Corner Transfer Matrix Approach to the Yang-Lee Singularity in the 2D Ising Model

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A thesis submitted for the degree of
Doctor of Philosophy



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December, 2023

DECLARATION

This dissertation is an account of research undertaken between April 2018 and November 2023 at the Research School of Physics, The Australian National University, Canberra, Australia.

Except where acknowledged in the customary manner, all material presented in this dissertation including figures are original and have not been submitted in whole or part for a degree in any university.

Bryte Hagan
December 29, 2023

PUBLICATIONS

Peer-Reviewed articles

V. Mangazeev, **B. Hagan** and V. Bazhanov (2023). "Corner Transfer Matrix Approach to the Yang-Lee Singularity in the 2D Ising Model in a magnetic field" [49].

Dedicated to my family

ACKNOWLEDGEMENTS

This work is dedicated to the people who have been pivotal in supporting me along the far-too-many days for its completion. Without their unwavering assistance, constant reassurance and endless support I would not have been able to complete this work. The submission of this project is as much a testament to my efforts as it is to their aid.

I must first thank my parents. You have each been a lifelong inspiration for me, and any heights which I reach are built upon foundations you have laid. Thank you for not only enabling me but also encouraging me to achieve my dreams.

To my brilliant, ever-smiling and boundlessly helpful uncle Stewart, I thank you. Despite living hundreds of kilometers away, it never felt like you were any further than down the road. I will always treasure your understanding and compassionate ear.

I would like to thank my sisters, Aba and Nana. You have exemplified to me that through any difficult period, your family will be there for you. Thank you for always having my back. Your little brother appreciates you and the guidance that you both offer.

One of the last of the named thank you I would like to give is to my partner, Caitlin. This project has been the most difficult undertaking of my life and every day you helped me in innumerable ways. Despite not having a physics degree, you were always an ear to discuss with and a relentless source of encouragement. Every day you kept me on track, even on days when I was ready to give up. You carried me across the finish line many times over; I absolutely could not have done this without you. Thank you.

And of course, the lucky-last thanks must be given to our adorable little Teddy. He may not be able to understand the contents of this document, but he understands the importance of routine, ceaseless companionship and a good walk. Thank you for always sticking to the routine and keeping me sane, Ted.

There are many more people whose support and friendship along the journey were greatly valued. I do not have the space to thank you all, but I will always recognise your contributions. From the bottom of my heart I thank all of you, and I dedicate this to work you. Your help will forever be appreciated.

ABSTRACT

The goal of this work is to investigate the complex magnetic field analytic continuation of the 2D Ising model near the Yang-Lee singularity. The exact location of the singularity is not known precisely, and one of the results produced in this work is an improved quality estimate of its location $i\xi_0 = i0.18935060551(3)$. Another primary result is the numerical verification of the scaling function conjecture by Fonseca & Zamolodchikov in [31] regarding the structure of the free energy scaling function near the Yang-Lee singularity, as well as proposed logarithmic operators in the Ising free energy at order H^2.

In accomplishing the above results, this thesis starts by detailing the slice of the Ising model's history pertinent to this work. For an established model such as the Ising model it would be impractical to cover every branch and generalisation, so this work focuses on the standard 2D Ising model with magnetic field in both the square and triangular cases. The relevant historical developments covered focus on the Ising scaling theory, general renormalisation arguments and conformal field theory (and the more modern logarithmic extensions) used to underpin our current understanding of the model. This thesis then details the theory and implementation details for the main numerical technique used: the Corner Transfer Matrix Renormalisation Group (CTMRG) method.

The Ising susceptibility data obtained in [56, 22] plays a critical role in providing numerical evidence for the extended logarithmic operators proposed in this work. These operators are predicted by the theory of a logarithmic minimal model $\mathcal{LM}(3,4)$ for a conformal field theory of central charge $c = 1/2$ [44] which describes the Ising model at the critical point. The operators appear as the result of the integer difference in conformal weight between the identity $[I]$ and energy $[\epsilon]$ conformal families for the $c = 1/2$ CFT [58], and are also proposed from the theory of low Q Potts model [54, 72] (a generalisation of the Ising model). These extended logarithmic operators are used in conjunction with numerical data collected through the Corner Transfer Matrix Renormalisation Group method to obtain a high precision estimate of the free energy scaling function. CTMRG is a powerful numerical technique with high convergence, compatible with studying the Ising model in the complex realm through an extension developed in this work.

The scaling function has been characterised extensively near the thermodynamic critical point in prior work [48, 31, 8, 71, 77] with highly accurate expansion coefficients up to order ξ^8 and less accurate estimates for terms as high as order ξ^{14}. This work aims to provide numerical verification for the conjectured form of the scaling function given in [31] for the region near the Yang-Lee singularity, and to act as a condensed resource for those tackling the vast body of knowledge associated with the Ising model.

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CHAPTER 1

INTRODUCTION

> A scientist is happy, not in resting on his attainments but in the steady acquisition of fresh knowledge.
>
> Max Planck

The study of models is fundamental in all fields of research. Even though we, as researchers, are materially concerned with understanding nature, we do not test nature directly. Instead, we construct a model which encapsulates a vector of interest, test said model, extrapolate, and only then attribute the results to nature. It is a subtle detail to make this process explicit, as fundamentally, no alternative approach can ever exist and so these extra steps are an unimportant afterthought when describing physics research. It is brought up here, however, to highlight the importance of models, and to motivate our study of them. By thoroughly studying models and uncovering as much detail about a given model as possible, our knowledge of any physical system becomes enriched whenever the model can be applied.

In the field of statistical physics, the Ising model is a popular, historic and successful model. Evidence of its popularity is found in its many variations and generalisations [50, 27]. Its ubiquitous presence in undergraduate and graduate textbooks gives it universal familiarity. Over 400 unique proofs [13] have been documented for re-deriving Onsager's famous solution for the free energy of the model. The history of the model plays hand-in-hand with its popularity; being over a century old, the model is incredibly well-studied.

The last and perhaps most important adjective is "successful". Success in this context is attributed to the fact that the model relates to a wide array of physical systems and areas of study in physics. The most rudimentary example is using the Ising model to study ferromagnets, but the model has also been applied to lattice gases and diatomic lattices. Any system of two binary states where neighbouring interactions dominate can be first approximated as an Ising system.

Aside from physical utility, mathematical aspects are a standalone reason to study the model. The zero-field Ising model is an exactly solved model—the holy grail in any field of physics. Having exact results to compare generalisations against is a strong advantage when studying a given system. In addition, any applicable external theory can be directly and easily tested by knowing an exact formula; a reoccurring benefit.

The Ising model is an integrable model that is scale invariant (in fact, *conformally* invariant) at its two critical points: one point is well established numerically and experimentally, while the

other is strongly believed based on reasonable assertions and conjectures, but ultimately is less well understood. The model also belongs to a particular universality class (the Ising universality class; earning the class' name due to the model's fame). This universality class is composed of seemingly unrelated models which converge on the same dynamics at their respective critical points. This means that the Ising model acts as a case study for not only statistical physics, but integrable field theory, conformal field theory, universality and even renormalisation. Building our understanding of the Ising model strengthens our understanding of each of these fields.

Each of these fields are important in their own regard. Their relationship to the Ising model will be outlined in this thesis. The base model will first be established, followed by applying the universality hypothesis to explain experimental results and then exploring implications of renormalisation. Based on some straightforward and direct analysis, the ideas of conformal field theory are shown to be applicable, and the relevant foundational theory is stated. This then allows us to discuss the integrable field theory results pertinent to the work, which is where the main results of this thesis lie.

The continuum Ising field theory is integrable if at least one of the two lattice-derived variables—the inverse temperature β and the external magnetic field H—are held at their critical values [82]. The region for $H = H_c = 0$ corresponds to the region described by Onsager's exact formula mentioned above, while the region $\beta = \beta_c$ is the magnetic Ising theory. This latter region exhibits structure of the E_8 Lie algebra [28]. In [14], the authors note that the dilute A_3 model (a lattice model also within the Ising universality class) manifestly contains massive particles described by E_8. This makes the dilute A_3 theory a promising candidate for interpreting this region and is yet another model now related back to the Ising model. Both regions are conjectured to contain an infinite tower of integrals of motion, with several of the lightest particle mass ratios having been solved in [82].

If both of the lattice variables are non-critical then the integrals of motion are known to no longer exist. This region is very non-trivial and few exact results are known; a lot of the efforts in the field are spent on understanding this region. An important result in this space is the Yang-Lee circle theorem, which is a mathematical result that analyses the partition function as a polynomial and argues that for real β, the partition function zeroes must be located at purely imaginary $H = iH_0$ (which lie on a circle for the fugacity $z = e^H$). While this result is well-known, it is unfortunately not constructive: the exact value of H_0 is not determined by the process. This work aims to improve upon the current estimates for this value through numerical simulations of the Ising model utilising the *Corner Transfer Matrix Renormalisation Group* (CTMRG) algorithm, extended for complex arguments.

The location of the Yang-Lee singularity depends on both β and H and is given in terms of the scaling variable $\xi = h/|m|^{15/8}$, where $m = m(\beta, H)$ and $h = h(\beta, H)$ are Aharony-Fisher nonlinear variables [6]. These variables (historically denoted as g_t, g_h or u_t, u_h) were constructed to recast the lattice variables into an appropriately scaling form, but they now have been related to coupling constants used to obtain the massive Ising field theory from the Ising conformal field theory [82]. The coupling constants are related to the lightest masses appearing in the field theory [25, 28].

The final theory section of this thesis covers the main numerical algorithm utilised to generate the results. Transfer matrices are a common method to study statistical models, as they allow one to translate the calculation of thermodynamic variables into eigenvalue calculations of the transfer matrices. These matrices under a Wick rotation (which associates real time evolution with an imaginary temperature variable) correspond to quantum operators. This process can be made precise through Suzuki-Trotter step algorithm and is called the *quantum-to-classical correspondence*. This correspondence is at the heart of the popular formulation of the Ising

model as free fermions, and a slightly less refined version of this process is essentially how Onsager originally solved the model in the 1940s.

While theoretically fruitful, the row transfer matrix approach is intractable as the size of each matrix scales exponentially as the lattice grows, and the number of rows also increases linearly. In practice these two factors heavily limit the applicability of direct transfer matrix simulations to lattices of sizes $N \sim 10^1$. In the 1970s, Baxter developed an alternative form of transfer matrix, with the key insight being to divide the square lattice into four, equal-sized corners (a slightly modified algorithm exists for other lattices). These were aptly named *corner transfer matrices*.

While technically still intractable, the static number of matrices fixes one of the scaling issues. Baxter also showed that the eigenvalues decay exponentially with distance to the critical point and thus the vast majority of the matrix information is stored in the dominant few eigenvalues [9] away from the critical points. This observation, coupled with the recently popularised Density Matrix Renormalisation Group (DMRG) method by White [74], later prompted Nishino & Okunishi to develop the CTMRG algorithm [53]. This algorithm iteratively grows a lattice and truncates the corner transfer matrices by deleting the smaller half of eigenvalues and the corresponding eigenvectors. The memory footprint is kept static through this truncation, and since the number of matrices is also fixed and the information loss per iteration is minimal (for suitable choices of β and H), the algorithm converges quite rapidly and accurately. The convergence is assured by the variational principle, established by Baxter [11]. Chapter 5 discusses Baxter's variational analysis of corner transfer matrices and explains the CTMRG algorithm in detail.

CHAPTER 2

ISING SCALING THEORY

"Ising"? Did you mean "Using"?

Google

2.1 2D Ising Model

The Ising model is the prototypical *toy* model in statistical physics. It is most commonly used as a simplified model for a lattice of classical ferromagnets. The qualities that classify the Ising model as a "toy" model is that typically contains only a simplified subset of the physical parameters associated with real ferromagnets. The key simplifications are:

1. Interactions are limited to only nearest neighbours;
2. Sites are allowed to exist in one of two, mutually exclusive states.

The Hamiltonian, $\mathcal{H} = \mathcal{H}(\beta, H)$, and partition function, $\mathcal{Z} = \mathcal{Z}_N^N(\beta, H)$, can be stated as

$$\begin{aligned}
\mathcal{Z}_{[x]} &= \sum_{\{\sigma\}} e^{\mathcal{H}_{[x]}(\beta,H,\{\sigma\})} \\
\mathcal{Z}_{[\mathrm{sq}]} &= \sum_{\{\sigma\}} \exp\left[\beta \sum_{i,j}^{N,N} \sigma_i^j \sigma_{i+1}^j + \beta \sum_{i,j}^{N,N} \sigma_i^j \sigma_i^{j+1} + H\sigma_i^j\right] \\
\mathcal{Z}_{[\mathrm{tr}]} &= \sum_{\{\sigma\}} \exp\left[\beta \sum_{i,j}^{N,N} \sigma_i^j \sigma_{i+1}^j + \beta \sum_{i,j}^{N,N} \sigma_i^j \sigma_i^{j+1} + \beta \sum_{i,j}^{N,N} \sigma_i^j \sigma_{i+1}^{j+1} + H\sigma_i^j\right]
\end{aligned} \tag{2.1}$$

The variable $\sigma \in \{1, -1\}$ is the binary state variable. In the context of modelling a ferromagnet, the states would correspond to spin-up and spin-down states. $\beta \equiv \tilde{J}/k_B T$ is the inverse temperature parameter (paired with coupling strength $\tilde{J}$ between neighbouring spins) and $H \equiv \tilde{H}/k_B T$ is an external magnetic field or self-energy parameter. Since this 2D system is overdetermined between the three variables $(\tilde{J}, \tilde{H}, T)$, we use β as the temperature variable and counterbalance any temperature dependence in H through behind-the-scenes manipulation of $\tilde{J}$ and $\tilde{H}$, allowing us to treat β and H as independent variables. The sum over $\{\sigma\}$ ranges over all configurations of the lattice, as is typical in a partition function calculation.

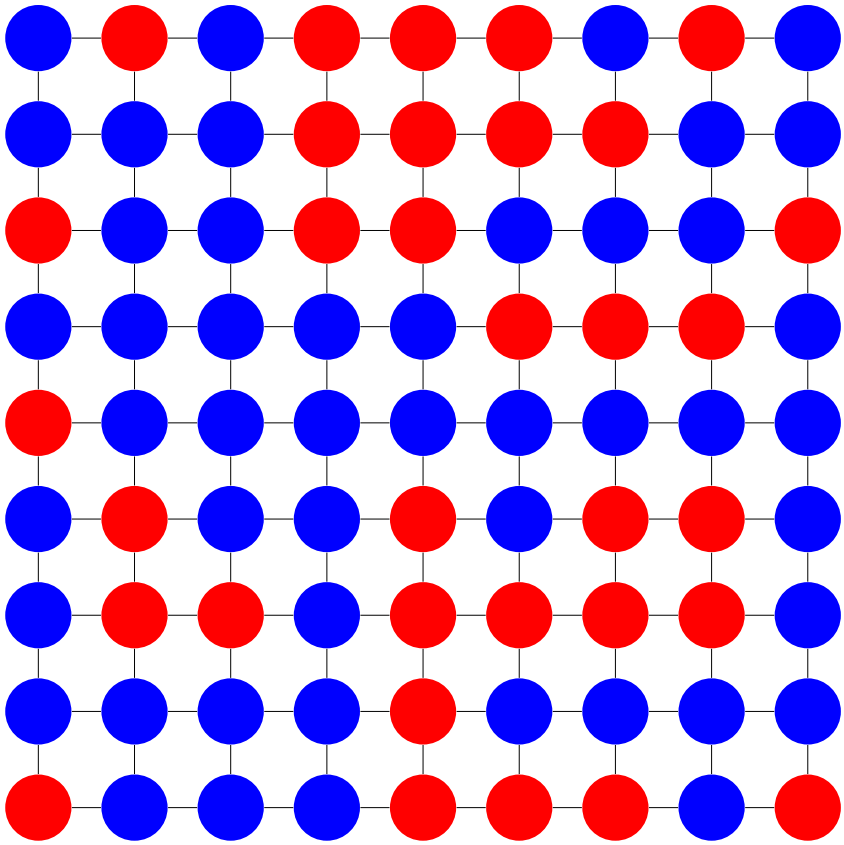


Figure 2.1: The self-dual square Ising lattice.

The lattices studied in this work are the square and triangular lattices. The Ising model is typically formulated on a square lattice for theoretical purposes, and this work primarily adopts this viewpoint. However, for the practical implementation of this work, the triangular lattice has important benefits owing to its rotational symmetry that provides better numerical convergence. Thus, the triangular lattice will also be kept in mind and discussed where relevant. A key concept in this body of work is that two lattices are equivalent at the critical points we intend to study anyway.

Lastly, one can impose periodic, free or other such boundary conditions, but in the large scale limit around the model's critical point that this work considers, the distinction becomes irrelevant. Periodic boundary conditions are presumed for theoretical simplicity.

Part of the beauty and intrigue of the Ising model is that despite the relative simplicity of the model—only allowing two variable states on an unglamorous lattice with nearest neighbour interactions—the mathematical structures of the model have surprising depth. One of the earliest major results for the 2D Ising model is the Kramers-Wannier duality relationship. This result showed that for $H = 0$, the model exhibits a duality relationship between lattices that are dual to one another, with high and low temperatures exchanged according to a direct relationship. The dual lattice is obtained by interchanging the role of vertices (position of spins) and faces (relationship between neighbouring spins) in the lattice. The square lattice (where this result was first proven) is dual to itself, and the triangular lattice is dual to the hexagonal lattice figs. 2.1 and 2.2. In the context of this work the duality between hexagonal and triangular lattices makes them effectively equivalent, hence only the triangular lattice was studied.

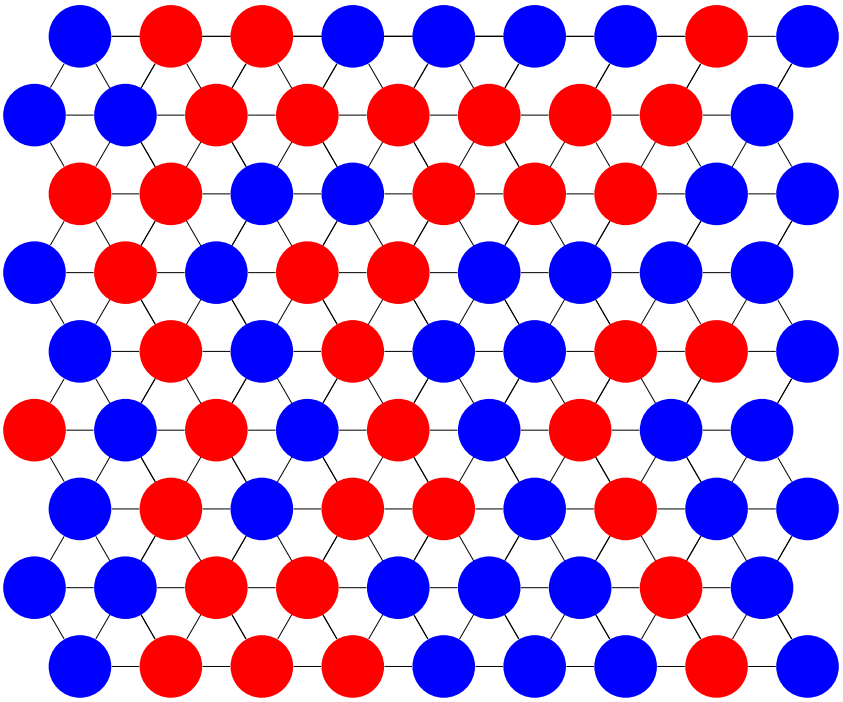


Figure 2.2: The triangular Ising lattice. The hexagonal dual is constructed from each of the faces.

2.1.1 Lattice Symmetries

Motivated by the KW-duality, one replaces the lattice temperature variable β with one that makes the symmetry much more apparent. The variable is denoted τ and is given in the lattice-agnostic form

$$\tau(k) = \frac{1}{2}\left(\sqrt{k} - \frac{1}{\sqrt{k}}\right) \tag{2.2}$$

for both lattices, and the lattice dependence emerges in the elliptic parameterisation variable k [22]

$$\begin{aligned} k_{[\mathrm{sq}]} &= \frac{1}{s^2} && (s \equiv \sinh 2\beta) \\ k_{[\mathrm{tr}]} &= \frac{4u^{3/2}}{(1-u)^{3/2}(1+3u)^{1/2}} && \left(u \equiv e^{-4\beta}\right) \end{aligned} \tag{2.3}$$

This relationship permits two inverse relations

$$\begin{aligned} k(\tau) &= \left(\tau + \sqrt{1+\tau^2}\right)^2 \\ k^*(\tau) &= \left(\tau - \sqrt{1+\tau^2}\right)^2 = 1/k(\tau) = k(-\tau) \\ k(0) &= k^*(0) = 1 \end{aligned} \tag{2.4}$$

The region of $\tau > 0$ corresponds to the high temperature regime $0 < \beta < \beta_c$ and $\tau < 0$ corresponds to the low temperature regime $\beta > \beta_c$. We strictly consider the ferromagnetic regime $\beta > 0$ in this work. The KW-duality manifests quite clearly in this redefinition as for $\tau^* = -\tau$ we have $\tau^*(k^*) = \tau(k)$ and $k^*(\tau^*) = k(\tau)$.

The critical point is the point where the system undergoes a phase transition. For $H = 0$ this corresponds the point which is invariant under the KW-duality, which simply corresponds to $\tau_c = 0$. In terms of β the critical point is [48]

$$\begin{aligned}\beta_c^{[\mathrm{sq}]} &= \frac{1}{2}\log\left[1+\sqrt{2}\right] = \frac{1}{2}\operatorname{arsinh}[1] = 0.441\ldots \\ \beta_c^{[\mathrm{tr}]} &= \frac{1}{3}\log[4] = 0.275\ldots\end{aligned} \tag{2.5}$$

This result is obtained straightforwardly in the square case due to self-duality, whereas in the triangular/hexagonal case the relation must first be symmetrised between the two lattices. This symmetrisation was abstracted and generalised by Baxter as the *star-triangle relation*; a powerful tool in the study of integrable systems.

The benefits of this redefinition are immediate, as not only does this shift the critical point to the origin, $\left(\tau_c^{[x]}, H_c^{[x]}\right) = (0,0)$, it elevates the KW-duality to a clear symmetry condition of the model that is non-obvious when expressed purely in lattice variables. In addition to the KW-symmetry, the Ising model exhibits another symmetry through $\mathcal{Z}(\tau, H) = \mathcal{Z}(\tau, -H)$, but luckily this one is easily verified as it is a direct result of the summation over states $\{\sigma\}$. These two symmetries are also used to characterise the three families of conformal operators in the Ising conformal field theory, as the identity family $[\mathbb{I}]$ is H-even and τ-even, the energy family $[\epsilon]$ is H-even and τ-odd while the spin family $[\sigma]$ is H-odd and not symmetric under τ inversion. This is summarised symbolically using the language of the fusion algebra eq. (3.142) as

$$\begin{aligned}[\mathbb{I}]_{-H} &= [\mathbb{I}]_H & [\mathbb{I}]_{-\tau} &= [\mathbb{I}]_\tau \\ [\epsilon]_{-H} &= [\epsilon]_H & [\epsilon]_{-\tau} &= -[\epsilon]_\tau \\ [\sigma]_{-H} &= -[\sigma]_H\end{aligned} \tag{2.6}$$

This guides the series expansions of such operators. For example, a spin family operator O is identified as an operator with the expansion

$$O(\tau, H) = O_1(\tau)H + O_2(\tau)H^3 + \ldots \tag{2.7}$$

around $H = 0$. This analysis is detailed further in section 3.5.2.

2.1.2 Exact Solutions

An important feature of the Ising model is that it is a non-trivial model that is also integrable, albeit only in two restricted cases. In the case where the magnetic field variable H is confined to its critical value $H = H_c = 0$, the model (in the square case) was famously solved by Onsager in the 1940s [55]. The triangular case was solved in the years that followed in the 1950s [73]. The infinite scale free energy (density) is given by the double integrals [55, 73]

$$\begin{aligned}f_{[\mathrm{sq}]}(\tau,0) &= -\frac{1}{2}\log[4\sinh(2\beta)] + \frac{1}{8\pi^2}\iint_0^{2\pi}\log[2\sqrt{1+\tau^2} - \cos\phi_1 - \cos\phi_2]\,\mathrm{d}\phi_1\,\mathrm{d}\phi_2 \\ f_{[\mathrm{tr}]}(\tau,0) &= -\frac{1}{2}\log[4\sinh(2\beta)] - \frac{1}{8\pi^2}\iint_0^{2\pi}\log[3+\tau^2 - \cos\phi_1 - \cos\phi_2 - \cos(\phi_1+\phi_2)]\,\mathrm{d}\phi_1\,\mathrm{d}\phi_2\end{aligned} \tag{2.8}$$

or, through some algebraic tricks and identifications (derivation in [60, 66]), as single integrals in various forms [47]

$$f_{[\mathrm{sq}]}(\tau(\beta),0) = -\log[2\cosh(2\beta)] - \frac{1}{2\pi}\int_0^{\pi} \log\left[1+\left(1-\frac{\cos^2\theta}{1+\tau^2}\right)^{1/2}\right]\mathrm{d}\theta$$
$$f_{[\mathrm{sq}]}(\beta,0) = -\log[2\cosh(2\beta)] - \frac{1}{2\pi}\int_0^{\pi/2} \log\left[\frac{1+\sqrt{1-q^2(\beta)\sin^2\phi}}{2}\right]\mathrm{d}\phi \tag{2.9}$$

with $q(\beta) \equiv 2\sinh(2\beta)/\cosh^2(2\beta)$, noting that $q(\beta_c) = 1$. There is a practical advantage to single integrals over double integrals as the former is significantly faster to compute numerically.

The temperature derivatives of these expressions is carried out in [60], giving the exact solutions in the square case

$$E_{[\mathrm{sq}]}(\beta,0) \equiv \frac{\partial f_{[\mathrm{sq}]}}{\partial\beta} = -J\coth(2\beta)\left[1+\frac{2}{\pi}\left(2\tanh^2(2\beta)-1\right)\mathrm{K}(q)\right]$$
$$\begin{aligned} C_{[\mathrm{sq}]}(\beta,0) &\equiv \frac{\partial^2 f_{[\mathrm{sq}]}}{\partial\beta^2} \\ &= \frac{4}{\pi}(\beta\coth(2\beta))^2\times \\ &\quad \left[\mathrm{K}(q)-\mathrm{E}(q)-(1-\tanh^2(2\beta))\left(\frac{\pi}{2}+(2\tanh^2(2\beta)-1)\mathrm{K}(q)\right)\right] \end{aligned} \tag{2.10}$$

where $\mathrm{K}(q)$ and $\mathrm{E}(q)$ are complete elliptic functions of the first and second kind respectively

$$\mathrm{K}(q) = \int_0^{\pi/2}\frac{\mathrm{d}\phi}{\sqrt{1-q^2\sin^2\phi}} \qquad \mathrm{E}(q) = \int_0^{\pi/2}\mathrm{d}\phi\sqrt{1-q^2\sinh^2\phi} \tag{2.11}$$

K logarithmically diverges for $q \to 1$ while $\mathrm{E}(1) = 1$.

These temperature-dependent expressions were derived through the transfer matrix method, wherein one expresses the summations in the Hamiltonian as matrix multiplications of appropriately selected matrices. The partition function in the case of periodic boundary conditions then corresponds to a matrix trace and matrix power, reducing the problem to eigenanalysis. For other boundary conditions, the results from eigenanalysis dominate in the large N limit. These eigenvalues can be evaluated at $H = 0$ as the transfer matrices have relatively simple quaternionic structure—isomorphic to that of free fermions—allowing the eigenvalues to be determined by symmetry arguments. This is called the *free fermion* approach.

The simple quaternionic structure does not survive for generic $H \neq 0$, which is ultimately why the Ising model has not been completely solved already. Exact results for the magnetic derivatives can still be obtained from the transfer matrix method, which is explored in [66]. The magnetisation can be expressed as a ratio of transfer matrix traces which similarly reduce to eigenanalysis. For a transfer matrix such that the partition function is expressed as a trace

$$\mathcal{Z} = \mathrm{Tr}\{e^{\mathcal{H}(\beta,H)}\} \tag{2.12}$$

the magnetisation is

$$\begin{aligned} M &= -\frac{\partial f}{\partial H} \\ &= -\frac{1}{V}\frac{\mathrm{Tr}\left\{\sum_\sigma \sigma e^{\mathcal{H}(\beta,H)}\right\}}{\mathrm{Tr}\left\{e^{\mathcal{H}(\beta,H)}\right\}} \end{aligned} \tag{2.13}$$

with $V = N^2$. Since $\sigma \in \{1, -1\}$, the finite magnetisation vanishes identically at $H = 0$. The non-trivial magnetisation in the thermodynamic limit is therefore obtained by first evaluating $N \to \infty$ *and then* $H \to 0$ [66]. The expression then no longer vanishes for the high temperature $\beta > \beta_c$ regime.

The cyclic structure of the problem means that the eigenvalues correspond to Toeplitz matrices, which can be evaluated via the first Szegő limit theorem. The end result is [66, 48, 59, 22]

$$M = \begin{cases} [1 - k^2(\tau)]^{1/8} & \tau < 0 \\ 0 & \tau > 0 \end{cases} \tag{2.14}$$

which holds for both lattice types.

Similar to the critical $H = 0$ phase, when restricted to the critical temperature $\tau = \tau_c = 0, H \neq 0$ the model is integrable. In [82] Zamolodchikov studied the Ising field theory and showed that it possesses a host of integrals of motion. The Ising conformal field theory exists at exactly the critical point $(\tau, H) = (0, 0)$ and the massive field theory is obtained by perturbing from this point by one or more relevant perturbation parameters. Of the two non-trivial relevant fields, perturbation by the energy field coincides with the zero-field Ising model ($H = 0$), while perturbation by the spin field has structure corresponding to the exceptional Lie Algebra E_8 [28]. Under perturbation by two or more fields the integrals of motion no longer survive, and the model is no longer integrable. In addition, a lattice in the Ising universality class (discussed next) is the dilute A_3 model. This model was shown in [14] to recover the E_8 Lie Algebra in the scaling limit.

2.2 Universality

An interesting property of statistical theories is the notion of universality, whereby the dynamics of distinct models coincide in the vicinity of a critical point. Universality is organised into *universality classes*, which are classified by *critical exponents*. These exponents control the critical behaviour of various thermodynamic functions. The main critical exponents[1] are $\{\alpha, \beta, \gamma, \delta, \eta, \nu\}$ which feature as powers of normalised critical deviation $t \equiv \frac{\beta_c - \beta}{\beta} = T/T_c - 1$ The first four exponents arise from partial derivatives of the free energy

$$\begin{aligned} C = \frac{\partial^2 f}{\partial \beta^2} &\propto \frac{1}{|t|^\alpha} \\ M = -\frac{\partial f}{\partial H} &\propto \begin{cases} |t|^\beta & \text{for } t < 0, H \to 0^+ \\ 0 & \text{for } t > 0, H \to 0^+ \end{cases} \\ M &\propto H^{1/\delta} \text{ for } t = 0, H \neq 0 \\ \chi = -\frac{\partial^2 f}{\partial H^2} &\propto \frac{1}{|t|^\gamma} \end{aligned} \tag{2.15}$$

The magnetisation is distinguished as the *order parameter* of the Ising model, as it has qualitatively different behaviour in the high and low temperature phases and can therefore be used to identify which phase the model is in. The remaining critical exponents come from studying the

[1] Note that β in this set is unrelated to the inverse temperature variable.

correlations of the model [35, 25]

$$\langle\sigma(x)\sigma(0)\rangle_c \sim \frac{e^{-|x|/\xi}}{|x|^{(d-1)/2}} \qquad \langle\sigma(x)\sigma(0)\rangle \sim \frac{1}{|x|^{d-2-\eta}}$$
$$\xi \sim |t|^{-\nu} \tag{2.16}$$

Here $\sigma(x)$ is a spin located at some position x distance away from $\sigma(0)$ at the centre of the lattice. The isotropy of the lattice means we don't have to be particularly careful about defining position variables. ξ here is the correlation length[2]. It controls the rate of exponential decay of the connected correlation function

$$\langle A(x)A(0)\rangle_c \equiv \langle A(x)A(0)\rangle - \langle A(x)\rangle\langle A(0)\rangle \tag{2.17}$$

This variable describes how local fluctuations affect other parts of the system.

In principle the critical exponents can be different on either side of the critical point, but in practice for the Ising model they are almost all the same except for the magnetisation which behaves differently on either side of the critical point.

These critical exponents form the basis of a *universality class*. Many seemingly different models that possess the same set of critical exponents therefore behave the same in the critical limit, allowing one to bridge a link between otherwise separate models. This fact is the basis for linking study of the square, triangular and hexagonal Ising model (as each have the same critical exponents) along with the Ising conformal field theory in section 3.7. The critical exponents for the Ising universality class are

α	β	γ	δ	ν	η
0	1/8	7/4	15	1	1/4

(2.18)

The evidence for these critical exponents are both theoretical and experimental. For example, from the exact formulae for the magnetisation eq. (2.14) and eq. (2.2) one can readily verify that $\tau \sim t$ and $M \sim t^{1/8}$. The specific heat around the critical point can be approximated as

$$C \sim -\frac{8\beta_c^2}{\pi}\ln t \tag{2.19}$$

which is expected from the logarithmic divergence of $\mathrm{K}(q)$. Critical exponents feature when thermodynamic variables obey power law relations, but this logarithmic structure can be seen as a limiting case of a special power law. Using the limit definition of the logarithm

$$\lim_{\alpha\to 0}\frac{1}{\alpha}\left(t^{-\alpha}-1\right) = -\ln t \tag{2.20}$$

and $t = T/T_c - 1$ means that the logarithmic structure can be seen as the limiting behaviour of a power law for $\alpha \to 0$.

Given that these quantities are either derivatives of a common function or can be linked through renormalisation arguments, they are not fully independent. The famous identities linking the exponents together are named

$$\begin{aligned} \alpha + 2\beta + \gamma &= 2 && \text{Rushbrooke's Identity} \\ \delta - 1 &= \gamma/\beta && \text{Widom's Identity} \\ \gamma &= (2-\eta)\nu && \text{Fisher's Identity} \\ 2 - \alpha &= d\nu && \text{Josephson's Identity} \end{aligned} \tag{2.21}$$

[2]Again, ξ here is not to be confused with the scaling variable $\xi(m,h)$ encountered in the Ising field theory in section 3.7 or the transfer matrix eigenvalue ratio in chapter 5

These identities are known as *scaling relations*, with the last identity in particular being known as a *hyperscaling relation* due to additionally incorporating the dimension of the space d. These relations mean that the set of critical exponents can be reduced to ν, η and the dimension of the system d, which are the typically chosen independent variables

$$\begin{aligned}\alpha &= 2 - \nu d \\ \beta &= \frac{1}{2}\nu(d - 2 + \eta) \\ \gamma &= \nu(2 - \eta) \\ \delta &= \frac{d + 2 - \eta}{d - 2 + \eta}\end{aligned} \tag{2.22}$$

2.3 Scaling Hypothesis

An explanation for the source of the power law behaviour is the **Scaling Hypothesis**. This hypothesis supposes that the free energy (and its derivatives) are homogeneous functions near the critical point. This assumption alone is enough to generate the power law behaviour.

The assumption of homogeneity means that in the vicinity of the critical point the free energy can be described by a single, homogeneous function. A homogeneous function is one that satisfies a scaling relation of the form

$$f(\lambda^a t, \lambda^b H) = \lambda f(t, H) \tag{2.23}$$

In words, a homogeneous function is one where a rescaling of the input variables corresponds to an overall rescaling of the output.

A direct consequence of this property is that the variables t and H themselves cannot be fully independent. Their dependence is expressed through the *scaling variable* y which reduces the dimensionality of the free energy by 1. To see this, first note that the function $g(t, H) \equiv t^{-1/a} f(t, H)$ is invariant under the transformation

$$t \to t' = \lambda^a t \qquad\qquad H \to H' = \lambda^b H$$

$$g(t', H') = g(t, H) \tag{2.24}$$

With this, if we then fix the rescaling by setting $\lambda^a = 1/t \Rightarrow \lambda = 1/t^{1/a}$ then

$$\begin{aligned}f(t, H) &= t^{1/a} g(t, H) \\ &= t^{1/a} g(\lambda^a t, \lambda^b H) \\ &= t^{1/a} g(1, H/t^{b/a}) \\ &= t^{1/a} G_f(y)\end{aligned} \tag{2.25}$$

where we introduce the scaling variable $y = H/t^{b/a}$, along with the all-important scaling function G which is a function of a single variable.

The criteria of a homogeneous function also has implications for its derivatives. Namely, the derivative of a homogeneous function is itself homogeneous with an associated scaling function

$$\begin{aligned}\frac{\partial f}{\partial t} &= \frac{t^{1/a-1}}{a} G_f(y) + t^{1/a} G_f'(y) \frac{\partial y}{\partial t} \\ &= t^{1/a-1} G_E(y)\end{aligned} \tag{2.26}$$

and similarly for other derivatives

$$\frac{\partial^2 f}{\partial t^2} = t^{1/a-2} G_C(y) \qquad \frac{\partial f}{\partial H} = t^{(1-b)/a} G_M(y) \qquad \frac{\partial^2 f}{\partial H^2} = t^{(2-b)/a} G_\chi(y) \tag{2.27}$$

2.3.1 Renormalisation Theory

To connect the above scaling arguments to theory, we need to find theoretical grounding to define λ, a and b. To do this we will explore the idea of renormalisation theory and see how this motivates the scaling definitions. We will first briefly discuss a naïve but intuitive renormalisation method (and its limitations) in block-spin renormalisation, after which we will explore a more general but less precise framework in the Ginzburg-Landau phenomenological model.

1D Block-Spin Renormalisation

Block-spin is a relatively simple form of renormalisation, so we will cover it here to give a concrete foundation for the idea. The procedure is exact for the 1D Ising model, so we will first study this model and then explore the shortcomings of its generalisations to the 2D model. This will motivate the search for more sophisticated methods beyond it.

For the 1D Ising model in zero external field (this approach works even for $H \neq 0$ as seen in [69], but its inclusion isn't any more or less illuminating, so we ignore it for now), the partition function (defined on an even sized lattice for convenience) is

$$\begin{aligned} \mathcal{Z} &= \sum_{\{\sigma\}} \exp\left\{ \sum_{i=1}^{2N} \mathcal{H}\left(\beta; \sigma_i, \sigma_{i+1}\right) \right\} \\ &= \sum_{\{\sigma\}} \exp\left\{ \beta \sum_{i=1}^{2N} \sigma_i \sigma_{i+1} \right\} \end{aligned} \tag{2.28}$$

with periodic boundary conditions $\sigma_{2N+1} = \sigma_1$ for simplicity. We can employ block-spin renormalisation by "integrating out" chosen degrees of freedom to reduce the dimension of the model. In this scheme, we will sum over odd nodes by calculating

$$\sum_{\sigma_3} \exp\{\beta\left(\sigma_2\sigma_3 + \sigma_3\sigma_4\right)\} = \exp\{g(\beta)\sigma_2\sigma_4 + h(\beta)\} \tag{2.29}$$

where it is straightforward to verify

$$g(\beta) = \frac{1}{2}\ln[4\cosh(2\beta)] \qquad h(\beta) = \frac{1}{2}\ln[\cosh(2\beta)] \tag{2.30}$$

is the solution. This works equally for all odd sites, so to tidy things up further and prepare for recursion we define

$$\sigma_i' \equiv \sigma_{2i} \qquad \beta' \equiv g(\beta) \qquad \lambda' \equiv e^{h(\beta)}$$

$$\lambda' \exp\left\{\mathcal{H}'(\beta'; \sigma_i', \sigma_{i+1}')\right\} \equiv \sum_{\sigma_{2i+1}} \exp\{\mathcal{H}(\beta; \sigma_i, \sigma_{i+1}) + \mathcal{H}(\beta; \sigma_{i+1}, \sigma_{i+2})\} \tag{2.31}$$

With this renormalisation scheme, the original partition function can be calculated via

$$\mathcal{Z} = \sum_{\{\sigma'\}} \lambda' \exp\left\{ \sum_{i=1}^{N} \mathcal{H}'(\beta'; \sigma'_i, \sigma'_{i+1}) \right\} \tag{2.32}$$

giving the same answer for the partition function as before. Important to note here is that the renormalised Hamiltonian is *statistically similar* to the original, as it features only pair-wise interactions between sites and is therefore also an Ising model.

Even though in principle this function is just as difficult to evaluate as the original, we can recursively apply this procedure to obtain

$$\begin{aligned} \sigma'' &\equiv \sigma_{4i} \\ \beta'' &\equiv g(\beta') = g(g(\beta)) \\ \lambda'' &\equiv e^{h(\beta')}\lambda'\lambda' = e^{h(g(\beta))+2h(\beta)} \end{aligned} \tag{2.33}$$

with the partition function sum now executed over every $4th$ site in the original lattice. Iterative applications of this procedure generates the *renormalisation beta function*

$$\beta^{(n)} = \overbrace{g \circ \cdots \circ g}^{n\text{times}}(\beta) \tag{2.34}$$

which defines the *renormalisation group flow*. Renormalisation group[3] flow describes how the parameter space of the system changes in response to the as the scale of the system changing. Analysis of the beta function leads to *renormalisation fixed points*, which are any points which satisfy $g(\beta) = \beta$. The critical point of the Ising model is a fixed point of the renormalisation group flow. In 1D, it is known that the Ising model in zero field has no phase transition, and this is supported by the fact that the fixed points for g are complex, obtained by simply solving the quadratic $e^{2\beta} = 2e^{2\beta} + 2e^{-2\beta}$.

2D Model

Generalising this technique to higher dimensions, we can define the parity of a site by the sum of its coordinates. That is, the site σ_i^j will be considered even (odd) if $i + j$ is an even (odd) integer. This creates a checkerboard pattern across the lattice. Proceeding as before, we define the five-site Hamiltonian

$$\mathcal{H}(\beta; \sigma_i^j; \sigma_i^{j+1}, \sigma_{i-1}^j, \sigma_{i+1}^j, \sigma_i^{j-1}) \equiv \frac{\beta}{2}\left(\sigma_i^j\sigma_{i+1}^j + \sigma_i^j\sigma_{i-1}^j + \sigma_i^j\sigma_i^{j+1} + \sigma_i^j\sigma_i^{j-1}\right) \tag{2.35}$$

which contains every interaction between a chosen odd site σ_i^j $(i + j = 2n + 1)$ and its four even neighbours, with an additional weighting factor of $\frac{1}{2}$ to account for overcounting in the partition function. However, if we try to perform the block-spin renormalisation scheme, we immediately encounter the problem that the result is not an Ising model. In 2D this renormalisation scheme does not produce a statistically similar model.

The Hamiltonian defined above is more tedious to evaluate directly, as we cannot use simple identities to reduce it to known functions. Instead, we note that $\mathcal{H}(\beta; \sigma_i^j; a, b, c, d)$ is totally symmetric under any permutation of the odd sites, so in general the result is something of the

[3]Technically, the algebra defined here is a semigroup as it does not, a priori, have an inverse.

form

$$\sum_{\sigma_i^j} \exp\{\mathcal{H}(\beta; \sigma_i^j; a, b, c, d)\} =$$
$$\exp\{A(\beta)\,(ab + ac + bd + cd) + B(\beta)(ad + bc) + C(\beta)abcd + D(\beta)\} \tag{2.36}$$

The renormalisation approach rotates the Cartesian lattice by 45°, turning horizontal and vertical pairs into diagonal ones.

Unfortunately, this renormalised Hamiltonian is *not* an Ising model; it features diagonal couplings (the $B(\beta)$ terms, which were vertical/horizontal next-nearest neighbours in the original lattice) and four-site terms ($C(\beta)$ terms). The scaling factor $D(\beta)$ is as before in the 1D case.

There are a few ways to proceed from this point. One approach is to charge headstrong and declare that $C(\beta) = 0$, completely ignoring the four-site terms. The diagonal couplings can be interpreted as increased nearest neighbour couplings, e.g. $B(\beta)(ad + bc) \to B(\beta)/2(ab + ac + bd + cd)$. This approach is analysed in the lecture notes [3] and, unsurprisingly, the resulting beta function gives the wrong critical point. It calculates $\beta_c \approx 0.507$ when the true value is $0.4407\ldots$. However, an answer that is still within $\sim 15\%$ error is still instructive as a crude, first approximation. Another method is to change renormalisation scheme. A numerically successful method analysed in the same reference (or in [43] for a peer-reviewed reference) is the *majority rule* scheme.

Majority rule renormalisation replaces the explicit mathematical operation of summation with the operation of choosing the most common spin value across an odd-sized block (either 5 as above or blocks of 3). Even sized blocks are permissible with an appropriate tie-break scheme—such as randomly picking a winner (which averages out to 0).

This scheme is more successful in the sense that the beta function it defines calculates the Ising critical point and critical exponents closer to the known values. However, the more fruitful approach is actually to ignore lattice-level details (which is exactly what universality suggests) and instead argue the structure of the free energy based on symmetry principles. This is the underlying idea of the *Ginzburg-Landau* approach. This is a powerful idea that can also be bolstered by our understanding of conformal field theory, as we will eventually see.

2.3.2 Phenomenological Model

We have seen how explicit renormalisation schemes are ineffective when applied to the 2D Ising model as the statistical self-similarity of the scheme cannot be guaranteed. In fact, it is a complete coincidence that an explicit method even worked at all in the 1D case. Relying on a framework that requires explicit tracking of variables through parameter space does not lead to a universal understanding of models under renormalisation. This is not surprising, as many-body problems generally become intractable in the thermodynamic limit. Some sort of microscopic averaging procedure is needed if we want to sensibly talk about macroscopic variables (which are the ones that we ultimately care about).

An alternative approach is to abandon hope for an analytically derived theory and instead construct *phenomenological* theories based on symmetries. Phenomenological models only need to respect whichever symmetries are expected to be present in the system. The variables of the theory no longer have to be physical in origin or directly interpretable; they can later be physically interpreted through experiment and additional theoretical study. When the model or a parameter within it is found to not obey a given symmetry, this is an indication that the set of variables that have been ascribed to the theory are incomplete in one way or another, leading to the potential for new physics.

Ginzburg and Landau were the first to implement this idea in their work studying the mean-field theory of superconductors. Between the two of them, they constructed the Ginzburg-Landau model. This is a phenomenological model founded solely on the basis of an analyticity assumption and on respecting translational & rotational symmetries (and any other relevant symmetries; in the original papers on superconductors there was $U(1)$ gauge symmetry), as well as locality. The free energy was expressed as a function of the *order parameter*—a variable which distinguishes between different phases of the model across a phase transition.

We can construct an equivalent model for the Ising model, whose order parameter is its magnetisation. A priori, we do not know the explicit dependence of the free energy on the magnetisation, so we presume it is a functional relation of the form

$$f_{\mathrm{GL}}[m] = \int \mathrm{d}^2x \; tm^2(x) + um^4(x) + \cdots + J\left(\frac{\partial m}{\partial x}\right)^2 + K\left(\frac{\partial^2 m}{\partial x^2}\right)^2 + \cdots - Hm \tag{2.37}$$

This model analytically depends on the parameters $\{t, u, J, K, \dots\}$ which are the phenomenological variables; these variables do not need to have physical interpretations (yet). Only even powers of m appear for $H = 0$ as the Ising model is symmetric under the $\mathbb{Z}_2$ symmetry of a total spin-flip across the lattice (i.e. $m \to -m$).

When the Ginzburg-Landau model is restricted to quadratic powers, it is a *Gaussian model*. Gaussian models are particularly convenient as they can be directly solved by Fourier transform. Accordingly, much of the discussion takes place in the context of Fourier modes in frequency-space, with "real-space renormalisation" reserved as the alternative formulation. Although simplified, the Gaussian Hamiltonian produces critical exponents in agreement with mean-field theory (another simplification process) in the cases of $d \geq 4$ [35]. From the analysis one finds that the quartic coupling is relevant for $d < 4$, irrelevant for $d > 4$ and marginal for $d = 4$, which explains the correspondence.

This idea was greatly expanded upon by Wilson in [75], whose work underpins the modern perspective of renormalisation. Wilson's work considered the addition of the m^4 term as a perturbation from the solved Gaussian model and investigated the resulting renormalisation flow. He introduced the idea of integrating the theory up to a *cutoff scale*—which represents the maximum sensitivity of the detection device. Beyond the cutoff scale we lose the luxury of explicitly tracking the fine details, and our models should incorporate this limitation.

Even though Wilson's ideas were profound and won him a Nobel Prize in 1982, we will neither explore them nor the Wilson-Ginzburg-Landau model beyond this brief introduction. For the purposes of this work, we are only interested a cursory overview these ideas and the concept of phenomenological parameters. These ideas are the origin for the concept of relevant and irrelevant operators, which are of considerable importance in this work.

2.3.3 Renormalisation Fixed points

With the concepts of phenomenology and renormalisation introduced we will now explore their intersection. This primarily involves exploring the implications of scaling for the phenomenological free energy.

Consider a free energy defined by a set of phenomenological parameters $\mathbf{S} \equiv (S_1, S_2, S_3, \dots) = (t, u, J, \dots)$ and define the renormalisation operation by the operator $\mathbf{\Lambda}(\lambda)$. Under renormalisation, we expect this set to change $\mathbf{S}' = (t', u', J', \dots) = \mathbf{\Lambda}(\lambda)\mathbf{S}$ where each new parameter is some function of the previous iteration, i.e. $t' = t'(\mathbf{S})$ etc. We saw this for the Hamiltonian explicitly in the block-spin renormalisation scheme through the beta

function $\beta' = g(\beta)$. This operation has the properties of a semigroup under composition

$$\mathbf{\Lambda}(\lambda)\mathbf{\Lambda}(\lambda') = \mathbf{\Lambda}(\lambda\lambda') \tag{2.38}$$

with the identity operation

$$\mathbf{\Lambda}(1) = \mathbf{I} \tag{2.39}$$

Suppose there is a fixed point under this renormalisation $\mathbf{S}^*$ given by $\mathbf{\Lambda}(\lambda)\mathbf{S}^* = \mathbf{S}^*$. Note that since the correlation length (ξ) is a function of the Hamiltonian parameters ($\xi = \xi(\mathbf{S})$), it will scale under renormalisation. In order for the correlation length to remain fixed at this point, it must be 0 or ∞. A correlation length of 0 describes completely independent fluctuations and therefore corresponds to complete order for zero temperature and complete disorder for infinite temperature. An infinite correlation length describes a critical point, which is the case that we are studying here for the Ising critical point.

In general the action of $\mathbf{\Lambda}(\lambda)$ is not linear, but near the critical point it can be linearised

$$S_i^* + \delta S_i' = S_i^* + \sum_j A_{ij}\delta S_j + \dots \qquad\qquad A_{ij} \equiv \left.\frac{\partial S_i'}{\partial S_j}\right|_{\mathbf{S}^*} \tag{2.40}$$

We label the eigenvectors of $\mathbf{A}$ as $\{O_i\}$ with corresponding eigenvalues $\{\lambda_i\}$. The semigroup properties above mean that the eigenvalues are exponential and of the form $\lambda_i \equiv \lambda^{y_i}$. The renormalisation group map is diagonal in terms of these eigenvectors

$$\mathbf{S} = \mathbf{S}^* + \sum_i g_i \mathbf{O}_i \qquad\qquad \mathbf{S}' = \mathbf{S}^* + \sum_i \lambda^{y_i} g_i \mathbf{O}_i \tag{2.41}$$

meaning the scaling analysis in eq. (2.23) directly applies and y_i are the scaling exponents $a, b, \dots$.

In physics language, the eigenvectors are called **scaling directions** of the fixed point $\mathbf{S}^*$ and the eigenvalues are **anomalous dimensions** or simply **RG eigenvalues**. The RG eigenvectors have qualitatively different behaviours based on the value of the corresponding eigenvalue

- For $y_i > 0$, g_i *increases* under scaling and $\mathbf{O}_i$ is called a **relevant operator**
- For $y_i < 0$, g_i *decreases* under scaling and $\mathbf{O}_i$ is called an **irrelevant operator**
- For $y_i = 0$, g_i is a **marginal operator**, and higher order terms are needed to determine its behaviour.

These operators can be further studied by investigating a mathematical framework which deals with scale invariance in physics. The framework is known as *Conformal Field Theory* (CFT), as scale invariance is a type of conformal transformation.

Conformal field theory allows us to place constraints on the scaling parameter λ and the scaling exponents $(a, b, \dots)$. Conformal field theories place strict constraints on these scaling parameters. This is useful to us as there is plenty of numerical and experimental evidence to support the idea that conformal field theories can be applied to the Ising model near the critical points.

For a direct example of applying CFT to the Ising model, it is known that the correlation length of the Ising model becomes infinite at the critical point. Since the correlation length is inversely proportional to mass in the model, the theory is massless—this is a necessity for

a conformally invariant model. The relationship between correlation length and mass can be observed by representing the connected correlation function eq. (2.16) as a sum over n-particle states [25, 77]

$$\langle \sigma(x)\sigma(0)\rangle_c = \sum_n |\langle 0|\sigma|n\rangle|^2 e^{-E_n|x|} \tag{2.42}$$

therefore correlation length scales inversely to the mass of the lightest state in the thermodynamic limit.

When constructing a phenomenological free energy, one should include contributions from all know relevant operators (these can be determined from CFT analysis, if applicable), and include as many characterised irrelevant operators as possible. In principle there can be infinitely many irrelevant operators whose contributions occur at varying degrees of coupling strength, and higher precision analysis must account for their presence. Consider the renormalisation $x \to x/\lambda$ on a parameter of the form

$$f[m] \sim \int \mathrm{d}^2x \; g_i O_i(x) \tag{2.43}$$

where $O(\mathbf{x})$ is an eigenvector of the linearised scaling operation (later, we will identify these eigenvectors with primary and secondary operators in conformal field theory). In practice, O_i could be anything allowed by the symmetry considerations above, such as $m(x)$, a derivative term like ∇m or $(\nabla m)^2$, or even linear combinations thereof. Near the critical point, the transformation is linearised as

$$O(x) \to O'(x') = \lambda^{\Delta_O} O(x) \tag{2.44}$$

Just as we saw in the block renormalisation scheme, we expect the coupling constant to absorb this emergent term to recover an Ising model, hence it must scale as

$$g \to g' = \lambda^{\Delta_g} g \tag{2.45}$$

with $\Delta_g = d - \Delta_O$ and $d = 2$ for us.

In the next chapter we will establish the foundations of conformal field theory, focusing on concepts necessary to discuss the main results in the literature for the Ising field theory.

CHAPTER 3

CONFORMAL FIELD THEORY

> All of physics is either impossible or trivial. It is impossible until you understand it, and then it becomes trivial.
>
> Ernest Rutherfort

A **Conformal Field Theory** (CFT) is a **Quantum Field Theory**[1] (QFT) that is invariant under the four conformal transformations: translations, rotations, scaling and special conformal transformations (which are generalised circle inversions). Invariance under these transformations is quite a strict requirement which leads to constraints on the correlation functions of the theory. This in turn has many implications for the operators in the theory, and allows us to extract useful quantities; a prime example being the renormalisation group eigenvalues discussed in the chapter prior.

The conserved charges in a CFT have an associated *central charge*, which parameterises different CFTs in a direct way through the Virasoro algebra. Specific values of central charge have restrictions on the conformal dimension of the operators in the theory, induced by the associated Virasoro operator algebra, and implications for the unitarity of the CFT. The Ising model at its critical points corresponds to conformal field theories, with the Onsager solution $(\beta, H) = (\beta_c, 0)$ being a CFT with central charge $c = 1/2$ and the Yang-Lee imaginary partition function zeroes believed to correspond to a CFT with central charge of $c = -22/5$. Both of these central charges correspond to minimal models, which are an example of a *Rational Conformal Field Theory* (RCFT), meaning they feature only finitely many operators. This makes minimal models especially convenient to study.

The central charge of $c = 1/2$ corresponds to the minimal model $\mathcal{M}_{p,q} = \mathcal{M}_{3,4}$ while $c = -22/5$ is the model $\mathcal{M}_{2,5}$. A difference of $|p - q| = 1$ indicates a theory is unitary, and the Yang-Lee CFT is assumed to be non-unitary [15]. In addition, the $c = 1/2$ case features the energy conformal family $[\epsilon]$ with conformal dimension $(\Delta_\epsilon + \bar{\Delta}_\epsilon) = 1$. This family is an integer difference from the identity family $[I]$ of dimension 0, which indicates degeneracies in differential equations (DEs) satisfied by higher degree ($n \geq 4$) correlation functions and a non-diagonalisable Virasoro operator L_0 [39]. These degeneracies yield the logarithmic operators that we see in the Ising

[1] In the unitary case, at the very least. Non-unitary CFTs arise naturally in statistical theories (e.g. through decay rates) that do not correspond to QFTs as they fail the positivity postulate [62].

scaling function ansatz utilised in this work and the susceptibility data analysed. The theoretical framework for this is known as the logarithmic Ising minimal model $\mathcal{LM}_{3,4}$ [58, 64] and is characterised by representations that are reducible but not indecomposable [63]. However, the most thorough theoretical underpinning of the logarithmic operator content has emerged from studying the Q-state Ising model [54, 72] for low values of $Q < 4$. $Q = 2$ corresponds to the Ising model.

This chapter will outline the theory required to discuss conformal field theory and the emergent logarithmic fields. The main references are the infamous "Big Yellow Book" by Francesco et al. [35], Ginsparg's CFT lecture notes [37], as well as David Tong's candid explanations in the CFT section of his string theory notes [70]. Additional references will be given within the relevant sections.

This chapter will not be a comprehensive cover of all CFT or LCFT, as the subjects are both enormously large. Instead, we will cover a curated subsection of topics relevant to this work.

3.1 Conformal Transformations

We begin study of conformal field theory by first defining conformal transformations and studying them in detail.

The set of conformal transformations is colloquially referred to as "angle preserving" transformations. These are: translations, rotations, dilations (scale transformations) and special conformal transformations (generalised circle inversions). In 2D, each conformal transformation can be represented readily by a Möbius transformation, so to simplify the discussion we introduce the holomorphic coordinate system $(z, \bar{z})$ given by

$$z = x^1 + ix^2 = x + iy \qquad\qquad \bar{z} = x^1 - ix^2 = x - iy \tag{3.1}$$

with (x, y) or (x^1, x^2) being the coordinates on the underlying space (both notations are used). In a general CFT one can consider Euclidean, Minkowski or a more general curved spacetime. However, perturbations in Euclidean space automatically satisfy the Cauchy-Riemann equations, making them especially convenient to work with. This motivates the name "holomorphic coordinates" and the Euclidean case is the main focus here.

We define the following derivative operators

$$\begin{aligned} \partial \equiv \partial_z &= \frac{1}{2}\left(\frac{\partial}{\partial x} + \frac{\partial}{i\partial x}\right) & \bar{\partial} \equiv \partial_{\bar{z}} &= \frac{1}{2}\left(\frac{\partial}{\partial x} - \frac{\partial}{i\partial y}\right) \\ &= \frac{1}{2}\left(\partial_x - i\partial_y\right) & &= \frac{1}{2}\left(\partial_x + i\partial_y\right) \end{aligned} \tag{3.2}$$

These operators are called *Wirtinger derivatives*, and they satisfy the rules $\partial z = \bar{\partial}\bar{z} = 1$ and $\partial\bar{z} = \bar{\partial}z = 0$. These derivatives are quite useful for studying holomorphic functions, which will be done often in this chapter. Lastly, the Euclidean line element is expressed in holomorphic coordinates as $\mathrm{d}s^2 = \mathrm{d}x^2 + \mathrm{d}y^2 = \mathrm{d}z\,\mathrm{d}\bar{z}$.

Note that in general one may wish to explore a complexified underlying space where $x^1, x^2 \in \mathbb{C}$ (as we will do so in this work in the Ising model near the Yang-Lee singularity). In this realisation, an arbitrary point in the space would be an element of $\mathbb{C}^2$ and z and $\bar{z}$ would *not* be complex conjugates of one another. With this in mind we, a priori, do not assume z and $\bar{z}$ are complex conjugates of one another and instead treat them as independent variables. The reason for introducing the coordinates is that the structure of the CFT is much simpler in the language

of holomorphic coordinates, as the space decomposes into independently moving holomorphic and antiholomorphic parts, also called 'left-moving' and 'right-moving' to emphasise their independence. We will first see this explicitly in the Witt and the Virasoro Algebras.

3.1.1 Global Transformations

In 2D, the set of global conformal transformations can all be represented by Möbius transformations on the Riemann sphere $\widehat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$. These are transformations of the following form

$$M(z) = \frac{az+b}{cz+d} \qquad \bar{M}(\bar{z}) = \frac{\bar{a}\bar{z}+\bar{b}}{\bar{c}\bar{z}+\bar{d}} \tag{3.3}$$

with $a, \bar{a}, b, \bar{b}, c, \bar{c}, d, \bar{d} \in \mathbb{C}$ and we enforce $ad - bc = \bar{a}\bar{d} - \bar{b}\bar{c} = 1$. For specific choices of the four parameters, one can capture each of the conformal transformations by

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \Rightarrow \begin{cases} \begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix} & \text{Translations } (z \to z+b) \\ \begin{pmatrix} e^{i\theta/2} & 0 \\ 0 & e^{-i\theta/2} \end{pmatrix} & \text{Rotations } \left(z \to e^{i\theta} z\right) \\ \begin{pmatrix} \sqrt{\lambda} & 0 \\ 0 & \frac{1}{\sqrt{\lambda}} \end{pmatrix} & \text{Dilations } (z \to \lambda z) \\ \begin{pmatrix} 1 & 0 \\ c & 1 \end{pmatrix} & \text{Special Conformal Transformations } \left(z \to \frac{z}{cz+1}\right) \end{cases} \tag{3.4}$$

The reason why this is the only globally defined conformal transformation isn't too difficult to argue. To be a group, such transformations must at least be invertible. If we have a general transformation M then the presence of any branch points or essential singularities would ruin invertibility. This means M can be, at most, a meromorphic function, expressed as a ratio of holomorphic functions which share no common zeroes

$$M(z) = \frac{P(z)}{Q(z)} \tag{3.5}$$

Now we argue that P and Q are at most linear polynomials. If P has multiple roots at a point z_0, then $M^{-1}(0)$ is not single valued, and similarly for Q and $M^{-1}(\infty)$. Thus, $P(z) = (z-b')^n$ and $Q(z) = (z-d')^m$ with $n, m \in \mathbb{N}$. However, if $n > 1$ then $z = b'$ is a branch point for the inverse function M^{-1} and hence it is not single valued in a region around b' (same argument holds for m and Q). Thus, $P(z) = z - b'$, $Q(z) = z - d'$ which by convention we relabel $P(z) = az - b$ and $Q(z) = cz - d$ to get the standard form of a Möbius transform eq. (3.3). The case where the root from P and the pole from Q coincide corresponds to $z_0 = b/a = d/c$ which means $ad - bc = 0$. In this case, M collapses to a constant and is no longer invertible. Note that M is invariant under a rescaling $\{a, b, c, d\} \to \{\lambda a, \lambda b, \lambda c, \lambda d\}$, so we can always rescale the condition $ad - bc \neq 0$ to the standardised form $ad - bc = 1$ as given above.

3.1.2 Local Transformations

Conformal transformations can also be defined locally (infinitesimally) with respect to how the metric changes under the transformation. For a change of coordinates $x^\sigma \to x'^\sigma = x'^\sigma(x)$, the metric transforms as

$$g'_{\sigma\rho}(x') = \frac{\partial x^\mu}{\partial x'^\sigma}\frac{\partial x^\nu}{\partial x'^\rho} g_{\mu\nu}(x) \qquad \text{(Passive Transformation)} \tag{3.6}$$

with $\partial'_\sigma x^\mu \partial'_\rho x^\nu$ being the Jacobian of the transformation. A change of coordinates is a passive transformation; it is a change of reference for the same point in space (or spacetime), meaning the line element must be the same in both reference frames

$$\mathrm{d}s^2 = g_{\sigma\rho}(x)\,\mathrm{d}x^\sigma\,\mathrm{d}x^\rho = g'_{\sigma\rho}(x')\,\mathrm{d}x'^\sigma\,\mathrm{d}x'^\rho = \mathrm{d}s'^2 \tag{3.7}$$

An active transformation on the other-hand takes an object at a point x and moves it to another point x'. Active transformations vary inversely compared to passive transformations, hence we have

$$g'_{\sigma\rho}(x') = \frac{\partial x'^\mu}{\partial x^\sigma}\frac{\partial x'^\nu}{\partial x^\rho} g_{\mu\nu}(x) \qquad \text{(Active Transformation)} \tag{3.8}$$

with the inverse Jacobian $\partial_\sigma x'^\mu \partial_\rho x'^\nu$. Since the points x and x' are physically distinguished points, we do not expect the line element to be invariant, so $\mathrm{d}s^2 \neq \mathrm{d}s'^2$ in general. This is a subtle point, but the following calculations do not work unless the correct definitions are chosen above, so it is worth taking a moment to make this point crystal clear. Many introductory CFT texts tend to brush over this point.

Under an arbitrary transformation, if the resulting transformation on the metric amounts to an overall scale multiplication then the transformation is said to be **conformal**. This means that for a transformation $x \to x' = x'(x)$, we have

$$g'_{\sigma\rho}(x') = \Omega(x) g_{\sigma\rho}(x) \tag{3.9}$$

where $\Omega(x) > 0$ is the positive scale factor. Conformal transformations are the set of transformations that satisfy this property. The condition is similar when expressed in holomorphic coordinates where for $(z, \bar{z}) \to (z', \bar{z}') = (f(z), \bar{f}(\bar{z}))$, the metric transforms as

$$\begin{aligned} g_{\sigma\rho}(z) \to g'_{\sigma\rho}(z') &= \frac{\partial f}{\partial z}\frac{\partial \bar{f}}{\partial \bar{z}} g_{\mu\nu} \\ &= \Omega(z, \bar{z}) g_{\mu\nu}(z) \end{aligned} \tag{3.10}$$

This is immediately satisfied if f is a holomorphic function of z and $\bar{f}$ is an antiholomorphic function. Since f is analytic it can be expanded in Taylor series

$$f(z) = \sum_n c_n z^n \tag{3.11}$$

and we define the antiholomorphic counterpart $\bar{f}$

$$\bar{f}(\bar{z}) = \sum_n \bar{c}\bar{z}^n \tag{3.12}$$

which is a holomorphic function of $\bar{z}$. Returning to the plane $\mathbb{C}^2 \to \mathbb{R}^2$ is accomplished by the identification $\bar{z} = z^*$ and $\bar{f} = f^*$; this identification means $\Omega = \left|\frac{\partial f}{\partial z}\right|^2 \in \mathbb{R}_{\geq 0}$ is satisfied, making our theory inherently conformal.

For translations ($z \to z + b, \bar{z} \to \bar{z} + \bar{b}$) and rotations ($z \to e^{i\theta} z, \bar{z} \to e^{-i\bar{\theta}} \bar{z}$), the metric is unchanged ($\Omega = 1$). When scaling by a factor of λ the metric changes as $\Omega = \lambda\bar{\lambda}$ and for special conformal transformations such as $z \to -1/z$, the metric transforms as $\Omega(z, \bar{z}) = 1/(z\bar{z})^2$. In flat spacetime (as opposed to Euclidean), the subset of transformations satisfying $\Omega(x) = 1$ is the Poincaré group.

Conformal field theories are invariant under all conformal transformations. Informally this means that the physics can only depend on relative angles between objects and looks the same at all length scales. Scale invariance implies that conformal field theories have no preferred length, and hence can only appear when the theory is massless. The mass term in the continuum Ising model is defined proportionally to critical deviation, hence at the critical point the Ising theory is massless. Equivalently, the spectrum of the continuum Hamiltonian is gapless at the critical point.

We will also see that in two dimensions specifically, conformal field theories are special as their symmetry group is infinite dimensional. This ultimately results in a level of solubility enjoyed by 2D CFTs that is not shared by higher dimensions, and for us this eventually manifests as the theory of minimal models.

The typical starting point for formally studying CFTs is to consider an infinitesimal transformation[2]

$$x'^{\rho} = x^{\rho} + \epsilon^{\rho}(x) + \mathcal{O}(\epsilon^2) \tag{3.13}$$

with $\epsilon \ll 1$. The derivative of this transformation is

$$\frac{\partial x'^{\sigma}}{\partial x^{\mu}} = \delta^{\sigma}_{\mu} + \partial_{\mu}\epsilon^{\sigma} \tag{3.14}$$

If we consider how the metric in flat space (with $g_{\sigma\rho}(x) = \eta_{\sigma\rho}$ which does not depend on x) transforms under eq. (3.13), we have

$$\begin{aligned} \eta'_{\sigma\rho} = \frac{\partial x'^{\sigma}}{\partial x^{\mu}} \frac{\partial x'^{\rho}}{\partial x^{\nu}} \eta_{\mu\nu} &= \Omega(x)\eta_{\mu\nu}(x) \\ \eta_{\mu\nu} + (\partial_{\mu}\epsilon_{\nu} + \partial_{\nu}\epsilon_{\mu}) &= \Omega(x)\eta_{\mu\nu} \end{aligned} \tag{3.15}$$

to first order in ϵ. This means for the transformation to be conformal the sum must be proportional to the metric

$$\partial_{\mu}\epsilon_{\nu} + \partial_{\nu}\epsilon_{\mu} = (\Omega(x) - 1)\eta_{\mu\nu} \tag{3.16}$$

By multiplying both sides by $\eta^{\mu\nu}$ we get

$$\Omega(x) - 1 = \frac{2}{d}\partial^{\nu}\epsilon_{\nu} \tag{3.17}$$

introducing a proportionality relation with the dimension of the space, which we have inserted into the calculation to highlight why 2D is a special case. If we inject this result back into eq. (3.16) and multiply by ∂^{ν}, then

$$\begin{aligned} d\partial^{\nu}\left(\partial_{\mu}\epsilon_{\nu} + \partial_{\nu}\epsilon_{\mu}\right) &= 2\partial^{\nu}\eta_{\mu\nu}\left(\partial^{\nu}\epsilon_{\nu}\right) \\ d\partial_{\mu}\left(\partial^{\nu}\epsilon_{\nu}\right) + d\left(\partial^{\nu}\partial_{\nu}\right)\epsilon_{\mu} &= 2\partial_{\mu}\left(\partial^{\nu}\epsilon_{\nu}\right) \\ d\left(\partial^{\nu}\partial_{\nu}\right)\epsilon_{\mu} &= (2-d)\partial_{\mu}\left(\partial^{\nu}\epsilon_{\nu}\right) \end{aligned} \tag{3.18}$$

[2]All transformations will be active transformations from here onwards.

and we can see the uniqueness of the $d = 2$ case. For $d = 2$ the transformation satisfies

$$(\partial^\nu \partial_\nu)\, \epsilon_\mu = 0 \tag{3.19}$$

indicating that the transformation satisfies Laplace's equation when taken over a Euclidean space. There is a well-known link between solutions to Laplace's equation (harmonic functions) and holomorphic functions. In particular, under the holomorphic transformation eq. (3.1), Laplaces equation eq. (3.19) becomes the Cauchy-Riemann equations

$$\partial_1 \epsilon_1 = \partial_2 \epsilon_2 \qquad\qquad \partial_1 \epsilon_2 = -\partial_2 \epsilon_1 \tag{3.20}$$

which was probably much of the initial motivation for the introduction of holomorphic coordinates once upon a time. This identification will ultimately enable the power of Cauchy's Integral Theorem for analytic functions. With this we will construct and simplify many contour integrals in following calculations. We consequently define holomorphic and antiholomorphic representations of the symmetry transformations

$$\epsilon(z) = \epsilon^1 + i\epsilon^2 \qquad\qquad \bar{\epsilon}(\bar{z}) = \bar{\epsilon}^1 - i\bar{\epsilon}^2 \tag{3.21}$$

Next, we discuss the conserved currents associated with conformal symmetries. This is used to define the generalised stress tensor and the all-important central charge. The Laurent expansion of the stress tensor generates the Virasoro algebra, which is the symmetry algebra of the theory. This is an infinite dimensional algebra, and is a feature of 2D CFTs specifically which makes study of 2D uniquely fruitful.

3.2 Stress Tensor

The action functional in a field theory (classical or quantum) is the usual integral over a Lagrangian of some field $\phi(x)$ and its derivative

$$\mathcal{S}[\phi] = \int d^2x\ \mathcal{L}(\phi(x), \partial_\sigma \phi(x)) \tag{3.22}$$

We proceed by considering symmetries on the system and observing how the Lagrangian changes in response to the symmetry in order to keep the action unchanged. This will give us the definition of conserved currents, conserved charges and the stress tensor. This is Noether's theorem.

A generalised symmetry transformation takes the linearised form [52, 61]

$$x'^\sigma = x^\sigma + \epsilon_a \frac{\delta x^\sigma}{\delta \epsilon_a} + \mathcal{O}(\epsilon^2) \tag{3.23}$$

which ranges over the set of symmetries $\{\epsilon_a(x)\}$ and summation over a is implied, even though it is not a spacetime index. This generates the field transformation given by

$$\phi'(x') = \phi(x) + \epsilon_a \frac{\delta F}{\delta \epsilon_a}(x) \tag{3.24}$$

where F relates the new field ϕ' evaluated in the new coordinates to the old field in the old coordinates: $\phi'(x') = F(\phi(x))$ and $\partial'_\sigma \phi'(x') = \frac{\partial x^\rho}{\partial x'^\sigma} \partial_\rho F(\phi(x))$. For a symmetry given by ϵ_a, the

corresponding *generator* G_a is given by the difference between the two fields[3] *evaluated at the same point*

$$\phi'(x) - \phi(x) \equiv -i\epsilon_a G_a \phi(x) \tag{3.25}$$

where we have

$$iG_a\phi = \frac{\delta x^\mu}{\delta \epsilon_a}\partial_\mu \phi - \frac{\delta F}{\delta \epsilon_a} \tag{3.26}$$

with two, oppositely acting contributions from both the active field transformation and the passive underlying space transformation.

Under this transformation, the action has the form

$$\begin{aligned}
\mathcal{S}' = \mathcal{S}[\phi'] &= \int d^2x' \ \mathcal{L}\left(\phi'(x'), \partial'_\sigma \phi'(x')\right) \\
&= \int d^2x \left|\frac{\partial x'}{\partial x}\right| \mathcal{L}\left(F(\phi(x)), \frac{\partial x^\sigma}{\partial x'^\rho}\partial_\sigma F(\phi(x))\right) \\
&= \int d^2x \ \left[1 + \partial_\sigma\left(\epsilon_a \frac{\delta x^\sigma}{\delta \epsilon_a}\right)\right] \mathcal{L}\left(\phi + \delta\phi, \partial\phi + \delta\partial\phi\right)
\end{aligned} \tag{3.27}$$

The next step is to expand to first order in ϵ_a and $\partial_\sigma \epsilon_a$ and substitute the appropriate terms. The terms proportional to 1 and ϵ_a sum to zero, which is easy to see as in the case where the transformation is a simple translation ($\frac{\delta F}{\delta \epsilon} = 0$) the variation in the action $\delta S \equiv S' - S$ would be exactly zero. The terms proportional to $\partial\epsilon_a$ are present in the three remaining higher order conformal symmetries and are collected to define the conserved current J_a^σ

$$J_a^\sigma = -\mathcal{L}\frac{\delta x^\sigma}{\delta \epsilon_a} + \frac{\partial \mathcal{L}}{\partial(\partial_\sigma \phi)}\partial_\rho \phi \frac{\delta x^\rho}{\delta \epsilon_a} - \frac{\partial \mathcal{L}}{\partial(\partial_\sigma \phi)}\frac{\delta F}{\delta \epsilon_a} \tag{3.28}$$

With this, the variation in the action has the form

$$\begin{aligned}
\delta\mathcal{S} &= -\int \mathrm{d}^2x \ J_a^\sigma \partial_\sigma \epsilon_a \\
&= \int \mathrm{d}^2x \ \epsilon_a \partial_\sigma J_a^\sigma + \text{boundary term}
\end{aligned} \tag{3.29}$$

We will neglect boundary terms which do not contribute to the extrema.

Considering stationary solutions ϕ that satisfy the Euler-Lagrange equation, the variation δS vanishes for *any* perturbation, including symmetry transformations. In this case, the conserved charge obeys the continuity equation

$$\partial_\sigma J_a^\sigma = 0 \tag{3.30}$$

We now define the stress tensor as the variation of the action under an arbitrary transformation $x'^\sigma = x^\sigma + \omega^\sigma$

$$\delta\mathcal{S} = -\int \mathrm{d}^2x \ T^{\sigma\rho}\partial_\sigma \omega_\rho \tag{3.31}$$

[3]The factor of i is a Physicist convention so the terms are Hermitian.

Under a simple (only one symmetry) conformal transformation $x'^{\sigma} = x^{\sigma} + \epsilon^{\sigma}$, from eq. (3.29) we can identify

$$J_{\sigma} = T_{\sigma\rho}\epsilon^{\rho} \tag{3.32}$$

so, for our purposes, the stress tensor is identified as the other component of the conserved current in a conformal transformation ϵ. If we again consider just the simplest case of translations we find that from the continuity equation eq. (3.30)

$$\begin{aligned} 0 &= \partial^{\sigma} J_{\sigma} \\ &= \partial^{\sigma} \left(T_{\sigma\rho}\epsilon^{\rho}\right) \\ &= \partial^{\sigma} \left(T_{\sigma\rho}\right) \epsilon^{\rho} \end{aligned} \tag{3.33}$$

so $\partial^{\sigma} T_{\sigma\rho} = 0$.

It is worth noting that the definition of the stress tensor in eq. (3.31) is not symmetric as one would expect. However, we can recover symmetry adding divergence terms to the definition (for details, see [61]), which gives the *Belinfante* stress tensor, which *is* manifestly symmetric. We will ignore this minor detail and act as if $T_{\sigma\rho}$ is symmetric, and just make a note in the followng calculation which requires it.

For more general conformal symmetries, the continuity equation implies that the stress tensor is *traceless*

$$\begin{aligned} 0 &= \partial^{\sigma} J_{\sigma} \\ &= \left(\partial^{\sigma} T_{\sigma\rho}\right) \epsilon^{\rho} + T_{\sigma\rho} \partial^{\sigma} \epsilon^{\rho} \\ &= 0 + \frac{1}{2} T_{\sigma\rho} \left(\partial^{\sigma} \epsilon^{\rho} + \partial^{\rho} \epsilon^{\sigma}\right) \\ &= \frac{1}{d} T^{\sigma}_{\sigma} (\partial^{\rho} \epsilon_{\rho}) \end{aligned} \tag{3.34}$$

In these steps we have explicitly utilised eq. (3.16), which is only true for conformal transformations.

We have shown that the stress tensor, born from symmetry requirements of the action, is of supreme importance. From the stress tensor, we are able to determine the *central charge* of a conformal field theory, which is an object which parameterises different conformal field theories. For CFT, the central charge is a complex number. In a wider mathematical sense, it is an operator that commutes with all other symmetry operators. For us, the central charge is the sole parameter which determines which conformal field theories can be "solved" by method of minimal models. In addition to computing the central charge, the stress tensor also provides a litmus test for determining which operators in a theory are *primary*, which are the building blocks of a CFT. All other operators are derived from the set of primary operators, and minimal models have finitely many primary operators, which is the sense under which one can consider them solvable.

Lastly, the stress tensor generates the symmetry algebra for a given conformal field theory. The algebras are collectively known as "Virasoro Algebras", and are parameterised through their commutation relations by the central charge.

3.2.1 Ward-Takahashi Identities

So far the discussion has been classical field theory. To upgrade to a quantum field theory, we now need to talk about the path integral. By applying Noether's theorem to the quantum path

integral we derive the quantum analogue. This is known as the Ward-Takahashi identities, or commonly as just the Ward identities. We will find that the corresponding statement about conserved currents in the quantum realm is about correlation functions instead, highlighting the importance of studying correlation functions in QFT.

The analysis starts by considering a quantum path integral

$$\mathcal{Z} = \int \mathcal{D}\phi \; e^{-\mathcal{S}[\phi]} \tag{3.35}$$

A symmetry in this context is one that leaves the path integral invariant. This can be accomplished a transformation[4]

$$\phi'(x) = \phi(x) + \epsilon(x)\delta\phi(x) \tag{3.36}$$

that leaves both the action and the measure invariant

$$\mathcal{S}[\phi'] = \mathcal{S}[\phi] \qquad\qquad \mathcal{D}\phi\,' = \mathcal{D}\phi \tag{3.37}$$

This definition for invariance is actually overkill, as we only need the combination $\mathcal{D}\phi \; e^{-S[\phi]}$ to be invariant. However, this shortcut is perfectly suitable for the level of CFT being explored here. The cases where the measure fails to be invariant gives rise to *anomalies*, which are beyond the scope of this thesis.

Under this transformation and utilising our past results for $\delta\mathcal{S}$, the path integral becomes (using $\int$ as shorthand for $\int \mathrm{d}^2x$)

$$\begin{aligned}
\mathcal{Z} &= \int \mathcal{D}\phi' \; e^{-\mathcal{S}[\phi']} \\
&= \int \mathcal{D}\phi' \; e^{-\mathcal{S}[\phi] - \int \partial_\sigma J^\sigma \epsilon} \\
&= \int \mathcal{D}\phi' \; e^{-\mathcal{S}[\phi]} \left(1 - \int \partial_\sigma J^\sigma \epsilon\right) \\
&= \int \mathcal{D}\phi \; e^{-\mathcal{S}[\phi]} \left(1 - \int \partial_\sigma J^\sigma \epsilon\right) \\
&= \mathcal{Z} - \int \mathcal{D}\phi \; e^{-\mathcal{S}[\phi]} \int \partial_\sigma J^\sigma \epsilon
\end{aligned} \tag{3.38}$$

where we expanded the exponential, expanded again via Binomial series and then only kept terms up to first order in ϵ. We also employed the measure invariance and swapped $\mathcal{D}\phi' \to \mathcal{D}\phi$. The whole expression is still equal to $\mathcal{Z}$, as all we've really done is change a dummy variable of integration. This implies that the last term must be zero

$$\int \mathcal{D}\phi \; e^{-\mathcal{S}[\phi]} \left(\int \partial_\sigma J^\sigma \epsilon\right) = 0 \tag{3.39}$$

This expression must hold if we vary ϵ, meaning the rest of the expression must be zero

$$\int \mathrm{d}^2x \; \partial_\sigma \langle J^\sigma \rangle = 0 \tag{3.40}$$

[4]The symmetry here is implemented at the field level rather than the coordinate level, so the variation is proportional to a generator.

Realising that $\mathcal{Z}$ is just the (unnormalised) vacuum correlation function, we can play the same game with more fields. For one field, its correlation function is given by

$$\langle \phi(x) \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi \; e^{-\mathcal{S}[\phi]} \; \phi(x) \tag{3.41}$$

if we take the same symmetry $\phi'(x) = \phi(x) + \epsilon\delta\phi(x)$ (which leaves the correlation function invariant [52]), then we have by the same process above

$$\begin{aligned} \langle \phi'(x') \rangle &= \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi' \; e^{-\mathcal{S}[\phi']} \phi'(x') \\ &= \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi \; 'e^{-\mathcal{S}[\phi']} (\phi(x') + \epsilon\delta\phi(x')) \\ &\dots \\ &= \langle \phi(x') \rangle + \langle \delta\phi(x')) \rangle - \int \langle \partial_\sigma J^\sigma(x) \phi(x') \epsilon \rangle + \mathcal{O}\left(\epsilon^2\right) \end{aligned} \tag{3.42}$$

The first two terms cancel as $\delta\phi$ is a symmetry, so we are left with

$$\langle \delta\phi(x') \rangle \equiv - \langle i\epsilon G \phi(x') \rangle = \int \mathrm{d}^2 x \; \partial_\sigma \langle J^\sigma(x) \phi(x') \epsilon \rangle \tag{3.43}$$

If we utilise the delta function

$$f(x') = \int \delta(x' - x) f(x) \, \mathrm{d}x \tag{3.44}$$

we can relate the coefficients of ϵ under the integrals

$$i\delta(x - x') \langle G\phi(x') \rangle = -\partial_\sigma \langle J^\sigma(x) \phi(x') \rangle \tag{3.45}$$

Performing the same process but generalised for multiple fields, we get

$$i \sum_{i=1}^{n} \delta(x - x_i) \langle \phi_1(x_1) \dots G\phi_i(x_i) \dots \phi_n(x_n) \rangle = -\partial_\sigma \langle J^\sigma(x) \phi_1(x_1) \dots \phi_n(x_n) \rangle \tag{3.46}$$

which is the titular *Ward-Takahashi Identity* (i.e. Noether's theorem of Quantum Field Theory). Where we once had a statement about the derivative of the current vanishing, we now have a statement about the derivative of the correlation functions *almost* vanishing. Instead of disappearing outright, we have delta-functions with support at the position where the current is defined. The equation can be generalised to an arbitrary linear combination of symmetries by making the promotions $(\epsilon, G, J) \to (\epsilon_a, G_a, J_a)$.

3.2.2 Conformal Ward-Takahashi Identity

The Ward-Takahashi relationship is true for an arbitrary symmetry in QFT. We can specialise the relationship to conformal symmetries by considering the properties unique to conformal symmetries.

We will now introduce the notion of primary and quasi-primary fields. A primary field is one that, under a scaling transformation $z \to \lambda z, \bar{z} \to \bar{\lambda}\bar{z}$, the field transforms as

$$\phi'(\lambda z, \bar{\lambda}\bar{z}) = \lambda^{-\Delta} \bar{\lambda}^{-\bar{\Delta}} \phi(z, \bar{z}) \tag{3.47}$$

where $\Delta, \bar{\Delta}$ are *conformal dimensions*[5] and their sum is the eigenvalue of the dilation operator $\mathbf{D}$.

There is another, less restrictive notion which is that of *quasi-primary* fields. These fields obey the more general transformation rule under a global conformal transformation $z \to w(z), \bar{z} \to \bar{w}(\bar{z})$

$$\phi'(w, \bar{w}) = \left(\frac{\partial w}{\partial z}\right)^{-\Delta} \left(\frac{\partial \bar{w}}{\partial \bar{z}}\right)^{-\bar{\Delta}} \phi(z, \bar{z}) \tag{3.48}$$

All primary fields automatically satisfy the quasi-primary condition, but the reverse is not true. All other types of fields (called *secondary*) are linear combinations of primary and quasi-primary fields as well as their derivatives [37]. The local version of eq. (3.48) for the transformation $z \to \epsilon(z), \bar{z} \to \bar{\epsilon}(\bar{z})$ leads to

$$\delta\phi \equiv \phi'(z, \bar{z}) - \phi(z, \bar{z}) = -\left[(\Delta \partial\epsilon + \epsilon\partial) + (\bar{\Delta}\bar{\partial}\bar{\epsilon} + \bar{\epsilon}\bar{\partial})\right] \phi(z, \bar{z}) \tag{3.49}$$

which gives us a first-order expression for the variation in terms of the symmetry transformation. Let us compare this to the variation given in the Ward-Takahashi identity. To accomplish this, take Stokes' theorem

$$\int_\Sigma \mathrm{d}\omega = \int_{\partial\Sigma} \omega \tag{3.50}$$

which relates the integral of an exterior deriavative over a region to the integral of the function over the boundary. The RHS of (the integral version of) eq. (3.45) is in the correct form to be interpreted as the exterior derivative of a 2-form, so we have

$$\begin{aligned} \int_\Sigma \mathrm{d}x^1 \mathrm{d}x^2 \ \left\langle \left(\partial_1 J^1 + \partial_2 J^2\right) \phi \right\rangle &= \int_{\partial\Sigma} \mathrm{d}x^2 \ \langle J_1 \phi \rangle - \int_{\partial\Sigma} \mathrm{d}x^1 \ \langle J_2 \phi \rangle \\ &= \frac{1}{2} \int_{\partial\Sigma} \mathrm{d}z \ \langle J_{\bar{z}} \phi \rangle - \frac{1}{2} \int_{\partial\Sigma} \mathrm{d}\bar{z} \ \langle J_z \phi \rangle \end{aligned} \tag{3.51}$$

where we have made the following substitutions

$$\begin{aligned} \mathrm{d}x^1 &= \frac{1}{2}(\mathrm{d}z + \mathrm{d}\bar{z}) & \mathrm{d}x^2 &= \frac{1}{2i}(\mathrm{d}z - \mathrm{d}\bar{z}) \\ J_1 &= \frac{1}{2}(J_z - J_{\bar{z}}) & J_2 &= \frac{1}{2i}(J_z + J_{\bar{z}}) \end{aligned} \tag{3.52}$$

which is consistent with the differences between raised and lowered complex indices as in eq. (3.2). This can be then expressed in terms of the stress tensor, however one would first need to explicitly symmetrise the equation to cancel cross terms by employing the Belinfante stress tensor as mentioned before. Ultimately we obtain

$$\langle \delta\phi \rangle = \int_{\partial\Sigma} \frac{\mathrm{d}z}{2\pi i} \ \langle T(z)\epsilon(z)\phi \rangle + \int_{\partial\Sigma} \frac{\mathrm{d}\bar{z}}{2\pi i} \left\langle \bar{T}(\bar{z})\bar{\epsilon}(\bar{z})\phi \right\rangle \tag{3.53}$$

[5] Often these are denoted $h, \bar{h}$ in modern literature, but I will use the slightly older notation to avoid conflicting with the Ising field theory perturbation parameter h later in the chapter.

with the following definitions

$$\begin{aligned} T_{zz} &= \frac{1}{4}\left(T_{11} - T_{22} - 2iT_{12}\right) & T_{\bar{z}\bar{z}} &= \frac{1}{4}\left(T_{11} - T_{22} + 2iT_{12}\right) \\ T_{z\bar{z}} &= T_{\bar{z}z} = \frac{1}{4}\left(T_{11} + T_{22}\right) & & \\ \epsilon^z &= \left(\epsilon^1 + i\epsilon^2\right) & \epsilon^{\bar{z}} &= \left(\epsilon^1 - i\epsilon^2\right) \\ T(z) &\equiv 2\pi T_{zz} & \bar{T}(\bar{z}) &\equiv 2\pi T_{\bar{z}\bar{z}} \\ \epsilon(z) &\equiv \epsilon^z = e_{\bar{z}} & \bar{\epsilon}(\bar{z}) &\equiv \epsilon^{\bar{z}} = e_z \end{aligned} \tag{3.54}$$

As promised, this equation decouples into independent holomorphic and antiholomorphic sectors. This is a direct consequence of the symmetry of the stress tensor and its traceless property, which in holomorphic coordinates corresponds to $T_{z\bar{z}} = T_{\bar{z}z} = 0$. This means that while the stress tensor was traceless in Euclidean coordinates, it is diagonal in holomoprhic coordinates. It is worth noting that T is not necessarily traceless in the presence of a dynamical spacetime metric $g_{\sigma\rho}(x)$ [70], but here we are only interested in a flat metric. Expressed in holormophic coordinates, the result $\partial_\sigma T^{\sigma\rho} = 0$ translates to

$$\bar{\partial} T_{zz} = \partial T_{\bar{z}\bar{z}} = 0 \tag{3.55}$$

so these functions are holomorphic and antiholomorphic respectively.

To compare this to eq. (3.49), we employ Cauchy's integral formula

$$f^{(n)}(w) = n! \int_{\partial\Sigma} \frac{\mathrm{d}z}{2\pi i} \frac{f(z)}{(z-w)^{n+1}} \tag{3.56}$$

then we can express the local symmetries as contour integrals

$$\begin{aligned} \epsilon(w) &= \int_{\partial\Sigma} \frac{\mathrm{d}z}{2\pi i} \frac{\epsilon(z)}{(z-w)} \\ \partial_w \epsilon(w) &= \int_{\partial\Sigma} \frac{\mathrm{d}z}{2\pi i} \frac{\epsilon(z)}{(z-w)^2} \end{aligned} \tag{3.57}$$

We can then compare the variation of a quasi-primary operator eq. (3.49) with the general expression for the variation under a general symmetry transformation eq. (3.43) to investigate the effects of conformal symmetry. Comparing integrals and equating coefficients of $\epsilon(z)$ and $\bar{\epsilon}(\bar{z})$ in each equation (which are treated as independent), we arrive at

$$\begin{aligned} \langle T(z)\phi(w,\bar{w})\rangle &= \left(\frac{1}{z-w}\partial_w \langle\phi\rangle + \frac{\Delta}{(z-w)^2}\langle\phi\rangle\right) + \dots \\ \left\langle \bar{T}(\bar{z})\phi(w,\bar{w})\right\rangle &= \left(\frac{1}{\bar{z}-\bar{w}}\partial_{\bar{w}} \langle\phi\rangle + \frac{\bar{\Delta}}{(\bar{z}-\bar{w})^2}\langle\phi\rangle\right) + \dots \end{aligned} \tag{3.58}$$

where "$\dots$" represents regular terms that do not contribute to the contour integrals. Just as before, this can be generalised to a product of multiple fields $\Phi(\mathbf{w},\bar{\mathbf{w}}) \equiv \phi_1(w_1,\bar{w}_2)\dots\phi_n(w_n,\bar{w}_n)$

$$\begin{aligned} \langle T(z)\Phi(\mathbf{w},\bar{\mathbf{w}})\rangle &= \sum_i \left(\frac{1}{z-w_i}\partial_{w_i} \langle\Phi\rangle + \frac{\Delta}{(z-w_i)^2}\langle\Phi\rangle\right) + \dots \\ \left\langle \bar{T}(\bar{z})\Phi(\mathbf{w},\bar{\mathbf{w}})\right\rangle &= \sum_i \left(\frac{1}{\bar{z}-\bar{w}_i}\partial_{\bar{w}_i} \langle\Phi\rangle + \frac{\bar{\Delta}}{(\bar{z}-\bar{w}_i)^2}\langle\Phi\rangle\right) + \dots \end{aligned} \tag{3.59}$$

This is the *Conformal Ward-Takahashi Identity* and is an example of an *Operator Product Expansion* (OPE) of two (or more) fields. An OPE is generically given by

$$\langle \phi_i(z,\bar{z})\phi_j(w,\bar{w})\rangle = \sum_{k=-\infty}^{\infty} C_{ij}^k(z-w,\bar{z}-\bar{w})\,\langle \phi_k(w,\bar{w})\rangle \tag{3.60}$$

where the C_{ij}^k are a set of translationally invariant functions capturing the singular nature while the expectation values $\langle\phi_k\rangle$ are analytic. The expansion was originally an ansatz by Wilson [76] for the general form of the product of operators which incorporated the singular behaviour as fields were brought together. This equation is often written without explicit expectation values, in which case it is implicitly understood that the equality does not make sense without them. More operators can be present in eq. (3.60), but by contour deformation in eqs. (3.49) and (3.53) one can integrate in a small region around w as $z \to w$ to ignore their contribution.

The OPE in eq. (3.58) between the stress tensor and a primary field is an important one due to the terms at order $(z-w)^{-2}$ and $(\bar{z}-\bar{w})^{-2}$. This actually forms an alternate definition for a primary field, as quasi-primary and secondary fields will always include lower order terms, but primary operators will truncate at this order. In particular, the stress-energy tensor itself includes one such additional term

$$\begin{aligned} T(z)T(w) &= \frac{c/2}{(z-w)^4} + \frac{2T(w)}{(z-w)^2} + \frac{\partial T(w)}{z-w} + \dots \\ \bar{T}(\bar{z})\bar{T}(\bar{w}) &= \frac{\bar{c}/2}{(z-w)^4} + \frac{2\bar{T}(\bar{w})}{(\bar{z}-\bar{w})^2} + \frac{\partial \bar{T}(\bar{w})}{\bar{z}-\bar{w}} + \dots \end{aligned} \tag{3.61}$$

which demonstrates that the stress-energy tensor is not a primary operator unless $c = \bar{c} = 0$.

There is a great deal of information contained in the OPE. The conformal dimensions $\Delta, \bar{\Delta}$ (which describe the transformation of the field under scaling transformations and are linked to the first-order renormalisation in eq. (2.40)) feature as the coefficient of the $(z-w)^{-1}, (\bar{z}-\bar{w})^{-1}$ terms. The central charges, $c, \bar{c}$, can be read off from the coefficient of $(z-w)^{-4}$ and $(\bar{z}-\bar{w})^{-4}$. The central charges are an important parameter which is used to parameterise different CFTs. In this work we only investigate CFTs where $c = \bar{c}$, but in principle these can be independent parameters. In a sense, the central charge can be seen to characterise the "degrees of freedom" of the model. For example, for a free scalar field, the central charges are $c = \bar{c} = 1$. With n non-interacting fields, the central charges are $c = \bar{c} = n$. But in general, the central charge does not have to be an integer, half-integer or even positive, so the analogy is not exact. Another interpretation—distinguished by the alternate name *conformal anomaly*—comes from observing that the parameter naturally emerges when comparing the stress tensor on the plane vs cylinder of circumference L

$$T_{\text{cyl.}}(w) = \left(\frac{2\pi}{L}\right)^2 \left\{ T_{\text{pl.}}(z)z^2 - \frac{c}{24} \right\} \tag{3.62}$$

As the boundary L introduces a macroscopic length scale, the conformal anomaly can be seen as the system's reaction to the setting of said scale.

3.2.3 Lattice-Continuum Connection

With the groundwork of CFT established, it is worth taking a moment to see how to connect back to the lattice and to see how these results bolster the original model we are trying to study. Correlation functions are a natural place to form associations between the lattice and

continuum theories. In any discrete theory, the expectation of an operator O^{lat} is given as a weighted sum with respect to a probability distribution $\{p_i\}$

$$\left\langle O^{\text{lat}} \right\rangle \equiv \sum_i p_i o_i \tag{3.63}$$

where $\{o_i\}$ are the observable outcomes of the operator. Due to the laws of thermodynamics, in statistical physics the probability of a given state p_i is inversely proportional to the exponential of the energy associated with that state, with equality given by normalising through summing over all states: $p_i = e^{-\mathcal{H}_i}/\mathcal{Z}_{\text{lat}}$

$$\left\langle O^{\text{lat}} \right\rangle = \frac{1}{\mathcal{Z}_{\text{lat}}} \sum_i o_i e^{\mathcal{H}_i} \tag{3.64}$$

A lattice theory such as the Ising model is enumerated by lattice configurations $\{\sigma\} \equiv \{\sigma(r_1), \ldots, \sigma(r_n)\}$ with $\sigma \in \{1, -1\}$, and in particular we focus on correlation functions that are a product of N local observables $O^{\text{lat}} \equiv \phi_1^{\text{lat}} \ldots \phi_N^{\text{lat}}$ located at positions $\{r_1, \ldots, r_N\}$

$$\left\langle \phi_1^{\text{lat}}(r_1) \ldots \phi_N^{\text{lat}}(r_N) \right\rangle = \frac{1}{\mathcal{Z}_{\text{lat}}} \sum_{\{\sigma\}} \phi_1^{\text{lat}}(r_1) \ldots \phi_N^{\text{lat}}(r_N) e^{-\mathcal{H}(\{\sigma\})} \tag{3.65}$$

An analogous definition exists in quantum field theory through the path integral approach

$$\langle \phi_1(r_1) \ldots \phi(r_N) \rangle \equiv \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi \; \phi_1(r_1) \ldots \phi_N(r_N) e^{-\mathcal{S}[\phi]} \tag{3.66}$$

which is defined with respect to the Euclidean action functional $\mathcal{S}[\phi]$ instead of the Hamiltonian H. The action is linked even more directly to the free energy functional $f[m]$ in eq. (2.37). One could also define continuum correlation functions as a limit of the discrete case eq. (3.65), however as is typical when dealing with infinity, there are additional subtleties to achieve convergence.

As argued by Cardy in [15], we can obtain the scaling limit by fixing certain lattice observables (such as the correlation length) and considering the limit as the number of sites goes to infinity $n \to \infty$ whilst the lattice separation goes to zero $a \equiv |r_i - r_{i+1}| \to 0$. This is constructed such that the domain D also remains fixed and maintains the same topological structure. In this limit we do not expect eq. (3.65) to converge, but from our understanding of renormalisation theory (think: critical exponents eq. (2.15)) and perturbative analysis of QFTs at a scale cutoff, we can expect the renormalised limit

$$\langle \phi_1(r_1) \ldots \phi_N(r_N) \rangle = \lim_{a \to 0} a^{-\sum_j^N y_j} \left\langle \phi_1^{\text{lat}}(r_1) \ldots \phi_N^{\text{lat}}(r_N) \right\rangle \tag{3.67}$$

to exist for a certain set of values $\{y_j\}$. By comparison with the CFT we have detailed so far, we will identify these variables with the conformal dimensions $\{\Delta_j\}$.

If we presume that this limit exists, then we should be able to rescale the lattice spacing by $a \to a/\lambda$ and obtain an equally sensible result but with an overall multiplicative factor $\lambda^{\sum_j^N y_j}$. A shrinking lattice spacing a/λ and fixed domain D is functionally equivalent to a fixed lattice spacing a and expanded domain λD, which implies that the correlation functions satisfy

$$\langle \phi_1(\lambda r_1) \ldots \phi_N(\lambda r_N) \rangle_{\lambda D} = \lambda^{\sum_j^N y_j} \langle \phi_1(r_1) \ldots \phi_N(r_N) \rangle_D \tag{3.68}$$

which is to say that they are *scale covariant*. We can further claim this scale covariance occurs at the field level

$$\phi_j(\lambda r) = \lambda^{y_j}\phi_j(r) \tag{3.69}$$

which is the homogeneity condition seen before in eq. (2.23). We can promote scale covariance to full *conformal covariance* if we introduce

$$\langle \phi_1(r_1') \dots \phi_N(r_N') \rangle_{D'} = \prod_j^N b(r_j)^{y_j} \langle \phi_1(r_1) \dots \phi_N(r_N) \rangle_D \tag{3.70}$$

where $b(r) = |\partial r'/\partial r|$ is the Jacobian of the conformal transformation $r \to r'$ and D' is the image of D under the same transformation. This relation holds exactly for conformal transformations (as we know from eq. (3.9) that conformal transformations are the subset of transformations that locally look like scale transformations) and only for primary fields ϕ from eq. (3.47).

It is also worth noting that from the operator product expansions eq. (3.60), we expect correlation functions in CFT to be singular as $|r_i - r_j| \to 0$, so it is not at all surprising that the scaling limit of eq. (3.65) does not generically converge.

The important observation to link CFT to our concrete lattice model is that since the scale invariance property in CFT implies that the theory is massless (the presence of a mass term would break scale invariance as masses set a preferred length scale). This in turn implies an infinite correlation length as mass scales inversely to correlation length, $m \sim \xi^{-1}$. A key observation of the Ising model at the critical point, the correlation length diverges $\xi \to \infty$, indicating that CFT is a candidate framework to study the scaling limit at the critical points.

3.2.4 Correlation Functions

Correlation functions are an important object to study in any field theory—conformal or not. Correlation functions are physically observable objects that can be measured in experiments, so they provide a critical link between theory and experiment. For conformally invariant field theories in particular, the constraint of satisfying conformal invariance greatly limits the allowable forms that the correlation functions can take. This is to the point where that the two- and three-point functions are completely determined (up to normalisation). The four-point function and beyond can be reduced to functional dependence on the so-called anharmonic ratios, which, at least for small n, reduce the degrees of freedom from n to $n(n-3)/2$.

Generically, by eq. (3.48) we expect the correlation function

$$\langle \phi_1 \dots \phi_n \rangle \equiv \int \mathcal{D}\phi \; e^{-\mathcal{S}[\phi]} \phi_1 \dots \phi_n \tag{3.71}$$

of the n (not necessarily distinct) quasi-primary fields $\phi_1, \dots, \phi_n$ under the transformation $z \to z'$ to transform according to

$$\langle \phi_1(z_1) \dots \phi_n(z_n) \rangle = \left(\frac{\partial z_1'}{\partial z_1}\right)^{\Delta_1} \dots \left(\frac{\partial z_n'}{\partial z_n}\right)^{\Delta_n} \langle \phi_1(z_1') \dots \phi_n(z_n') \rangle \tag{3.72}$$

where the antiholomorphic part has been suppressed to make the equation fit on one line, as it merely contributes simple-to-track multiplicative factors of $(\partial \bar{z}_i'/\partial \bar{z}_i)^{\bar{\Delta}_i}$.

We will now explore how the four different conformal transformations $z \to z'$ impose conditions on the form of these functions.

3.2.5 Two-Point Function

Considering the case of only two fields, rotation invariance of the two-point function means that it should be a function of an absolute value, $|z|^2 = zz^*$, which means it should be a function of a complex modulus. We allow for a richer theory by constructing functions that depend on two variables: $z, \bar{z}$, then enforce $\bar{z} = z^*$ at the end to recover rotation invariance. Thus, the two-point correlation function is a function of the variables

$$\langle \phi_1(z, \bar{z}) \phi_2(w, \bar{w}) \rangle \tag{3.73}$$

If we also include translation invariance then this implies that the two-point function is of the form

$$\langle \phi_1(z, \bar{z}) \phi_2(w, \bar{w}) \rangle = G(z - w, \bar{z} - \bar{w}) \tag{3.74}$$

Under scale covariance this function obtains the further restriction that

$$G(\lambda(z - w), \bar{\lambda}(\bar{z} - \bar{w})) = \lambda^{-\Delta_1 - \Delta_2} \bar{\lambda}^{-\bar{\Delta}_1 - \bar{\Delta}_2} G(z - w, \bar{z} - \bar{w}) \tag{3.75}$$

which implies that $\langle \phi_1 \phi_2 \rangle$ has exponential dependence on the conformal dimension. Combining these two properties implies the form

$$G(z - w, \bar{z} - \bar{w}) = \frac{c_{12}}{(z - w)^{\Delta_1 + \Delta_2} (\bar{z} - \bar{w})^{\bar{\Delta}_1 + \bar{\Delta}_2}} \tag{3.76}$$

where c_{12} is a constant related to the fields ϕ_1 and ϕ_2 and cannot be determined by conformal symmetries alone. It is often arbitrarily set to unity as a normalisation scale. In order to satisfy eq. (3.72), in the case of circle inversion of the form $z \to -1/z, w \to -1/w$ one must have $\Delta_1 = \Delta_2 = \Delta$ and $\bar{\Delta}_1 = \bar{\Delta}_2 = \bar{\Delta}$, whilst rotations $(z, w) \to e^{i\theta}(z, w), (\bar{z}, \bar{w}) \to e^{-i\theta}(\bar{z}, \bar{w})$ imply that the conformal spins $s \equiv \Delta - \bar{\Delta}$ sum to zero, $s_1 + s_2 = 0$ (this is more relevant for correlators with more spins).

With these considerations, the general two-point function has the form

$$\langle \phi_1(z, \bar{z}) \phi_2(w, \bar{w}) \rangle = \delta_{\Delta_1, \Delta_2} \delta_{\bar{\Delta}_1, \bar{\Delta}_2} \frac{c_{12}}{(z - w)^{2\Delta} (\bar{z} - \bar{w})^{2\bar{\Delta}}} \tag{3.77}$$

This says that the only non-trivial correlations are between fields that have matching conformal dimension, the behaviour is singular as $z \to w$ if $\Delta, \bar{\Delta} > 0$.

Three-Point Function

The effect of conformal symmetry can similarly be explored for the three-point function. The process is slightly more involved than for the two-point function, but the result is that the most general form is

$$\langle \phi_1(z_1) \phi_2(z_2) \phi_3(z_3) \rangle = \frac{c_{123}}{z_{12}^{\Delta_1 + \Delta_2 - \Delta_3} z_{23}^{\Delta_2 + \Delta_3 - \Delta_1} z_{31}^{\Delta_3 + \Delta_1 - \Delta_2}} \tag{3.78}$$

with $z_{ij} \equiv z_i - z_j$ and an analogous factor for the antiholomorphic part. This is again very constrained, however four-point functions and onwards are considerably less trivial.

Four-Point & n-Point Function

For the four-point function, conformal symmetry alone is not enough to constrain the equation completely. As such, the general form allowed by conformal symmetry

$$\langle \phi_1(z_1)\phi_2(z_2)\phi_3(z_3)\phi_4(z_4)\rangle = F\left(x, 1-x\right)\prod_{i<j} z_{ij}^{-\Delta_i-\Delta_j+\Delta/3} \tag{3.79}$$

where F is a function of the two, independent cross-ratios (or anharmonic ratios) $x = \frac{z_{12}z_{34}}{z_{13}z_{24}}, 1-x = \frac{z_{14}z_{23}}{z_{13}z_{24}}$ and $\Delta = \sum_i \Delta_i$. The cross-ratios are invariant under conformal symmetries and hence symmetry alone cannot further decompose F. For n fields, the $n-$point functions are functions of $n(n-3)/2$ independent cross-ratios. The function F can be decomposed into what are called *conformal blocks*. Determination of these blocks is important for analytically studying conformal field theories; this approach is called *conformal bootstrap*.

Conformal blocks are difficult to determine in full generality, but as we will see below it can be shown that they satisfy certain ODEs; namely the hypergeometric differential equation. For particular values of the central charge (e.g. the well-studied case of $c = -2$), this ODE has degenerate solutions which directly lead to logarithmic terms that appear in the theory. For $c = 1/2$—which is the conformal field theory that describes the Onsager critical point for the Ising model—logarithmic terms present are proposed based on studying the $Q-$state Potts model for low values of Q [54, 72] and from numerical studies of the susceptibility [56, 22].

3.3 Radial Quantisation

We have seen that conformal field theory takes place most naturally on the Riemann sphere where Möbius transformations are invertible. We will now associate the sphere space to a Minkowski space, which allows us to utilise the machinery of quantum field theory. We will then relate operators with states through the aptly named *operator-state correspondence*.

In spacetime, one distinguishes between time and space through the metric signature. In a Minkowski space (τ, ξ), this is easily read off from the Lorentzian signature present in the spacetime interval

$$\mathrm{d}s^2 = -\,\mathrm{d}\tau^2 + \mathrm{d}\xi^2 \tag{3.80}$$

In QFT, one partitions spacetime into slices of equal time τ through a process formally known as *foliation*[6]. One then defines the familiar unitary time evolution operator which moves operators between time slices

$$A(\xi, \tau) = e^{i\mathcal{H}\tau}A(\xi, 0)e^{-i\mathcal{H}\tau} \tag{3.81}$$

In Euclidean space there is no inherent time dimension, so we can arbitrarily choose how we partition our space. Being a complex space it would be wise to leverage contour integration, hence we choose to foliate our space *radially*. We do this by defining the relationship

$$z = re^{i\theta} = e^{\tau+i\xi} \qquad\qquad \bar{z} = re^{-i\theta} = e^{\tau-i\xi} \tag{3.82}$$

which associates our CFT defined on the Riemann sphere with a compactified Minkowski theory defined on the cylinder $\tau \in \mathbb{R}, \xi \in [0, 2\pi)$. We can now explore how traditional QFT objects

[6] Foliation is the formal process by which a $d+1$ dimensional space is decomposed into a set of d dimensional spaces.

manifest on the Riemann sphere. In particular, the analogue of the Minkowski time translation generator (the Hamiltonian)

$$\mathbf{H} = \partial_\tau \tag{3.83}$$

is the dilation operator

$$\begin{aligned}\mathbf{D} &\equiv r\partial_r \\ &= x\partial_x + y\partial_y \\ &= z\partial + \bar{z}\bar{\partial}\end{aligned} \tag{3.84}$$

while the generator of rotations in a Euclidean space (x, y) is given by

$$\begin{aligned}\mathbf{R} &= -i(x\partial_y - y\partial_x) \\ &= (z\partial - \bar{z}\bar{\partial})\end{aligned} \tag{3.85}$$

which is also the momentum operator in the Minkowski space $\mathbf{P}_\xi$. The eigenvalues of these operators are *conformal dimension* and *conformal spin* respectively

$$D \equiv \Delta + \bar{\Delta} \qquad\qquad s \equiv \Delta - \bar{\Delta} \tag{3.86}$$

The Euclidean space momentum operator is

$$\begin{aligned}\mathbf{P}_x &= -i\partial_x & \mathbf{P}_y &= -i\partial_y \\ &= -i(\partial + \bar{\partial}) & &= \partial - \bar{\partial}\end{aligned} \tag{3.87}$$

while the last type of global conformal symmetry, circle inversions, in Euclidean and holomorphic coordinates is

$$\begin{aligned}\mathbf{K}_x &= i(2x[x\partial_x + y\partial_y] - [x^2 + y^2)\partial_x] & \mathbf{K}_y &= i(2y[x\partial_x + y\partial_y] - [x^2 + y^2)\partial_y] \\ &= i(z^2\partial + \bar{z}^2\bar{\partial}) & &= z^2\partial - \bar{z}^2\bar{\partial}\end{aligned} \tag{3.88}$$

where the quadratic structure is essentially due to the Jacobian of the transformation $z \to w = -1/z$, i.e. $\partial_w = z^2\partial$.

3.3.1 Time Evolution Operator

In QFT, correlation functions are implicitly time-ordered. This can be made explicit by defining the *time ordering operator*

$$\mathcal{T}\{A(\tau_1)B(\tau_2)\} \equiv \theta(\tau_1 - \tau_2)A(\tau_1)B(\tau_2) + \theta(\tau_2 - \tau_1)B(\tau_2)A(\tau_1) \tag{3.89}$$

with θ the Heaviside theta function. In the context of CFT, time-ordering now becomes *radial ordering* with the corresponding radial ordering operator

$$\mathcal{R}\{A(z)B(w)\} \equiv \theta(r_z - r_w)A(z)B(w) + \theta(r_w - r_z)B(w)A(z) \tag{3.90}$$

The main way in which radial ordering manifests is through the ordering of contour integrals. That is to say the equal time commutator of a local operator A and a spatial integral of an operator B becomes the contour integral of a radially ordered product, $[A, \int \mathrm{d}x\, B]_{\text{E.T.}} \to \oint \mathrm{d}w\, \mathcal{R}(A(z)B(w))$. Contour integrals, unless otherwise stated, are assumed to be taken around a contour centred at the origin.

3.3.2 Conserved Charges

In QFT a conserved charge Q, at the most general level, is an object which is conserved under time translation. These can be systematically obtained from each of the conserved currents J

$$Q_a(\tau) \equiv \int \mathrm{d}\xi \, J_a^\tau(\xi, \tau) \tag{3.91}$$

for which the time derivative naturally vanishes

$$\begin{aligned} \partial_\tau Q_a(\tau) &= \int \mathrm{d}\xi \, \partial_\tau J_a^\tau \\ &= -\int \mathrm{d}\xi \, \partial_\xi J_a^\xi \\ &= \text{boundary term} \\ &= 0 \end{aligned} \tag{3.92}$$

and the second equality holds from $\partial_\alpha J^\alpha = \partial_\tau J^\tau + \partial_\xi J^\xi = 0$, the third holds by Stokes' theorem (i.e. integration by parts) and the boundary term vanishes as we take our region of integration over all space. Conserved charges generate symmetry translations [52, 61]

$$[Q, \phi] = \delta\phi = -i\omega G\phi \tag{3.93}$$

3.4 Virasora Algebra

The stress tensor uncovers a great deal of structure about a given CFT. We can expand the stress tensor in a Laurent series

$$T(z) = \sum_{n\in\mathbb{Z}} \frac{L_n(w)}{(z-w)^{n+2}} \tag{3.94}$$

and similarly for the right-moving sector $\bar{T}(\bar{z})$. Inverting this expression by taking a contour integral gives

$$L_n(w) = \oint \frac{\mathrm{d}z}{2\pi i}(z-w)^{n+1}T(z) \tag{3.95}$$

which allows for the definition of L_n acting on the fields directly via

$$\begin{aligned} (L_n\phi)(w,\bar{w}) &\equiv \oint_w \frac{\mathrm{d}z}{2\pi i}(z-w)^{n+1}\phi(w,\bar{w})T(z) \\ (\bar{L}_n\phi)(w,\bar{w}) &\equiv_{\bar{w}} \oint \frac{\mathrm{d}\bar{z}}{2\pi i}(\bar{z}-\bar{w})^{n+1}\phi(w,\bar{w})\bar{T}(\bar{z}) \end{aligned} \tag{3.96}$$

Without loss of generality, we typically set $w = 0$ and instead use the shorthand expansion

$$L_n = \oint \frac{\mathrm{d}z}{2\pi i} z^{n+1}T(z) \tag{3.97}$$

If we expand $\epsilon(z)$ in Laurent series as well

$$\epsilon(z) = \sum_{n\in\mathbb{Z}} \epsilon_n z^{n+1} \tag{3.98}$$

where the somewhat odd choices of powers mean that the conserved charges are simply given by

$$Q = \sum_{n\in\mathbb{Z}} \epsilon_n L_n \tag{3.99}$$

This can be derived by considering the conformal Ward identities, the commutation relationship between charges and generators in eq. (3.93) and how the time variable maps to a radial variable in the Riemann sphere. This procedure is done explicitly in [61].

These operators form an algebra under the commutator bracket known as the *Virasoro Algebra*. The algebra is naturally realised by contour deformation, given that $T(z)$ is holomorphic

$$[L_m, L_n] = \left(\oint \frac{\mathrm{d}z}{2\pi i}\oint \frac{\mathrm{d}w}{2\pi i} - \oint \frac{\mathrm{d}w}{2\pi i}\oint \frac{\mathrm{d}z}{2\pi i}\right) z^{m+1}T(z)w^{n+1}T(w) \tag{3.100}$$

We then fix one of the variable, say w, and perform the integral over z, which combines the two integrals into one integral over a contour surrounding the point w. This then results in

$$\begin{aligned}[L_m, L_n] &= \oint \frac{\mathrm{d}w}{2\pi i}\oint_w \frac{\mathrm{d}z}{2\pi i} z^{m+1}w^{n+1}T(z)T(w) \\ &= \oint \frac{\mathrm{d}w}{2\pi i}\mathrm{Res}_z\left[z^{m+1}w^{n+1}\left(\frac{c/2}{(z-w)^4} + \frac{2T(w)}{(z-w)^2} + \frac{\partial T(w)}{z-w} + \dots\right)\right]\end{aligned} \tag{3.101}$$

where "..." signifies additional regular terms which will not contribute to the residue calculation. Expanding $z^{m+1}(w)$ as a Taylor series in w gives

$$\begin{aligned}z^{m+1} = w^{m+1} &+ (m+1)w^m(z-w) + \frac{1}{2}m(m+1)w^{m-1}(z-w)^2 \\ &+ \frac{1}{6}m(m^2-1)w^{m-2}(z-w)^3 + \dots\end{aligned} \tag{3.102}$$

Substituting and evaluating the residue gives

$$[L_m, L_n] = \oint \frac{\mathrm{d}w}{2\pi i} w^{n+1}\left[w^{m+1}\partial T(w) + 2(m+1)w^m T(w) + \frac{c}{12}m(m^2-1)w^{m-2}\right] \tag{3.103}$$

We can now make some identifications using the definition of the Virasoro operators eq. (3.97). The first and second terms are expansions of L_{n+m}, while the last term is a simple contour integral that vanishes for all powers except w^{-1}. This gives the standard form of the Virasoro algebra

$$[L_m, L_n] = (m-n)L_{m+n} + \frac{c}{12}m(m^2-1)\delta_{m,-n} \tag{3.104}$$

The infamous factor of "1/12" can sometimes be appear in similar calculations and be attributed to due to the (negative of the) limit of the sum of natural numbers, but here we see it unceremoniously emerges from $\frac{1}{2!\times 3!}$. The right-moving sector follows an equivalent derivation, giving

$$\left[\bar{L}_m, \bar{L}_n\right] = (m-n)\bar{L}_{m+n} + \frac{\bar{c}}{12}m(m^2-1)\delta_{m,-n} \tag{3.105}$$

and

$$\left[L_m, \bar{L}_n\right] = 0 \tag{3.106}$$

as the OPE $T(z)\bar{T}(\bar{w})$ has no power-law singularities.

The Virasoro Algebra is the central extension of the *Witt Algebra* (i.e. the algebra for $c = \bar{c} = 0$), which is the algebra of local conformal transformations (infinitesimal versions of translations, rotations, dilations and SCTs). The central charge, more generally, is a term in an algebra (which is not always a scalar or a multiple of the identity) that commutes with all operators in an algebra.

3.4.1 Verma Modules

We will now turn our attention to the claim that specific values of the central charge have only finitely many primary operators, as well as determination of the allowed primary operators based on conformal dimension. To see this we formalise the concept of a *Verma Module*, which is a collection of states generated from a primary field and states that can be obtained by the action of Virasoro operators. Analysis of this algebraic structure will give us our desired properties.

Consider a primary field $\phi(w,\bar{w})$ with conformal weights $\Delta,\bar{\Delta}$. As given in eq. (3.58), the OPE with the stress-energy tensor $T(z)$ is

$$T(z)\phi(w,\bar{w}) = \frac{\Delta}{z-w}\phi(w,\bar{w}) + \frac{1}{(z-w)^2}\partial\phi(w,\bar{w}) \tag{3.107}$$

On the other-hand, substituting the Laurent expansion for T gives

$$T(z)\phi(w,\bar{w}) = \sum_n \oint \frac{\mathrm{d}z}{2\pi i}\frac{1}{z}T(z)\phi(w,\bar{w}) \tag{3.108}$$

and due to radial quantisation we can relate contour integrals to commutation relations,

$$\oint_w \frac{\mathrm{d}z}{2\pi i}\frac{1}{z}T(z)\phi(w,\bar{w}) = [L_n,\phi(w,\bar{w})] \tag{3.109}$$

Equating coefficients of $(z-w)$ we get the commutation relations

$$\begin{aligned}[L_n,\phi(w,\bar{w})] &= \oint_w \mathrm{d}z\, z^{n+1}T(z)\phi(w,\bar{w}) \\ &= \Delta(n+1)w^n\phi(w,\bar{w}) + w^{n+1}\partial\phi(w,\bar{w})\end{aligned} \tag{3.110}$$

The ground state in a quantum field theory is the state of lowest energy. The vacuum state, denoted $|0\rangle$, is a ground state that is additionally invariant under the relevant global symmetry group of the theory, which for CFT is $SL(2,\mathbb{R})$. This requirement turns out to be equivalent to requiring that $|0\rangle$ is regular at $z=0$ [37]. With this in mind, we can see that the effect of the stress tensor acting on the vacuum state

$$T(z)\,|0\rangle = \sum_n \frac{L_n}{z^{n+2}}\,|0\rangle \tag{3.111}$$

at $z=0$ necessarily implies $L_n\,|0\rangle = 0$ for all $n > -1$.

If we consider the limit $w,\bar{w}\to 0$ along with the vacuum state $|0\rangle$, we see that by defining the asymptotic state

$$\left|\Delta,\bar{\Delta}\right\rangle \equiv \phi(0,0)\,|0\rangle \tag{3.112}$$

along with our requirement for regularity at $w=\bar{w}=0$, then $\left|\Delta,\bar{\Delta}\right\rangle$ is an eigenvalue of L_0 and $\bar{L}_0$ with eigenvalues Δ and $\bar{\Delta}$

$$\begin{aligned} &L_0\left|\Delta,\bar{\Delta}\right\rangle = \Delta\left|\Delta,\bar{\Delta}\right\rangle && \bar{L}_0\left|\Delta,\bar{\Delta}\right\rangle = \bar{\Delta}\left|\Delta,\bar{\Delta}\right\rangle \\ &L_n\left|\Delta,\bar{\Delta}\right\rangle = 0 && \bar{L}_n\left|\Delta,\bar{\Delta}\right\rangle = 0 \qquad (n>0)\end{aligned} \tag{3.113}$$

The fact that the theory conveniently decouples into holomorphic and antiholomorphic parts means we can use the simplified notation $|\Delta\rangle$. The antiholomorphic component is still present and can be recovered simply by analogy with the holomorphic part.

By the commutation relations of the Virasoro algebra eq. (3.104) we can see that the action of L_{-n} (and similarly for $\bar{L}_{-n}$) on $|\Delta\rangle$ creates another eigenstate of L_0 and increases the conformal dimension by an integer amount

$$\begin{aligned} [L_0, L_{-n}] &= nL_{-n} \\ \Rightarrow L_0 L_{-n} |\Delta\rangle &= (h+n) L_{-n} |\Delta\rangle \end{aligned} \tag{3.114}$$

Thus we see that while the operators L_n annihilate $|\Delta\rangle$, the operators L_{-n} act as raising operators and raise the energy of the state. L_n are lowering operators and satisfy $L_{-n}^\dagger = L_n$. This leads to a tower of states generated by successively applying raising operators of various degrees, exactly the same as the ladder operators for angular momentum in $\mathfrak{su}(2)$, albeit more generalised as there are now infinitely many ladder operators instead of just a single raising and lowering one. The correspondence with the representation theory of $\mathfrak{su}(2)$ is that the ladder operators $\{L_-, L_z, L_+\}$ are analogous to the closed subset $\{L_{-1}, L_0, L_1\}$.

Because of the commutation relation eq. (3.104), the operators can be arranged in a canonical, ascending order. This collection of states is known as the *Verma Module* which is denoted $\mathcal{V}_{c,h}$ as it is parameterised by both the central charge of the CFT and the weight of the state $|\Delta\rangle$. There is an analogous antiholomorphic module $\bar{\mathcal{V}}_{c,\bar{h}}$. In this context, the state $|\Delta\rangle$ is *defined* as the eigenvector of L_0, and is called a **highest weight state**. This name derives from highest weight representations in representation theory.

The states in a Verma module are organised into *levels* corresponding to conformal dimension

Level	**Dimension**	**States**
0	Δ	ϕ
1	$\Delta + 1$	$L_{-1}\phi$
2	$\Delta + 2$	$L_{-2}\phi, L_{-1}^2\phi$
3	$\Delta + 3$	$L_{-3}\phi, L_{-2}L_{-1}\phi, L_{-1}^3\phi$
...	...	...
n	$h + n$	$P(n)$ fields

Here, $P(n)$ is the *partition number* which counts the number of ways to partition n positive integers. This number arises from the canonical ordering due to the commutation relations. It can be explicitly calculated from the generating function[7]

$$\frac{1}{\prod_{n=1}^{\infty}(1-q^n)} = \sum_{k=0}^{\infty} P(k) q^k \tag{3.115}$$

with the low order terms of the sequence (for $n = 0, 1, \dots$) given by $P(n) = 1, 1, 2, 3, 5, 11, \dots$

For diagonal L_0, basic theory of linear algebra guarantees that states belonging to different dimensions (that is, the eigenvalue under the action of L_0) are orthogonal. A logarithmic CFT, however, is characterised by a non-diagonalisable L_0 with non-trivial Jordan blocks, so this can no longer be guaranteed in that case.

3.4.2 Singular Vectors

While the highest weight state $|\Delta\rangle$ is annihilated by all lowering operators, there can sometimes be other states with this property. Suppose we have a state $|\chi\rangle$ which is *not* a highest weight

[7] This definition often includes a factor of q^{-24} to correspond to the Dedekind eta function, which is an important function encountered when quantising the theory on the torus.

state, yet it still satisfies

$$L_n |\chi\rangle = 0 \qquad \text{for all } n > 0 \tag{3.116}$$

Such a state is called a *null state* or *singular vector*. If this state exists at level $N > 0$ in our Verma Module, then the descendants of this state are also null and form a submodule. In this case, the state $|\chi\rangle$ is orthogonal to all states in the Verma module

$$\begin{aligned} \langle\chi| \left[L_{-J} |\Delta\rangle\right] &= \left[\langle\chi| L_J\right] |\Delta\rangle \\ &= 0 \end{aligned}$$

which in turn implies $\langle\chi|\chi\rangle = 0$. Singular vectors can therefore be identified by searching for states with zero norm. In this notation, the capitalised index implies J is a *multi-index*, used as shorthand for

$$J = \{j_1, \ldots, j_n\} \qquad j_1 \geq j_2 \geq \cdots \geq j_n$$

$$\begin{aligned} L_{-J} &\equiv L_{-j_1} \ldots L_{-j_n} \\ L_J &\equiv L_{j_n} \ldots L_{j_1} \end{aligned} \tag{3.117}$$

where the ordering is allowed by the Virasoro commutation relations and arranged so that $L_{-J}^\dagger = L_J$.

If $|\chi\rangle$ is a singular vector at level N, then all its descendants $\{L_{-J} |\chi\rangle\}$ are also singular. Taken together they form a submodule within $\mathcal{V}_{c,h}$. This implies that the Verma module is **reducible**. In representation theory, a representation is said to be **irreducible** if it cannot be expressed as a direct sum of smaller representations, and reducible otherwise. Irreducibility is a desirable quality, as reducibility implies redundancy in our mathematical description. Even though singular vectors may be present, luckily there is a lemma which states that irreducible Verma modules can be obtained as a quotient of reducible ones. In physicist language, this is described as "setting singular vectors to zero".

In addition to reducibility, a related (and equivalent, in the case of finite groups) condition is that of decomposability. A representation is indecomposable if it does not contain any non-trivial proper subrepresentations, and decomposable otherwise. Irreducibility implies indecomposability, but not the other way around for an infinite-dimensional representation. This distinction is important as logarithmic Verma modules are characterised as reducible but indecomposable [63].

3.4.3 Kac Determinant

A systematic way to search for singular states is to construct the *Gram matrix* $G_{ij}^{(N)} = \langle i|j\rangle$. This is a matrix constructed from the basis vectors at a given level of the Verma module. It is fully determined by the level and the parameters of the Verma module itself: central charge c and weight h. For example, at level 2 there are two basis vectors $\{L_{-1}^2 |h\rangle, L_{-2} |h\rangle\}$. The Gram matrix for this level is

$$\begin{aligned} G^{(2)}(c,h) &= \begin{pmatrix} \langle\Delta|L_1^2 L_{-1}^2|\Delta\rangle & \langle\Delta|L_1^2 L_{-2}|\Delta\rangle \\ \langle\Delta|L_2 L_{-1}^2|\Delta\rangle & \langle\Delta|L_2 L_{-2}|\Delta\rangle \end{pmatrix} \\ &= \begin{pmatrix} 4\Delta(1+2\Delta) & 6\Delta \\ 6\Delta & 4\Delta + \frac{c}{2} \end{pmatrix} \end{aligned} \tag{3.118}$$

which is evaluated by considering the commutation relations eq. (3.104), "sandwiching" the expressions with $\langle\Delta|\Delta\rangle$ and noting that any terms of the form $\langle\Delta|L_{-I}L_J|\Delta\rangle$ vanish. This is completely analogous to the interaction between ladder operators and normally ordered products in, say, the quantum harmonic oscillator. However, we cannot call operators in the form $L_I L_{-J}$ normally ordered as CFT also leverges the traditional definition of normal ordering through Wick's theorem and temporally/radially ordered fields. This understanding is therefore left implicit in the literature.

The norm of any state can be obtained from the Gram matrix. An arbitrary state at level N is expressed as a linear combination of the basis states $|a\rangle = \sum_i a_i |i\rangle$ and its norm can be obtained readily from the Gram matrix [35]

$$\langle a|a\rangle = a^\dagger G^{(N)} a \tag{3.119}$$

The existence of zero eigenvalues of $G^{(N)}$ imply there are zero norm states and thus singular vectors. Similarly, negative eigenvalues imply the presence of negative norm states, meaning the theory is non-unitary. However, the converse is not true as a non-unitary theory with an even number of negative eigenvalues still has a positive determinant.

The eigenvalues of $G^{(N)}$ are not trivial to determine, however a general formula was developed by Kac [42]. The determinant of this matrix is called the *Kac determinant*

$$\det G^{(N)}(c,h) = A_N \prod_{\substack{r,s\geq 1\\ rs\leq N}} (h - h_{r,s})^{\mathcal{P}(N-rs)} \tag{3.120}$$

with A_N a positive constant (explicitly calculated in [35]) independent of c and Δ and with solutions $\Delta_{r,s}$. This determinant gives complete information about singular vectors in a Verma module, as the determinant vanishes for Verma module $\mathcal{V}_{c,\Delta}$ with weight $\Delta = \Delta_{r,s}$. In this case, a singular vector first appears at level $N = rs$. The order of the Kac determinant as a polynomial in Δ is the sum of the first N partition numbers, which can be viewed on the Online Encylopedia of Integer Sequences [2]. The first few terms are $\{0, 1, 3, 6, 12, 20, 35, 54, 86, 128, 192, 275, 399, \dots\}$

The parameterisation of the roots $\Delta_{r,s}$ is dictated by the variable t, which is in turn obtained from the central charge

$$\begin{aligned} \Delta_{r,s}(t) &= \frac{t}{4}\left(r^2-1\right) + \frac{1}{4t}\left(s^2-1\right) - \frac{1}{2}\left(rs-1\right) \\ c(t) &= 13 - 6\left(t + \frac{1}{t}\right) \end{aligned} \tag{3.121}$$

If $t = p/q$ is rational, then the roots can be expressed as

$$\Delta_{r,s}(p,q) = \frac{(pr-qs)^2 - (p-q)^2}{4pq} \tag{3.122}$$

where (p, q) are coprime integers given by the central charge

$$\frac{p}{q} = \frac{\sqrt{25-c} + \sqrt{1-c}}{\sqrt{25-c} - \sqrt{1-c}} \tag{3.123}$$

and the central charge is

$$c(p,q) = 1 - 6\frac{(p-q)^2}{pq} \tag{3.124}$$

This parameterisation is especially useful for identifying unitary representations. A Verma module is a non-unitary representation if $c < 0$ or $h < 0$. For $c \geq 1, h \geq 0$ the representation is unitary. The remaining region of $c \in [0, 1)$ is only unitary exactly for the cases where c matches the form of eq. (3.124) *and* $|p - q| = 1$ [17]. The particular cases that we are interested in are $c = 1/2$ (with $\{p, q\} = \{4, 3\}$) and $c = -22/5$ (with $\{p, q\} = \{5, 2\}$), with the latter being non-unitary. Central charges which are of this form are known as **minimal models** and have been fully characterised in terms of the ADE classification.

Independent to whether a representation is unitary or not, another feature of a representation is whether it is rational or non-rational. Rational CFTs feature a finite number of operators and have rational values for c and h, which can otherwise be arbitrary complex numbers [17]. Rational CFTs encompass a larger set of CFTs than just minimal models, but we are only interested in minimal models in this work.

3.5 Finite Operators

Here we will derive the fact that, at least for minimal models, only finitely many primary operators are present. To start, note that eq. (3.122) is manifestly invariant under the simultaneous substitutions

$$r \to r + q \qquad\qquad s \to s + p \tag{3.125}$$

which is a *periodicity property*. This periodicity means we can relax the condition of $r, s \geq 1$ to simply $r, s \neq 0$. When coupled with periodicity this means $r \neq kq, s \neq np$ for $k, n \in \mathbb{Z}$. Due to this property, weights can be identified

$$\Delta_{r+q,s+p} = \Delta_{r,s} \tag{3.126}$$

Incrementing either of the indices independently induces positive integer terms

$$\begin{aligned} \Delta_{r+2q,s} - \Delta_{r,s} &= (q + r)(p - s) + rs \\ \Delta_{r,s+2p} - \Delta_{r,s} &= (q - r)(p + s) + rs \end{aligned} \tag{3.127}$$

which is a *translation property*. The terms are positive when $r < q$ and $s < p$ and if not then we can repeatedly apply the above rules, as we will see below. k repeated applications of either of these rules amounts to the simultaneous replacements $\{p, q\} \to \{kp, kq\}$ in the above equations. Of note is that for half integer shifts $k \in \mathbb{Z} + \frac{1}{2}$ (which still produce integer indices) the translation property induces whole, half and quarter integer additive terms (depending on the parity of p and q). To induce only integer terms, an alternative approach is taken which utilises other properties.

Another useful property is that under inversion of one of the indices independently, one induces an additive term rs

$$\Delta_{-r,s} - \Delta_{r,s} = rs \tag{3.128}$$

which is again an integer and works equivalently for either index choice

$$\Delta_{-r,s} = \Delta_{r,-s} \tag{3.129}$$

This rule is sometimes called the *reflection property*. Combining two reflections produces two terms that cancel, hence

$$\Delta_{-r,-s} = \Delta_{r,s} \tag{3.130}$$

which is sometimes called the *symmetry property*. Lastly, reflection and translation together yield

$$\Delta_{2q-r,s} = \Delta_{r,2p-s} = \Delta_{r,s} + (q-r)(p-s) \tag{3.131}$$

which will be labelled the *inversion property*. Although these properties are presented for the sake of completion, the additive terms imply that periodicity and only two out of inversion, reflection and translation are necessary to derive the rest.

These rules are (more than) enough to characterise the degeneracy present. It is simple to show that any index not in the range $(r,s) \notin [1,q) \times [1,p)$ can always be reduced to a set in the range $(r,s) \in [1,q) \times [1,p)$ via successive applications of these rules, with only a positive integer part left over. The integer part is unimportant as this simply indicates descendant states via eq. (3.114). That is, $\mathcal{V}_{c,h+k} \subset \mathcal{V}_{c,h}$ for $k > 1$ and the integer terms induced are always positive.

Suppose we have an index of the form $\{r+kq, s+np\}$ with $k,n \in \mathbb{Z}$. The case of $k = n$ is already handled by k applications of eq. (3.125), so we assume $k \neq n$ and w.l.o.g. we assume $k < n$ (the same result holds by symmetry for the case of $k > n$). Under k applications of eq. (3.125) we obtain the index $\{r, s+(n-k)p\}$. Since $k < n$ the difference $n-k$ is positive and has two cases: even ($n-k = 2m$) and odd ($n-k = 2m-1$). In the even case, we apply eq. (3.127) m times to obtain indices $\{r,s\}$ with a positive integer part (since $r < q$ and $s < p$) left over and we are done. In the odd case, we also apply the same rule eq. (3.127) m times to obtain the indices $\{r, s+p\}$. Define the index $s' \equiv p - s$ so we have $\{r, 2p-s'\}$, which is equivalent to $\{r,s'\}$ in the desired range (up to an integer term) via the inversion property eq. (3.131).

This calculation demonstrates that the only unique solutions are contained within the range $(r,s) \in [1,q) \times [1,p)$, and by symmetry and periodicity we also learn that a further half of these solutions are redundant. This in turn means that only finitely many primary operators will be present in a minimal model, which was the main result we wanted to show. This procedure only works for the central charges of the form eq. (3.124) which are minimal models, but more generally one can show that all CFTs with finitely many operators have rational Δ and c [65, 16, 36, 7] (note that this is a one-way implication).

Next, we will examine various n-point correlation functions and the implications on the corresponding operators in the theory.

3.5.1 Descendant Correlation Functions

We can re-express the correlators involving descendant fields in terms of correlators with primary fields and an appropriate differential equation. For the correlation function $\langle L_{-n}\phi(z)\Phi(\mathbf{w})\rangle$ with $L_{-n}\phi(z) \equiv (L_{-n}\phi)(z)$, if we use the contour definition of the Virasoro generators eq. (3.95), the OPE eq. (3.59) and the residue theorem, this can be expressed as a differential equation

$$\begin{aligned}
\langle L_{-n}\phi(z)\Phi(\mathbf{w})\rangle &= \oint_z \frac{\mathrm{d}\zeta}{2\pi i}(\zeta - z)^{1-n} \langle T(\zeta)\phi(z)\Phi(\mathbf{w})\rangle \\
&= -\sum_i \oint_{w_i} \frac{\mathrm{d}\zeta}{2\pi i}(\zeta - z)^{1-n} \left[\frac{1}{(\zeta - w_i)}\partial_{w_i} + \frac{1}{(\zeta - w_i)^2}\Delta_i\right] \langle \phi(z)\Phi(\mathbf{w})\rangle \\
&= \mathcal{L}_{-n} \langle \phi(z)\Phi(\mathbf{w})\rangle
\end{aligned} \tag{3.132}$$

where we have defined the differential operator

$$\mathcal{L}_{-n} \equiv \sum_i \left[\frac{n-1}{(w_i - z)^n}\Delta_i - \frac{1}{(w_i - z)^{n-1}}\partial_{w_i}\right] \tag{3.133}$$

This demonstrates that the correlators involving descendant fields reduce to correlators of primary fields. This result generalises to a sequence of Virasoro operators $L_{-j_1} \dots L_{-j_n}$—as one would expect—to the corresponding sequence of differential operators $\mathcal{L}_{-j_1} \dots \mathcal{L}_{-j_n}$, thus the result holds for an arbitrary descendant field. This means that primary fields are the key object to study and that correlators of descendant fields can be transcribed to correlators involving only primary fields.

We now consider the differential equations associated with singular vectors. These differential equations will drastically constrain the primary fields that can exist, generating the *fusion rules* in the three-point case and giving some motivation for logarithmic operators in the four-point case.

3.5.2 Singular Vector Differential Equations

Suppose there is a singular vector at level N

$$|\chi(z)\rangle = \sum_J \alpha_J L_{-J}\phi(z)\,|0\rangle \tag{3.134}$$

using the multi-index notation eq. (3.117). Since the null state $|\chi\rangle$ is orthogonal to any state, the associated correlator with any field mush also vanish

$$\begin{aligned} \langle \chi(z)\Phi(\mathbf{w})\rangle &= 0 \\ \Rightarrow \sum_J \alpha_J \mathcal{L}_{-J} \langle \phi(z)\Phi(\mathbf{w})\rangle &= 0 \end{aligned} \tag{3.135}$$

If this singular vector occurs at level 2 then it is of the form $|\chi\rangle = \left(L_{-2} + aL_{-1}^2\right)|h\rangle$. To satisfy $L_1|\chi\rangle = 0$ some simple algebra leveraging the commutation relations eq. (3.104) reveals we must have $a = -\frac{3}{2(2h+1)}$. Evaluating $L_2|\chi\rangle = 0$ also reveals a relationship between c and h. Therefore, at level 2 the correlator must be a solution to an ODE of the form

$$\begin{aligned} \left\{\mathcal{L}_{-2} - \frac{3}{2(2h+1)}\mathcal{L}_{-1}^2\right\}\langle\phi(z)\Phi(\mathbf{w})\rangle &= 0 \\ \left\{\left[\sum_{i=2}^{N}\frac{1}{z-w_i}\partial_{w_i} + \frac{\Delta_i}{(z-w_i)^2}\right] - \frac{3}{2(2h+1)}\partial_z^2\right\}\langle\phi(z)\Phi(\mathbf{w})\rangle &= 0 \end{aligned} \tag{3.136}$$

This degree 2 ODE places additional restrictions on the conformal dimensions that can appear in the theory. This, in turn, limits the general OPE eq. (3.60) and the correlation functions. An ODE of degree N exists if there exists a singular vector at level N. The Ising and Yang-Lee CFTs have singular vectors first occuring at level 1 and 2.

We can now systematically explore the effect that satisfying this ODE has on N-point functions.

3.5.3 Singular Vectors and Two-Point Functions

To study the 2-point function we set $\Phi(\mathbf{w}) = \phi(w)$

$$\left\{\frac{1}{z-w}\partial_w + \frac{\Delta}{(z-w)^2} - \frac{3}{2(2h+1)}\partial_z^2\right\}\langle\phi(z)\phi(w)\rangle = 0 \tag{3.137}$$

This equation is already satisfied by the general 2-point function in eq. (3.77) allowed by conformal symmetry, $\langle\phi(z)\phi(w)\rangle = (z-w)^{-2\Delta}$ (see [35] for details), so we gain nothing new other than the satisfaction of passing a sanity check.

3.5.4 Singular Vectors and Three-Point Function

For the 3-point function with $\Phi(\mathbf{w}) = \phi(w_2)\phi(w_3)$, conformal symmetry analysed in eq. (3.78) finds that the general (antiholomophric suppressed) three-point function is of the form

$$\langle \phi_1(z_1)\phi_2(w_2)\phi_3(w_3)\rangle = \frac{c_{123}}{(z_1-w_2)^{\Delta_1+\Delta_2-\Delta_3}(w_2-w_3)^{\Delta_2+\Delta_3-\Delta_1}(w_3-z_1)^{\Delta_1+\Delta_3-\Delta_2}} \tag{3.138}$$

The solution to the corresponding three-point ODE from eq. (3.136) implies that this correlation function must satisfy

$$2(2\Delta_1+1)(\Delta_1+2\Delta_3-\Delta_2) = 3(\Delta_1-\Delta_2+\Delta_3)(\Delta_1-\Delta_2+\Delta_3+1) \tag{3.139}$$

with an equivalent condition on the antiholomorphic parts. This has the explicit solutions[8]

$$\Delta_3 = \frac{1}{6} + \frac{1}{3}\Delta_1 + \Delta_2 \pm \frac{2}{3}\sqrt{\Delta_1^2 + 3\Delta_1\Delta_2 - \frac{1}{2}\Delta_1 + \frac{3}{2}\Delta_2 + \frac{1}{16}} \tag{3.140}$$

meaning that the existence of a null state at level 2 has imposed additional constraints on the three-point function. For the three point function $\langle\phi(z_1)\phi(w_2)\phi(w_3)\rangle$, the dimensions of two operators Δ_1, Δ_2 determine the third Δ_3. For fixed Δ_1, Δ_2 there are two solutions for Δ_3 each given by $\pm$. This relationship is summarised symbolically using the notation of the *fusion rules*

$$[\phi_1] \times [\phi_2] = [\phi_3^+] + [\phi_3^-] \tag{3.141}$$

where ϕ_3^+ and ϕ_3^- represent the two solutions to eq. (3.140). We note that this notation is commutative as the original equation was (after some algebra) symmetric under $\Delta_2 \leftrightarrow \Delta_3$. From our earlier analysis we learned that the conformal dimensions can be parameterised in terms of the integers r and s. If we incorporate this knowledge and set $\Delta_1 = \Delta_{2,1}$ (or $\Delta_1 = \Delta_{1,2}$) and $\Delta_2 = \Delta_{r,s}$, then the solutions to eq. (3.140) have the form

$$\begin{aligned}[\phi_{2,1}] \times [\phi_{r,s}] &= [\phi_{r-1,s}] + [\phi_{r+1,s}] \\ [\phi_{1,2}] \times [\phi_{r,s}] &= [\phi_{r,s-1}] + [\phi_{r,s+1}]\end{aligned} \tag{3.142}$$

and we start to see the motivation for the notation. We see that the operators $\phi_{2,1}$ ($\phi_{1,2}$) act as pseudo-ladder operators. That is, the fields only produce non-vanishing three-point correlations when paired with operators of conformal dimension one lower or higher in the first (second) parameterisation index.

If we recursively repeat this process, noting that the indices of the operators on the RHS always differ by 2, then we can obtain the general solution known as the **fusion fules**

$$[\phi_{rs}] \times [\phi_{r's'}] = \sum_{r''\overset{2}{=}|r-r'|+1}^{r+r'-1} \sum_{s''\overset{2}{=}|s-s'|+1}^{s+s'-1} [\phi_{r''s''}] \tag{3.143}$$

The sums here increment by 2 each time, symbolised by the notation $\overset{2}{=}$. This equation, coupled with the conformal dimension parameterisation eq. (3.122), tells us exactly which primary operators we expect to exist in a theory. The object $[\phi]$ is called a **conformal family**, and it represents a primary field and all its descendants.

This result coupled with the finitely many primary operators derived in the previous section allow us to conclude that fusion operation is *closed*. One can formalise the ideas here and construct a *Fusion Algebra* as an axiomatic generalisation of these rules. This is useful to discuss the fusion of CFTs with more complex correlation functions at a higher level.

[8] Rest assured, this solution is symmetric if we had solved for Δ_2 instead.

3.6 Logarithmic CFT

3.6.1 Singular Vectors and Four-Point Function

Just as restrictions on the correlation functions and operator algebra were garnered by examining the three-point function, one can examine the four-point correlation function and the associated ODE to draw additional constraints. Study of the four-point function is incredibly fruitful, leading to analysis of conformal blocks as a constructive formulation of CFTs, as well as giving the first theoretical pieces of evidence for the emergence of logarithmic operators. These logarithimic operators are a crucial component of this work, as they are present in the free energy scaling ansatz [31] and have numerical evidence from analysis of the susceptibility in [56, 22], which this work builds upon.

These logarithmic terms, however, do not have as thorough a theoretical basis as the rest of the theory established so far. They were originally proposed based on experimental observations (see [38] for a review). The modern theoretical standpoint for the logarithmic operators comes from study of the Q-state Potts model as a generalisation of the Ising model (which is recovered by setting $Q = 2$) and studying the emergence of such operators in that context [72]. As an illustrative and constructive example, we will first examine the $c = -2$ CFT which is the simplest minimal model in which logarithmic operators can be immediately derived.

Euler-Cauchy ODE

Logarithmic terms can be shown to emerge naturally from degenerate ODEs. We will follow the example explored in [34] and consider the Euler-Cauchy 2nd order differential equation in $y = y(x)$

$$\mathcal{L}y = x^2y'' + pxy' + qy = 0 \tag{3.144}$$

with p, q constants. As an ansatz, one uses a trial solution of the form $y = x^\alpha$

$$\begin{aligned} \mathcal{L}y = \left(\alpha(\alpha-1) + p\alpha + q\right) x^\alpha &= 0 \\ \left(\alpha - \alpha_+\right)\left(\alpha - \alpha_-\right) x^\alpha &= 0 \\ f(\alpha)x^\alpha &= 0 \end{aligned} \tag{3.145}$$

for $\alpha \in \mathbb{R}$. $f(\alpha)$ is known as the *indicial equation*. The two roots, $\alpha_\pm$, depend on p and q. In the non-degenerate case, the two, linearly independent solutions are given by $y_\pm(x) = A_\pm x^{\alpha_\pm}$. On the other-hand, if these constants are such that the solution is degenerate ($\alpha_+ = \alpha_- = \alpha_0$) then the polynomial $f(\alpha) = (\alpha - \alpha_0)^2$ has a single root and the solutions are no longer linearly independent. However, it is clear that the derivative $f'(\alpha)$ still has a root at $\alpha = \alpha_0$. This motivates looking for a second, linearly independent solution from the indicial derivative $\partial_\alpha y$

$$\begin{aligned} \mathcal{L}\partial_\alpha y = \partial_\alpha \mathcal{L}y &= 0 \\ \partial_\alpha\left[f(\alpha)x^\alpha\right] &= 0 \\ \left(f(\alpha)\log x + f'(\alpha)\right)x^\alpha &= 0 \\ g(\alpha, x)x^\alpha &= 0 \end{aligned} \tag{3.146}$$

where we commute the operators as x and α are clearly independent. $g(\alpha, x)$ still has a root at $\alpha = \alpha_0$, so we have found a second, linearly independent solution to $\mathcal{L}y = 0$. The general solution is therefore

$$y = Ax^{\alpha_0} + Bx^{\alpha_0}\log x \tag{3.147}$$

and we see that logarithms emerge naturally as a consequence of the linear independence of the derivative solution and the fact that derivatives share roots with the original equation in degenerate cases. This perspective is the one held in the literature, as the logarithmic operators are operators described as derivatives with respect to conformal dimension [54, 44].

Frobenius Method

This same game can be played for the more general case where p and q are promoted from constants to analytic functions, given in series form $p(x) = \sum_n p_n x^n$, $q(x) = \sum_n q_n x^n$

$$\mathcal{L}y(x) = x^2 y'' + p(x)xy' + q(x)y = 0 \tag{3.148}$$

In this case, we use the Frobenius method which involves a series trial solution of the form $y(x) = \sum_i a_i x^{i+\alpha}$. Define an analytic function by the action of the differential operator on the powers x^α

$$\mathcal{L}x^\alpha = f(\alpha, x)x^\alpha \tag{3.149}$$

where $f(\alpha, x)$ is analytic in x

$$\begin{aligned} f(\alpha, x) &= \sum_j f_j(\alpha)x^j \\ f_j(\alpha) &\equiv \begin{cases} \alpha(\alpha-1) + p_0\alpha + q_0 & j = 0 \\ p_j\alpha + q_j & j > 0 \end{cases} \end{aligned} \tag{3.150}$$

Note the familiar zeroth order equation exactly matches the previous analysis. The full Frobeius solution is

$$\begin{aligned} \mathcal{L}y = \sum_i a_i(\mathcal{L}x^{i+\alpha}) &= 0 \\ \sum_i a_i f(i+\alpha, x)x^{i+\alpha} &= 0 \\ \sum_i \sum_j a_i f_j(i+\alpha)x^i x^j x^\alpha &= 0 \end{aligned} \tag{3.151}$$

Upon evaluation of the sums, the coefficient of $x^{n+\alpha}$ is explicitly given by

$$\sum_{k=0}^{n} a_{n-k} f_k([n-k]+\alpha) \tag{3.152}$$

which gives us a system of equations to solve. For $y(x)$ to be a solution, all coefficients must independently and simultaneously vanish for some value of α

$$\begin{aligned} f_0(\alpha)a_0 &= 0 \\ f_0(\alpha+1)a_1 + f_1(\alpha)a_0 &= 0 \\ f_0(\alpha+2)a_2 + f_1(\alpha+1)a_1 + f_2(\alpha)a_0 &= 0 \\ &\vdots \end{aligned} \tag{3.153}$$

where the zeroth order term is the familiar indicial equation. From these equations one can construct a recursion relation between series terms a_n, which may then be solved by recursive

techniques. To capture this, we promote $a_n \to a_n(\alpha)$ to highlight that the series coefficients are ultimately defined by α through the recurrence relation.

Since we are interested in two linearly independent solutions for $y(x)$, there are now three cases to consider.

- If the two **solutions to the indicial equation, $f_0(\alpha)$, are equal**, we obtain logarithmic terms in a very similar manner as seen before

$$y(x) = Ax^{\alpha_0} \sum_n a'_n(\alpha_0)x^n + B\log(x)x^{\alpha_0} \sum_n a_n(\alpha_0)x^n \tag{3.154}$$

- If the **roots differ by a non-integer**, then the two solutions are again guaranteed to be linearly independent

$$y(x) = Ax^{\alpha_+} \sum_n a_n(\alpha_+)x^n + Bx^{\alpha_-} \sum_n a_n(\alpha_-)x^n \tag{3.155}$$

- However, the new case is now **when the roots differ by an integer**, that is $f_0(\alpha) = (\alpha - \sigma)(\alpha - (\sigma + s))$ for some positive integer $s \in \mathbb{N}_{>0}$. In this case, the two solutions $y_1(x) = x^{\alpha_0} \sum_n a_n x^n$ and $y_2(x) = x^{\alpha_0} \sum_n b_n x^{n+s}$ are clearly not linearly independent as one can simply identify $b_n = a_{n+s}$. Thankfully, this case actually just mimics the degenerate case and similar (but more involved) analysis reveals the solution is the form

$$y(x) = Ax^{\alpha_0+s} \sum_n a'_n(\alpha_0 + s)x^n + B\log(x)x^{\alpha_0} \sum_n a_n(\alpha_0)x^n \tag{3.156}$$

The net takeaway is that for the indicial equation of an ODE with roots that differ by an integer, logarithmic terms naturally arise when one attempts to use a Frobenius series as a trial solution. This is hinted at by the Ising CFT, as the conformal dimension of the identity operator ($\Delta_{\mathbb{I}} + \bar{\Delta}_{\mathbb{I}} = 0$) and the energy operator ($\Delta_\epsilon + \bar{\Delta}_\epsilon = 1$) differ by an integer.

3.6.2 Logarithmic Ising Model

We will now examine the singular vector ODE associated with the four-point function and observe the indicial equation degeneracy immediately present for $c = -2$. The four-point correlation function eq. (3.79) of four of the same field can be decomposed as in [44]

$$\langle \phi(z_1)\phi(z_2)\phi(z_3)\phi(z_4)\rangle = \frac{1}{|z_{12}z_{34}|^{4\Delta}} \sum_{i,j} U_{ij} F^i(x) F^j(\bar{x}) \tag{3.157}$$

The four-point function is associated with the following ODE due to the level 2 singular vector (after several algebraic manipulations; details in [35])

$$x(1-x)\frac{\partial^2 F}{\partial x^2} + [d - (a+b+1)x]\frac{\partial F}{\partial x} - abF = 0 \tag{3.158}$$

which is the *hypergeometric differential equation*. The Frobenius solution to this equation is the Gauss hypergeometric function, defined as

$${}_2F_1(a, b; d; z) \equiv \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(d)_n} \frac{z^n}{n!} \tag{3.159}$$

for complex z lying inside the unit circle $|z| < 1$ and $(x)_n \equiv \Gamma(x+1)/\Gamma(x-n+1)$ the *Pochhammer falling factorial*. The usual parameter c has been replaced to avoid potential confusion with the central charge. In this instance of four repeated fields the hypergeometric parameters $\{a, b, d\}$ can be related to the central charge

$$a = \frac{B}{24} \qquad b = -1 + \frac{B}{8} \qquad d = \frac{B}{12} \tag{3.160}$$

with $B \equiv \left(\sqrt{1-c} - \sqrt{25-c}\right)^2$. Thus, for $c = -2$, the hypergeometric parameters are

$$B = 12 \qquad a = \frac{1}{2} \qquad b = \frac{1}{2} \qquad d = 1 \tag{3.161}$$

The indicial equation for the ODE eq. (3.158) is

$$\alpha(\alpha - 1 + d) = 0 \tag{3.162}$$

and it has two linearly independent solutions given by

$$\begin{aligned} F_1 &= {}_2F_1\left(a, b; d; x\right) \\ F_2 &= x^{1-d}{}_2F_1\left(a-d+1, b-d+1; 2-d; x\right) \end{aligned} \tag{3.163}$$

meaning for the $c = -2$ case we have degeneracy. This is reconciled by promoting the second solution to include a multiplicative logarithmic factor, which is exactly what we wanted to observe.

The Ising scenario is not quite as simple as the case study here. Substituting $c = 1/2$ or $c = -22/5$ gives a non-degenerate hypergeometric ODE, but that does not rule out the possibility of other ODEs generated from mixed or higher order correlation functions creating logarithms. Theory aside, there is a plethora of experimental evidence to warrant the inclusion of logarithmic terms to fit numerical data. The key dataset in this work is the susceptibility data [56, 22] wherein a polynomial-time algorithm was used to generate the zero-field susceptibility. The susceptibility was numerically fitted to the data using many orders of logarithmic terms. This is discussed further in chapter 4.

The presence of logarithmic terms are associated with non-diagonalisable Virasoro generators [44]. The operators have a Jordan block structure

$$\begin{aligned} L_0 \left|C\right\rangle &= h \left|C\right\rangle \\ L_0 \left|D\right\rangle &= h \left|D\right\rangle + \left|C\right\rangle \end{aligned} \tag{3.164}$$

for the logarithmic pair of operators C and D. This is further linked to Verma modules that are reducible but indecomposible [63].

3.6.3 Yang-Lee Conformal Field Theory

Yang-Lee Effective Free Energy

In [15] it was first proposed that the effective action for the Ising model at the Yang-Lee singularity should be of the form

$$f = \int \mathrm{d}^2x \ (\nabla m(\mathbf{x}))^2 + i(H - H_c)m(\mathbf{x}) + igm(\mathbf{x})^3 \tag{3.165}$$

The presence of imaginary terms makes this theory non-unitary. The paper goes on to associate the $d = 2$ theory with the $c = -22/5$ non-unitary conformal field theory. This CFT is a minimal model with $\{q, p\} = \{5, 2\}$ and hence $r = 1$ and $s \in [1, 4]$

$$h_{1,1} = 0 \qquad h_{1,2} = -\frac{1}{5} \qquad h_{1,3} = -\frac{1}{5} \qquad h_{1,4} = 0 \tag{3.166}$$

The fusion rules for $\mathcal{L}_{5,2}$ are

$$\begin{aligned} \mathbb{I} \times \mathbb{I} &= \mathbb{I} \\ \Phi \times \mathbb{I} &= \Phi \\ \Phi \times \Phi &= \mathbb{I} + \Phi \end{aligned} \tag{3.167}$$

This form relates to the famous result by Yang and Lee. In [45] it was proven—quite generally—that a certain class of polynomials must have roots along the unit circle in the complex plane. In particular by introducing the fugacity variable $z = e^{-2H}$, the partition function can be expressed as

$$\mathcal{Z} \propto \sum_n P_n z^n \tag{3.168}$$

where P_n is the contribution to the partition function at $H = 0$ from configurations with n spin down sites. As a polynomial in z, $\mathcal{Z}$ has zeroes along the unit circle, corresponding to the case where H is purely imaginary. In the thermodynamic limit where $N \to \infty$, the zeroes condense in the complex H plane between two values iH_0 and $-iH_0$: the Yang-Lee singularities. One typically takes a branch cut between these two points passing through infinity. This theorem is known as the Yang-Lee circle theorem and the branch cut is the Yang-Lee edge singularity in the thermodynamic limit.

3.7 Ising Field Theory

Perturbatively expanding away from a massless conformal field theory gives a quantum field theory. As mentioned above eq. (2.42), correlation length is inversely proportional to critical deviation, and mass in the continuum Ising model is proportional to correlation length. Therefore, when moving away from the critical point, one expects to induce mass and generate a field theory.

The perturbative approach was first presented by Zamolodchikov in [82] wherein he studied the Hamiltonian

$$\mathcal{H} = \mathcal{H}_{c=1/2} + \lambda \int \mathrm{d}^2x \; \phi(x) \tag{3.169}$$

which is perturbed from the critical point by one primary field. Building upon this work, in [31] Fonseca & Zamolodchikov explicitly studied

$$\mathcal{H}_{\mathrm{IFT}} = \mathcal{H}_{c=1/2} + \lambda_\epsilon \int \mathrm{d}^2x \; \epsilon(x)x + \lambda_\sigma \int \mathrm{d}^2x \; \sigma(x) \tag{3.170}$$

allowing for perturbation by two fields. These Hamiltonians (in particular the second one) are known as the *Ising Field Theory* (IFT), which are Euclidean quantum field theories. The

$c = 1/2$ case is the unperturbed Ising conformal field theory studied above, with primary field OPE normalisation set as

$$\langle \epsilon(x)\epsilon(0)\rangle = \frac{1}{|x|^2} \qquad \langle \sigma(x)\sigma(0)\rangle = \frac{1}{|x|^{1/4}} \tag{3.171}$$

in the limit $x \to 0$. Under perturbation by one field, Zamolodchikov originally proved in [82] that if one expresses the resulting field theory as a power series in λ, then only *finitely* many powers are present in *local* expressions such as the equations of motion. This is essentially the observation that allowed Zamolodchikov to assert that perturbations by only one field remain integrable, while the same cannot be said for multiple perturbations.

3.7.1 Single Field Perturbation

To briefly recount the work of Zamolodchikov, we first start by recalling the action of the Virasoro algebra on the space of local fields (primary *and* secondary), $A \in \mathbf{A}$, was defined in eq. (3.96) and is repeated here

$$(L_n A)(w,\bar{w}) \equiv \oint_w \frac{\mathrm{d}z}{2\pi i}(z-w)^{n+1}A(w,\bar{w})T(z) \tag{3.172}$$

The space of fields decomposes according to conformal classes

$$\mathbf{A} = \bigoplus_{\alpha} [\phi_\alpha] \tag{3.173}$$

where each class is a direct product of left and right moving sectors: $[\phi] = \phi \otimes \bar{\phi}$. We saw above that the Verma module is the collection of eigenvalues of the generator L_0, but it was not necessarily irreducible without constructing an appropriate factor space by singular vectors. Here we sidestep this discussion and directly define the *Virasoro module*, Λ

$$\Lambda = \bigoplus_{s=0}^{\infty} \Lambda_s \tag{3.174}$$

as the sum of irreducible representations with highest weight 0 (that is, acting on the identity $A = I$), enumerated by the spin variable s.

Now, recall from eq. (3.55) that the continuity equation $\partial_\mu T^{\mu\nu} = 0$ when expressed in holomorphic coordinates vanishes

$$\bar{\partial} T = 0 \tag{3.175}$$

Because of this condition, the action of the Virasoro generators in eq. (3.172) implies that L_n are *integrals of motion* (IM). Each field $T_s \in \Lambda_s$ has an associated IM

$$\oint_z \mathrm{d}w\, T_s(w)(w-z)^{n+s-1} \tag{3.176}$$

However, these operators are not linearly independent as some fields in Λ are total derivatives. To obtain linearly independent IMs, we construct the factor space $\hat{\Lambda} = \Lambda / L_{-1}\Lambda$ where $L_{-1}\Lambda \subset \Lambda$ is the subspace consisting of total derivatives. This space factorises similarly to the original Virasoro module

$$\hat{\Lambda} = \bigoplus_{s=0}^{\infty} \hat{\Lambda}_s \tag{3.177}$$

The dimension of these spaces are given by the the *character formula*

$$\sum_{s=0}^{\infty} q^s \dim(\hat{\Lambda}_s) = (1-q)\chi_0(q) + q \tag{3.178}$$

where χ_0 is the character for the module. There are subtle considerations to be made for rational, unitary CFTs (i.e. minimal models with central charge satisfying eq. (3.124)) to do with dimensional resonance, but the low order dimensionalities are

$$\begin{aligned} &\dim(\hat{\Lambda}_0) = 1 \qquad \dim(\hat{\Lambda}_2) = 1 \qquad \dim(\hat{\Lambda}_4) = 1 \qquad \dim(\hat{\Lambda}_6) = 2 \\ &\dim(\hat{\Lambda}_1) = 0 \qquad \dim(\hat{\Lambda}_3) = 0 \qquad \dim(\hat{\Lambda}_5) = 0 \end{aligned} \tag{3.179}$$

noting that in particular the odd orders vanish. In this augmented space, for $\hat{T}_s \in \hat{\Lambda}_s$ the following are linearly independent integrals of motion

$$\hat{\mathcal{L}}_{s,n} A(z,\bar{z}) \equiv \oint_z \mathrm{d}w\, \hat{T}_s(w)(w-z)^{n+s-1} A(z,\bar{z}) \tag{3.180}$$

In [82], Zamolodchikov was able to prove they can still exist for perturbed field theories, meaning the resulting field theories are integrable.

Under the perturbation eq. (3.169) by a relevant field ϕ (which is, in practice, primary) with coupling strength λ, we define the analogue of the Virasoro module eq. (3.174)

$$\Phi = \bigoplus_{s=0}^{\infty} \Phi_s \tag{3.181}$$

The continuity equation $\partial_\mu T^{\mu\nu} = 0$ no longer vanishes in holomorphic coordinates, as it instead reads

$$\bar{\partial} T = \partial \Theta \tag{3.182}$$

where $\Theta = \lambda(\Delta - 1)\phi$. Now, we again construct the factor space of the Virasoro module $\hat{\Phi}_s = \Phi_s / L_{-1}\Phi_s$ to recover linearly independent IMs. Due to the modified continuity equation eq. (3.182), we now have that for $\hat{T}_{s+1} \in \hat{\Lambda}_{s+1}$ and $\hat{\Theta}_{s-1} \in \hat{\Phi}_{s-1}$, if a particular operator $B_s : \Lambda_s \to \hat{\Phi}_{s-1}$ exists such that $B_{s+1} T_{s+1} = 0$, then the operators obey the relationship

$$\bar{\partial} \hat{T}_{s+1} = \partial \hat{\Theta}_{s-1} \tag{3.183}$$

The operator is decomposed as the following sequence of operators

$$B_s \equiv \Pi_s D_{0,s} \qquad D_{0,s} : \Lambda_s \to \Phi_s \qquad \Pi_s : \Phi_s \to \hat{\Phi}_s \tag{3.184}$$

To look for a non-vanishing kernel for B_s, using the generalisation of the character formula eq. (3.178)

$$\sum_{s=0}^{\infty} q^{s+\Delta} \dim(\hat{\Phi}_\Delta) = (1-q)\chi_\Delta(q) \tag{3.185}$$

one can calculate that for $\phi = \phi_{1,2} = \sigma$ with conformal dimension $\Delta = 1/16$, the dimensions of the low order spaces are

$$\begin{aligned} &\dim(\hat{\Phi}^\sigma_1) = 0 \quad \dim(\hat{\Phi}^\sigma_3) = 1 \quad \dim(\hat{\Phi}^\sigma_5) = 1 \quad \dim(\hat{\Phi}^\sigma_7) = 2 \quad \dim(\hat{\Phi}^\sigma_9) = 4 \quad \dim(\hat{\Phi}^\sigma_{11}) = 6 \\ &\dim(\hat{\Phi}^\sigma_2) = 0 \quad \dim(\hat{\Phi}^\sigma_4) = 1 \quad \dim(\hat{\Phi}^\sigma_6) = 2 \quad \dim(\hat{\Phi}^\sigma_8) = 5 \quad \dim(\hat{\Phi}^\sigma_{10}) = 8 \end{aligned} \tag{3.186}$$

while for $\phi = \phi_{1,3} = \epsilon, \Delta = 1/2$, the dimension of the spaces are

$$\begin{array}{lllll} \dim(\hat{\Phi}_1^\epsilon) = 0 & \dim(\hat{\Phi}_3^\epsilon) = 0 & \dim(\hat{\Phi}_5^\epsilon) = 1 & \dim(\hat{\Phi}_7^\epsilon) = 2 & \dim(\hat{\Phi}_9^\epsilon) = 4 \quad \dim(\hat{\Phi}_{11}^\epsilon) = 7 \\ \dim(\hat{\Phi}_2^\epsilon) = 1 & \dim(\hat{\Phi}_4^\epsilon) = 2 & \dim(\hat{\Phi}_6^\epsilon) = 3 & \dim(\hat{\Phi}_8^\epsilon) = 5 & \dim(\hat{\Phi}_{10}^\epsilon) = 8 \end{array} \tag{3.187}$$

By comparing the dimension of $\hat{\Phi}_{s-1}$ above and $\hat{\Lambda}_s$ from eq. (3.179), we can see that the compatible dimensions are $s = 1, 5, 7, 11, ...$ for σ and $s = 1, 3, 5, 7, ...$ for ϵ. The existence of the operator B_s in these dimensions in turn implies that

$$P_s \equiv \oint \mathrm{d}z \ \hat{T}_{s+1} + \oint \mathrm{d}\bar{z} \ \hat{\Theta}_{s-1} \tag{3.188}$$

survive as IMs from the $c = 1/2$ CFT with the prescribed values of s above (note $s = 1$ is the standard conservation of momentum). The densities P_s only appear under perturbation by at most a single primary field ϕ in eq. (3.169). Because of the existence of these IMs, the resulting field theories are naturally integrable.

Massive field theories (QFT) are equivalent to relativistic scattering theories, which are in turn completely determined by specifying the *S-matrix*. Through analysis of S-matrix theory carried out by Zamolodchikov, it was determined that these IMs lead to multiple massive particles. The masses of these particles are given as mass ratios

$$\frac{m_2}{m_1} = 2\cos\left(\frac{\pi}{5}\right) \qquad \frac{m_3}{m_1} = 2\cos\left(\frac{\pi}{30}\right) \qquad \frac{m_4}{m_2} = 2\cos\left(\frac{7\pi}{30}\right) \qquad \dots \tag{3.189}$$

The lowest mass term, $m \equiv m_1$, is singled out as the parameter for the ϵ perturbation.

Lastly, the final important result of the paper was that the perturbations by primary fields were identified with the standard Ising model in various forms. For $\phi = \epsilon$, noting that the model is solvable with an infinite set of integrals of motion, this regime is identified with the zero-field Ising model $\tau \neq 0, H = 0$, and we designate the perturbation parameter as $\lambda \to m \sim \tau + \mathcal{O}(\tau^3)$. For the primary field $\phi = \sigma$, the model is identified with the critical-temperature Ising model $\tau = 0, H \neq 0$. The perturbation parameter in this case is $\lambda \to h \sim H + \mathcal{O}(H^3)$ and both parameters embody the $\mathbb{Z}^2$ symmetries under $\tau \to -\tau$ and $H \to -H$ expected by their respective conformal classes.

In [28] Fateev explores the relationship between the perturbation parameter λ and the mass of the lightest particle, m. After some intense group theoretic analysis, the main result from the work is that for a field with conformal dimension $\Delta = \frac{p-2}{4(p+1)}$, the perturbation parameter relates to the mass via

$$\begin{aligned} \lambda^2 &= \frac{\gamma^2\left(\frac{p}{4(p+1)}\right)\gamma\left(\frac{1}{p+1}\right)}{4\pi^2\gamma\left(\frac{2}{p+1}\right)}\left(\frac{m\Gamma\left(\frac{2}{3}\right)\Gamma\left(\frac{2(p+1)}{3(p+2)}\right)}{2\Gamma\left(\frac{p}{3(p+2)}\right)}\right)^{\frac{3(p+2)}{p+1}} \\ \gamma(x) &\equiv \frac{\Gamma(x)}{\Gamma(1-x)} \end{aligned} \tag{3.190}$$

For each of our fields, $p = 3$ recovers $\Delta = \frac{1}{16}$ and under the substitution $p \to -p - 1$ one finds that $p = -4$ gives $\Delta = \frac{1}{2}$. This relationship and substitution essentially come from the fact that it is common to describe unitary minimal models by a single parameter as $\mathcal{L}_{p,p+1}$, and then noting that all expressions in eq. (3.122) are invariant under $(p, q) \to (-p, -q)$. The formula

above yields

$$\begin{aligned} \lambda_\epsilon &= \frac{m}{2\pi} & \lambda_\sigma &= m^{15/8} \frac{\Gamma\left(\frac{3}{16}\right)\Gamma\left(\frac{1}{4}\right)^{1/2}\left[\Gamma\left(\frac{2}{3}\right)\Gamma\left(\frac{8}{15}\right)\right]^{15/8}}{4\times 2^{7/8}\pi\Gamma\left(\frac{13}{16}\right)\Gamma\left(\frac{3}{4}\right)^{1/2}\Gamma\left(\frac{1}{5}\right)^{15/8}} \\ &\approx m\times 0.15915494\ldots & &\approx m^{15/8}\times 0.08401070\ldots \end{aligned} \tag{3.191}$$

meaning the perturbations have mass dimension 1 and 15/8 respectively, also given by $m^{d-2\Delta}$.

3.7.2 Multiple Field Perturbation

As explored above, the integrals of motion eq. (3.188) only exist for a single perturbation. In the case of multiple perturbations, the analytic study was carried out by Fonseca and Zamolodchikov in [31]. The Ising field theory studied within was (using the notation of [47, 48])

$$\mathcal{H}_{\text{IFT}} = \mathcal{H}_{c=1/2} + \frac{m}{2\pi}\int \mathrm{d}^2x\ \epsilon(x) + h\int \mathrm{d}^2x\ \sigma(x) \tag{3.192}$$

The relative mass dimensions of the parameters promote the definition of dimensionless *scaling parameters*

$$\xi(m,h) = \frac{h}{|m|^{15/8}} \qquad \eta(m,h) = \frac{m}{|h|^{8/15}} \tag{3.193}$$

The scaling parameters were first met in a theoretical setting in the previous chapter on the lattice scaling theory. In the scaling field theory, the free energy near the critical point is given by

$$\begin{aligned} f(m,h) &= \frac{m^2}{8\pi}\log m^2 + |h|^{16/15}\Phi(\eta) \\ f(m,h) &= \frac{m^2}{8\pi}\log m^2 + m^2 G(\xi) \end{aligned} \tag{3.194}$$

where the choice of appropriate representation corresponds to the region under consideration; $G(\xi)$ for small ξ and $\Phi(\eta)$ in the limit $\xi\to\infty$. $G(\xi)$ is the preferred parameterisation for the region we are considering, as we operate in a region where ξ is small and the series representation for $G(\xi)$ is convergent. This region is along the renormalisation flow from the Onsager critical point to the Yang-Lee critical point located at $i\xi_0 = i0.18935060551(3)$, estimated in this work and in [31] as $i0.18930(5)$.

The scaling function $G(\xi)$ is piecewise defined

$$G(\xi) = \begin{cases} G_{\text{high}}(\xi) & m<0 \\ G_{\text{low}}(\xi) & m>0 \end{cases} \qquad G(0) = G_{\text{high}}(0) = G_{\text{low}}(0) = 0 \tag{3.195}$$

with separate functions to describe the behaviour in the two regions, each corresponding to the *high temperature* and *low temperature* regions in the lattice Ising model. This split reflects the broken symmetry in the magnetism observed in the lattice eq. (2.15) for $\tau>0$ and $\tau<0$. The work of Fonseca and Zamolodchikov [31] explored the analytic continuation of both functions to the complex plane, making their work a suitable framework for studying the region near the Yang-Lee singularity, which is purely imaginary.

The high temperature scaling function G_{high}—reflecting the lattice H symmetry—is expressed as an even function of ξ around 0

$$G_{\text{high}}(\xi) = G_2\xi^2 + G_4\xi^4 + G_6\xi^6 + \dots \tag{3.196}$$

and is thus real for pure imaginary ξ. The lowest order term, G_2, is known as an integral representation [8]. Estimates for the next terms have been numerically generated in [31, 47, 48, 20, 8]

	Ref. [31]	Ref. [48]	Ref. [47]	Ref. [8]
G_2	-1.8452283	-1.84522807823(1)	-1.8452280782328(2)	-1.845228078232...
G_4	8.33410	8.3337117508(1)	8.333711750(5)	—
G_6	-95.1884	-95.16897(3)	-95.16896(1)	—
G_8	1458.21	1457.8(2)	1457.62(3)	—
G_{10}	-25889	—	-25891(2)	—
G_{12}	5.02×10^5	—	—	—
G_{14}	-1.04×10^7	—	—	—

The Yang-Lee singularity determines the radius of convergence for the series expansion for G_{high}.

The low temperature scaling function, G_{low}, is not studied in this work, but it is given as a series expansion (which is neither even nor odd)

$$G_{\text{low}}(\xi) = \tilde{G}_1\xi + \tilde{G}_2\xi^2 + \tilde{G}_3\xi^3 + \dots \tag{3.197}$$

and coefficients estimated in [31, 47, 48, 8]

	Ref. [31]	Ref. [48]	Ref. [47]	Ref. [8]
$\tilde{G}_1$	-1.35783835	-1.357838341706595(2)	-1.3578383417066(1)	-1.35783834170659...
$\tilde{G}_2$	-0.0489589	-0.048953289720(2)	-0.048953289720(1)	-0.048953289720...
$\tilde{G}_3$	0.0388954	0.0388639290(1)	0.038863932(3)	—
$\tilde{G}_4$	-0.0685060	-0.068362121(1)	-0.068362119(2)	—
$\tilde{G}_5$	0.18453	0.18388371(1)	0.18388370(1)	—
$\tilde{G}_6$	-0.66215	-0.659170(1)	-0.6591714(1)	—
$\tilde{G}_7$	2.952	2.93763(2)	2.937665(3)	—
$\tilde{G}_8$	-15.69	-15.57(2)	-15.61(1)	—

The lowest order term is known exactly [51]

$$\tilde{G}_1 = -2^{1/12}e^{1/8}\mathcal{A}^{3/2} = -1.357838341706595\dots \tag{3.198}$$

where $\mathcal{A} = 1.282427\dots$ is the Glaisher constant. Similarly to the high temperature case, the coefficient $\tilde{G}_2$ has an integral representation [8].

Tackling the problem from the other side, however, we can construct the Yang-Lee QFT by perturbing the Yang-Lee CFT by the relevant primary field

$$\mathcal{H}_{\text{YL}} = \mathcal{H}_{c=-22/5} + \lambda_\phi \int \mathrm{d}^2x\ \phi(x) + \dots \tag{3.199}$$

From $m^{2-2\Delta}$, we see that the mass dimension of λ_ϕ is 12/5. The "..." here contains contributions from an infinite tower of irrelevant operators, the highest order being $T\bar{T}$.

It is assumed that the series expansion around the Yang-Lee singularity is of the form [31]

$$G_{\text{high}}(\xi) = \mathcal{G}_A(\xi) + (\xi_0^2 + \xi^2)^{5/6}\mathcal{G}_B(\xi) + (\xi_0^2 + \xi^2)^{5/3}\mathcal{G}_C(\xi) + \dots \tag{3.200}$$

with each of $\mathcal{G}_A, \mathcal{G}_B, \mathcal{G}_C, \dots$ being analytic functions at the singularity. The structure of this expansion is guided by the Yang-Lee edge exponent. In [29], Fisher showed that under a power law assumption for the density of zeroes for the partition function (ρ), around the Yang-Lee critical point (which is $\pm iH_0(\beta)$ in lattice variables and corresponds to $\pm i\xi_0 = \xi(\tau(\beta), \pm iH_0(\beta))$) the magnetisation has a similar power law behaviour. If we parameterise the deviation in the imaginary direction from the Yang-Lee critical point as the real variable $\mathfrak{h} \equiv \text{Im}(H) - H_0(\beta)$ then the density of zeroes has the form

$$\rho(\mathfrak{h}) \sim |\mathfrak{h}|^{1/\delta} \tag{3.201}$$

while the magnetic deviation $m \equiv M - M(\beta, iH_0)$ has the form

$$m \sim (H - iH_0(\beta))^{1/\delta} \tag{3.202}$$

The edge exponent $(1/\delta)$ can be determined by scaling arguments mentioned briefly in eq. (2.21). It has the form and value

$$\begin{aligned} \frac{1}{\delta} &= \frac{d - 2 + \eta}{d + 2 - \eta} \\ &= -\frac{1}{6} \end{aligned} \tag{3.203}$$

as $\eta = 2(\Delta + \bar{\Delta}) = -4/5$ for the Yang-Lee scaling theory. This implies that the magnetisation should observe branch points at $\pm iH_0(\beta)$ (and hence $\pm i\xi_0$). In the ξ-plane, a branch cut is made along $(i\xi_0, i\infty) \cup (-i\infty, -i\xi_0)$. This is called the *Yang-Lee edge*.

The ultimate goal of this work is to improve on the estimate of the Yang-Lee singularity. This is accomplished by combining data of the Ising susceptibility function from [56, 22] with data obtained through the CTMRG method. The relevance of the susceptibility is explained in the next chapter, as is the CTMRG method, and the final chapter recounts and analyses the results obtained.

CHAPTER 4

SUSCEPTIBILITY

> It has been written that the shortest and best way between two truths of the real domain often passes through the imaginary one.
>
> Jaques Hadamard

This work leverages the extended susceptibility data obtained in [56] by Orrick, Guttmann, Nickel and Perk for the square lattice and [22] by Chan, Guttmann, Nickel and Perk for the triangular lattice. In their work they developed a polynomial time algorithm for computing pair correlation functions, which in turn can be used to calculate the susceptibility. The polynomial time algorithm was used to generate terms over $\mathcal{O}(\tau^{300})$ which is well beyond what was utilised in this work, but allowed us to extend the free energy scaling ansatz dramatically.

4.1 OGNPC Susceptibility

The expectation value of an arbitrary operator O is defined as a weighted sum over states, with the weight of a state of energy E given by the Boltzmann probability density $P(E) = \frac{1}{\mathcal{Z}} e^{-\beta E}$

$$\langle O \rangle = \frac{1}{\mathcal{Z}} \sum_{\{\sigma\}} O e^{\mathcal{H}(\beta, H, \{\sigma\})} \tag{4.1}$$

With this, it is not too hard to show that the logarithmic derivative of the partition function and its derivative can be expressed as a sum of pairwise correlation functions evaluated over all

pairs of sites in the lattice

$$\begin{aligned}\chi(\beta, H) &\equiv \frac{\partial^2 \log \mathcal{Z}}{\partial H^2} \\ &= \frac{\partial}{\partial H}\left[\frac{\partial_H \mathcal{Z}}{\mathcal{Z}}\right] \\ &= \frac{\mathcal{Z}\partial_H^2 \mathcal{Z} - (\partial_H \mathcal{Z})^2}{\mathcal{Z}^2} \\ &= \sum_i^N \sum_j^N \langle \sigma_i \sigma_j \rangle - N^2 \langle \sigma_0 \rangle^2 \end{aligned} \tag{4.2}$$

The observation that derivatives of the partition function take the form of expectation values is why the partition function is so important in the first place, and equivalently is why studying correlation functions is so fruitful. With this reframing, we see that the difficulty of evaluating the susceptibility translates to the difficulty of evaluating the pair correlation functions $C(i,j) \equiv \langle \sigma_i \sigma_j \rangle$.

In the 80s, these correlation functions were shown be shown to satisfy a rather complicated set of nonlinear partial difference equation [40] and these difference equations (with some later simplifications) can be evaluated in polynomial time. The authors of [56] evaluated the difference equations—noting that a time complexity of $\mathcal{O}(N^6)$ was observed in practice—and efforts were made to reduce complexity. Even on machines that are two decades old, they reported being able to match series coefficients up to τ^{323}. They repeated their experiment a decade later [22] for the triangular / honeycomb lattices, obtaining terms of order τ^{2000}. The difference equations require correlation functions evaluated on the dual lattice, which is why these two lattices were studied simultaneously.

The partial difference equations are excellent for obtaining numerical results, but even more structure could be obtained by studying another theoretical framing. The susceptibility can be expressed as a determinant of Toeplitz matrices [51], and the elements of these matrices are given as integrals corresponding to hypergeometric functions. As we will explore in more detail below, hypergeometric function have an asymptotic expansion with a divergent logarithmic part and a regular part given in terms of the digamma function. Because of the presence of this logarithm term, the ONGP group in [56] conjectured that the structure of the $H = 0$ Ising susceptibility has the following form

$$\chi^{[x]}_{\text{ONGPC}}(\tau, 0) = C^{[x]}_{0,\pm} |\tau|^{-7/4} \mathcal{F}^{[x]}_{\pm}(\tau) + \sum_{q=0}^{\infty} \sum_{p=0}^{\lfloor \sqrt{q} \rfloor} \tilde{b}^{[x]}_{pq} \left(\log |\tau|\right)^p \tau^q \tag{4.3}$$

There are several prominent features of this proposal. First, even though the model has temperature symmetric terms in $|\tau|$, it also has phase dependent terms which behave differently in the ferromagnetic[1] ($\tau > 0$) and antiferromagnetic ($\tau < 0$) regions. This is encapsulated in the regular functions $\mathcal{F}_{\pm}(\tau)$, which, up to τ^2, has equal expansions for both lattice types. The divergence at τ^4 is because the irrelevant operators that contribute are non-rotationally invariant[2] [19], meaning they appear at order $\mathcal{O}(\tau^{4n})$ in the square lattice and order $\mathcal{O}(\tau^{6n})$ in the triangular lattice.

[1] We are adopting the language of [56] and subtly referring to ferromagnetism with respect to the critical point $T = T_c$, rather than the typical lattice ferromagnetism relative to $T = 0$, the latter of which determines whether energy states on the lattice are bounded from above or below.

[2] They have a non-zero value for conformal spin $s \equiv \Delta - \bar{\Delta}$ which means they transform non-trivially under the rotation operator $R \equiv i(\partial_z - \partial_{\bar{z}})$.

The second interesting thing of note is the presence of the logarithms. However, this form is actually to be expected, as we saw from studying logarithmic conformal field theory. Since the energy conformal family $[\epsilon]$ has conformal dimension 1 and the identity family $[I]$ has conformal dimension 0, the integer difference leads to degenerate solutions in the ODE associated with the four-point correlation functions. This degeneracy in the ODE solution is solved by the addition of linearly independent terms that take the form of logarithms.

The work by the ONGPC groups provided the coefficients for constructing series representations of $\mathcal{F}_{+}^{[x]}$ and $\tilde{b}_{pq}^{[x]}$ for both lattices in the paper directly to order $\sim \tau^{14}$, $\log[\tau]^3$ for the square and $\log[\tau]^5$ for the triangular lattice, and also to significantly higher order ($\sim \tau^{2000}$) in the source code [21] on the Arχiv repository. The source code coefficients require further analysis to parse as they are given in their elliptic form, but only the paper values were necessary to match the accuracy of the data used in this work. We used this data to extend the scaling ansatz of the free energy density.

4.2 The Free Energy

The scaling ansatz of the Ising free energy density we use in this research is

$$f(\tau, H, \{u_j\}) = f_{\text{reg}}(\tau, H) + f_{\text{sing}}(m(\tau, H), h(\tau, H), \{u_j\}) + f_{\text{sub}}(\tau, H, \{u_j\}) \tag{4.4}$$

where the right-hand side includes the regular part of the free energy, the singular scaling part already discussed and subleading terms which are singular but not as severe as those in f_{sing}. We include the possibility of contributions from irrelevant operators $\{u_j\}$ in the non-analytic components of the free energy, but the operators are not classified in this work and henceforth explicit $\{u_j\}$ reference will be suppressed. Instead, the presence of the irrelevant operators manifests in the deviations of the free energy from scaling ansatz.

The scaling ansatz with only the leading singular and regular parts were used in previous work in the field [56, 48, 31, 47]. The subleading terms come directly from studying the susceptibility and are included to match the accuracy of the free energy data obtained from the CTMRG method. They are predicted by the logarithmic conformal field theory for $c = 1/2$.

We will first review some known results surrounding these expansions. We start by stating definitions and presenting known both known results and results derived in this work in order to keep. As the lattice free energy is symmetric under $H \to -H$, the free energy is given by a Taylor series in H^2 and τ dependence given as series expansions in τ and $\log \tau$.

The regular part of the free energy is relatively straightforward. It is just a Taylor series of non-universal regular functions

$$f_{\text{reg}}^{[x]}(\tau, H) = A^{[x]}(\tau) + H^2 B^{[x]}(\tau) + \mathcal{O}(H^4) \tag{4.5}$$

and has no singularities. The singular part (for $\tau > 0$) is given by

$$f_{\text{sing}}(m(\tau, H), h(\tau, H)) = \frac{m^2}{8\pi} \log|m^2| + m^2 G_{\text{high}}(\xi(m, h)) \tag{4.6}$$

where each term is

$$\begin{aligned} m(\tau, H) &= -C_\tau a(\tau) + \mu_h b(\tau) H^2 + \mathcal{O}(H^4) \\ h(\tau, H) &= C_H c(\tau) H + e_h d(\tau) H^3 + \mathcal{O}(H^5) \\ \xi(m, h) &= \frac{h}{|m|^{15/8}} \\ G_{\text{high}}(\xi) &= G_2 \xi^2 + G_4 \xi^4 + G_6 \xi^6 + \dots \end{aligned} \tag{4.7}$$

for $\tau < 0$ the scaling function is replaced with the function $G_{\text{low}}(\xi)$. The series $a(\tau)$ is normalised[3] to $\mathcal{O}(\tau)$ and the series $b(\tau), c(\tau), d(\tau)$ are all normalised to $1 + \mathcal{O}(\tau)$. The subleading part is

$$f_{\text{sub}}^{[x]}(\tau, H) = H^2 \tau^{-7/4} F^{[x]}(\tau) + H^2 \sum_{i=2} F_i^{[x]}(\tau) \log[\tau]^i + \mathcal{O}(H^4) \tag{4.8}$$

4.2.1 Singular Free Energy

The singular free energy reproduces to the Onsager solution for $H = 0$. This can be seen through $h(\tau, 0) = 0$ & $m(\tau, 0) \neq 0$ for $\tau \neq 0$ and $\xi(m, 0) = 0$ for $m \neq 0$. This kills off the second term, while the first term reduces exactly to the Onsager integral eq. (2.8).

The zero-field term in $m(\tau, H)$, $a(\tau)$, is known exactly in the square case and to arbitrary series order in the triangular case. The method for its evaluation is also detailed in [22] but with a few minor errors that are corrected here. First, we consider the zero field internal energy $\partial f / \partial \beta$ (which is known exactly from differentiating Onsager's solution as seen in [60]) and integrating with respect to τ. This is effectively just the continuous version of the change of basis formula from elementary linear algebra [5], or a change of variable formula in calculus. The internal energy according to [22] is

$$\begin{aligned} \frac{\partial f^{[\text{sq}]}}{\partial \beta} &= \coth(2\beta)(1 - \tau I(\tau)) \\ \frac{\partial f^{[\text{tr}]}}{\partial \beta} &= \frac{1+u}{1-u}\left(1 - \frac{3u-1}{2\left[u^3(1-u)^3(1+3u)\right]^{1/4}} I(\tau)\right) \end{aligned} \tag{4.9}$$

where u was introduced when defining the elliptic parameterisation variable k for the triangular lattice in eq. (2.3) ($u = e^{-4\beta}$). For both lattices the integral term I corresponds to an elliptic integral of the first kind

$$\begin{aligned} I(\tau) &= \frac{2}{\pi} \int_0^{\pi/2} \frac{1}{\sqrt{\tau^2 + \sin^2\theta}} \, \mathrm{d}\theta \\ &= \frac{2}{\pi\sqrt{1+\tau^2}} \mathrm{K}\left(\frac{1}{1+\tau^2}\right) \end{aligned} \tag{4.10}$$

where the elliptic integral K was seen in eq. (2.11)

$$\mathrm{K}(m) \equiv \int_0^{\pi/2} \frac{1}{\sqrt{1 - m\sin^2(\theta)}} \, \mathrm{d}\theta \tag{4.11}$$

Note that there are two plausible definitions for K, and the one used in [22] corresponds to $\mathrm{K}_{\text{Chan}}(k) \equiv \mathrm{K}(k^2)$. The distinction is due to whether the elliptic parameter (m) or elliptic modulus (k) is used to define the function ($m \equiv k^2$). The reason for my choice of definition is that it is the definition used within `Mathematica` (the main numeric tool in this work) and it has easier identification with Gauss hypergeometric function $\mathrm{K}(m) = \frac{\pi}{2} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; m\right)$ (hypergeometric functions, thankfully, have only one, unambiguous definition in terms of series).

Given the definition of $I(\tau)$, it is easy to verify that the integrand is singular over the region of integration for $\tau = 0$. This singularity is a logarithmic divergence. The nature of logarithmic

[3] Note that many references normalise to $1 + \mathcal{O}(\tau)$ by factoring an additional τ to eq. (4.7).

divergences is such that a simple Taylor series is not sufficient to describe it, and instead an asymptotic expansion is needed. There are some neat tricks that can be played (see, for example, [80, 1, 4]) where one can split the hypergeometric functions into a logarithmic term and a regular part. The regular part is given in terms of the digamma function ($\digamma(x) \equiv \Gamma'(x)/\Gamma(x)$), which is an entire function with a singularity only at $x = \infty$ (by Liouville's theorem). This representation is very desirable for our purposes, as it matches the scaling ansatz for the free energy eq. (4.4) as having a regular part and a logarithmic singular part. Explicitly, the identity has the form (noting $1 - \frac{1}{1+\tau^2} = \frac{\tau^2}{1+\tau^2}$)

$$
\begin{aligned}
{}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{1+\tau^2}\right) = \frac{1}{\pi}\sum_{m=0}^{\infty}\left(\frac{\tau^2}{1+\tau^2}\right)^m\left(\frac{\left(\frac{1}{2}\right)_m}{m!}\right)^2 \\
\times\left[-\log\left(\frac{\tau^2}{1+\tau^2}\right)+2\digamma(1+m)-2\digamma\left(\frac{1}{2}+m\right)\right]
\end{aligned}
\tag{4.12}
$$

with $(a)_m$ the Pochhammer falling factorial. With this, we can split $I(\tau)$ into singular and regular parts

$$
\begin{aligned}
I(\tau) &= I_{\text{sing}}(\tau) + I_{\text{reg}}(\tau) \\
I_{\text{sing}}(\tau) &= -\frac{2}{\pi\sqrt{1+\tau^2}}\log(\tau)\sum_{m=0}^{\infty}\left(\frac{\left(\frac{1}{2}\right)_m}{m!}\right)^2\left(\frac{\tau^2}{1+\tau^2}\right)^m \\
&= -\frac{2}{\pi}\log(\tau){}_2F_1\left(\frac{1}{2},\frac{1}{2};1;-\tau^2\right)
\end{aligned}
\tag{4.13}
$$

where the hypergeometric simplification is known as a *Plaff transformation*, and we drop the $\log(1+\tau^2)$ terms as they don't contribute to finding $a(\tau)$. We can now integrate this to compare against f_{sing}. For $H = 0$, we expect the form for the free energy from the series expansions to be[4]

$$
f(\tau,0) = \frac{C_\tau \tau^2 a(\tau)^2}{4\pi}\log[\tau] + \dots \tag{4.14}
$$

where for the purpose of identifying $a(\tau)$ we only really care about the coefficient of $\tau^2\log\tau$ from this expression. Integrating the internal energy with respect to τ we obtain[5]

$$
\begin{aligned}
f^{[x]}_{\text{sing}}(\tau,0) &= \int_0^\tau \frac{\partial f^{[x]}}{\partial\beta}\frac{\mathrm{d}\beta}{\mathrm{d}\tau'}\,\mathrm{d}\tau' && \text{(singular part only)} \\
&= -\frac{2}{\pi}\int_0^\tau \mathrm{d}\tau'\,\frac{\mathrm{d}\beta}{\mathrm{d}\tau'}C_I^{[x]}\log\tau' \times {}_2F_1\left(\frac{1}{2},\frac{1}{2};1;-\tau'^2\right)
\end{aligned}
\tag{4.15}
$$

where $C_I^{[x]}$ is the lattice-dependent coefficient of $I_{\text{sing}}(\tau)$ originating from eq. (4.10). Performing integration by parts: $\int \mathrm{d}u\, v = uv - \int u\,\mathrm{d}v$ with the identification $v = \log\tau$ gives

$$
f^{[x]}_{\text{sing}}(\tau,0) = -\frac{2}{\pi}\log\tau\int_0^\tau \mathrm{d}\tau'\,\frac{\mathrm{d}\beta}{\mathrm{d}\tau'}C_I^{[x]} \times {}_2F_1\left(\frac{1}{2},\frac{1}{2};1;-\tau'^2\right) \tag{4.16}
$$

[4]Note $\log m(\tau,0) = \log\tau + \log(C_\tau a(\tau))$.

[5]This integral effectively amounts to a change of variable formula for $f(\beta,0) \Rightarrow f(\tau,0)$.

where the term $\int \mathrm{d}u\, v$ contributes to the regular part and the boundary case of $\tau = 0$ vanishes due to the condition that the singular free energy should vanish at $\tau = 0$. This allows us to identify

$$C_\tau a^{[x]}(\tau) = \sqrt{\int_0^\tau \mathrm{d}\tau' \, \frac{\mathrm{d}\beta}{\mathrm{d}\tau'} C_I^{[x]} \times {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; -\tau'^2\right)} \tag{4.17}$$

and upon evaluation we find[6]

$$\begin{aligned} C_\tau^{[\mathrm{sq}]} &= \sqrt{2} \\ C_\tau^{[\mathrm{tr}]} &= 3^{3/4} \times 2^{-1/2} \end{aligned} \tag{4.18}$$

For the square lattice [22]

$$\begin{aligned} C_I^{[\mathrm{sq}]} \frac{\partial \beta^{[\mathrm{sq}]}}{\partial \tau} &= \tau \coth[2\beta] \frac{1}{\partial \tau / \partial \beta} \\ &= \frac{\tau}{\sqrt{1+\tau^2}} \end{aligned} \tag{4.19}$$

and for the triangular lattice [22]

$$\begin{aligned} C_I^{[\mathrm{tr}]} \frac{\partial \beta^{[\mathrm{tr}]}}{\partial \tau} &= \tau - \frac{\tau^3}{2} + \frac{97\tau^5}{256} - \frac{327\tau^7}{1024} + \dots \\ &= \sum_{n=0}^{\infty} c_n \tau^{2n+1} \end{aligned} \tag{4.20}$$

where the triangular coefficients can be calculated by the three term recursion relation

$$0 = \left(n^2 + n + \frac{2}{9}\right) c_n + \left(2n^2 - \frac{11}{18}\right) c_{n-1} + \left(n^2 - n - \frac{11}{18} - \frac{15}{144(n^2-n)}\right) c_{n-2} \tag{4.21}$$

For non-zero H, we use the results of [56, 22] to calculate $b(\tau)$. This was done by comparing their expression for $\chi(\tau, 0)$ against $\partial^2 f / \partial H^2$ and matching coefficients of $\log \tau$, which recursively featured coefficients of the $b(\tau)$ series. A similar technique was employed in [47, 48].

The series $c(\tau)$ can be derived readily from the zero-field magnetisation, which is known in the anti-ferromagnetic region and has a simple form in terms of the elliptic parameterisation

$$M^{[x]}(\tau, 0) = \begin{cases} (1 - k^{[x]}(\tau)^2)^{1/8} & \text{for } \tau < 0 \\ 0 & \text{for } \tau \geq 0 \end{cases} \tag{4.22}$$

where the elliptic parameter $k^{[x]}$ contains the factors which distinguish between lattices. Differentiating eq. (4.4) by τ at $H = 0$ and equating to eq. (4.22) we obtain the relation for the only terms surviving the differentiation

$$c^{[x]}(\tau) = \frac{M^{[x]}(\tau, 0)}{(-4a^{[x]}(\tau))^{1/8}} \tag{4.23}$$

[6]The definition of $C_\tau^{[\mathrm{tr}]}$ differs from [48] and is due to differing definitions of τ. The conversion between both conventions is detailed in eq. (6.8).

After substituting the appropriate lattice terms, $c(\tau)$ can effectively be obtained exactly. The constant coefficient of $c(\tau)$ is given by

$$\begin{aligned} C_h^{[\mathrm{sq}]} &= \frac{-2^{3/16}}{G_1} \\ C_h^{[\mathrm{tr}]} &= \frac{-2^{5/16} \times 3^{-3/32}}{G_1} \end{aligned} \tag{4.24}$$

The final regular function, $d(\tau)$, is not known very precisely. It is estimated only to constant order in [48, 18]

$$\begin{aligned} d^{[\mathrm{sq}]}(\tau) &= -0.00728 + \mathcal{O}(\tau) \\ d^{[\mathrm{tr}]}(\tau) &= 0.00129 + \mathcal{O}(\tau) \end{aligned} \tag{4.25}$$

The imprecision in this variable dictated much of the considerations for the region of (τ, H) parameter space that was explored. Care was taken to suppress contributions from this term but keep better known terms present. That is, τH^3 was made to be small enough to be less than the precision of our final results, but large enough to keep H^2 relevant for many orders in τ.

4.2.2 Regular Free Energy

The regular part of the zero-field free energy, $A(\tau)$, is slightly more involved. It is the same calculation as above, but done whilst keeping track of all the regular parts that were discarded. The explicit series for $A(\tau)$ is given below in eq. (6.6). We have

$$I_{\mathrm{reg}}(\tau) = \frac{2}{\pi} \sum_{m=0}^{\infty} \left(\frac{\left(\frac{1}{2}\right)_m}{m!} \right)^2 \left(\frac{\tau^2}{1+\tau^2} \right)^m \left[\digamma(1+m) - \digamma\left(\frac{1}{2} + m \right) \right] \tag{4.26}$$

and the regular contributions are

$$\begin{aligned} f_{\mathrm{reg}}^{[x]}(\tau, 0) &= \int_0^\tau \frac{\partial f^{[x]}}{\partial \beta} \frac{\mathrm{d}\beta}{\mathrm{d}\tau'} \, \mathrm{d}\tau' \, (\text{regular parts only}) \\ f_{\mathrm{reg}}^{[\mathrm{sq}]}(\tau, 0) &= \int_0^\tau \frac{\tau' + I_{\mathrm{reg}}(\tau')}{\sqrt{1+\tau'^2}} \, \mathrm{d}\tau' + \frac{2}{\pi} \int_0^\tau \mathrm{d}\tau' \, \frac{\tau}{\sqrt{1+\tau^2}} \frac{1}{\tau} \times {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; -\tau'^2 \right) \end{aligned} \tag{4.27}$$

The 2nd order term, $B(\tau)$, was determined by comparison with the susceptibility, detailed below. We did not consider H^4 terms or higher, as this was beyond the precision of our numerics.

4.2.3 Subleading Free Energy

The subleading terms we have included appear in the free energy at order H^2. These are non-analytic contributions due to logarithmic corrections in the theory. Being of order H^2, they do not contribute to the zero field magnetisation, but they do contribute to the zero-field susceptibility. The form for the subleading part is

$$f_{\mathrm{sub}}^{[x]}(\tau, H) = H^2 \tau^{-7/4} F^{[x]}(\tau) + H^2 \sum_{i=2}^{3} F_i^{[x]}(\tau) \log[\tau]^i + \mathcal{O}(H^4) \tag{4.28}$$

where $F(\tau), F_2(\tau), F_3(\tau), \ldots$ are all regular functions of τ with series representations where the leading term in $F_i(\tau)$ is of order $\mathcal{O}(\tau^{(i^2)})$. For the precision and range of τ used in this work, we only include logarithmic factors of order 2 and 3. The familiar power $\tau^{-7/4}$ is the Ising susceptibility critical exponent.

A notable exclusion from this expression is a term of the form $F_1(\tau)$. This was intentionally omitted as its contributions would be indistinguishable from $b(\tau)$ in the next stage of analysis, as we did not classify or analyse any of these irrelevant operators. This is a possible source of error for this method and an important limitation to be mindful of.

Lastly, one could also very readily use the coefficients in [22] to apply this scheme to the anti-ferromagnetic case. However, this regime was out of the scope of this work. As such, we will also be relaxed and drop the explicit $|\tau| \to \tau$ as $\tau > 0$ in the ferromagnetic region.

4.3 Susceptibility Comparison

In order to evaluate $b(\tau)$, $B(\tau)$ and $F_i(\tau)$, we first differentiate the scaling ansatz eq. (4.4) and evaluate at $H = 0$ (which is the same procedure in [47] but with more logarithm terms coming from $\partial^2 f_{\text{sub}}/\partial H^2$)

$$\partial_H^2 f(\tau, 0) = G_2 \left[C_\tau \tau a(\tau)\right]^{-7/4} c(\tau)^2 + 2B(\tau) - \frac{C_\tau \tau a(\tau) \mu_h b(\tau)}{2\pi} \left(1 + 2\log[C_\tau \tau a(\tau)]\right) + 2\tau^{-7/4} F(\tau) + 2\sum_{i=2}^{3} F_i^{[x]}(\tau) \log[\tau]^i \tag{4.29}$$

Recalling that $a(\tau)$, $c(\tau)$ and G_2 are already known exactly, this can be compared directly to the susceptibility expression given by the ONGPC group in eq. (4.3) to evaluate the missing terms.

In comparing series expansions, there are three main forms of τ that appear in the expansion: integer powers (τ^i), rational powers ($\tau^{-7/4+i}$) and logarithm terms ($\tau^i \log[\tau]^j$). Some terms correspond exactly to terms in ONGPC, for example $\tilde{b}_{23}$ and F_{23} both appear only as the coefficient of $\tau^2 \log[\tau]^3$. But many powers of τ feature coefficients from multiple series. For example, the coefficient of τ^4 is $(b_4 + B_4)$. There is enough freedom to uniquely determine the B series in terms of b, but not the (omitted) F_1 series.

We first start by noting that coefficients $b(\tau)$ are the only that appear next to $\log \tau$ (we arbitrarily set $F_1 = 0$, hoping to recover it later). Each power of τ features progressively more coefficients from b, but one can evaluate the lowest order terms $b_0, b_1, ...$ and then recursively evaluate higher terms through substitution. This uniquely defines $b(\tau)$. This would not uniquely define $b(\tau)$ if we did not exclude the lowest order logarithmic terms F_1 from the subleading free energy, as they would appear at this order.

With $b(\tau)$ series obtained, the integer τ terms now only contain b_i coefficients and B_i coefficients. These can be solved by substituting values for b just obtained. Similarly, the $\log[\tau]^j$ terms feature contributions from both b and F_j, and can be evaluated using the b values obtained.

4.4 Implementation Details

This process was performed programmatically in `Mathematica` by leveraging the `Series[]`, `CoefficientList[]` and `Solve[]` functions as well as some clever replacements to manipulate `Mathematica`.

The process begins with calculating the free energy derivative eq. (4.29) which has the form

$$\begin{aligned}\chi_1(\tau) &\equiv -\partial_H^2 f(\tau,0)\\ &= \sum_i X_i\tau^i + \tau^{-7/4}\sum_i Y_i\tau_i + \sum_{ij} Z_{ij}\tau^i\log[\tau]^j\end{aligned} \tag{4.30}$$

as well as the ONGPC susceptibility

$$\begin{aligned}\chi_2(\tau) &\equiv \chi_{\text{ONGPC}}(\tau,0)\\ &= \sum_i \tilde{X}_i\tau^i + \tau^{-7/4}\sum_i \tilde{Y}_i\tau_i + \sum_{ij} \tilde{Z}_{ij}\tau^i\log[\tau]^j\end{aligned} \tag{4.31}$$

The term X_i includes the unknown series coefficients from $b(\tau)$ and $B(\tau)$, Y_i includes terms from $F(\tau)$ and Z_{ij} includes both $b(\tau)$ and $F_{ij}(\tau)$. The difference $\chi_D = \chi_1 - \chi_2$ is then an asymptotic expansion in τ^i, $\tau^{-7/4}\tau^i$ and $\tau^i\log[\tau]^j$ with coefficients that form a system of equations. `Mathematica` can easily solve a system of equations using the built-in function `Solve[]`, but there were some manipulations necessary before it could recognise χ_D as a system of equations.

The goal was to separate out each power of $\tau^i\log[\tau]^j$ and τ^i into individual cells in a 2D array. Each column in the array would correspond to a unique power of $\log[\tau]^i$ and `Solve[]` could be run on each column to evaluate the coefficients. The order of evaluation was important, as many of the terms depend on the series coefficients from $b(\tau)$. The system of equations was of the form (with coefficients suppressed)

$$\begin{bmatrix} 1 & \tau^{-7/4} & \log[\tau] & \log[\tau]^2 & \log[\tau]^3 \\ \tau^1 & \tau\times\tau^{-7/4} & \tau\log[\tau] & \tau\log[\tau]^2 & \tau\log[\tau]^3 \\ \tau^2 & \tau^2\times\tau^{-7/4} & \tau^2\log[\tau] & \tau^2\log[\tau]^2 & \tau^2\log[\tau]^3 \\ \tau^3 & \tau^3\times\tau^{-7/4} & \tau^3\log[\tau] & \tau^3\log[\tau]^2 & \tau^3\log[\tau]^3 \\ & & \vdots & & \end{bmatrix} \tag{4.32}$$

Converting a series to a matrix of coefficients is readily accomplished with the `CoefficientList[]` function. However, this function requires a polynomial input. The asymptotic expansion with rational terms, negative powers and logarithms did not fit the bill. In order to trick `Mathematica` to accept χ_D, I first ran the replacement

$$\chi_D'(\tau) = \tau^{11/4}\chi_D(\tau) \tag{4.33}$$

in order to remove negative powers. The power $\tau^{7/4}$ could not be used as a multiplier as this would lead to the lowest order coefficients from multiple series mixing at the new constant order. Next, the replacement $\gamma^j \equiv \log[\tau]^j$ transformed the asymptotic expansion into a bivariate series,

$$\chi_D''(\tau,\gamma) = \tau^{11/4}\sum_i \tilde{\tilde{X}}_i\tau^i + \tau\sum_i \tilde{\tilde{Y}}_i\tau^i + \tau^{11/4}\sum_{ij} \tilde{\tilde{Z}}_{ij}\tau^i\gamma^j \tag{4.34}$$

and lastly the replacement $\tau \to \tau^4$

$$\chi_D'''(\tau,\gamma) \equiv \chi_D''(\tau^4,\gamma)$$

resulted in a polynomial which could be decomposed with `CoefficientList[]`. The final coefficient matrix was

$$\begin{bmatrix} \tau^{11} & \tau^4 & \gamma & \gamma^2 & \gamma^3 \\ \tau^4 \times \tau^{11} & \tau^4 \times \tau^4 & \tau^4 \times \tau^{11} \times \gamma & \tau^4 \times \tau^{11} \times \gamma^2 & \tau^4 \times \tau^{11} \times \gamma^3 \\ \tau^8 \times \tau^{11} & \tau^8 \times \tau^4 & \tau^8 \times \tau^{11} \times \gamma & \tau^8 \times \tau^{11} \times \gamma^2 & \tau^8 \times \tau^{11} \times \gamma^3 \\ \tau^{12} \times \tau^{11} & \tau^{12} \times \tau^4 & \tau^{12} \times \tau^{11} \times \gamma & \tau^{12} \times \tau^{11} \times \gamma^2 & \tau^{12} \times \tau^{11} \times \gamma^3 \\ & & \vdots & & \end{bmatrix} \tag{4.35}$$

The second column was recursively solved to find coefficients of the $b(\tau)$ series, which were in turn then used to solve the remaining series for $B(\tau), F_2(\tau), F_3(\tau)$ and $F_4(\tau)$.

The results of this section are collected in section 6.1. In the next chapter we detail the other main numerical algorithm of this thesis: the CTMRG algorithm, along with the relevant theoretical background.

CHAPTER 5

CORNER TRANSFER MATRIX RENORMALISATION GROUP

> In theory, theory and practice are the same. In practice, they are not.
>
> Albert Einstein

We will begin this chapter by recapping the well known transfer matrix method for the Ising model, which translates the thermodynamic problem of determining the partition function into one of eigenanalysis. An established solution for this method is the *free fermion* approach, which is obtained by exploiting an implicit quaternionic structure present in the model. This method solves the model exactly in the 1D case, but fails to be sufficient in the 2D case when a magnetic field is applied, as the quaternionic structure breaks down.

An alternative approach presents itself in Baxter's variational method, which takes a different approach to solving the eigenvalue problem. The variational method is an eigenvalue approximation method based on guessing the eigenvector of the largest eigenvalue and minimising around this to find the true largest eigenvector. Baxter uses a trial solution of a half-plane eigenvector based on the limiting behaviour of the eigenvector. Given that a half-plane divides the plane into equal partitions, this allows Baxter to once again apply the variational method on each half-plane. This produces the four titular corners of the *corner transfer matrices*. Analysis of these matrices is used to find the solution to the variational method.

The last section of this chapter describes how large corner transfer matrices (CTMs) can be well approximated by truncating eigenvalues. The size of each CTM grows exponentially with the number of rows in the lattice as the CTM is of size $2^N \times 2^N$. Increasing the rows and columns by 1 therefore doubles the number of eigenvalues. Baxter showed that these eigenvalues decay exponentially with distance away from the critical point, thus the vast majority of the information content is stored in the dominant few eigenvalues. This is the basis for the **Corner Transfer Matrix Renormalisation Group** algorithm by Nishino & Okunishi, which grows the CTM by doubling its size then truncates by deleting the smaller half of eigenvalues. This approximates the lattice of size $(N+1) \times (N+1)$ while keeping the size of the matrices static. This process loses minimal information content and is a very good approximation. These steps can be repeated to reasonably approximate lattices of order $N \sim 10^2 - 10^3$ on a consumer-grade computer.

5.1 1D Transfer Matrices

The transfer matrix method is ubiquitous for studying the partition function of the Ising model. In 1D the transfer matrix method solves the model, as the partition function calculation reduces to calculating the trace of a simple 2×2 matrix known as the **transfer matrix**

$$\begin{aligned} T_{\sigma_i\sigma_j} &= e^{\beta\sigma_i\sigma_j + H/2(\sigma_i+\sigma_j)} \\ &= \begin{pmatrix} e^{\beta+H} & e^{-\beta} \\ e^{-\beta} & e^{\beta-H} \end{pmatrix} \end{aligned} \tag{5.1}$$

Here we have symmetrised the linear contributions $H\sigma_i \to \frac{H}{2}(\sigma_i + \sigma_{i+1})$ and assumed periodic boundary conditions $\sigma_{N+1} \equiv \sigma_1$ for simplicity (boundary effects become unimportant in the thermodynamic limit). In terms of this transfer matrix the partition function can be expressed as

$$\begin{aligned} \mathcal{Z}_{\text{1D}} &= \sum_{\{\sigma\}} \prod_i e^{\beta\sigma_i\sigma_{i+1} + H/2(\sigma_i+\sigma_{i+1})} \\ &= \sum_{\{\sigma_1\}} \cdots \sum_{\{\sigma_N\}} T_{\sigma_1\sigma_2} \dots T_{\sigma_N\sigma_1} \\ &= \operatorname{Tr} T^N \\ &= \lambda_+^N + \lambda_-^N \\ &= \lambda_+^N \left(1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right) \\ &\sim \lambda_+^N \text{ as } N \to \infty \end{aligned} \tag{5.2}$$

In anticipation of generalising to the 2D case, we express the transfer matrix in terms of Pauli matrices [66, 60]

$$\begin{aligned} T &= \begin{pmatrix} e^{H/2} & 0 \\ 0 & e^{-H/2} \end{pmatrix} \begin{pmatrix} e^{\beta} & e^{-\beta} \\ e^{-\beta} & e^{\beta} \end{pmatrix} \begin{pmatrix} e^{H/2} & 0 \\ 0 & e^{-H/2} \end{pmatrix} \\ &= e^{H/2\mathbf{Z}} \left(\mathbf{I}e^{\beta} + \mathbf{X}e^{-\beta}\right) e^{H/2\mathbf{Z}} \end{aligned} \tag{5.3}$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{X}$ and $\mathbf{Z}$ are Pauli matrices

$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \mathbf{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \mathbf{Y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \mathbf{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{5.4}$$

The transfer matrix is traditionally factorised in terms of the following matrices

$$V_1 = \begin{pmatrix} e^{\beta} & e^{-\beta} \\ e^{-\beta} & e^{\beta} \end{pmatrix} \qquad V_2 = \begin{pmatrix} e^{H} & 0 \\ 0 & e^{-H} \end{pmatrix} \tag{5.5}$$

so that the transfer matrix has the symmetric form

$$T = V_2^{1/2} V_1 V_2^{1/2} \tag{5.6}$$

Note that V_2 is already diagonal and V_1 can be simplified by exploiting the dual lattice

$$\begin{aligned} V_1 &= \mathbf{I}e^{\beta} + \mathbf{X}e^{-\beta} \\ &= e^{\beta}\left(\mathbf{I} + \mathbf{X}e^{-2\beta}\right) \\ &= e^{\beta}\left(\mathbf{I} + \tanh\beta^*\mathbf{X}\right) \\ &= \frac{e^{\beta}}{\cosh\beta^*}e^{\beta^*\mathbf{X}} \\ &= \frac{1}{\sinh^{1/2}\beta^*\cosh^{1/2}\beta^*}e^{\beta^*\mathbf{X}} \\ &= (2\sinh 2\beta)^{1/2}e^{\beta^*\mathbf{X}} \end{aligned} \tag{5.7}$$

where β^* is the temperature of the dual lattice, defined by satisfying the relation $\tanh\beta^* = e^{-2\beta}$ (which equivalently is $\sinh 2\beta \sinh 2\beta^* = 1$). In step 4, we explicitly utilised the exponential of a hyperbolic quaternion. That is, given a hyperbolic quaternion $q = a + b\hat{\imath} + c\hat{\jmath} + d\hat{k} = a + \mathbf{v}$ where $\hat{\imath}^2 = \hat{\jmath}^2 = \hat{k}^2 = 1$ (instead of the usual -1, as this now matches the structure of the Pauli matrices $\mathbf{X}^2 = \mathbf{Y}^2 = \mathbf{Z}^2 = \mathbf{I}$), we can express the hyperbolic version of Euler's formula for quaternions

$$\begin{aligned} q &= \|q\|e^{\hat{v}\theta} \\ &= \|q\|\left(\cosh\theta + \hat{v}\sinh\theta\right) \end{aligned} \tag{5.8}$$

with $\hat{v} = \frac{\mathbf{v}}{\|v\|}$ the unit vector of $\mathbf{v}$ and θ is the hyperbolic angle given by $\cosh\theta = \frac{a}{\|q\|}$. We have also made use of the hyperbolic double-angle formula in step 5. The eigenvalues can be determined directly

$$\lambda_{\pm} = e^{\beta}\cosh H \pm \sqrt{e^{2\beta}\sinh^2 H + e^{-2\beta}} \tag{5.9}$$

so the partition function per site and the free energy are

$$\begin{aligned} \kappa_{1\mathrm{D}} &\equiv \mathcal{Z}_{1\mathrm{D}}^{1/N} \\ &= e^{\beta}\cosh H + \sqrt{e^{2\beta}\sinh^2 H + e^{-2\beta}} \\ -f_{1\mathrm{D}} &= \ln\kappa_{1\mathrm{D}} \end{aligned} \tag{5.10}$$

The unique properties 1D that allow for this direct solution is the fact that the transfer matrix has a static size and can be easily diagonalised. In fact, this feature is quite general, and often classical problems in 1D map to 0D quantum problems. This concept is known as the **classical-to-quantum correspondence**. The correspondence occurs at arbitrary dimension. There is a mapping between $(n+1)$-dimensional statistical physics and n-dimensional quantum physics by associating statistical transfer matrices and quantum operators.

In 2D, however, the scenario is not so simple. The original Onsager solution for $H = 0$ explicitly exploits the transfer matrix being a direct product of quaternionic algebras. The insolubility of the $H \neq 0$ regime can be pinned on the fact that T is no longer a simple product of Pauli matrices. In some sense, the parameter $H \neq 0$ can be seen as a parameterisation of the model deviating from a factorised quaternionic form, and this viewpoint helps to elucidate why a seemingly innocuous inclusion of the linear H term into the model breaks integrability.

5.2 2D Transfer Matrices

The approach taken in the 1D case falls short when applied to higher dimensional models as the transfer matrix method reduces the 2D statistical problem to a 1D quantum problem that still grows infinitely large in the thermodynamic limit. The quantum problem also has a complicated structure that is not easy to diagonalise in general. In 2D, the square partition function has the form

$$\mathcal{Z} = \sum_{\{\sigma\}} \exp\left[\beta \sum_i \sum_j \sigma_i^j \sigma_{i+1}^j + \sigma_i^j \sigma_i^{j+1} + H \sum_i \sum_j \sigma_i^j\right] \tag{5.11}$$

which has been split into vertical and horizontal interactions (rows are lower indices and columns are upper indices), with individual site contributions being symmetrised as in the 1D case and grouped (arbitrarily) with the horizontal summation. The generalisation of eq. (5.6) is constructed by considering two adjacent rows (the i^{th} and $(i+1)^{th}$ rows) across the lattice, and defining the appropriate transfer matrix analogue [66]

$$\begin{aligned} V_1 &= (2\sinh 2\beta)^{N/2} \exp\left(\beta^* \sum_i \mathbf{X}_j\right) \\ V_2 &= \exp\left(\beta \sum_i \mathbf{Z}_i \mathbf{Z}_{i+1}\right) \\ V_3 &= \exp\left(H \sum_j \mathbf{Z}_i\right) \end{aligned} \tag{5.12}$$

and

$$T = (V_2 V_3)^{1/2} V_1 (V_2 V_3)^{1/2} \tag{5.13}$$

such that the partition function is again expressed as a matrix trace

$$\begin{aligned} \mathcal{Z} &= \sum_{\{\boldsymbol{\sigma}\}} (T)_{\boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2} \cdots (T)_{\boldsymbol{\sigma}_N \boldsymbol{\sigma}_1} \\ &= \mathrm{Tr}\left[T^N\right] \\ &= \lambda_1^N \left(1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N + \ldots\right) \\ \kappa &\sim \lambda_1 \text{ as } N \to \infty \end{aligned} \tag{5.14}$$

The original and famous $H = 0$ solution produced by Onsager [55] then leverages the direct product and quaternionic structure of T and V to diagonalise them, ultimately leading to the solution eq. (2.8). One can consult [60] for a straightforward and complete re-derivation of this result with more modern notation.

As brilliant as Onsager's approach was, the same route cannot be exploited for $H \neq 0$ due to the lack of factorised quaternionic structure. Thus, alternate methods are required to study this regime.

5.3 Variational Principle — Square Lattice

As seen in eq. (5.14), the partition function can be written as the product of row transfer matrices

$$\begin{aligned} \mathcal{Z} &= \mathrm{Tr}\big[T^N\big] \\ &\sim \lambda_1^N \end{aligned} \tag{5.15}$$

Given that the transfer matrix T is symmetric (swapping rows and columns in the lattice has no overall effect), one can employ the *variational principle* to rephrase the calculation of an eigenvalue to a maximisation over eigenvectors. Although the search for an eigenvector is in general just as intractable as an eigenvalue one in the large scale limit, one can leverage physically motivated and symmetry arguments better in the context of eigenvectors over eigenvalues. For the Ising model, the variational principle leads to an exceptional approximation method utilising Corner Transfer Matrices, which are the method's namesake.

To state the variational principle, we first define the Rayleigh quotient of a symmetric matrix M with respect to an arbitrary vector $\mathbf{x}$

$$\mathcal{R}(M, \mathbf{x}) = \frac{\mathbf{x}^{\mathrm{T}} M \mathbf{x}}{\mathbf{x}^{\mathrm{T}} \mathbf{x}} \tag{5.16}$$

It is simple to show that $\mathcal{R}(M, \mathbf{x})$ is bounded between the largest and smallest eigenvalues of M. Since M is symmetric it has an orthogonal decomposition given by $D = P^{\mathrm{T}} M P$ with $P^{\mathrm{T}} P = I$. If the eigenvectors of M are given by the basis $\{\mathbf{v}_i\}$, then by setting $\mathbf{y} = P^{\mathrm{T}} \mathbf{x}$ we have

$$\begin{aligned} \frac{\mathbf{x}^{\mathrm{T}} M \mathbf{x}}{\mathbf{x}^{\mathrm{T}} \mathbf{x}} &= \frac{\mathbf{y}^{\mathrm{T}} P^{\mathrm{T}} M P \mathbf{y}}{\mathbf{y}^{\mathrm{T}} P^{\mathrm{T}} P \mathbf{y}} \\ &= \frac{\mathbf{y}^{\mathrm{T}} D \mathbf{y}}{\mathbf{y}^{\mathrm{T}} \mathbf{y}} \\ &= \frac{\sum_i \lambda_i y_i^2}{\sum_j y_j^2} \\ &= \sum_i \lambda_i \hat{y}_i^2 \end{aligned} \tag{5.17}$$

with the normalised quantities $\hat{y}_i^2 \equiv y_i^2 / \sum_j y_j^2$ and $0 \leq \hat{y}_i^2 \leq 1$. We see that the quantity on the RHS is therefore a weighted average of the eigenvalues of M. It equals the largest eigenvalue, λ_1, in the case where $\mathbf{y} = \mathbf{y}_1 \propto (1, 0, \ldots, 0)^{\mathrm{T}}$, meaning $\mathbf{x}_1 \propto \mathbf{v}_1$ is an eigenvector of M. This follows by examining

$$\begin{aligned} \frac{\mathbf{y}_1^{\mathrm{T}} D \mathbf{y}_1}{\mathbf{y}_1^{\mathrm{T}} \mathbf{y}_1} - \frac{\mathbf{y}^{\mathrm{T}} D \mathbf{y}}{\mathbf{y}^{\mathrm{T}} \mathbf{y}} &= \lambda_1 - \sum_i \lambda_i \hat{y}_i^2 \\ &= \sum_i (\lambda_1 - \lambda_i)\, \hat{y}_i^2 \\ &\geq 0 \end{aligned} \tag{5.18}$$

and similarly for the minimum eigenvalue. The variational principle thus states that $\mathcal{R}(M, \mathbf{x})$ is bounded between the largest (λ_1) and smallest (λ_N) eigenvalues, and by maximising (minimising) $\mathcal{R}(M, \mathbf{x})$ with respect to $\mathbf{x}$, one can therefore find the corresponding largest (smallest) eigenvalue.

It is summarised as

$$\lambda_1 = \max_{\substack{\mathbf{x}\in\Lambda(M)\\ \mathbf{x}\neq 0}} \frac{\mathbf{x}^{\mathrm{T}} M \mathbf{x}}{\mathbf{x}^{\mathrm{T}}\mathbf{x}} \tag{5.19}$$

where $\Lambda(M)$ is the spectrum of M and the maximisation is over all non-zero vectors $\mathbf{x}$.

It is important to note there is some nuance in applying this result to the complex Ising model studied in this work. The row transfer matrix in the Ising model is symmetric, so the result applies directly in the real case that Baxter studied. In the complex case however, the correct generalisation of Rayleigh quotient upgrades M to a Hermitian matrix, exchanges T for † and promotes P from orthogonal to unitary. This poses a potential problem, since T is not a Hermitian matrix (it remains symmetric) in the complex case, it is not unitarily diagonalisable and thus this modification does not necessarily apply. It is still somewhat possible to blindly apply the same result to a complex symmetric matrix, but for an arbitrary complex vector $\mathbf{y}$ since we no longer have $y_i^2 \geq 0$, we cannot interpret the RHS of eq. (5.17) as a weighted average. This means we cannot guarantee that the maximum eigenvalue corresponds to the maximal eigenvector using the same logic as above. However, in practice using the half-plane ansatz as the maximal eigenvector that Baxter proposes (discussed below) still converges rapidly to the maximal eigenvector, despite this theoretical hiccup. That is, vectors $\mathbf{x}$ for which $\mathcal{R}(M,\mathbf{x}) \geq \mathcal{R}(M,\mathbf{v}_1)$ (only possible in the complex case) are still somewhat "close" to $\mathbf{v}_1$.

While the variational principle can be a simplification in some cases, it is generally still difficult to maximise $\mathcal{R}(M,\mathbf{x})$ directly. Optimising the Rayleigh quotient involves finding a maximal eigenvector, which can be just as difficult as the original problem of finding the maximal eigenvalue. However, one can employ physical and symmetry arguments to describe an eigenvector more easily than one can for a scalar like an eigenvalue, so this reframing still has benefits.

It is typical in the variational method approach to reduce the scope of the search for optimal solutions by maximising over a subset of possible vectors, or by simply guessing a trial solution using symmetry arguments or otherwise. In Baxter's original work [11] he used the ansatz (and later justified) that the maximal eigenvector of T should be a half-plane, given as a product of pairwise operators over neighbouring spins in the lattice connected to T

$$\psi_{\boldsymbol{\sigma}} = \mathrm{Tr}[F(\sigma_1,\sigma_2)F(\sigma_2,\sigma_3)\dots F(\sigma_N,\sigma_1)] \tag{5.20}$$

with $\boldsymbol{\sigma} = (\sigma_1,\dots\,\sigma_n)$ being the vector of free spins along one row of T. The trace operation is used to match the periodic boundary conditions typically employed for convenience when studying the row transfer matrix method. The structure of $F(a,b)$ is not yet defined, but it will be defined by conditions induced by the variational principle. We do however impose a symmetry condition of the form $F(a,b)_{ij} = F(b,a)_{ji}$ which is also sometimes represented in the literature by $F^{\mathrm{T}}(a,b) = F(b,a)$ (which we note is a *slightly* ambiguous notation used in the literature and thus won't be used here) or $F(a,b)^{\mathrm{T}} = F(b,a)$ (which is less ambiguous and will be used). This is the only external restriction we place on F, and we do so in order to recursively apply the variational principle one additional time.

It is worth taking a moment to note the frequent abuse of mathematical terminology that is common in this subject (before we mostly disregard it). The quantities

$$C_\rho \quad C(a,b)_\mu \quad C_{ij} \quad C(a,b)_{kl} \tag{5.21}$$

are a 2^{2N+2} vector, a $2\times 2\times 2^{2N}$ tensor, a $2^{N+1}\times 2^{N+1}$ square matrix and a $2\times 2\times 2^N\times 2^N$ tensor respectively. By rearranging indices appropriately and keeping track of dimensions, the

same quantity can be represented equally by any of the three forms, and we will frequently switch between them depending on the demands of the calculation at hand. Even though strictly speaking the only matrix is the term C_{ij}, one almost always refers to $C(a)_{ij}$ as a matrix in the literature (even though it is more accurately a *set* of matrices, a.k.a. a tensor or an array). In this work, each of the different representations will be denoted through the use of concatenated indices. An example of these indices is

$$(i, a, j) \equiv (i_1, \ldots, i_N, a, j_1, \ldots, j_N) \tag{5.22}$$

and so on. In this case one can graphically interpret the indices (i, a, j) as forming a straight line along the lattice in the specified order.

In this work the roman letters $a, b, c, d, \ldots$ will be used to represent single spins, while the roman letters $i, j, k, l, m, \ldots$ are used to signify vectors of spins $i \equiv (i_1, i_2, \ldots, i_N)$. Greek letters $\mu, \nu, \rho, \ldots$ are used to signify a spin vector concatenated with an extra spin, so one can generally interpret $\mu = (a, i)$.

With this in mind, the tensor $F(a, b)_{ij}$ can be flattened a matrix $F_{(a,i)(b,j)}$, and the symmetry condition then corresponds to $F_{(a,i)(b,j)} = F_{(b,j)(a,i)}$, or even $F^{\mathrm{T}} = F$.

A heuristic understanding of the half-plane ansatz is presented in [11] which is paraphrased as follows. The effect of T on a half-plane is to add an extra row. Thus, given a half-plane ψ_N on a lattice of size N, we would expect $\psi_{N+1} \equiv T\psi_N$ to behave as $\psi_{N+1} \sim \psi_N$ in the large scale limit. The addition of a single extra row becomes increasingly insignificant for large N, as we would expect.

With this ansatz, the partition function per site can be found through the variational argument

$$\kappa = \mathcal{Z}^{1/N^2} \sim \lambda_1^{1/N} = \left(\frac{\psi^{\mathrm{T}} T \psi}{\psi^{\mathrm{T}} \psi}\right)^{1/N} \tag{5.23}$$

Analysing each of the components of the RHS, we can see

$$\begin{aligned}
\psi^{\mathrm{T}}\psi &= \sum_{\boldsymbol{\sigma}} \mathrm{Tr}[F(\sigma_1, \sigma_2) \ldots F(\sigma_N, \sigma_1)] \, \mathrm{Tr}[F(\sigma_N, \sigma_{N-1}) \ldots F(\sigma_1, \sigma_N)] \\
&= \sum_{\boldsymbol{\sigma}} \left[\sum_{\boldsymbol{\rho}} F(\sigma_1, \sigma_2)_{\rho_1\rho_2} \ldots F(\sigma_N, \sigma_1)_{\rho_N\rho_1}\right] \left[\sum_{\boldsymbol{\mu}} F(\sigma_N, \sigma_{N-1})_{\mu_N\mu_{N-1}} \ldots F(\sigma_1, \sigma_N)_{\mu_1\mu_N}\right] \\
&= \sum_{\boldsymbol{\sigma}} \sum_{\boldsymbol{\rho}} \sum_{\boldsymbol{\mu}} F(\sigma_1, \sigma_2)_{\rho_1\rho_2} F(\sigma_2, \sigma_1)_{\mu_2\mu_1} \ldots F(\sigma_N, \sigma_1)_{\rho_N\rho_1} F(\sigma_1, \sigma_N)_{\mu_1\mu_N}
\end{aligned} \tag{5.24}$$

where terms and summations have been rearranged as this is an index equation and not a matrix equation. We then group the terms sharing $\sigma_i\sigma_j$ indices and define the column transfer matrix by the tensor equation

$$\begin{aligned}
R_{(i,a,k),(j,b,l)} &\equiv F(a, b)_{(i,j)} F(b, a)_{(l,k)} \\
&= F(a, b)_{ij} F(b, a)_{lk}
\end{aligned} \tag{5.25}$$

with concatenated indices given by

$$\begin{aligned}
(i, a, k) &= (i_1, \ldots, i_N, a, k_1, \ldots, k_N) \\
(j, b, l) &= (j_1, \ldots, j_N, b, l_1, \ldots, l_N)
\end{aligned} \tag{5.26}$$

and so on. Note that since the spins i, a and k form a straight line along the lattice (and similarly for j, b and l) there is no matrix product between the F terms. This is strictly a tensor equation.

This auxiliary matrix means that we can recognise the product $\psi^{\mathrm{T}}\psi$ as a power of a matrix trace and employ eigenanalysis

$$\begin{aligned}\psi^{\mathrm{T}}\psi &= \mathrm{Tr}\big[R^N\big] \\ &= \xi_1^N\left(1+\left(\frac{\xi_2}{\xi_1}\right)^N+\dots\right) \\ \big(\psi^{\mathrm{T}}\psi\big)^{1/N} &\sim \xi_1 \text{ as } N\to\infty\end{aligned} \tag{5.27}$$

where $\{\xi_i\}$ are the eigenvalues of R. The same argument holds for analysing the term $\psi^{\mathrm{T}}T\psi$, which has the form

$$\begin{aligned}\psi^{\mathrm{T}}T\psi &= \mathrm{Tr}\big[S^N\big] \\ &= \eta_1^N\left(1+\left(\frac{\eta_2}{\eta_1}\right)^N+\dots\right) \\ (\psi^{\mathrm{T}}T\psi)^{1/N} &\sim \eta_1 \text{ as } N\to\infty\end{aligned} \tag{5.28}$$

with the matrix S defined from

$$\begin{aligned}S_{(i,a,c,k)(j,b,d,l)} &= w\begin{pmatrix}a & b\\ c & d\end{pmatrix}F(a,b)_{(i,j)}F(d,c)_{(l,k)} \\ &= w\begin{pmatrix}a & b\\ c & d\end{pmatrix}F(a,b)_{ij}F(d,c)_{lk}\end{aligned} \tag{5.29}$$

for similarly defined concatenated spin vectors as before, and eigenvalues $\{\eta_i\}$. The new w term comes from the additional face included from the row transfer matrix T when taking a slice across a column of the lattice formed by $\psi^{\mathrm{T}}T\psi$. One can readily define the row transfer matrix as a product of adjacent w lattice faces

$$T\begin{pmatrix}\boldsymbol{\sigma}\\ \boldsymbol{\rho}\end{pmatrix} = w\begin{pmatrix}\sigma_1 & \sigma_2\\ \rho_1 & \rho_2\end{pmatrix}w\begin{pmatrix}\sigma_2 & \sigma_3\\ \rho_2 & \rho_3\end{pmatrix}\dots w\begin{pmatrix}\sigma_N & \sigma_1\\ \rho_N & \rho_1\end{pmatrix} \tag{5.30}$$

with

$$w\begin{pmatrix}a & b\\ c & d\end{pmatrix} = \exp\left\{\frac{\beta}{2}(ab+ac+bd+cd)+\frac{H}{4}(a+b+c+d)\right\} \tag{5.31}$$

This term is not arbitrary like F since it is defined from the lattice. In fact, $w\begin{pmatrix}a & b\\ c & d\end{pmatrix}$ is the most important transfer matrix in this study. It is called the Boltzmann matrix, and the whole partition function is generally given in terms of this transfer matrix.

$$\mathcal{Z} = \sum_{\{\sigma\}}\prod_{ij} w\begin{pmatrix}\sigma_i^j & \sigma_i^{j+1}\\ \sigma_{i+1}^j & \sigma_{i+1}^{j+1}\end{pmatrix} \tag{5.32}$$

In some sense, the Boltzmann matrix describes the "unit cell" of the lattice, and other lattices can be described by simply changing the definition of this matrix.

5.3.1 Recursive Variational Principle

As we have now transcribed the calculation of $\lambda_1^{1/N}$ into the eigenanalysis of η_1/ξ_1, we can again employ the same variational principle to each of $\eta \equiv \eta_1$ and $\xi \equiv \xi_1$, assuming that R and S are themselves symmetric. This assumption is true if F is symmetric, explaining the symmetry condition placed on F.

The variational principle applied to ξ gives

$$\begin{aligned}
\xi &= \frac{X^{\mathrm{T}} R X}{X^{\mathrm{T}} X} \\
&= \frac{\sum_{ab} \sum_{ijkl} X_{(k,a,i)} R_{(i,a,k)(j,b,l)} X_{(j,b,l)}}{\sum_a \sum_{ik} X_{(k,a,i)} X_{(i,a,k)}} \\
&= \frac{\sum_{ab} \sum_{ijkl} X(a)_{ki} F(a,b)_{ij} F(b,a)_{lk} X(b)_{jl}}{\sum_a \sum_{ik} X(a)_{ki} X(a)_{ik}} \\
&= \frac{\sum_{ab} \sum_{ijkl} X(a)_{ki} F(a,b)_{ij} X(b)_{jl} F(b,a)_{lk}}{\sum_a \sum_{ik} X(a)_{ki} X(a)_{ik}} \\
&= \frac{\sum_{ab} \mathrm{Tr}\{X(a)F(a,b)X(b)F(b,a)\}}{\sum_a \mathrm{Tr}\{X^2(a)\}}
\end{aligned} \tag{5.33}$$

and similarly for η

$$\begin{aligned}
\eta &= \frac{Y^{\mathrm{T}} S Y}{Y^{\mathrm{T}} Y} \\
&= \ \ldots \\
&= \frac{\sum_{abcd} w \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mathrm{Tr}\{Y(c,a)F(a,b)Y(b,d)F(d,c)\}}{\sum_{ac} \mathrm{Tr}\{Y(c,a)Y(a,c)\}}
\end{aligned} \tag{5.34}$$

where X and Y are the dominant eigenvectors of R and S respectively. We can rearrange the indices of the components slightly by defining

$$\begin{aligned}
X(a)_{(i,k)} &\equiv X_{(i,a,k)} & Y(a,b)_{(i,k)} &\equiv Y_{(i,a,b,k)} \\
R(a,b)_{(i,k)(j,l)} &\equiv R_{(i,a,b,k)(j,c,d,l)} & S(a,b)_{(i,k)(j,l)} &\equiv S_{(i,a,b,k)(j,c,d,l)}
\end{aligned} \tag{5.35}$$

This reshuffling amounts to representing the length 2^{2N+1} vector $X_{(i,a,j)}$ as a (2×2^{2N}) rectangular matrix $X(a)_{(i,j)}$, and so on.

The eigenvalue equation for the eigenpair (ξ, X) is given by

$$\begin{aligned}
\xi X_{(i,a,k)} &= \sum_b \sum_{jl} R_{(i,a,k)(j,b,l)} X_{(j,b,l)} \\
\Rightarrow \xi X(a)_{ik} &= \sum_b \sum_{jl} F(a,b)_{ij} F(b,a)_{lk} X(b)_{jl} \\
&= \sum_b \sum_{jl} F(a,b)_{ij} X(b)_{jl} F(b,a)_{lk} \\
&= \sum_b \left[F(a,b)X(b)F(b,a)\right]_{ik}
\end{aligned} \tag{5.36}$$

In purely matrix notation this equation reads

$$\xi X(a) = \sum_b F(a,b)X(b)F(b,a) \tag{5.37}$$

and we note that by premultiplying this equation by $X(a)$, taking a trace, and undergoing some slight algebraic manipulation one reobtains the original variational equation eq. (5.33). This means that eq. (5.37) equation can be used to garner some geometric intuition for the variational principle itself. Equation (5.37) is the direct result of the expected large scale behaviour of the lattice. For a large lattice where $N \sim N+1$, the addition of a single column to an already large half-plane is negligible and approximately generates another half-plane. The largest eigenvalue is a scaling ratio between the two half-planes, which are two transfer matrices with approximately the same entries just scaled by a factor ξ.

Similar analysis and interpretation holds for (η, Y), leading to

$$\eta Y(a,c) = \sum_{bd} w \begin{pmatrix} a & b \\ c & d \end{pmatrix} F(a,b)Y(b,d)F(d,c) \tag{5.38}$$

The eigenvalue equations eqs. (5.36) and (5.38) give conditions that help to define F, but do not do so uniquely. These conditions are all invariant under the scaling transformations

$$\begin{aligned} X(a) &\to \alpha X(a) \\ Y(a,b) &\to \beta Y(a,b) \end{aligned} \tag{5.39}$$

and also the paired similarity transforms

$$\begin{aligned} X(a) &\to P(a)^{\mathrm{T}} X(a) P(a) \\ Y(a,b) &\to P(a)^{\mathrm{T}} Y(a,b) P(b) \\ F(a,b) &\to P(a)^{\mathrm{T}} F(a,b) P(b) \end{aligned} \tag{5.40}$$

for orthogonal matrices $P(a)$.

Both of these invariance facts are important for the Corner Transfer Matrix Renormalisation Group algorithm (discussed below) which is the main technique used in this research. The first condition allows us to set the normalisation for the matrices (which the algorithm normalises each matrix by its leading eigenvalue to keep numbers within machine precision), and the second condition allows us to diagonalise the symmetric corner transfer matrices, which are symmetric matrices and generate orthogonal matrices $P(a)$.

5.3.2 Critical Point

To prove the assumption eq. (5.20) for the form of the half-plane eigenvector ψ, we need to show that the variation of κ with respect to ψ is zero, indicating a stationary point. ψ dependence can be transferred to F dependence, so we instead focus on showing

$$\frac{\partial \kappa}{\partial F} = 0 \tag{5.41}$$

This object is a scalar differentiated with respect to a tensor, which, according to the rules of matrix calculus, gives a tensor with the entries

$$\frac{\partial \kappa}{\partial F}(a,b)_{ij} = \frac{\partial \kappa}{\partial F(a,b)_{ij}} \tag{5.42}$$

Expressing $\kappa = \eta/\xi$, the stationary point is then given by

$$\begin{aligned} \frac{\partial}{\partial F}\left(\frac{\eta}{\xi}\right) = \frac{\eta'\xi - \eta\xi'}{\xi^2} = 0 \\ \Rightarrow \frac{\eta}{\xi} = \frac{\eta'}{\xi'} \end{aligned} \tag{5.43}$$

where $\eta' = \partial\eta/\partial F$ and $\xi' = \partial\xi/\partial F$ are both matrices, $1/\xi' = (\xi')^{-1}$ and there is an implied I matrix multiplying η/ξ.

Proving that F satisfies eq. (5.43) is an exercise in matrix calculus manipulations. To make life much easier, we first note that since X and Y are the maximal eigenvectors of R and S, which in turn depend on F, we have for free that $\partial X/\partial F = \partial Y/\partial F = 0$. This follows from the chain rule, noting that one solution of $\mathrm{d}g\left(f(x)\right)/\,\mathrm{d}x = 0$ is simply given by $\mathrm{d}f\,/\,\mathrm{d}x = 0$. Evoking our usual strategy of evaluating the easier of the two expressions (ξ') and then arguing by similarity for the other (η'), we get the following expression

$$\begin{aligned}
\frac{\partial\xi}{\partial F} &= \frac{\partial}{\partial F}\left[\frac{\sum_{ab}\mathrm{Tr}\{X(a)F(a,b)X(b)F(b,a)\}}{\sum_a \mathrm{Tr}\{X^2(a)\}}\right] \\
&= \frac{1}{\sum_a \mathrm{Tr}\{X(a)^2\}}\frac{\partial}{\partial F}\sum_{ab}\mathrm{Tr}\{X(a)F(a,b)X(b)F(b,a)\} \\
&= \frac{1}{\sum_a \mathrm{Tr}\{X(a)^2\}}\sum_{ab}\mathrm{Tr}\left\{X(a)\frac{\partial F(a,b)}{\partial F}X(b)F(b,a) + X(a)F(a,b)X(b)\frac{\partial F(b,a)}{\partial F}\right\} \\
&= \frac{2}{\sum_a \mathrm{Tr}\{X(a)^2\}}\sum_{ab}\mathrm{Tr}\left\{X(a)F(a,b)X(b)\frac{\partial F(b,a)}{\partial F}\right\} \qquad (5.44)
\end{aligned}$$

the last line follows from the linearity of the trace, the invariance of the trace under cyclic permutations and by a relabelling of the indices $a \leftrightarrow b$ for half of the equation to match the other half.

For this expression we now evoke

$$\frac{\partial F}{\partial F} \equiv \frac{\partial F(b,a)_{li}}{\partial F(c,d)_{nm}} = \delta_{bc}\delta_{ad}\delta_{ln}\delta_{im} \qquad (5.45)$$

which is the matrix derivative of a matrix with respect to itself. This expression is in slight contrast to the one used in [23], so I will take a brief moment to discuss this difference in the hopes of mitigating the propagation of the error.

The reference [23] (and others in the literature) uses a popular definition for the "symmetric matrix derivative" as seen in [41], which is

$$\frac{\mathrm{d}f(A)}{\mathrm{d}A} \overset{?!}{=} \frac{\partial f(A)}{\partial A} + \left[\frac{\partial f(A)}{\partial A}\right]^{\mathrm{T}} - \mathrm{diag}\left(\frac{\partial f(A)}{\partial A}\right) \qquad (5.46)$$

for a scalar function of a matrix, $f(A)$. This definition is incorrect. There have been recent studies and experiments conducted exploring the legitimacy and origin of this definition ([68, 24]), and the conclusion is that the definition can be rigorously be proven to be incorrect, and that the results obtained by this definition are consistently wrong. The standard definition for a matrix derivative is already true for symmetric matrices, and there is no need for inclusion of additional structure unless one expects to be working with intermediate asymmetric objects. One then can symmetrise by including the transpose term (but *not* the dubious diagonal term) and halving to force any intermediate asymmetric matrices to generate symmetric derivatives. For purely symmetric matrices that already satisfy the symmetry condition $A = \frac{1}{2}(A + A^{\mathrm{T}})$ there is no need for this consideration.

This is a minor error ultimately, as this merely leads to a prefactor which appears for both the numerator and denominator of our original calculation eq. (5.43) and promptly cancels. Thus, the end result is unaffected.

Carrying on with the correct matrix derivative definition, we have

$$\begin{aligned}
\frac{\partial \xi}{\partial F(c,d)_{nm}} &= \frac{2}{\sum_a \mathrm{Tr}\{X(a)^2\}} \sum_{ab} \sum_{ijkl} X(a)_{ij} F(a,b)_{jk} X(b)_{kl} \frac{\partial F(b,a)_{li}}{\partial F(c,d)_{nm}} \\
&= \frac{1}{\sum_a \mathrm{Tr}\{X(a)^2\}} \sum_{ab} \sum_{ijkl} X(a)_{ij} F(a,b)_{jk} X(b)_{kl} \left(\delta_{bc}\delta_{ad}\delta_{ln}\delta_{im}\right) \\
&= \frac{2}{\sum_a \mathrm{Tr}\{X(a)^2\}} \sum_{jk} X(d)_{mj} F(d,c)_{jk} X(c)_{kn} \\
&= \frac{2}{\sum_a \mathrm{Tr}\{X(a)^2\}} \left[\{X(d)F(d,c)X(c)\}^{\mathrm{T}}\right]_{mn} \\
&= \frac{2}{\sum_a \mathrm{Tr}\{X(a)^2\}} \left[(X(c)^{\mathrm{T}} F(d,c)^{\mathrm{T}} X(d)^{\mathrm{T}}\right]_{nm} \\
&= \frac{2}{\sum_a \mathrm{Tr}\{X(a)^2\}} \left[(X(c)F(c,d)X(d)\right]_{nm} \\
\Rightarrow \frac{\partial \xi}{\partial F(a,b)} &= 2\frac{X(a)F(a,b)X(b)}{\sum_c \mathrm{Tr}\{X(c)^2\}} \\
\sum_{ab} \mathrm{Tr}\left\{\frac{\partial \xi}{\partial F(a,b)}\right\} &= 2\frac{\sum_{ab} \mathrm{Tr}\{X(a)F(a,b)X(b)\}}{\sum_c \mathrm{Tr}\{X(c)^2\}}
\end{aligned} \tag{5.47}$$

which utilises the symmetry of the half plane $X(a)^{\mathrm{T}} = X(a)$ and the assumed symmetry of F. In the last two steps we standardise the indices and take its trace to reduce it to a scalar, in anticipation of a future manipulation.

A similar analysis holds for $\partial\eta/\partial F$, giving

$$\begin{aligned}
\frac{\partial \eta}{\partial F(a,b)} &= 2\frac{\sum_{cd} w \begin{pmatrix} a & b \\ c & d \end{pmatrix} Y(a,b)F(b,d)Y(d,c)}{\sum_{cd} \mathrm{Tr}\{Y(c,d)Y(d,c)\}} \\
\Rightarrow \sum_{ab} \mathrm{Tr}\left\{\frac{\partial \eta}{\partial F(a,b)}\right\} &= 2\frac{\sum_{abcd} w \begin{pmatrix} a & b \\ c & d \end{pmatrix} Y(a,b)F(b,d)Y(d,c)}{\sum_{cd} \mathrm{Tr}\{Y(c,d)Y(d,c)\}}
\end{aligned} \tag{5.48}$$

meaning the critical point of $\partial\kappa/\partial F = 0$ corresponds to

$$\begin{aligned}
\frac{\eta}{\xi} &= \frac{\eta'}{\xi'} \\
&= \frac{\sum_c \mathrm{Tr}\{X(c)^2\} \sum_{cd} w \begin{pmatrix} a & b \\ c & d \end{pmatrix} Y(a,b)F(b,d)Y(d,c)}{X(a)F(a,b)X(b) \sum_{cd} \mathrm{Tr}\{Y(c,d)Y(d,c)\}}
\end{aligned} \tag{5.49}$$

To solve this final equation, we now insert some geometric intuition into our discussion

5.3.3 Geometric Intuition

This is the point where one can finally physically interpret all the transfer matrices discussed so far. Up until this point, only ψ, T and w had physical, geometric descriptions given by the

lattice, and everything else had been a (mostly) arbitrary object related to the lattice through the variational principle and conditions derived from it. What we will now show is that if we interpret X, Y and F as transfer matrices in the plane, then the criteria of $\partial\kappa/\partial F = 0$ is satisfied, justifying such an interpretation.

We interpret F as a half-column (or half-row when symmetry permits) transfer matrix. The transfer matrix $X(a)$ is therefore interpreted as a vertical half-plane, and broken into two adjacent corners

$$X(a) = A(a)^2 \tag{5.50}$$

Y will similarly be a horizontal half-plane with an additional column. This can be constructed from two corners "sandwiching" a row F

$$Y(a,b) = A(a)F(a,b)A(b) \tag{5.51}$$

With the definitions, eq. (5.49) above can be simplified by invoking the eigenvalue equations eqs. (5.36) and (5.38). Specifically, for each of the four terms in eq. (5.49) we have for the two scalar terms

$$\sum_c \mathrm{Tr}\big\{X(c)^2\big\} = \sum_c \mathrm{Tr}\big\{A(c)^4\big\} \tag{5.52}$$

and

$$\begin{aligned}
\sum_{cd} \mathrm{Tr}\{Y(c,d)Y(d,c)\} &= \sum_{cd} \mathrm{Tr}\{A(c)F(c,d)A(d)A(d)F(d,c)A(c)\} \\
&= \sum_c \mathrm{Tr}\left\{ A(c)\left[\sum_d F(c,d)X(d)F(d,c)\right] A(c)\right\} \\
&= \sum_c \mathrm{Tr}\{A(c)\left[\xi X(c)\right] A(c)\} \\
&= \xi \sum_c \mathrm{Tr}\big\{A(c)^4\big\}
\end{aligned} \tag{5.53}$$

while the matrix terms give

$$\begin{aligned}
\sum_{cd} w \begin{pmatrix} a & b \\ c & d \end{pmatrix} Y(a,b)F(b,d)Y(d,c) &= \sum_{cd} w \begin{pmatrix} a & b \\ c & d \end{pmatrix} A(a)F(a,b)A(b)F(b,d)A(d)F(d,c)A(c) \\
&= A(a)\left[\sum_{cd} w \begin{pmatrix} a & b \\ c & d \end{pmatrix} F(a,b)Y(b,d)F(d,c)\right] A(c) \\
&= A(a)\left[\eta Y(a,c)\right] A(c) \\
&= \eta A(a)^2 F(a,c) A(c)^2
\end{aligned} \tag{5.54}$$

and

$$X(a)F(a,b)X(b) = A(a)^2 F(a,b) A(b)^2 \tag{5.55}$$

As suggested by the manipulations above, the LHS of eq. (5.49) is invariant under taking the trace, thus we can reduce the matrix equations to scalars by taking the trace over appropriate pairs of free variables. Alternatively one can interpret the denominator as the matrix inverse of the numerator. In either case, substituting all these terms back into eq. (5.49), the equation reduces to $\eta/\xi = \eta/\xi$, thus finally confirming that the choice of F as a half-column, A as a corner and X, Y as half-planes does indeed result in the maximal choice given by the variational principles.

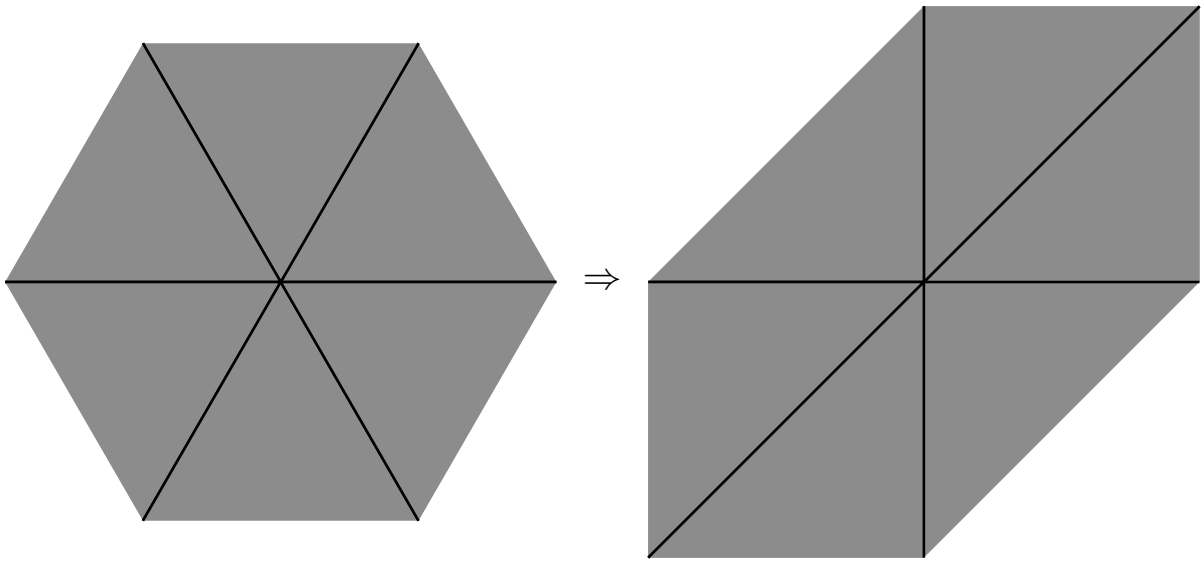


Figure 5.1: Mapping a 60° triangular lattice to a $90° - 45° - 45°$ lattice.

5.3.4 Partition Function Ratios

From the variational principle we have

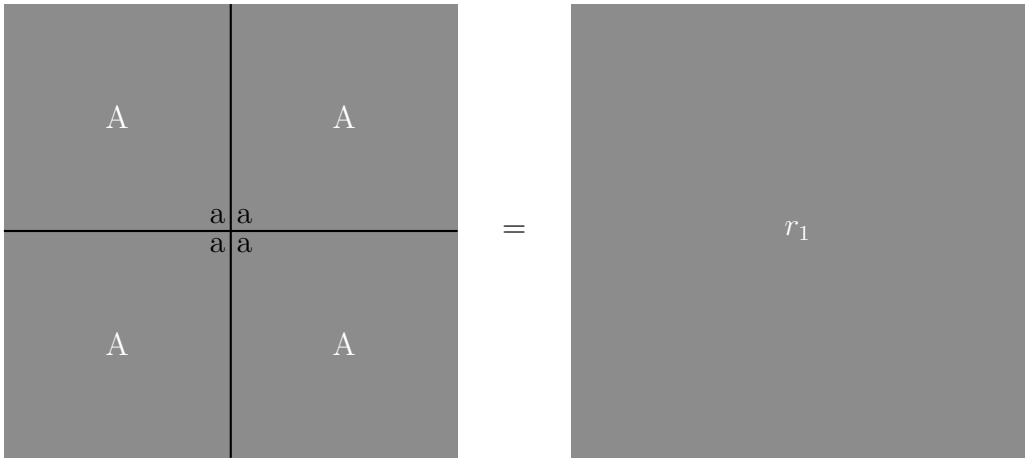
$$\begin{aligned} \frac{\eta}{\xi} &= \frac{Y^{\mathrm{T}} S Y}{Y^{\mathrm{T}} Y} \times \frac{X^{\mathrm{T}} X}{X^{\mathrm{T}} R X} \\ &= \frac{r_4 r_1}{r_2 r_3} \end{aligned} \tag{5.56}$$

Each of these terms has an interpretation with respect to partition functions of lattices of similar sizes. r_1 is the partition function of an $N \times N$ lattice, r_2 and r_3 are the partition functions of an $(N+1) \times N$ and $N \times (N+1)$ lattice respectively, while r_4 is a $(N+1) \times (N+1)$ lattice. They have a graphical representation, which is depicted in fig. 5.2. Each of these terms also correspond to the four terms in eq. (5.49) after taking the appropriate traces.

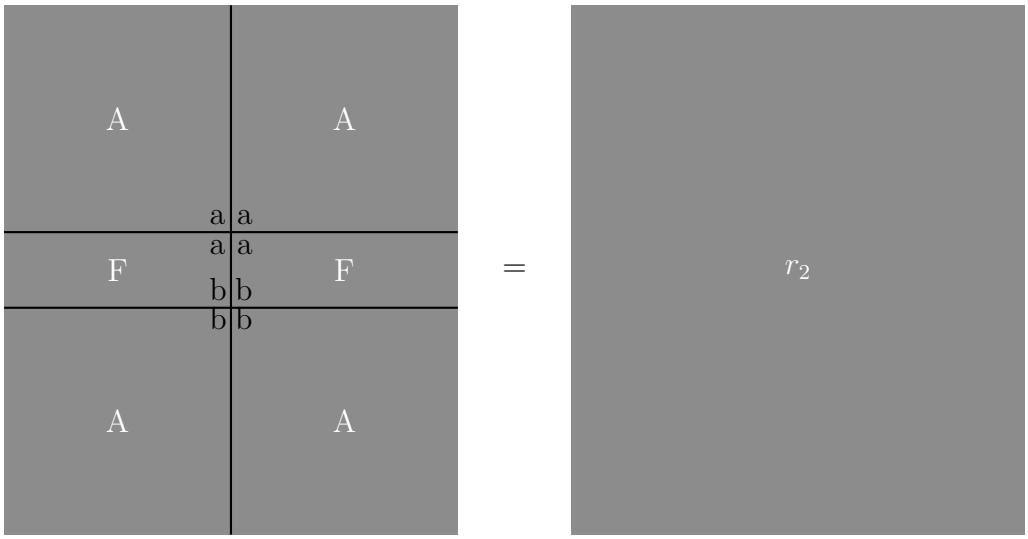
5.4 Variational Principle — Triangular Lattice

All the above arguments can be applied to the triangular lattice Ising model with slight modifications. In [10], Baxter and Tsang applied a generalised version of the variational principle to the Hard Hexagons problem, another statistical model with similar macro-level structure to the Ising model. The variational principle employed is identical to that used for the Ising model as only the difference between the two occurs in the explicit realisation of the transfer matrices F and A. The triangular variational method was similarly studied by Baxter again in [12] for the Chiral Potts model (a generalised Ising model) and for the Ising model explicitly by Malakis in [46].

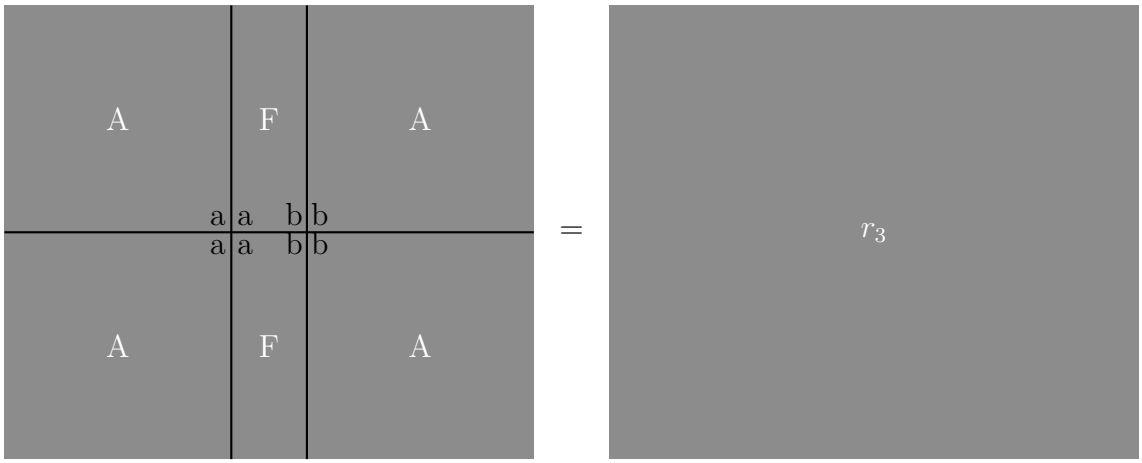
$$r_1 = \sum_a \mathrm{Tr}\{A(a)^4\} \tag{5.57}$$



$$r_2 = \sum_{ab} \mathrm{Tr}\big\{A(a)F(a,b)A(b)^2F(b,a)A(b)\big\} \tag{5.58}$$



$$r_3 = \sum_{ab} \mathrm{Tr}\big\{A(a)^2 F(a,b) A(b)^2 F(b,a)\big\} \tag{5.59}$$



$$r_4 = \sum_{abcd} w \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mathrm{Tr}\{A(a)F(a,c)A(c)F(c,d)A(d)F(d,b)A(b)F(b,a)\} \tag{5.60}$$

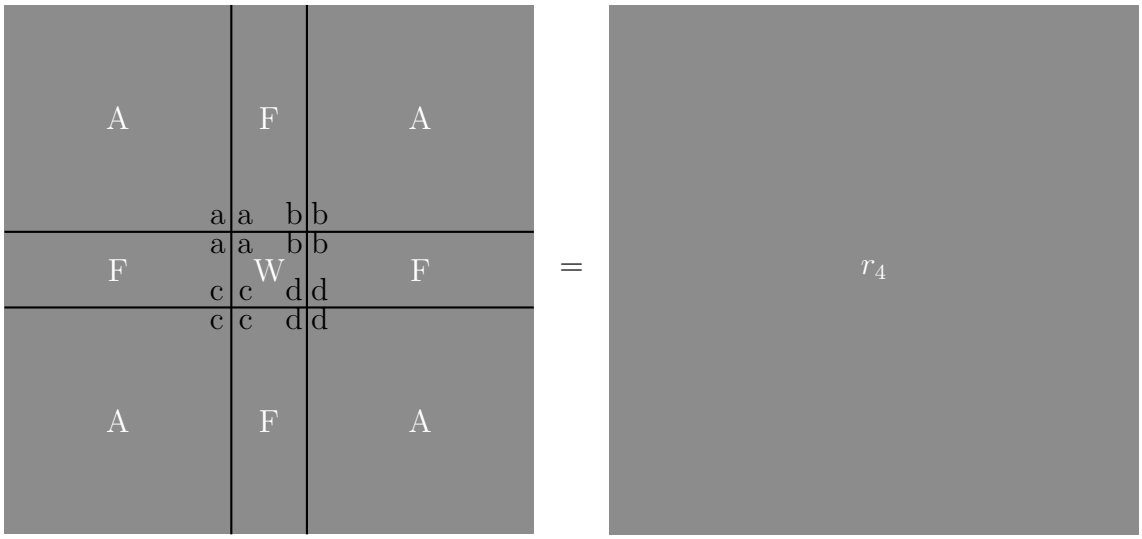


Figure 5.2: Square lattice partition functions.

There are two main ways to apply the variational principle in the triangular case that we will cover here. The first is the historical and exact approach employed by Baxter and others in the above references. The other approach is what is used in practice in this work which is to embed the triangular lattice inside a square lattice and apply the square principles above. Up to the boundary (seen in fig. 5.1), the embedded triangular lattice behaves as a square lattice with modified half-planes $X(a)$ and $Y(a,b)$, as well as partition function ratios.

This approach is not exact because due to the boundary, the resulting matrices are not symmetric. This means that the variational principle should not apply, but as we know the boundary becomes increasingly irrelevant in the large scale, we expect the variational principle to still converge to the desired result. The embedded triangular lattice is the preferred approach for this work as it is easier to implement, takes less additional theoretical development, and it is relatively easy to test against the square lattice for reference.

5.4.1 Baxter Triangulation

The first method is credited to Baxter and Tsang in [10]. In this paper, the authors developed a triangular version of the principle by defining appropriate corner and half-column transfer matrices. While the CTM A is the same as that used in this work (i.e. in the square-triangular method), the half-column is slightly different. We will denote Baxter's choice of half-column with the distinctive $\mathcal{F}$. Both definitions are equivalent, as one can define $\mathcal{F} = tFAF$ where t is a triangular unit cell (analogue of w), A is one of the six "corner" transfer matrices and F is a standard half-"column" transfer matrix.

The CTM $A(a)$ is now a triangular chunk of the lattice, shaped as a slice of cake that has been cut into 6 equal slices. As we saw in eq. (5.52)–(5.55) and eq. (5.56), it is entirely possible to derive the partition function per site ratio from the eigenvalue equations, so we will start the calculation from this point as Baxter does in [10]. The eigenvalue equations eqs. (5.36) and (5.38) have the corresponding triangular form

$$\xi A^4(a) = \sum_b \mathcal{F}(a,b)A(b)A(b)\mathcal{F}(b,a) \tag{5.61}$$

$$\eta A(a)\mathcal{F}(a,b)A(b) = \sum_c t\begin{pmatrix} & a & \\ b & & c \end{pmatrix} \mathcal{F}(a,c)A(c)\mathcal{F}(c,b) \tag{5.62}$$

with the three-site Boltzmann transfer matrix t defined as

$$t\begin{pmatrix} & a & \\ b & & c \end{pmatrix} = \exp\left\{\frac{\beta}{3}(ab+bc+ca) + \frac{H}{6}(a+b+c)\right\} \tag{5.63}$$

To isolate the eigenvalues in eqs. (5.61) and (5.62), we pre-multiply by the appropriate transfer matrices and perform traces as we did before

$$\begin{aligned}
\xi &= \frac{\sum_{ab} \operatorname{Tr} \mathcal{F}(a,b)A(b)A(b)\mathcal{F}(b,a)A(a)A(a)}{\sum_a \operatorname{Tr} A^6(a)} \\
&= \frac{r_2^*}{r_1^*} \\
\eta &= \frac{\sum_{abc} t\begin{pmatrix} & a & \\ b & & c \end{pmatrix} \mathcal{F}(a,b)A(b)\mathcal{F}(b,c)A(c)\mathcal{F}(c,a)A(a)}{\sum_{ab} \operatorname{Tr} \mathcal{F}(a,b)A(b)A(b)\mathcal{F}(b,a)A(a)A(a)} \\
&= \frac{r_4^*}{r_3^*}
\end{aligned} \tag{5.64}$$

These can be visualised in fig. 5.3, and similarly for the three other partition functions. The partition function per site is then given by

$$\begin{aligned}
\kappa^2 &= \frac{\eta^2}{\xi} \\
&= \frac{r_1^* r_4^{*2}}{r_2^* r_3^{*2}}
\end{aligned} \tag{5.65}$$

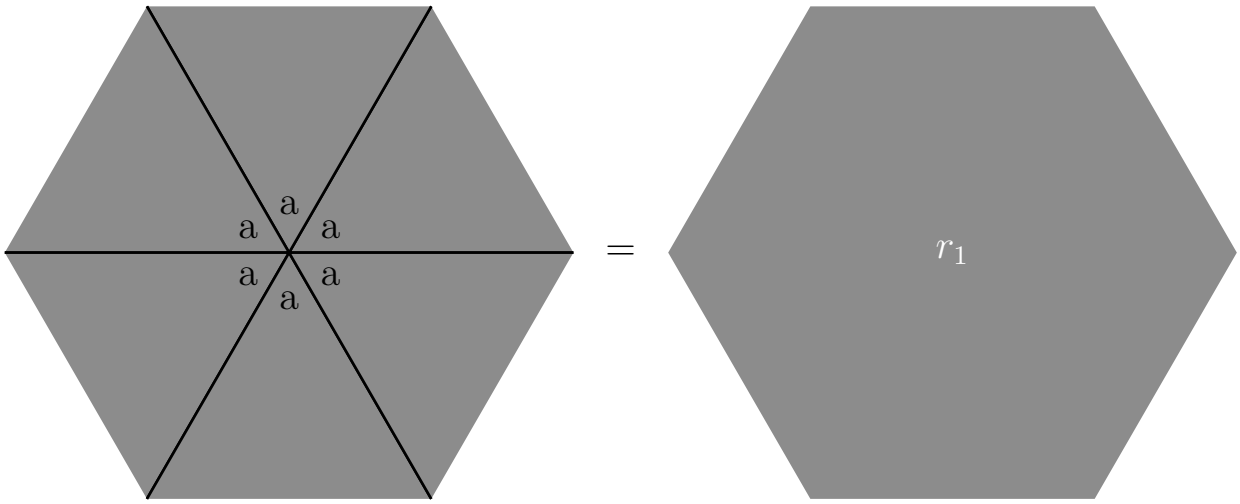


Figure 5.3: Triangular partition function ratio terms.

This is similar to the square case but with additional powers. These powers can be justified with a simple counting argument. For this argument, we choose to count faces instead of individual sites. The reasoning is that sites are shared between adjacent transfer matrices while faces are not, meaning there are no overcounting considerations to be made with faces.

If we suppose the number of faces in the CTM $A(a)$ is N, the number of faces in the HRTM $\mathcal{F}(a,b)$ is n and the number of faces in $t(a,b,c)$ is 1, then we can express the large-scale limit in terms of these values[1]. In the large site limit when the CTMs have stabilised, we expect that each site in the CTMs to contribute roughly κ to the overall partition function trace, so roughly speaking we expect $A \sim \kappa^N$, $\mathcal{F} \sim \kappa^n$ and $t \sim \kappa$. This in turn means that each partition functions featured in the ratios each scales as

$$\begin{aligned} r_1^* &\sim \kappa^{6N} \\ r_2^* = r_3^* &\sim \kappa^{4N+2n} \\ r_4^* &\sim \kappa^{3N+3n+1} \end{aligned} \tag{5.66}$$

Putting these all together

$$\begin{aligned} \frac{r_1^* r_4^{*2}}{r_2^* r_3^{*2}} &\sim \frac{\kappa^{6N}\kappa^{6N+6n+2}}{\kappa^{4N+2n}\kappa^{8N+4n}} \\ &\sim \kappa^2 \end{aligned} \tag{5.67}$$

gives the desired result. Clearly, setting the power of η to 1 to mimic the square case would not result in this cancellation, and the denominator would then out scale the numerator, making the result converge to 0.

5.4.2 Embedded Triangular Lattice

The preferred realisation is the embedded triangle approach, which is detailed by Dudalev in [26]. This case is depicted in fig. 5.4 as a right-angled triangular lattice. The main modification

[1] Of course, it is possible to write n as a function of N, but for this analysis such a level of granularity is unnecessary.

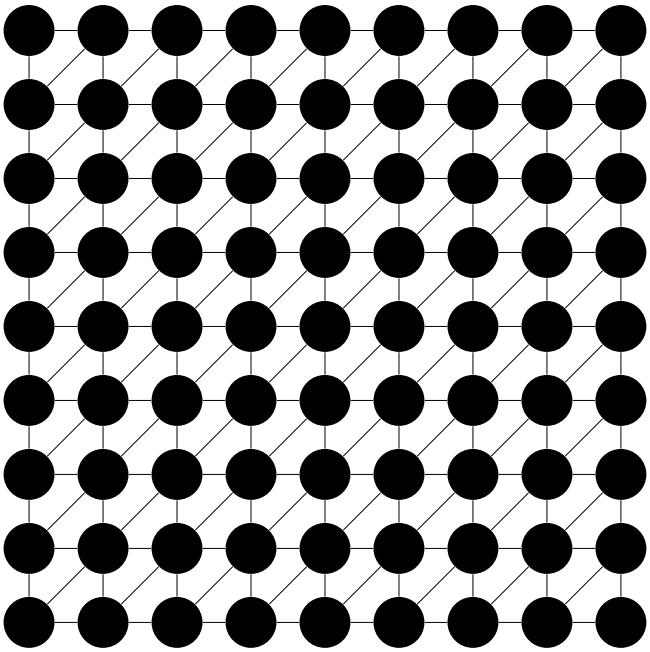


Figure 5.4: Triangular lattice embedded in a square lattice.

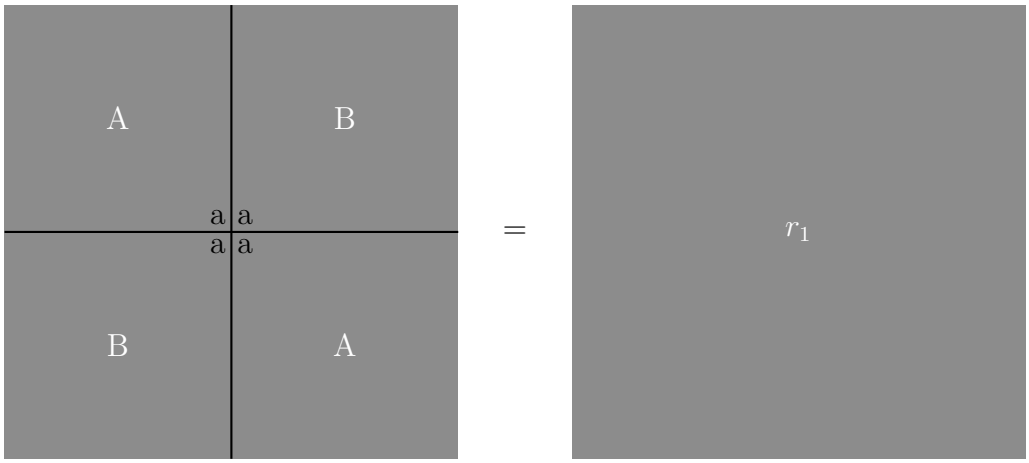
needed is to introduce an additional type of corner matrix $B(a)$ for the off-diagonal corners, along with the **half-row transfer matrix** $G(a,b) = F(a,b)^{\mathrm{T}}$. These additions require the new definitions

$$\begin{aligned} X(a) &= A(a)B(a) & X(a)^{\mathrm{T}} &= B(a)A(a) \\ Y(a,b) &= A(a)G(a,b)B(b) & Y(a,b)^{\mathrm{T}} &= B(a)F(a,b)A(b) \end{aligned} \tag{5.68}$$

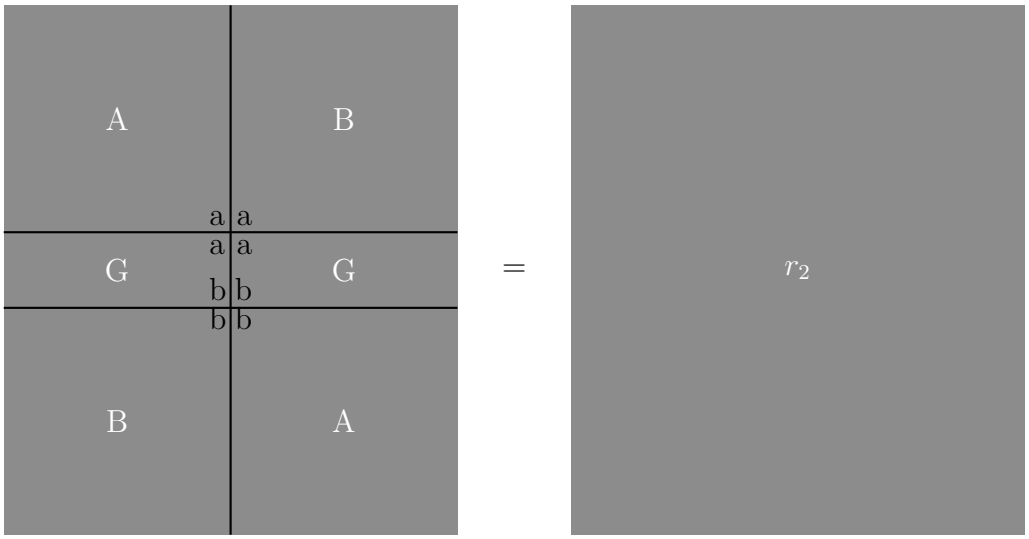
noting that A and B are themselves both symmetric but do not necessarily commute due to boundary effects. For large N when the boundary is unimportant, $B \approx A^2$. We also introduce the modified partition function ratios in fig. 5.5. These generalisations reduce back to the square definitions in fig. 5.2 since $X = X_{[\mathrm{sq}]}^{\mathrm{T}}$ and $Y = Y_{[\mathrm{sq}]}^{\mathrm{T}}$.

With the square and triangular variational theory established, the next step is to explicitly characterise the TMs. This chapter then concludes with an explanation of the corner transfer matrix renormalisation group algorithm.

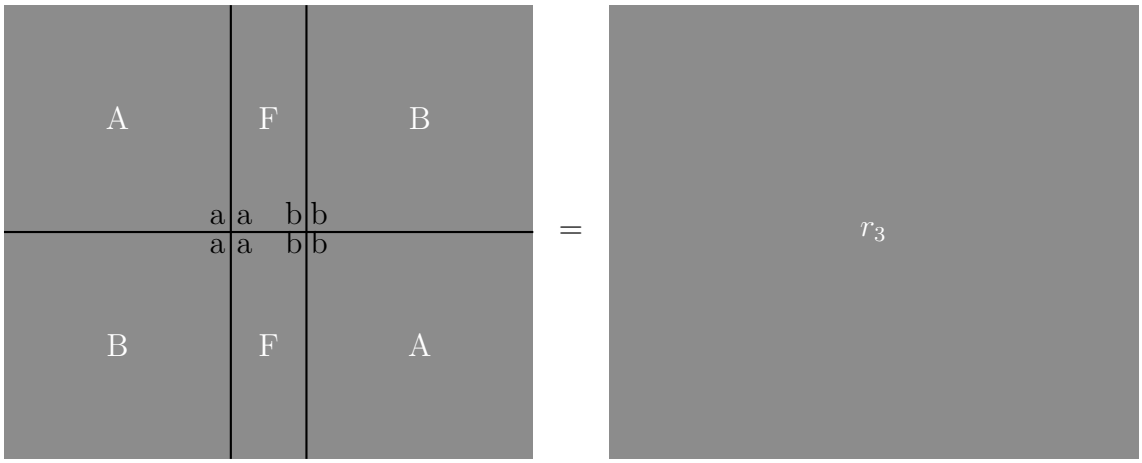
$$r_1^{[\mathrm{tr}]} = \sum_a \mathrm{Tr}[A(a)B(a)A(a)B(a)] \tag{5.69}$$



$$r_2^{[\mathrm{tr}]} = \sum_{a,b} \mathrm{Tr}[A(a)G(a,b)B(b)A(b)G(b,a)B(b)] \tag{5.70}$$



$$r_3^{[\mathrm{tr}]} = \sum_{a,b} \mathrm{Tr}[A(a)B(a)F(a,b)A(b)B(b)F(b,a)] \tag{5.71}$$



$$r_4^{[\mathrm{tr}]} = \sum_{abcd} w(a,b,c,d)\,\mathrm{Tr}\left[A(a)G(a,c)B(c)F(c,d)A(d)G(d,b)B(b)F(b,a)\right] \tag{5.72}$$

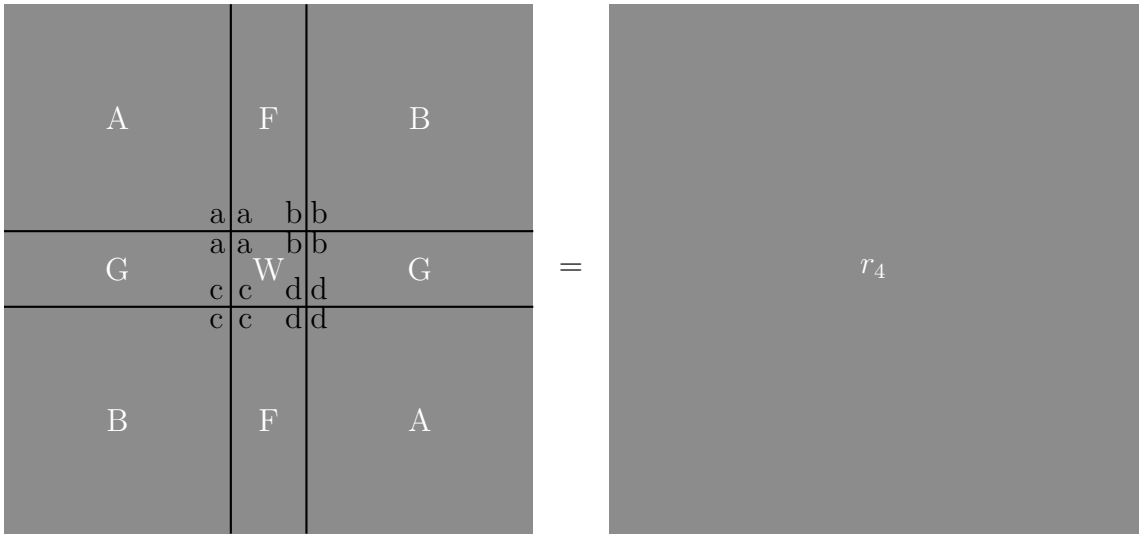


Figure 5.5: Square lattice partition functions.

5.5 Corner Transfer Matrices

In the 1960s, as part of developing the variational approach, Baxter created an alternative to the row or column transfer matrices: the **Corner Transfer Matrices** (CTM). We saw that this object emerged naturally as a result from the variational analysis. While the traditional row transfer matrix method partitions the lattice into N rows, the corner transfer matrix splits the lattice into four partitions of equal size. A numerical advantage of this is that while the number of row transfer matrices increases as the lattice increases in size, the number of corners remains fixed (4 for the square lattice, 6 for the triangular lattice). The size of all transfer matrices still grow exponentially, but as exploited by the CTMRG algorithm, the eigenvalues of the corner transfer matrices decay exponentially near the critical point and Yang-Lee singularity. This means that one can well-approximate CTMs by truncating the lower half of their eigenvalues. This property is leveraged by the algorithm to approximate the thermodynamic limit with finite memory.

5.5.1 Transfer Matrix Definitions

There are three major players in the CTM analysis. These are the *Boltzmann weight matrix*, w (which can be thought of as a **Single Face Transfer Matrix** [SFTM]), the **Corner Transfer Matrix** (CTM), A, and the **Half Column/Row Transfer Matrices** (HCTM / HRTM), F and G respectively.

Corner Transfer Matrix

The corner transfer matrix A is explicitly defined in the square case as

$$\begin{aligned} A(a)_{ij}^{[\mathrm{sq}]} = \; & \exp\left\{\frac{H}{4}a\right\}\times \\ & \exp\left\{\frac{\beta}{2}\left(ai^1 + i^1i^2 + \cdots + i^{N-1}i^N\right) + \frac{H}{2}\left(i^1 + \cdots + i^N\right)\right\}\times \\ & \exp\left\{\frac{\beta}{2}\left(aj_1 + j_1j_2 + \cdots + j_{N-1}j_N\right) + \frac{H}{2}\left(j_1 + \cdots + j_N\right)\right\}\times \\ & \sum_{k=0}^{2^{(N^2)}-1}\Bigg[\exp\left\{\beta\left(k_1^1k_2^1 + k_1^1k_1^2 + \cdots + k_{N-1}^Nk_{N-1}^N + k_N^{N-1}k_N^N\right)\right\}\times \\ & \exp\left\{H(k_1^1 + k_1^2 + k_2^1 + \cdots + k_N^N)\right\}\times \\ & \exp\left\{\beta\left(k_1^1i^1 + \cdots + k_1^Ni^N + k_1^1j_1 + \cdots + k_N^1j_N\right)\right\}\Bigg] \end{aligned} \tag{5.73}$$

which is graphically depicted in fig. 5.6. This expression is a partition function calculation with specific spins designated as free indices. The free indices for the matrix are the top-left corner (a index), the leftmost column (i index) and uppermost row (j index). These terms have their coupling parameters reduced ($H \to H/4, \beta \to \beta/2$) for overcounting reasons. For example, when computing the partition function r_1 in eq. (5.57), each of the four CTMs contribute $H/4$ to the centre spin while each pair of CTMs contribute $\beta/2$ along the cardinal seams. The remainder of the "fixed" spins are summed over with full weight as a standard partition function.

The embedded triangular case is similar but with two types of corners and an additional diagonal term per face. The embedded lattice approach keeps parity with the square case and

makes changing between each lattice much simpler. We have two types of CTM: CTMs along the lattice main diagonal (CTM type A with no diagonal couplings connecting to the free index a) and CTMs along the lattice anti-diagonal (CTM type B with couplings connecting to a). These are defined by adding diagonal couplings to each face of the square lattice via

$$\begin{aligned} A(a)_{ij}^{[\mathrm{tr}]} &= A(a)_{ij}^{[\mathrm{sq}]} \times \sum_{k=0}^{2^{(N^2)}-1} \exp\left\{\beta \sum_{\mu=0}^{N-1}\sum_{\nu=1}^{N} k_\mu^\nu k_{\mu+1}^{\nu-1}\right\} \\ B(a)_{ij}^{[\mathrm{tr}]} &= A(a)_{ij}^{[\mathrm{sq}]} \times \sum_{k=0}^{2^{(N^2)}-1} \exp\left\{\beta \sum_{\mu=0}^{N-1}\sum_{\nu=0}^{N-1} k_\mu^\nu k_{\mu+1}^{\nu+1}\right\} \end{aligned} \tag{5.74}$$

where for compactness we identify $k^0 \equiv i$, $k_0 \equiv j$ and $k_0^0 \equiv a$. Note that in the square case we simply have $B^{[\mathrm{sq}]} = A^{[\mathrm{sq}]}$. These are both depicted in figs. 5.7 and 5.8. All the additional terms added are full weight as these couplings aren't shared between multiple CTMs.

In both lattices, $i = (i^1, i^2, \ldots, i^N)$ is the shifted binary representation[2] of i with replacement $0 \to -1$ to coincide with the Ising spin variables. The variables j and k are similar, with k ranging over an $N \times N$ binary grid. The binary representation must use little-endian (the least-significant bit at the end) encoding on the free indices to ensure matrix operations are properly aligned with the lattice enumeration depicted in eq. (5.73). The i and j indices have the range $0 \leq i, j \leq 2^N - 1$ while k instead ranges over $0 \leq k \leq 2^{(N^2)} - 1$.

Each line in eq. (5.73) corresponds to a portion of the lattice partition function eq. (5.11). The first line is magnetic field term in the centre of the lattice (we always deal with odd-sized lattices of size $2N + 1$, so there is exactly 1 centre term). The second and third lines are the column and row interactions and are similarly weighted due to the fact that they are shared between neighbouring TMs. The first two lines of the summation over k corresponds exactly to a partition function of an $N \times N$ sized lattice, and the final line contains the remaining cross terms between the free indices (i, j) and the fixed index (k).

As a matrix, A is a $2 \times N \times N$ tensor which can be encoded in the diagonal block matrix

$$\mathbf{A} = \begin{pmatrix} A(0) & 0 \\ 0 & A(1) \end{pmatrix} \tag{5.75}$$

with diagonal entries $a = 0$ and $a = 1$ and zero matrices on the anti-diagonal.

While these definitions are relatively difficult to parse directly, there are very simple graphical interpretations available. In the square case, the CTM is fig. 5.6 and in the triangular case the matrices are figs. 5.6 to 5.8. The graphical representations have the advantage of being much easier to work with and connect to the tensor network approach for quantum many-body problems [57, 30].

The free index a corresponds to the spin in the centre of the lattice and the free indices i and j sum along the column and row respectively that connect to a. These free indices are used to combine CTMs together through computing matrix products. The index k is not a free index and instead iterates over internal spins that have been "summed over", forming a partition function for an $N \times N$ sublattice. The upper indices range across a column while the lower indices range over a row.

It is also worth noting that overall symmetry operations on the TMs do not affect their graphical representation. Symmetry operations such as rotations and reflections that leave the underlying matrix operations in the partition function calculations unchanged are permitted

[2]That is, for $N = 4$ and i equal to 7 for example, then $i = (i^1, i^2, i^3, i^4) = (-1, 1, 1, 1)$.

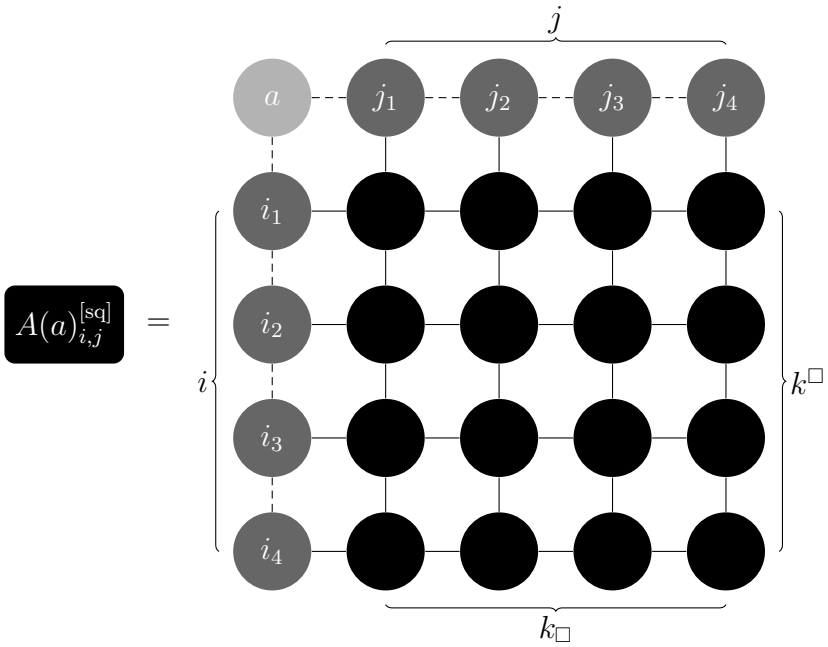


Figure 5.6: Square Corner Transfer Matrix $A(a)_{ij}$. The colouring scheme corresponds to the site weightings, with light grey denoting quarter contributions ($H/4$), dark grey being half contributions ($H/2$) and black being completely summed over (H). Dashed lines correspond to half contributions ($\beta/2$) and full lines are full contributions (β).

(eqs. (5.57) to (5.60)). CTMs can therefore be freely rotated (taking note of interacting free indices). Because of this, it is sometimes useful to rotate B by $3\pi/2$ to align with the free indices of A (as shown in fig. 5.9), and this property is implicitly used in the partition function ratios figs. 5.2 and 5.5.

Half-Column Transfer Matrix

The **Half-Column Transfer Matrix** (HCTM) F is explicitly defined in the square case as

$$\begin{aligned} F(a,b)^{[\mathrm{sq}]}_{ij} = \; & \exp\left\{\frac{H}{4}a + \frac{H}{4}b\right\}\times \\ & \exp\left\{\frac{\beta}{2}(ai^1 + i^1i^2 + \cdots + i^{N-1}i_N) + \frac{H}{2}(i^1 + \cdots + i^N)\right\}\times \\ & \exp\left\{\frac{\beta}{2}(aj^1 + j^1j^2 + \cdots + j^{N-1}j^N) + \frac{H}{2}(j^1 + \cdots + j^N)\right\} \end{aligned} \tag{5.76}$$

and has the graphical representation fig. 5.10.

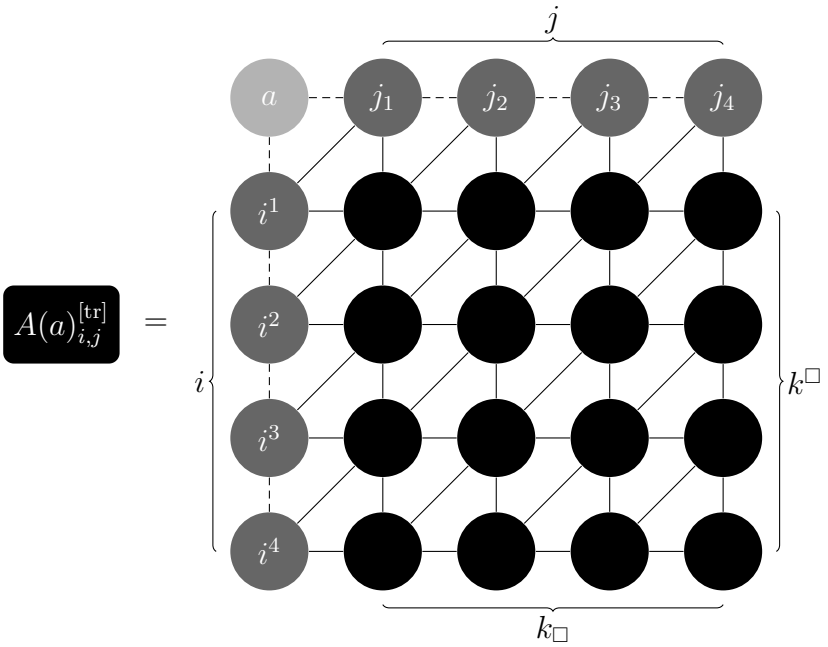


Figure 5.7: Triangular Corner Transfer Matrix $A(a)^{[\mathrm{tr}]}_{ij}$. This matrix is the main diagonal partition of the lattice.

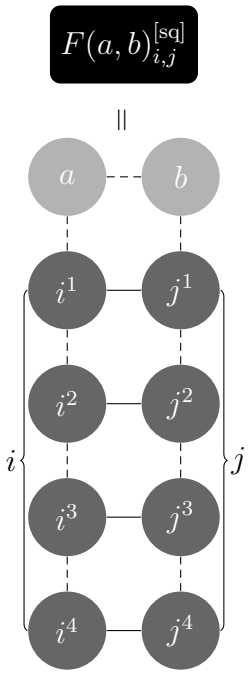


Figure 5.10: Square Half-Column Transfer Matrix $F(a,b)_{ij}$.

In the square case, the 90° rotational symmetry of the lattice means that half-column transfer matrices are equivalent to the row version. Therefore, in the square case they won't be distinguished and half-rows (HRTM) are also denoted by F. In the triangular case however, similar to the two types of corner partitions, the row and column TMs can be distinguished by whether they have diagonal interactions on their first free index (column TMs, $F(a,b)$) or

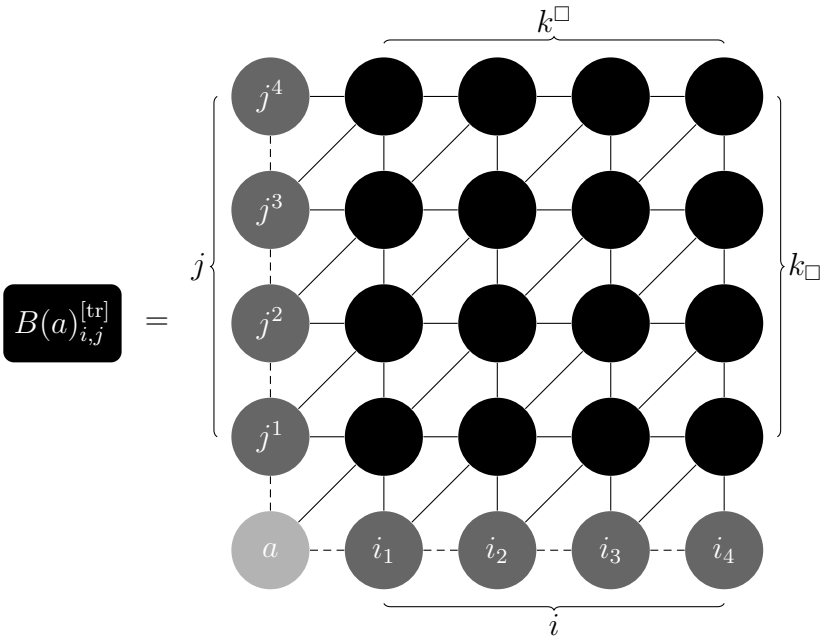


Figure 5.8: Triangular Corner Transfer Matrix $B(a)^{[\mathrm{tr}]}_{ij}$. This matrix is the anti-diagonal partition of the lattice.

their second free index (row TMs, $G(a,b)$). The triangular versions are defined by appending diagonal interactions to the square case

$$F(a,b)^{[\mathrm{tr}]}_{ij} = F(a,b)^{[\mathrm{sq}]}_{ij} \times \exp\left\{\beta\left(bi^1 + \sum_{\mu=1}^{N-1} i^{\mu+1}j^{\mu}\right)\right\} \tag{5.77}$$

with graphical representation fig. 5.11, and the row TM is

$$G(a,b)^{[\mathrm{tr}]}_{ij} = F(a,b)^{[\mathrm{sq}]}_{ij} \times \exp\left\{\beta\left(aj_1 + \sum_{\mu=1}^{N-1} i_{\mu}j_{\mu+1}\right)\right\} \tag{5.78}$$

with corresponding graphical representation fig. 5.12.

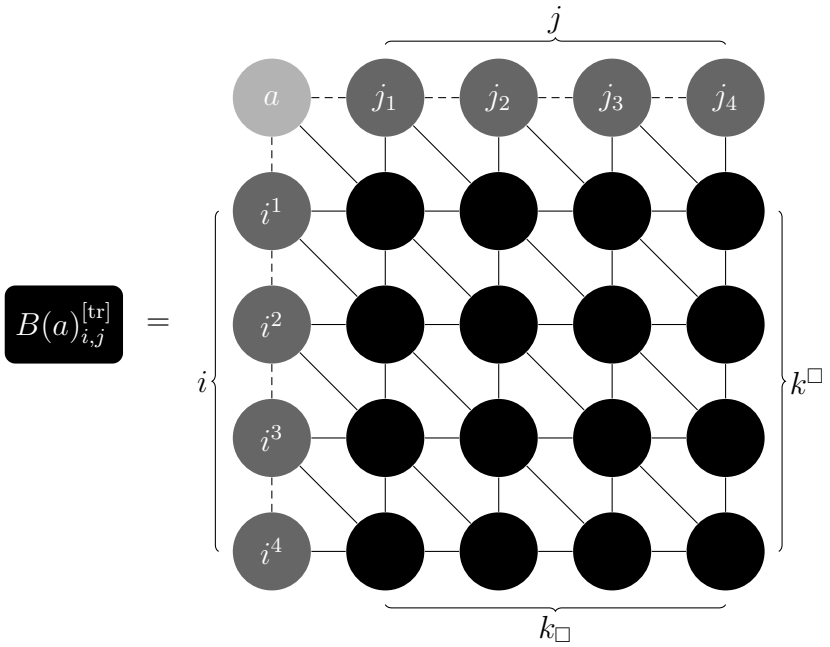


Figure 5.9: Triangular Corner Transfer Matrix $B(a)^{[\mathrm{tr}]}_{ij}$ rotated by $\frac{3\pi}{2}$.

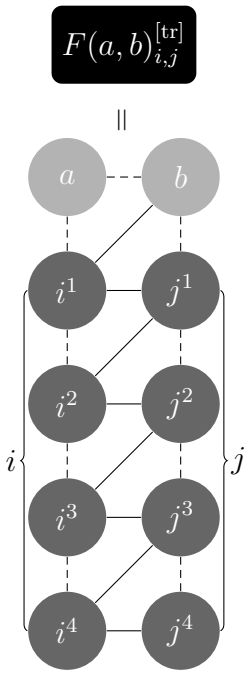


Figure 5.11: Half Column Transfer Matrix $F(a,b)_{ij}$.

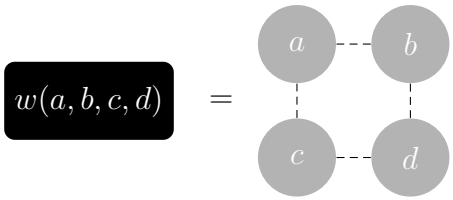


Figure 5.13: Square Single Face Transfer Matrix $w(a,b,c,d)^{[\mathrm{sq}]}$.

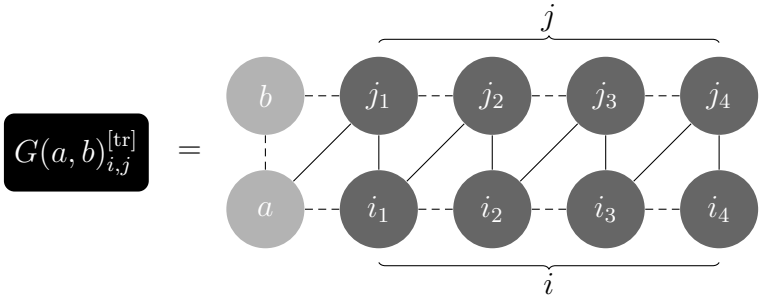


Figure 5.12: Half Row Transfer Matrix $G(a,b)_{ij}$.

These matrices all have block-matrix representations

$$\mathbf{F} = \begin{pmatrix} F(0,0) & F(0,1) \\ F(1,0) & F(1,1) \end{pmatrix}$$
$$\mathbf{G} = \begin{pmatrix} G(0,0) & G(0,1) \\ G(1,0) & G(1,1) \end{pmatrix} \tag{5.79}$$

and while F and G are not equal in the triangular case, by transposing all four indices they satisfy $\mathbf{F}^{\mathrm{T}} = \mathbf{G}$ which is equivalent to $F(a,b)^{\mathrm{T}} = G(b,a)$. This means that $\mathbf{F}$ is symmetric in the square case, which is not surprising given the rotational symmetry of the lattice.

Single Face Transfer Matrix

The last TM to be defined is the partial partition function of a single face and is the *Boltzmann transfer matrix* or the **Single Face Transfer Matrix** (SFTM), w. The definitions for both lattices are

$$w(a,b,c,d)^{[\mathrm{sq}]} = \exp\left\{\frac{\beta}{2}\left(ab+ac+bd+cd\right)\right\} \times \exp\left\{\frac{H}{4}\left(a+b+c+d\right)\right\}$$
$$w(a,b,c,d)^{[\mathrm{tr}]} = w(a,b,c,d)^{[\mathrm{sq}]} \times \exp\{\beta bc\} \tag{5.80}$$

and the graphical representations are depicted in section 5.5.1 Even though this is the simplest of the TMs, it is the most important. Through the expansion algorithm eq. (5.81), we will see that the physics of the lattices is entirely encoded in the SFTM eq. (5.80) and the two partition function calculations figs. 5.2 and 5.5 can be distinguished simply by modifying this matrix.

5.6 Corner Transfer Matrix Renormalisation Group

In the 90s, the Nishino group [53] successfully applied the techniques from **Density Matrix Renormalisation Group** (DMRG) [74] to corner transfer matrices. The algorithm they

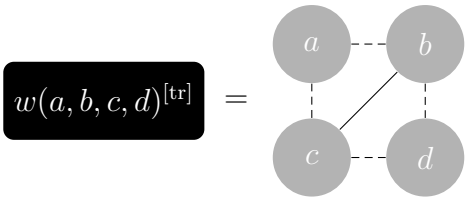


Figure 5.14: Triangular Single Face Transfer Matrix $w(a,b,c,d)^{[\mathrm{tr}]}$.

developed involves iteratively growing the size of CTMs and TMs then truncating and normalising to approximate large lattices. The effect of these steps is minimal on the calculation of κ as the normalisation cancels out.

5.6.1 Expansion Algorithm

The first part of the **Corner Transfer Matrix Renormalisation Group** (CTMRG) algorithm involves expanding the size of the lattice represented by the transfer matrices. The algorithm takes the form of a tensor equation. The CTMs and HTMs each have their own tensor equation. For CTMs, the equation is

$$\begin{aligned} A'(a)_{i(c),j(b)} &= \sum_{d}\sum_{kl} w(a,b,c,d) \times F(c,d)_{ik} A(d)_{kl} G(d,b)_{lj} \\ B'(c)_{i(d),j(a)} &= \sum_{b}\sum_{kl} w(a,b,c,d) \times G(d,b)_{ik} B(b)_{kl} F(b,a)_{lj} \end{aligned} \tag{5.81}$$

with $(c, i_1, \ldots, i_N)$ being the shifted binary representation for $i(c)$, and similarly for $j(b)$, etc. The CTM A' corresponds to a CTM that is 1 row and column larger A on the RHS. Graphically, the operation corresponds to "gluing" an additional row and column on to A and completing the square with the SFTM w. The expansion for A is the same for both the square and triangular case with the appropriate definition for w chosen from eq. (5.80). The summations along the indices b, c, d, k and l are the points where the four matrices join.

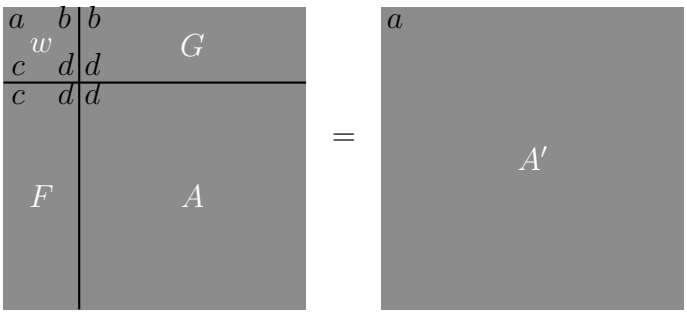


Figure 5.15: Expansion algorithm for growing corner transfer matrices $A(a)$ and $B(a)$.

HCTMs and HRTMs have the expansion algorithm

$$\begin{aligned} F'(a,b)_{i(c),j(d)} &= w(a,b,c,d) F(c,d)_{ij} \\ G'(c,a)_{i(d),j(b)} &= w(a,b,c,d) G(d,b)_{ij} \end{aligned} \tag{5.82}$$

noting the permuted indices between the two definitions to keep the orientation of w fixed.

F' and G' are two spins larger than the corresponding TM on the RHS. These equations have simple graphical interpretations, shown in fig. 5.15 and figs. 5.16 and 5.17.

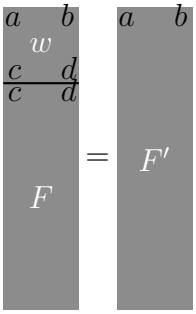


Figure 5.16: Expansion algorithm for growing half-column transfer matrices $F(a, b)$.



Figure 5.17: Expansion algorithm for growing half-row transfer matrices $G(c, a)$.

5.6.2 Iterative Transfer Matrix Definition

While in theory all the TMs can be generated directly using definitions in eqs. (5.73) and (5.74), in practice, CTMs are much more efficiently generated by beginning with a minimal 2x2 CTM and using the expansion procedure to generate the desired size. This is accomplished by defining the (2×2) CTMs and HTMs as

$$A(a)_{cb}^{[\mathrm{sq}]} = \sum_d \exp\left\{\frac{\beta}{2}(ab + ac + 2bd + 2cd) + \frac{H}{4}(a + 2b + 2c + 4d)\right\}$$

$$F(a, b)_{cd}^{[\mathrm{sq}]} = \exp\left\{\frac{\beta}{2}(ab + ac + 2bd + 2cd) + \frac{H}{4}(a + b + 2c + 2d)\right\} \tag{5.83}$$

and the asymmetrical triangular TMs are defined as

$$\begin{aligned} A(a)_{cb}^{[\mathrm{tr}]} &= A(a)_{cb}^{[\mathrm{sq}]} \times \exp\{\beta bc\} \\ B(a)_{cb}^{[\mathrm{tr}]} &= \sum_d A(a)_{cb}^{[\mathrm{sq}]} \times \exp\{\beta ad\} \\ F(a, b)_{cd}^{[\mathrm{tr}]} &= F(a, b)_{cd}^{[\mathrm{sq}]} \times \exp\{\beta bc\} \\ G(c, a)_{db}^{[\mathrm{tr}]} &= F(c, a)_{db}^{[\mathrm{sq}]} \times \exp\{\beta ad\} \end{aligned} \tag{5.84}$$

where b, c and d replace i and j for a single site in the appropriate definitions. The order of the parameters in A is specifically chosen to align with the matrix multiplications carried out shortly.

One then applies the expansion algorithms eqs. (5.81) and (5.82) $N-1$ times to generate TMs for a lattice of size $(2N+1)\times(2N+1)$. The tensors $\mathbf{A}$ and $\mathbf{B}$ will then be of physical size $2\times 2^N\times 2^N$ while $\mathbf{F}$ and $\mathbf{G}$ will be of size $2\times 2\times 2^N\times 2^N$. As matrix operations are generally quite fast, this method of generating large TMs is significantly faster than computing them directly. Additionally, since the algorithm converges rapidly, the actual entries chosen to initialise eq. (5.83) and eq. (5.84) can be chosen arbitrarily as they have very little effect on the final values in the full-sized tensor, and even less after renormalisation. The only term which affects the growth algorithm is the SFTM w, so changing between lattices is solely determined by how this tensor is defined.

5.7 Renormalisation Algorithm

In [53] the authors presented an improvement to the standard CTM algorithm, inspired by DMRG. The core of the algorithm relies on the insight that the eigenvalues of A decay exponentially, so the vast majority of the information about the CTMs is contained in the dominant eigenvalues. The expansion algorithm doubles the rows and columns of A and F, leading to exponentially increasing matrix sizes. However, since the majority of information is contained in the largest eigenvalues, the smaller half of eigenvalues can be discarded with minimal information loss (leading to a very good approximation) while reducing the size of the matrix to its original size and preventing the exponential blow up. The matrices $\mathbf{F}$ and $\mathbf{G}$ are also truncated with the same matrices, arranged so that the orthogonal matrices approximately cancel.

The algorithm can be summarised by the following set of instructions.

1. Begin with a small (2×2), arbitrarily initialised CTM (A) and HCTM (F).
2. Grow the TMs to appropriate sizes the computer can still handle within its cache size ($\sim 128\times 128$).
3. Expand all matrices using the growth algorithms eqs. (5.81) and (5.82), giving $A'(a)$ and $F'(a,b)$. These matrices have twice the rows and columns.
4. Eigendecompose $A'(a)=P(a)D(a)P(a)^{\mathrm{T}}$ (note that A is symmetric, so $P^{\mathrm{T}}=P^{-1}$). If A is complex, orthonormalise P to obtain $\hat{P}$ instead (discussed below).
5. Delete the smaller half of entries from each $D(a)$ to form $\tilde{D}(a)$. Delete the corresponding eigenvectors from $P(a)$ (or $\hat{P}(a)$) to form $\tilde{P}(a)$.
6. Approximate new TMs using the projection $A(a)\approx\tilde{D}(a)=\tilde{P}(a)^{\mathrm{T}}A'(a)\tilde{P}(a)$ and $F(a,b)\approx\tilde{P}^{\mathrm{T}}(a)F'(a,b)P(b)$. Note these matrices have the same number of matrix entries as A and F from step 2 but very closely approximate A' and F', which are one row and column larger.
7. Recurse the algorithm by repeating from step 3 with the new definitions $A(a)$ and $F(a,b)$.

Using this algorithm, one is able to approximate larger and larger transfer matrices with a static memory footprint. This algorithm relies on the fact that the bottom half of eigenvalues are significantly smaller than the larger half, which is true based on the decay of the eigenvalues. The exponential decay of the eigenvalues is controlled by the proximity to the critical point $(\tau(\beta),H)=(0,0)$ or the Yang-Lee singularity.

5.7.1 Modifications to the Algorithm

Complex Couplings

It is important to note that this algorithm is field agnostic, meaning it is suitable for lattices where the coupling constants are either real or complex. If β and/or H are complex, then A is complex—but it is still symmetric since this stems from isotropy of the lattice. This means that the eigenvectors of A are real orthogonal and are orthogonal with respect to the pseudo-inner product $v_i^{\mathrm{T}} v_j = \delta_{ij}$ instead of the typical Hermitian inner product $v_i^{\dagger} v_j = \delta_{ij}$.

In step 5 one normalises P by normalising each individual eigenvector. For each eigenvector v we define $\hat{v} = v/\|v\|$ and construct the columns of $\hat{P}$ from $\hat{v}$. This will be a complex matrix but nonetheless will satisfy $\hat{P}^{\mathrm{T}}\hat{P} = 1$ (note $\hat{P}\hat{P}^{\mathrm{T}} \neq I$ and $\hat{P}^{\dagger}\hat{P} \neq I$). $\hat{P}$ is now an orthonormalised, complex matrix of eigenvectors.

It would be tempting to generalise this algorithm to the complex case by promoting transposes to daggers and possibly using the SVD algorithm in place of eigendecomposition, but in practice the algorithm presented here converged much better. A rigorous dive into the reasoning behind its success was outside the scope of this work, but the suspected cause is the fact that A does not generalise to a Hermitian matrix in the complex case. This means that the necessary SVD modifications to the partition function per site calculations (detailed in [26]) are not faithful to Baxter's half-plane ansatz for the maximal eigenvector of the row transfer matrix, discussed in the next section. The SVD algorithm then has to overcome the additional inaccuracies introduced by complex conjugation through additional iterations, leading to a slow down in the convergence.

It was also theorised that a modified Ising model, comprised of four corners with off-diagonal corners having complex conjugate couplings relative to the diagonal corners, could explain the convergence discrepancy. Such a model would presumably be in the same Ising universality class and have similar scaling behaviour, but convergence of the CTMRG algorithm would be to this modified model rather than the original. This idea was not seriously explored in any numerical or theoretical detail due to time constraints and project scope.

Triangular Lattice

The modifications for the triangular lattice are relatively minor. When defining the TMs in step 1, one also constructs B and G (in the square case $B = A$ and $G = F$). In step 5, one also diagonalises $B'(a) = Q(a)\Delta(a)Q^{\mathrm{T}}(a)$ and orthonormalises if necessary. The truncation projection step 6 is then modified to

$$\begin{aligned} F(a,b) &= Q^{\mathrm{T}}(a)F'(a,b)P(b) \\ G(a,b) &= P^{\mathrm{T}}(a)G'(a,b)Q(b) \end{aligned} \tag{5.85}$$

The justification for this modification hinges on the fact that since $P^{\mathrm{T}}P = I_{n\times n}$ then $\tilde{P}^{\mathrm{T}}\tilde{P} \approx I_{\frac{n}{2}\times\frac{n}{2}}$ (and similarly for Q). This means that the truncation of F and G should be arranged such the products $\tilde{P}^{\mathrm{T}}\tilde{P}$ and $\tilde{Q}^{\mathrm{T}}\tilde{Q}$ are formed and approximately cancel.

CHAPTER 6

NUMERICAL RESULTS

> I have had my results for a long time:
> but I do not yet know how I am to arrive
> at them.
>
> Carl Friedrich Gauss

This chapter is dedicated to summarising the main numerical results obtained in this work. This mainly includes the series fits for $b(\tau)$, $B(\tau)$ and the subleading logarithmic terms $F(\tau)$ and $F_i(\tau)$. This section also describes the fitting procedure for the scaling function $G_{\text{high}}(\xi)$. The numerical derivative was utilised to help verify the original series conjecture and is within detailed.

6.1 Results

Below are the series expansions for data obtained through the susceptibility analysis chapter 4. The following are exact results for $a(\tau), c(\tau)$ and $A(\tau)$ which can all be readily computed to arbitrary degree using the calculations detailed in sections 4.2.1 and 4.2.2

6.1.1 Square lattice

$$a^{[\text{sq}]}(\tau) = \tau - \frac{3\tau^3}{16} + \frac{137\tau^5}{1536} - \frac{451\tau^7}{8192} + \frac{908071\tau^9}{23592960} - \frac{1214393\tau^{11}}{41943040} + \frac{5798332279\tau^{13}}{253671505920} - \frac{25264228033\tau^{15}}{1352914698240} + \frac{121964214040573\tau^{17}}{7792788661862400} - \frac{79440071562083\tau^{19}}{5937362789990400} + \mathcal{O}\left(\tau^{21}\right) \quad (6.1)$$

$$c^{[\text{sq}]}(\tau) = 1 + \frac{\tau}{4} + \frac{15\tau^2}{128} - \frac{9\tau^3}{512} - \frac{4333\tau^4}{98304} + \frac{1955\tau^5}{393216} + \frac{108949\tau^6}{4194304} - \frac{30211\tau^7}{16777216} - \frac{1745543057\tau^8}{96636764160} + \frac{234707983\tau^9}{386547056640} + \frac{18829207141\tau^{10}}{1374389534720} - \frac{1053009481\tau^{11}}{16492674416640} - \frac{728975795562971\tau^{12}}{66498463247892480} - \frac{11208070654159\tau^{13}}{53198770598313984} + \mathcal{O}\left(\tau^{14}\right) \quad (6.2)$$

$$A^{[\mathrm{sq}]}(\tau) = \left(-\frac{2C}{\pi} - \frac{\log(2)}{2}\right) + \frac{\tau}{2} - \frac{(1+5\log(2))\tau^2}{4\pi} - \frac{\tau^3}{12} + \frac{5(1+6\log(2))\tau^4}{64\pi} + \frac{3\tau^5}{80} + \frac{(-187-1230\log(2))\tau^6}{4608\pi} - \frac{5\tau^7}{224} + \frac{(1261+8820\log(2))\tau^8}{49152\pi} + \frac{35\tau^9}{2304} + \frac{(-531277-3892050\log(2))\tau^{10}}{29491200\pi} - \frac{63\tau^{11}}{5632} + \frac{(318667+2423025\log(2))\tau^{12}}{23592960\pi} + \frac{231\tau^{13}}{26624} + \mathcal{O}\left(\tau^{14}\right) \tag{6.3}$$

6.1.2 Triangular lattice

$$a^{[\mathrm{tr}]}(\tau) = \tau - \frac{3\tau^3}{16} + \frac{23\tau^5}{256} - \frac{229\tau^7}{4096} + \frac{25819\tau^9}{655360} - \frac{313083\tau^{11}}{10485760} + \frac{27876763\tau^{13}}{1174405120} - \frac{366781211\tau^{15}}{18790481920} + \frac{14139360979\tau^{17}}{858993459200} - \frac{1361651351923\tau^{19}}{96207267430400} + \mathcal{O}\left(\tau^{21}\right) \tag{6.4}$$

$$c^{[\mathrm{tr}]}(\tau) = 1 + \frac{\tau}{4} + \frac{15\tau^2}{128} - \frac{9\tau^3}{512} - \frac{1447\tau^4}{32768} + \frac{649\tau^5}{131072} + \frac{109293\tau^6}{4194304} - \frac{29803\tau^7}{16777216} - \frac{194751097\tau^8}{10737418240} + \frac{25036583\tau^9}{42949672960} + \frac{18921405429\tau^{10}}{1374389534720} - \frac{224111283\tau^{11}}{5497558138880} - \frac{27147912839129\tau^{12}}{2462906046218240} - \frac{2288621184617\tau^{13}}{9851624184872960} + \mathcal{O}\left(\tau^{14}\right) \tag{6.5}$$

$$A^{[\mathrm{tr}]}(\tau) = \left(\frac{5\,\mathrm{Im}\left(-\mathrm{Li}_2\left(\sqrt[3]{-1}\right) + \mathrm{Li}_2\left(-(-1)^{2/3}\right)\right)}{4\pi} - \frac{1}{4}\log\left(\frac{4}{3}\right)\right) + \frac{\tau}{2} + \frac{\left(-6\sqrt{3}+2\pi-3\sqrt{3}\log(1728)\right)\tau^2}{32\pi} - \frac{\tau^3}{12} + \frac{\left(15\sqrt{3}-7\pi+54\sqrt{3}\log(2)+27\sqrt{3}\log(3)\right)\tau^4}{256\pi} + \frac{3\tau^5}{80} + \frac{\left(-756\sqrt{3}+410\pi-2970\sqrt{3}\log(2)-1485\sqrt{3}\log(3)\right)\tau^6}{24576\pi} - \frac{5\tau^7}{224} + \frac{\left(1291\sqrt{3}-767\pi+5364\sqrt{3}\log(2)+2682\sqrt{3}\log(3)\right)\tau^8}{65536\pi} + \frac{35\tau^9}{2304} + \frac{\left(-734739\sqrt{3}+465160\pi-3180060\sqrt{3}\log(2)-1590030\sqrt{3}\log(3)\right)\tau^{10}}{52428800\pi} - \frac{63\tau^{11}}{5632} + \frac{\left(2677758\sqrt{3}-1778495\pi+11966670\sqrt{3}\log(2)+5983335\sqrt{3}\log(3)\right)\tau^{12}}{251658240\pi} + \frac{231\tau^{13}}{26624} + \mathcal{O}\left(\tau^{14}\right) \tag{6.6}$$

with $\mathcal{G} = \frac{1}{2}\int_0^1 \mathrm{K}(k^2)\,\mathrm{d}k \approx 0.91597\ldots$ being Catalan's constant and $\mathrm{Li}_2(x) = -\int_0^x \frac{\log(1-t)}{t}\,\mathrm{d}t$ the dilogarithm function.

It was often pertinent to utilise the inverse relationship to convert from values of τ to β. This is given exactly in the square case and as a high order series in the triangular case

$$\begin{aligned}\beta^{[\mathrm{sq}]}(\tau) =& -\frac{1}{2}\operatorname{arsinh}[\tau - \sqrt{1+\tau^2}] \\ \beta^{[\mathrm{tr}]}(\tau) =& \frac{\log(3)}{4} - \frac{\tau}{4} + \frac{\tau^2}{16} + \frac{11\tau^3}{192} - \frac{7\tau^4}{256} - \frac{39\tau^5}{1280} + \frac{205\tau^6}{12288} + \frac{1165\tau^7}{57344} - \frac{767\tau^8}{65536} \\ & - \frac{8887\tau^9}{589824} + \frac{11629\tau^{10}}{1310720} + \frac{548547\tau^{11}}{46137344} - \frac{355699\tau^{12}}{50331648} - \frac{2131113\tau^{13}}{218103808} + \mathcal{O}\left(\tau^{14}\right)\end{aligned} \tag{6.7}$$

Additionally, it is important to note that there are two plausible definitions for $\tau^{[\mathrm{tr}]}(\beta)$ seen in the triangular case in the literature. One is seen in [48] and the other in [22]. This work uses the definition given in [22], as this form better reflects the KW-symmetry. These definitions are not equivalent, but one can readily convert between the two.

Keeping our definition of τ as given in [22], we set the definition given in [48] as $\tau^* = \tau^{\mathrm{Dudalev}}$. The relationship is

$$\begin{aligned}\tau^*(\tau) =& \frac{3\tau}{2} - \frac{9\tau^3}{64} + \frac{249\tau^5}{4096} - \frac{4701\tau^7}{131072} + \frac{409065\tau^9}{16777216} - \frac{9655671\tau^{11}}{536870912} + \frac{480713253\tau^{13}}{34359738368} \\ & - \frac{12422113989\tau^{15}}{1099511627776} + \frac{2640207829737\tau^{17}}{281474976710656} - \frac{716604715111123\tau^{19}}{9007199254740992} + \mathcal{O}(\tau^{21}) \\ & + \frac{3956702460650583\tau^{21}}{576460752303423488} - \frac{1107553264101890 19\tau^{23}}{18446744073709551616} + O\left(\tau^{25}\right)\end{aligned} \tag{6.8}$$

This allows us to convert the result in [48]

$$a^*(\tau^*) = 1 - \frac{1}{24}(\tau^*)^2 + \frac{47}{10368}(\tau^*)^4 + \mathcal{O}((\tau^*)^6) \tag{6.9}$$

to be rectified and given in terms of τ

$$\begin{aligned}a^*(\tau^*(\tau)) &= 1 - \frac{3}{16}\tau^2 + \frac{23}{256}\tau^4 + \mathcal{O}(\tau^6) \\ &= a(\tau)\end{aligned} \tag{6.10}$$

This now matches the series coefficients in eq. (6.4). The leading coefficient of 3/2 accounts for the varying definitions of $C_\tau^{[\mathrm{tr}]}$ here vs $C_{\tau^*}^{[\mathrm{tr}]}$ given in [48].

Next are results calculated in this work. As noted above, we did not have time to characterise any potential logarithmic irrelevant operators at order $\log[\tau]$, so this would be a potential source of error. Future extensions of this work would likely include characterisation of these terms. A gradient descent style approach to evaluate these terms was in the process of being developed for this project but was omitted due to time constraints.

6.1.3 Square lattice

$$\begin{aligned}b^{[\mathrm{sq}]}(\tau) =& 1 + \frac{1}{2}\tau + 0.13397993\tau^2 + 1.767981279\tau^3 + 0.8820838362\tau^4 \\ & - 1.227894827\tau^5 - 0.8446316692\tau^6 + 0.9575843759\tau^7 + 0.7387874248\tau^8 \\ & - 0.8014734192\tau^9 - 0.64809119617\tau^{10} + \mathcal{O}\left(\tau^{11}\right)\end{aligned} \tag{6.11}$$

$$\mu_h^{[\mathrm{sq}]} = 0.07186867081 \tag{6.12}$$

$$\begin{aligned} B^{[\mathrm{sq}]}(\tau) = {} & 0.0520666225469 + 0.0769120341893\tau + 0.0360200462309\tau^2 \\ & - 0.00258792941465\tau^3 - 0.103373366270\tau^4 - 0.0449218744140\tau^5 \\ & + 0.0801266785935\tau^6 + 0.0476250390376\tau^7 - 0.0653467096773\tau^8 \\ & - 0.0454204414138\tau^9 + 0.0552135367913\tau^{10} + \mathcal{O}\left(\tau^{11}\right) \end{aligned} \tag{6.13}$$

$$\begin{aligned} F^{[\mathrm{sq}]}(\tau) = {} & 0.00184292514941\tau^4 + 0.000921462574703\tau^5 + 0.116445637962\tau^6 \\ & + 0.0579924533373\tau^7 - 0.100530191780\tau^8 - 0.0647056178135\tau^9 \\ & + 0.0864780877299\tau^{10} + 0.0630111809465\tau^{11} + \mathcal{O}\left(\tau^{12}\right) \end{aligned} \tag{6.14}$$

$$\begin{aligned} F_2^{[\mathrm{sq}]}(\tau) = {} & 0.00469578493557\log^2(\tau)\tau^4 - 0.00234789246779\log^2(\tau)\tau^5 \\ & + 0.00376098961449\log^2(\tau)\tau^6 + 0.00246746792419\log^2(\tau)\tau^7 \\ & - 0.00310781630608\log^2(\tau)\tau^8 - 0.00239466060481\log^2(\tau)\tau^9 \\ & + 0.00261864758381\log^2(\tau)\tau^{10} + 0.00228119502279\log^2(\tau)\tau^{11} \\ & - 0.00224870444041\log^2(\tau)\tau^{12} + \mathcal{O}\left(\tau^{13}\right) \end{aligned} \tag{6.15}$$

$$\begin{aligned} F_3^{[\mathrm{sq}]}(\tau) = {} & 7.8857845692 \times 10^{-6}\log^3(\tau)\tau^9 + 3.9428922846 \times 10^{-6}\log^3(\tau)\tau^{10} \\ & - 0.0000162283802393\log^3(\tau)\tau^{11} + \mathcal{O}(\tau^{12}) \end{aligned} \tag{6.16}$$

6.1.4 Triangular lattice

$$\begin{aligned} b^{[\mathrm{tr}]}(\tau) = {} & 1 + \frac{1}{2}\tau + 0.122460779015\tau^2 - 9.2284247711\tau^3 - 4.71090990756\tau^4 \\ & + 6.5481254798\tau^5 + 4.52874631568\tau^6 - 5.0599150755\tau^7 - 4.00945664230\tau^8 \\ & + 4.14543521741\tau^9 + 3.53508523262\tau^{10} + \mathcal{O}\left(\tau^{11}\right) \end{aligned} \tag{6.17}$$

$$\mu_h^{[\mathrm{tr}]} = -0.01047478007 \tag{6.18}$$

$$\begin{aligned} B^{[\mathrm{tr}]}(\tau) = {} & 0.0247805582609 + 0.0244432845027\tau + 0.0110251153619\tau^2 \\ & - 0.00128387180102\tau^3 - 0.0756757034728\tau^4 - 0.0346970708485\tau^5 \\ & + 0.0611443461008\tau^6 + 0.0371767877716\tau^7 - 0.0501408269600\tau^8 \\ & - 0.0349997455421\tau^9 + 0.0423937151580\tau^{10} + \mathcal{O}\left(\tau^{11}\right) \end{aligned} \tag{6.19}$$

$$\begin{aligned} F^{[\mathrm{tr}]}(\tau) = {} & 0.0966887515557\tau^6 + 0.0483443757779\tau^7 - 0.0853225031813\tau^8 \\ & - 0.0547473455351\tau^9 + 0.0730575283805\tau^{10} + 0.0532371240601\tau^{11} + \mathcal{O}(\tau^{12}) \end{aligned} \tag{6.20}$$

$$\begin{aligned} F_2^{[\mathrm{tr}]}(\tau) = {} & 0.00415078586899\log^2(\tau)\tau^4 - 0.00207539293450\log^2(\tau)\tau^5 \\ & + 0.00341306300278\log^2(\tau)\tau^6 + 0.00222537973501\log^2(\tau)\tau^7 \\ & - 0.00281678401085\log^2(\tau)\tau^8 - 0.00209690944138\log^2(\tau)\tau^9 \\ & + 0.00238873819476\log^2(\tau)\tau^{10} + 0.00192624549373\log^2(\tau)\tau^{11} \\ & - 0.00207409612301\log^2(\tau)\tau^{12} + \mathcal{O}(\tau^{13}) \end{aligned} \tag{6.21}$$

$$\begin{aligned} F_3^{[\mathrm{tr}]}(\tau) = {} & 4.12191321575\times10^{-6}\log^3(\tau)\tau^9 + 2.06095660787\times10^{-6}\log^3(\tau)\tau^{10} \\ & - 9.15472032775\times10^{-6}\log^3(\tau)\tau^{11} + \mathcal{O}(\tau^{12}) \end{aligned} \tag{6.22}$$

Although these terms have potentially been mischaracterised by the omission of a 1st order logarithm term from f_{sub}, in practice this form still produced an improved accuracy over the scaling ansatz without f_{sub} from testing. To test this, we compared against CTM data with $H \neq 0$ and larger τ (for better CTM convergence) The additional terms provided better convergence. There remains scope to improve the accuracy of the fitted terms and reintroduce the omitted logarithm in future works.

6.2 Numerical Derivative

The next sections utilise the numerical derivative, so we will briefly discuss the technique here. In a theoretical setting, the derivative is calculated by taking the limit of the standard forward difference quotient $f'(x) \approx (f(x+h) - f(x))/h$. In practice, this naïve approach is susceptible to numerical errors such as floating point errors and cancellation errors. These errors can be lessened by generalising the difference quotient to include additional data points, such as the 3-point forward derivative $f'(x) \approx (-f(x+2h) + 4f(x+h) - 3f(x))/(2h)$ which is accurate to $\mathcal{O}(h^2)$. The coefficients here (and the method in general) comes from Taylor expanding $f(x), f(x+h), f(x+2h), \ldots$ and simultaneously solving for $f'(x)$. The improved error estimate comes from the fact that the lower order terms cancel exactly in this procedure.

The full generalisation of the numerical n$^{\mathrm{th}}$ order derivative using a subset of $2m$ sample points[1] from a full data set of evenly spaced values $\{x_1, \ldots, x_N\}$ ($N \geq 2m$) is given by [26, 33, 32]

$$f^{(n)}(x_j) \approx \frac{1}{h^n}\sum_{k=0}^{2m} a_{n,s}^k f(x_j + (k + (m-s))h)$$

where the variable $s = \min(j-1, 2m, N-j)$ tracks how close the point x_j is to the edges of the data set and $h = |x_2 - x_1|$. The coefficients $a_{n,s}^k$ are defined by the relation

$$\sum_{k=0}^{2m} a_{n,s}^k x^k = \sum_{k=0}^{2m} \frac{(x-1)^k}{k!}\frac{\mathrm{d}^k}{\mathrm{d}y^k}\left[y^s(\log y)^n\right]\Big|_{y=1} \tag{6.23}$$

This formula is quite general and very adaptive, although it is possible to generalise it even further to an arbitrarily spaced grid [32, 33] by incorporating Lagrange interpolating polynomials (unnecessary for this work). For $s = 0$, this algorithm performs forward/backwards difference, and for $s = 2m$ it performs a symmetric difference. For points in between these two extremes, a skewed difference operation is performed. The accuracy of the n$^{\mathrm{th}}$ order derivative with $2m$ sample points is $\mathcal{O}(h^{2m-n})$.

[1] This formula is suitable for an even and odd number of sample points, but there are minor implementation modifications between the two cases so we assume even sample points.

6.3 Scaling Function Fitting

With the series $b(\tau), B(\tau)$ and terms in $f_{\text{sub}}(\tau, H)$ evaluated, we are able to use the new scaling ansatz to deviate into $H \neq 0$ territory. As mentioned, we are interested in the scaling function $G_{\text{high}}(\xi)$ in the vicinity of the Yang-Lee singularity. This singularity location is a function of both lattice parameters τ, H and is therefore best given in terms of the scaling variable. It had the approximate value $i\xi_0 = i0.1893(5)$ according to prior work in [31].

To study the scaling function, we start by rearranging eq. (4.4) for the scaling function

$$G_{\text{high}}(\xi(\tau, H)) = \frac{f(\tau, H) - f_{\text{reg}}(\tau, H) - f_{\text{sub}}(\tau, H)}{m(\tau, H)^2} - \frac{1}{8\pi} \log\big(m(\tau, H)^2\big) \tag{6.24}$$

Most of the terms on the RHS come from the susceptibility analysis except for the f term. This was supplied through data obtained from the CTMRG method, so $f = f_{\text{ctm}}$.

We consider the high-temperature regime $m < 0$ and fix the variable ξ. Then using (4.6) the scaling variable h can be written as

$$h(\tau, H) = \big(-m(\tau, H)\big)^{15/8} \xi \tag{6.25}$$

Combining this with (4.7) one can invert the series in H and obtain the following expansion

$$H(\tau) = \xi\, \tau^{15/8} \sum_{k=0}^{\infty} \xi^{2k} \tau^{11k/4} p_k(\tau) \tag{6.26}$$

where $p_k(\tau)$ are regular in τ. Then it is easy to see that the coefficients of a series expansion of $H(\tau)$ in powers of τ are finite polynomials in ξ. Thus, the variable ξ can be assigned to any fixed value—not necessarily small.

Substituting (6.26) into the RHS of (6.24) one obtains a function of two variables ξ and τ, which should not depend on τ. This is a highly nontrivial self-consistency test that determines the accuracy of the calculation of $G(\xi)$. Indeed, taking two different values of τ with a fixed ξ, one should get the same value of $G(\xi)$.

As explored in chapter 5, the CTM method can be applied to regular square, triangular, or even honeycomb lattices. As was shown in [19, 22], for the Ising model the CTF irrelevant operators contribute in the order τ^4 for the square lattice and in the order τ^6 for the triangular/honeycomb lattices. This implies that one can achieve much better accuracy for the triangular lattice [48]. For this reason, we restrict all further analysis to this case.

The precision of CTM calculations is limited by the machine accuracy, which in our case is 10^{-16}. As we shall see below, for the triangular lattice one can reliably control the series expansion coefficients in the RHS of (6.24) up to the order of τ^8. Therefore, there is an upper limit on the value of τ for which the unknown higher terms in (6.24) do not affect the precision of calculations. Having this in mind, one needs, nonetheless, to choose τ as large as possible to speed up the convergence of the CTM algorithm. The latter is mainly determined by the variable

$$\Delta\beta = \beta_c^{(t)} - \beta = \tfrac{1}{4}\tau + O(\tau^2) \tag{6.27}$$

Numerical experiments suggest that the optimal value of $\Delta\beta$ for the maximum precision calculatisons should be in the range

$$0.006 \leq \Delta\beta \leq 0.012 \tag{6.28}$$

where the lower bound is near the boundary of convergence of the CTM algorithm. To reach the numerical accuracy of 10^{-15} the calculations were performed with corner transfer matrices of the size $N = 170$.

Since the RHS of (6.24) contains an extra factor $1/m^2$, the accuracy of calculations of $G(\xi)$ is reduced by 4-5 decimal places. Therefore, one can expect the accuracy of the scaling function to be around 10^{-10}. Indeed, we calculated $G(\xi)$ for a large set of points ξ_i in the complex plane with three values of $\Delta\beta$,

$$\Delta\beta = 0.006,\ 0.007,\ 0.012 \tag{6.29}$$

corresponding to

$$\tau \simeq 0.024,\ 0.028,\ 0.048 \tag{6.30}$$

A difference between the values of $G(\xi)$ for these values of τ never exceeded $2. \times 10^{-10}$. Therefore, it suggests that this is the accuracy of our calculations of the scaling function $G(\xi)$.

6.4 Numerical Results

In this section, we describe numerical calculations used to generate and analyse the data for the scaling function in the region close to the Yang-Lee singularity. We will consider the high-temperature regime $m < 0$ with a complex magnetic field H. As mentioned before, the scaling function $G_{\rm high}(\xi)$ has two branch cuts $(-i\infty, -i\xi_0)$ and $(i\xi_0, +i\infty)$ with the value $i\xi_0 = i0.18930(5)$ estimated in [31].

Following [31], let us introduce the function $\Phi_{\rm imh}(z)$ (and a simply related function $G_{\rm YL}(z)$) via an analytic continuation of $G_{\rm high}(\xi)$ to purely imaginary ξ. Here we define

$$\Phi_{\rm imh}(z) = z^2 G_{\rm YL}(z) = z^2 G_{\rm high}(-iz^{-15/8}) \tag{6.31}$$

noting that our variable z is equal to $(-y)$ in the original definition of this function in eq.(3.38b) of ref. [31]. The relationship between z, ξ and the nonlinear scaling variables is captured by

$$z = (i\xi)^{-8/15} = -m(ih)^{-8/15} \tag{6.32}$$

The functions $\Phi_{\rm imh}(z)$ and $G_{\rm YL}(z)$ have a branch cut on the real axis for $0 < z < Z_0$, where Z_0 is the corresponding position of the YL singularity

$$Z_0 = 1/\xi_0^{8/15} \approx 2.4295 \tag{6.33}$$

For series expansions below it will be convenient to use the variable

$$v = (z - Z_0) = \frac{4}{15} Z_0^{19/4} u + \frac{38}{225} Z_0^{17/2} u^2 + \cdots \tag{6.34}$$

where $\xi = -iz^{-15/8}$ and

$$u = \xi^2 + \xi_0^2 = \frac{15}{4} Z_0^{-19/4} v - \frac{285}{32} Z_0^{-23/4} v^2 + \cdots \tag{6.35}$$

The scaling function $G_{\rm YL}(z)$ has a concise interpretation in terms of 2D Euclidean quantum field theory. Namely, it coincides with the vacuum energy density of the Ising Field Theory (IFT) in the vicinity of the Yang-Lee singularity. The IFT is defined as the $c = 1/2$ CFT perturbed by the energy and spin operators [31]

$$\mathcal{A}_{\rm IFT} = \mathcal{A}_{(c=1/2)} + \frac{m}{2\pi} \int \epsilon(x) d^2x + h \int \sigma(x) d^2x \tag{6.36}$$

where $\mathcal{A}_{(c=1/2)}$ stands for the action of the $c = 1/2$ CFT of free massless Majorana fermions, $\sigma(x)$ and $\epsilon(x)$ are primary fields of conformal dimensions $(1/16, 1/16)$ and $(1/2, 1/2)$. Their normalisation is fixed by the usual CFT convention

$$\left.\begin{aligned} x^2\langle\epsilon(x)\epsilon(0)\rangle &\to 1 \\ x^{1/4}\langle\sigma(x)\sigma(0)\rangle &\to 1 \end{aligned}\right\} \text{as } x \to 0 \tag{6.37}$$

The coupling constants m and h, appearing in (6.36), are the nonlinear scaling variables, related to the lattice model parameter τ and H via (4.7). Remarkably, the same field theory can also be defined (up to a constant shift of the vacuum energy density, see (6.45) below) as a model of perturbed minimal conformal field theory $\mathcal{M}_{2/5}$ (YLCFT)

$$\mathcal{A}_{\text{eff}} = \mathcal{A}_{\text{YLCFT}} + \lambda \int \phi(x) d^2x + \sum_i t_i \int O_i(x) d^2x \tag{6.38}$$

involving an infinite tower of irrelevant operators $O_i(x)$, with dimensions $(\Delta_i, \bar{\Delta}_i)$ such that $\Delta_i = \bar{\Delta}_i$ (see [78] for the details). In this work, we take into account the first few "least irrelevant" operators

$$\begin{aligned} \sum_i t_i \int O_i(x) d^2x = \frac{\alpha}{\pi^2} \int T\bar{T}(x) d^2x + \frac{\beta}{2\pi} \int \Xi(x) d^2x + \frac{\gamma}{2\pi} \int \Xi_6(x) d^2x \\ + \frac{\alpha_5}{\pi^2} \int (T\bar{T})^3(x) d^2x + \frac{\delta}{2\pi} \int \Xi_8(x) d^2x \\ + \text{higher irrelevant operators} \end{aligned} \tag{6.39}$$

The action (6.38) involves the $\mathcal{M}_{2/5}$ relevant primary operator ϕ with the conformal dimensions $(-1/5, -1/5)$ and the irrelevant operators $T\bar{T}$ and $(T\bar{T})^3$ with the dimensions $(2, 2)$ and $(6, 6)$ respectively; the operators Ξ, Ξ_6 and Ξ_8 with the dimensions $(19/5, 19/5)$, $(29/5, 29/5)$ and $(39/5, 39/5)$. The latter are the level four, level six and level eight descendants of the primary field ϕ. We will disregard all operators with the mass dimension greater than $78/5$, since their contribution is too small to be properly accounted for by our numerical data. Here we assume the same definitions and normalisations of these operators as in [78, 79].

The coupling constant λ carries the mass dimension $[\lambda] \sim [\text{mass}]^{12/5}$, while the constants α, β, γ and δ have negative mass dimensions, $\alpha \sim [\text{mass}]^{-2}$ and $\beta \sim [\text{mass}]^{-28/5}$, $\gamma \sim [\text{mass}]^{-48/5}$, and $\delta \sim [\text{mass}]^{-68/5}$. In IFT these coupling constants depend on the scaling parameter ξ or z, and admit convergent series expansion in powers of $v = (z - Z_0)$, in particular

$$\begin{aligned} \lambda(z) &= \sum_{k=1}^{\infty} \hat{\lambda}_k (z - Z_0)^k = \hat{\lambda}_1 v + \hat{\lambda}_2 v^2 + \cdots \\ \alpha(z) &= \sum_{k=0}^{\infty} \hat{\alpha}_k (z - Z_0)^k = \hat{\alpha}_0 + \hat{\alpha}_1 v + \cdots \\ \beta(z) &= \sum_{k=0}^{\infty} \hat{\beta}_k (z - Z_0)^k = \hat{\beta}_0 + \hat{\beta}_1 v + \cdots \\ \gamma(z) &= \sum_{k=0}^{\infty} \hat{\gamma}_k (z - Z_0)^k = \hat{\gamma}_0 + \hat{\gamma}_1 v + \cdots \\ \delta(z) &= \sum_{k=0}^{\infty} \hat{\delta}_k (z - Z_0)^k = \hat{\delta}_0 + \hat{\delta}_1 v + \cdots \end{aligned} \tag{6.40}$$

The QFT defined by the first two terms in the action (6.38) is called the Yang-Lee QFT. It is an integrable QFT containing one scalar particle with the mass

$$M_{\rm YL} = C_{\rm YL}\lambda^{5/12} \tag{6.41}$$

where [81]

$$C_{\rm YL} = \frac{2^{19/12}\sqrt{\pi}}{5^{5/16}}\frac{\left(\Gamma\left(\frac{3}{5}\right)\Gamma\left(\frac{4}{5}\right)\right)^{5/12}}{\Gamma\left(\frac{2}{3}\right)\Gamma\left(\frac{5}{6}\right)}. \tag{6.42}$$

With these notations the vacuum energy density of IFT defined by the action (6.38) reads

$$f_{\rm sing} = f_{\rm YL}M_{\rm YL}^2 + \sum_i c_i t_i M_{\rm YL}^{2\Delta_i} + \sum_{i,j} c_{ij}t_i t_j M_{\rm YL}^{2\Delta_i+2\Delta_j-2} + \cdots \tag{6.43}$$

where $f_{\rm YL} = -\sqrt{3}/12$ and numerical constants $c_i, c_{ij}, \ldots$ are expressed through the vacuum expectation values of the products of the operators $O_i(x)$. Remarkably, the contribution of the operator $T\bar{T}(x)$, generated by the first term in (6.39), can be calculated to all orders [67] in the coupling constant α in (6.39). The result is [78]

$$f_{\rm sing} = \frac{f_{\rm sing}^{(0)}}{1+\alpha f_{\rm sing}^{(0)}} \tag{6.44}$$

where $f_{\rm sing}^{(0)}$ is defined by (6.43) with $\alpha = 0$.

Next note, that the energy density $f_{\rm sing}$ defined above is, of course, a function of the scaling variable z, since the coupling constants (6.40) are the series in z. The scaling function $G_{\rm YL}(z)$ introduced in (6.31) can now be expressed as

$$G_{\rm YL}(z) = g(z) + f_{\rm sing}(z) \tag{6.45}$$

where the function $g(z)$ is analytic near $z = Z_0$

$$g(z) = \sum_{k=0}^{\infty}\hat{g}_k(z-Z_0)^k = \hat{g}_0 + \hat{g}_1(z-Z_0) + \cdots \tag{6.46}$$

it can be viewed as an "induced cosmological term" [78] for the IFT (6.38). Note, that $\hat{g}_0 = G_{\rm YL}(Z_0)$.

The formula (6.45) allows one to parameterize the scaling function $G_{\rm YL}(z)$ by the coefficients of the series expansions (6.40) and (6.46). Our aim is to determine the leading coefficients of these series by fitting the results of the numerical CTM calculations of the scaling function. Obviously, we need to reasonably truncate the series (6.40) so that the contribution of dropped terms does not exceed the error of the numerical data used for the fit (Looking ahead, we will drop all terms, contributing powers higher than $\mathcal{O}((z-Z_0)^8)$ into the series (6.45)).

Next, note that irrespective of such truncation, the series (6.40) contain an overdetermined set of coefficients, some of which cannot be found solely from the knowledge of the scaling function. To illustrate this point consider a few first terms in the expansion $f_{\rm sing}^{(0)}(z)$, given by (6.43) with $\alpha = 0$

$$f_{\rm sing}^{(0)} = f_{\rm YL}M_{\rm YL}^2 + c_\Xi\beta M_{\rm YL}^{38/5} + c_{\Xi_6}\gamma M_{\rm YL}^{58/5} + \mathcal{O}(M_{\rm YL}^{66/5}) \tag{6.47}$$

where the constants c_Ξ and c_{Ξ_6} are expressed via the vacuum expectation values of the corresponding operators, appearing in (6.39), see eq.(2.5) in [78]. Now, make the following transformations.

First, let us absorb the coefficients $\hat{\gamma}_k$, $k = 0, 1, 2, \ldots$ by redefining $\hat{\lambda}_{k+5}$ in the first term of (6.47). Next, since the coefficients $\hat{\lambda}_k$ also enter the second term via $M_{\rm YL}$ one can compensate their change there by redefining $\hat{\beta}_k$, $k = 4, 5, \ldots$. Therefore, the third term in (6.47) is "redundant" as it could be completely absorbed into the first two. Performing a similar analysis and omitting other redundant terms one can write $f^{(0)}_{\rm sing}$ as

$$f^{(0)}_{\rm sing} = f_{\rm YL} M^2_{\rm YL} + c_\Xi \beta M^{38/5}_{\rm YL} + c_{\Xi\Xi} \beta^2 M^{66/5}_{\rm YL} + c_{\Xi_8} \delta M^{78/5}_{\rm YL} + \mathcal{O}(M^{88/5}_{\rm YL}) \tag{6.48}$$

We would like to stress that the above reduction of the "redundant" terms does not mean that they do not contribute. We just state, that to write a series expansion for $f^{(0)}_{\rm sing}$ suitable for the fitting procedure, the contribution of these terms will be accounted for via a redefinition of the higher coefficients entering the remaining terms in (6.48). In particular, the modified coefficients $\hat{\lambda}_{k+5}$ and $\hat{\beta}_{k+4}$, with $k \geq 0$, will contain additions proportional to $\hat{\gamma}_k$. Moreover, the "induced cosmological term" (6.46) will have an addition proportional to $\sim (z - Z_0)^5 \alpha_5(z)$ coming from the contribution of the $(T\bar{T})^3$ term, contained in (6.39).

It is instructive to consider the series expansion of the scaling function (6.45). A simple (but a bit tedious) analysis of the possible powers of the variable $v = (z - Z_0)$ (to within the order of $\mathcal{O}(v^8)$) leads to the following expression

$$G_{\rm YL}(z) = s_0 v^{19/6} + \sum_{\substack{0 \leq 5k/6 + l \leq 8 \\ 0 \leq k \leq 5}} t_{k,l} v^{5k/6 + l} \tag{6.49}$$

It is worth noting that the coefficients in this formula will not be all independent, since, to within the same order in v, the expression (6.45) contains a lesser number of different coefficients than (6.49). Note also, that using (6.34) one could easily rewrite (6.49) as a series in the variable u defined in (6.35). The reason we prefer the variable v is because the expansion coefficients $t_{k,l}$ in (6.49) do not grow as fast as those for the corresponding expansion in u. Moreover, we could compare our results for the first coefficients $t_{k,l}$ with those obtained in [31].

Since only an approximate location of the singularity Z_0 is known, one must use a nonlinear fit to simultaneously determine the value of Z_0 and coefficients $t_{k,l}$ and b_0 in (6.49). Given this, we used the following iteration procedure.

Starting with some value of Z_0, initially given by (6.33), the function $\Phi_{\rm imh}(z)$ was calculated from (6.31) and (6.24) using the CTM method for about thirty points in the vicinity of Z_0. Then we used the `NonlinearModelFit` package from `Mathematica` to determine the coefficients in (6.49) and a new value of Z_0. Subsequently, the same procedure was repeated with an updated value of Z_0 on each step.

Quite remarkably, the above iterations quickly converge to a rather accurate value of Z_0

$$Z_0^{\rm init} = 2.429169172 \tag{6.50}$$

which was used as an initial value for subsequent calculations. Alternatively, we have also used the nonlinear formula (6.44) to simultaneously determine Z_0 and the coefficients (6.40), (6.46), but this led to the same result (6.50).

Next, we have generated approximately 2000 points in the neighbourhood of $Z_0^{\rm init}$

$$z = Z_0^{\rm init} + (\rho + \delta) e^{i\phi_j}, \quad \phi_j = \frac{\pi j}{6} \quad j = 0, 1, 2, 3 \tag{6.51}$$

with $0 < \rho < 1$, $\delta = 0.002$, and calculated the corresponding values of $\Phi_{\rm imh}(z)$ from (6.31) and (6.24). For further reference, it is convenient to split these points into the sets

$$\Delta_i = \{\, 0.1(i-1) + \delta < |z - Z_0| < 0.1 i + \delta \} \tag{6.52}$$

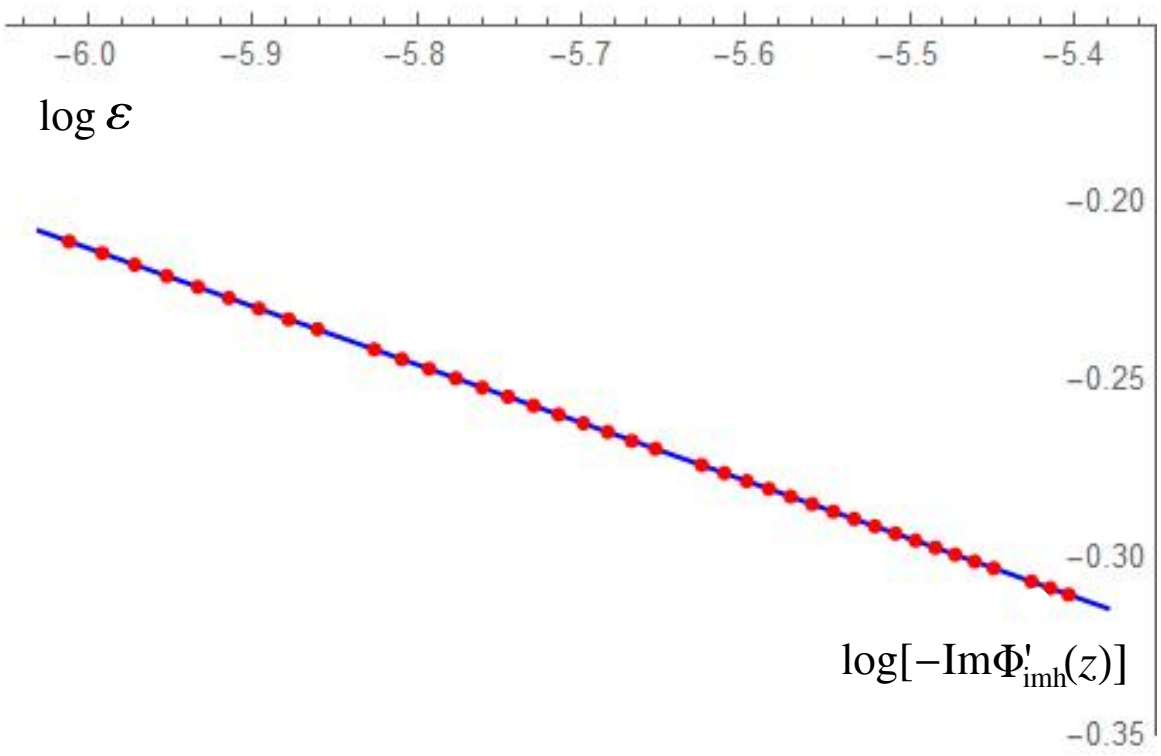


Figure 6.1: Numerical data points (red dots) for $\log[-\mathrm{Im}\Phi'_{\mathrm{imh}}(Z_0+i\epsilon)]$ fitted by eq.(6.54).

where $i=1,\ldots,10$, containing 200 points each. All calculations were done with several values of τ, given by (6.30), for each value of ξ (or z), as previously explained. A difference between the values of the scaling function with the same ξ (but different τ) never exceeded 2×10^{-10}, so we kept 10 decimal figures in our results for $\Phi_{\mathrm{imh}}(z)$.

The first test for our numerical analysis is to demonstrate the presence of the leading singular contribution $(z-Z_0)^{5/6}$ in (6.49) to confirm the CFT prediction (6.49). In doing this, we need to suppress the regular terms $t_{0,0}+t_{0,1}(z-Z_0)$ which smoothen the behaviour of $\Phi_{\mathrm{imh}}(z)$ near $z=Z_0$. This is achieved by differentiating (6.49) with respect to z and considering $\mathrm{Im}\Phi'_{\mathrm{imh}}(z)$ with $z=Z_0+i\epsilon,\ \epsilon>0$ (here the prime denotes the z-derivative). Since we expect $t_{1,0}$ to be real, a simple calculation gives

$$\mathrm{Im}\Phi'_{\mathrm{imh}}(Z_0+i\epsilon)=-\frac{5Z_0^2}{6}t_{1,0}\sin\frac{\pi}{12}\epsilon^{-1/6}+\mathcal{O}\left(\epsilon^{2/3}\right) \tag{6.53}$$

Using a very accurate numerical differentiation, we have calculated the data points for $\mathrm{Im}\Phi'_{\mathrm{imh}}(z)$ in the range $2.5\times10^{-3}<\epsilon<4.5\times10^{-3}$ and obtained the following fit

$$\log[-\mathrm{Im}\Phi'_{\mathrm{imh}}(Z_0+i\epsilon)]=-0.1650\log(\epsilon)-1.204+0.2197\epsilon^{5/6}+\mathcal{O}(\epsilon) \tag{6.54}$$

which also takes into account the correction term in (6.53). The fitting function (6.54) together with numerical data points is shown in Fig.6.1 in the logarithmic scale.

As expected, the plot is very close to the straight line with the slope $-\frac{1}{6}$ with a small deviation due to the next order corrections in (6.53). The result confirms the CFT prediction for the exponent (5/6) of the leading singular term in (6.49) to within 0.2% accuracy (our value is 5.010/6). For the subsequent fits, we used the nonlinear formula obtained from (6.45) and (6.44), with truncated series (6.40) and (6.46) dropping all terms whose contributions into (6.49)

are of the orders higher than $\mathcal{O}\left((z-Z_0)^8\right)$. As follows from our estimates, the coefficients $t_{k,l}$ for such terms appear be of the order 10^{-2} and smaller. This means that for $|z-Z_0|<0.2$ contributions of the discarded terms are expected to be of the order of 10^{-9} or less.

For this reason the main nonlinear fit for $\Phi_{\rm imh}(z)$ we used 400 points (6.51) with $0<\rho<0.2$, i.e., for which $z\in(\Delta_1\cup\Delta_2)$, as defined in (6.52). Subsequently, the accuracy of the fit was tested for all subsets (6.52) of calculated data points. The Table 6.1 contains the maximum difference (error) between the value of the fit and a numerical value of $\Phi_{\rm imh}(z)$ calculated with the CTM method,

$$\Sigma_i=\max_{z\in\Delta_i}|\Phi_{\rm imh}(z)-\Phi^{\rm CTM}_{\rm imh}(z)| \tag{6.55}$$

Table 6.1: The maximum error between $\Phi^{\rm trun}_{\rm imh}(z)$ and $\Phi^{\rm CTM}_{\rm imh}(z)$ for the points $z\in\Delta_i$.

i	1	2	3	4	5	6	7	8	9	10
Σ_i	1.1×10^{-10}	4.3×10^{-11}	1.8×10^{-8}	3.0×10^{-7}	1.8×10^{-6}	1.6×10^{-5}	1.2×10^{-4}	6.5×10^{-4}	3.1×10^{-3}	1.3×10^{-2}

Since the points $z\in\{\Delta_1\cup\Delta_2\}$ were used for the fit, it is not surprising that for $i=1,2$ the error is of the order of 10^{-10} or less. In fact, it coincides with the accuracy of our numerical calculations of $\Phi_{\rm imh}(z)$. The same accuracy also holds for the location of the singularity

$$Z_0=2.4291691718(2). \tag{6.56}$$

arising from our final fit. The corresponding position of the singular point ξ_0 for $G_{\rm high}(\xi)$ is

$$i\xi_0=i0.18935060551(3) \tag{6.57}$$

Further, Table 6.1 shows that for the subsequent sets $z\in\Delta_i$, with $i\geq3$, the accuracy of the fit drops down, which is natural due to an increasing effect of truncation of the series (6.49). Nevertheless, the value of Z_0, given in (6.56), remains stable, even if points $z\in\Delta_i$, with $i\geq3$, are included in the fit.

The final fit for the coefficients $\hat{g}_k$, $\hat{\lambda}_k$ and $\hat{\alpha}_k$ from (6.40) and (6.46) is shown in Table 6.2. Let us notice that the higher coefficients may be correct only up to 1-2 significant digits due to the series truncation. The lower coefficients should be still correct up to 8-9 digits. It is hard to estimate the number of correct digits in each coefficient, so we left them as they were produced by `Mathematica`.

Let us comment on this in more detail. We need to use all digits in coefficients in Table 6.2 to produce accurate values for $\Phi_{\rm imh}(z)$ from Appendix. Any truncation will cause a significant deviation from the values given there. It seems that this contradicts the statement from the previous paragraph. The explanation is that the series (6.49) contains too many independent powers in v with a very small separation of exponents. As a result, one can construct another fit for $\Phi_{\rm imh}(z)$ which will reproduce the data from Appendix with 10^{-10} accuracy, but higher coefficients will coincide only up to 1-2 significant digits. In other words, one needs the data with much higher precision to get reliable information about coefficients with $k>2$ in Table 6.2.

Now let us give coefficients $t_{k,l}$ of the series expansions (6.49) for the function $G_{\rm YL}(z)$. They are shown in Table 6.3. The coefficient s_0 coming from the leading power in the second term of (6.48) is estimated as

$$s_0=0.0623126407. \tag{6.58}$$

Let us notice that to get the series expansion for $\Phi_{\rm imh}(z)$ from $G_{\rm YL}(z)$ we could use (6.31). However, due to the presence of the extra factor $(Z_0+v)^2$, coefficients for $\Phi_{\rm imh}(z)$ will be in the range $(0.1,0.5)$.

Table 6.2: Coefficients $\hat{g}_k$, $\hat{\lambda}_k$ and $\hat{\alpha}_k$

k	$\hat{g}_k$	$\hat{\lambda}_k$	$\hat{\alpha}_k$
0	0.0928378351	—	-1.3478038278
1	0.1035665061	0.1720881869	0.0845043112
2	-0.0406336255	-0.0530975348	-0.1988535226
3	-0.1021530341	-0.0432647893	0.1096925182
4	0.0622170621	-0.0060926724	0.0588155481
5	-0.0427391325	0.0015477546	-0.0907062356
6	0.0367166751	-0.0026569648	0.0650203209
7	0.0120039152	-0.0046983681	—
8	-0.0179189367	-0.0050775498	—

We can also get an estimate for the term $c_\Xi \beta(z)$ in (6.48)

$$c_\Xi \beta(z) = 0.01015847 + 0.0070108v + 0.009344v^2 + 0.006279v^3 - 0.00058v^4 + \dots \tag{6.59}$$

where $v = z - Z_0$. From the third term in (6.48) we can estimate $c_{\Xi\Xi}$

$$c_{\Xi\Xi} \approx 7.69 c_\Xi^2. \tag{6.60}$$

Finally, from the expansion for the fourth term in (6.49) we obtain

$$c_{\Xi_8} \delta(z) = -0.00064 - 0.00094(z - Z_0) + \dots \tag{6.61}$$

It appears, that the values in (6.59-6.61) should be understood only as an order-of-magnitude estimate.

Note that the value of $t_{1,0}$ can also be estimated from (6.54)

$$t_{1,0} \approx -\frac{6}{5Z_0^2 \sin(\pi/12)} \exp(-1.204) \approx -0.236 \tag{6.62}$$

which is below the more accurate value

$$t_{1,0} = 2 f_{\rm YL} C_{\rm YL}^2 \hat{\lambda}_1^{5/6} = -0.232638\dots \tag{6.63}$$

The discrepancy is mostly caused by the fact that (6.54) contains an approximate "fitted" value of the leading coefficient $-1/6$, while in (6.49) the related exponent $5/6$ is set to its exact value.

Next, we present a few coefficient functions $G_k(u)$ in the expansion of $G_{\rm high}(\xi)$ near $\xi = \pm i\xi_0$ in terms of variable $u = \xi^2 + \xi_0^2$

$$G_{\rm YL}(\xi) = G_0(u) + G_1(u) u^{\frac{5}{6}} + G_2(u) u^{\frac{5}{3}} + G_3(u) u^{\frac{5}{2}} + \cdots \tag{6.64}$$

$$\begin{aligned} G_0(u) &= 0.09284 + 1.871u + 19.8u^2 - 371u^3 + \dots \\ G_1(u) &= -2.5947 - 26.154u - 172u^2 + \dots \\ G_2(u) &= 9.076 + 171.35u + 2091u^2 + \dots \\ G_3(u) &= -31.75 - 878.7u + \dots . \end{aligned} \tag{6.65}$$

Table 6.3: Coefficients $t_{k,l}$ of the truncated scaling function $G_{\rm YL}(z)$ from (6.49)

l \ k	0	1	2	3	4	5
0	0.0928378351	-0.2326384010	0.0729439864	-0.0228716546	0.0071714285	-0.0201278728
1	0.1035665061	0.0598168387	-0.0420846767	0.0205105351	-0.0087246739	-0.0105062255
2	-0.0406336255	0.0502778268	-0.0135928541	0.0012416359	0.0012912732	-0.0151031033
3	-0.1021530341	0.0095546595	-0.0076813505	0.0222269546	-0.0081326053	-0.036304106
4	0.0231406896	0.0184911041	-0.0070095153	-0.0314395832	0.0212048796	
5	-0.0183244972	-0.0135214010	0.0173465826	0.0001177947		
6	0.0426269803	0.0054321576	-0.0088442156			
7	0.0237701200	-0.0002697285				
8	0.0032474000					

It is instructive to compare the previous results [47] for the scaling function $G_{\rm high}(\xi)$ (given in (3.196) and Table 3.7.2) and our new results for the function $G_{\rm YL}(\xi)$ for purely imaginary values of the argument $\xi = ix$ in the interval $x \in (0, 0.2)$. As shown in Fig. 6.2, the two functions match very well in the intermediate region and deviate from each other towards the ends of the interval.

Finally, note that our results for the leading coefficients of the coupling constant

$$\lambda(z) = \hat{\lambda}_1 v + \hat{\lambda}_2 v^2 + \ldots = \lambda_1 u + \lambda_2 u^2 + \ldots \tag{6.66}$$

are in excellent agreement with the results of [31, 78] (the variables v and u are defined in (6.34) and (6.35)). Indeed, our values

$$\lambda_1 = 3.10916(2) \qquad \lambda_2 = 37.6(8) \tag{6.67}$$

corresponding to $\hat{\lambda}_1, \hat{\lambda}_2$ from Table 6.2, perfectly match the values $\lambda_1 = 3.089 \pm 0.008$ $\lambda_2 = 38.4 \pm 1.6$, given by eq.(4.7) of [78]. Similarly, their values for $f_0 = 0.092746\ldots$ (denoted here as $\hat{g}_0$) and for $\hat{\alpha}_0 = -1.32 \pm 0.05$, given in their eqs. (3.10) and (4.8), respectively, match our values presented in Table 6.2.

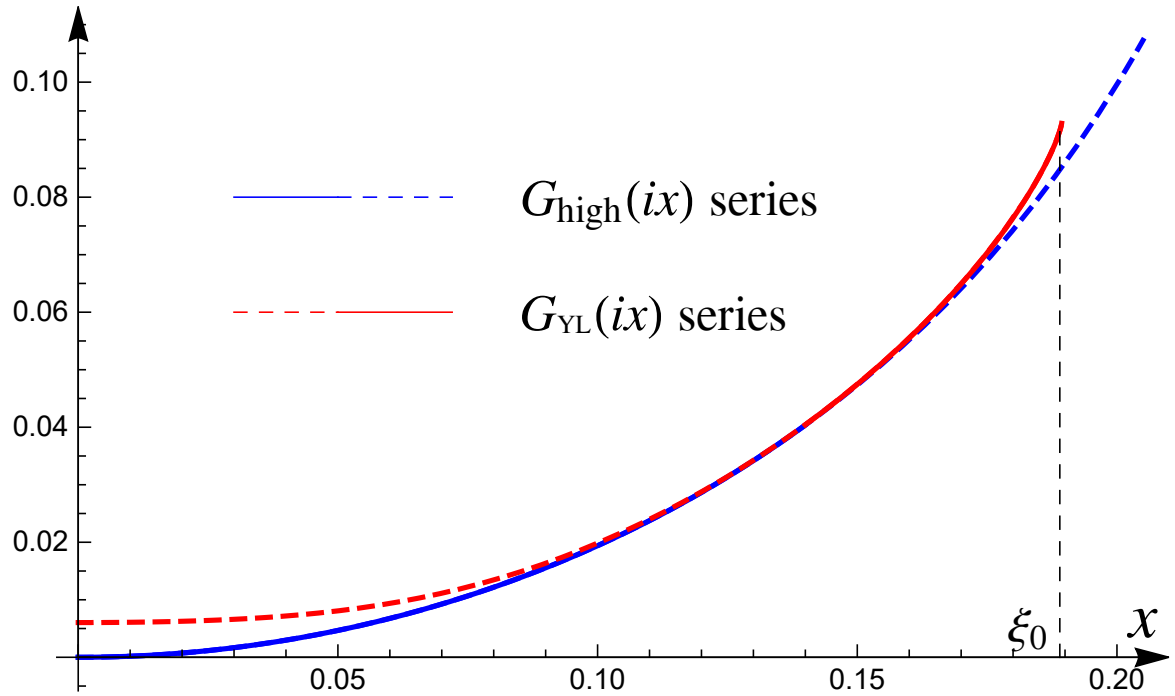


Figure 6.2: A comparison of $G_{\text{high}}(\xi)$ and $G_{\text{YL}}(\xi)$ along the imaginary axis $\xi = ix$

CHAPTER 7

CONCLUSION

This project set out to contribute an improved quality estimate of the location of the Yang-Lee singularity for the 2D Ising model. It has presented an improved estimate at $i\xi_0 = i0.18935060551(3)$. Further, it has generated numerical verification of the scaling function conjecture of Fonseca & Zamolodchikov [31] regarding the structure of the free energy scaling function near the Yang-Lee singularity. Lastly, it presents an updated free energy scaling ansatz that incorporates logarithmic operators at order H^2 evidenced by the susceptibility data [56, 22].

To accomplish these results, this project covered the salient slice of the Ising model's history in chapter 2, with attention to the Ising scaling theory, universality and renormalisation. In doing so we demonstrated the problem set presented by the Ising model—the prototypical "toy" model in statistical physics—delving into its surface simplicity but deeper, complex mathematical structures.

Chapters 3 and 4 covered key theoretical groundwork and tools used to unpack our analysis. Chapter 3 contained a study of conformal field theory fundamentals—drawing in particular on the infamous "Big Yellow Book" [35]. After establishment these tools were immediately utilised to navigate the Yang-Lee singularity, logarithmic conformal field theory and the Ising field theory of Zamolodchikov [82, 31].

Chapter 4 outlined the relevance of susceptibility to the project as a key apparatus. From the extended susceptibility data we were able to enumerate series expansions for key components of the Ising free energy scaling ansatz.

Chapters 5 and 6 prepare and present the main numerical results. In chapter 5 we surveyed supporting methodologies and theories for the main numerical technique used, the Corner Transfer Matrix Renormalisation Group (CTMRG) method, a method developed from the marriage of Baxter's variational analysis [11] and White's Density Matrix Renormalisation Group (DMRG) algorithm [74] by Nishino & Okunishi [53]. Using the CTMRG method, we produced a high accuracy partition function per site κ estimate for the region of interest, near $i\xi_0$. The free energy and scaling function could be extracted from this data. The data was analysed and tests were performed to verify the conjectured Yang-Lee expansion for the scaling function. Already established results for this expansion combined with the high accuracy CTMRG data yielded an improved estimate for the singularity ξ_0. The field would further benefit from supplementary analysis of the first order logarithmic operators that fell outside the scope of this project.

The door is wide open for continued exploration of the 2D Ising model. While the real domain is relatively well understood, the analytic continuation still lacks deep exploration

and categorisation. Through thoroughly studying key areas of interest such as the Yang-Lee singularity, we hope to delineate the subject and work towards the goal of obtaining a complete understanding of the model. An exhaustive understanding of the Ising model would undoubtedly bolster our understanding of statistical theories at large, integrable systems and many other important fields of study.

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