapter 4 all these techniques are applied to the numerical data obtained using algorithms from Chapter 2. Three regular lattices are studied thoroughly: the square, triangular and honeycomb lattices. While as expected all lattice values, magnetisation and internal energy have different values, all non-universal functions (Aharony-Fisher scaling fields and a regular part of the free energy) are different, but the function that lies at the heart of these functions, that is the scaling function, is absolutely the same for the three lattices, and coincides with the function obtained from IFT. This equality is demonstrated with unprecedented precision, that moves beyond any doubt the validity of the universality hypothesis. While it is very difficult to analyse high-order contributions of irrelevant operators, we also are able to partially confirm conjectures about the first irrelevant operators, i.e. their contribution to the fourth next to the leading order

in zero-field susceptibility of the square lattice Ising model.

In the final chapter, Chapter 5, we describe additional lattice models, namely the three-state Ising model and Blume-Capel model and present some basic results obtained with a simple extension of the algorithm to models with more than two states per spin. Not a lot of new results are described there, but we independently confirmed some earlier results (that were obtained by different methods specific to the models) using CTMRG (which is a rather general method). For models known much less well than the Ising model that is of great value. Also this chapter demonstrates how important it is to know some exact results in order to get the most from the numerical data; the precision of calculations was quite high, but because of the absence of knowledge of the exact critical temperature, the high precision data yielded a precision for the critical parameters and exponents that provides very little improvement over pre-existing results.

The Conclusion outlines two important things. The first are missing parts of the current research, plus a list of what could be usefully included in the current work or what was started, but wasn't finished or included. The second part contains the most promising directions for future research, albeit the plausibility of all the proposed research ideas needs careful assessment.