

Imperial College London
Department of Department of Mathematics

On Topics in Equilibrium and Non-Equilibrium Statistical Physics

Gary Willis

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Supervised by Andrew Parry and Gunnar Pruessner

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Declaration

I herewith certify that all material in this thesis which is not my own work has been properly acknowledged.

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Gary Willis

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List of Symbols

Chapter 1

- N - The linear extent of the system being studied
 B - The dilation factor used in the coarse graining procedure
 T_c - Critical temperature
 t - Reduced temperature given by $\frac{|T-T_c|}{T_c}$
 λ - Eigenvalues of the Jacobian Matrix
 Z - The partition sum
 k_B - Boltzmann's constant
 β - Inverse temperature or $\frac{1}{k_B T}$
 H - Magnetic Field
 h - Reduced magnetic field given by $\frac{H}{k_B T}$
 s_i - The state of the i^{th} spin of a system
 S_I - The coarse grained equivalent of s_i
 $\{s_i\}$ - Information about the state of every spin in a system, giving its state
 J - Strength of nearest neighbour interactions in Ising Model
 ξ - Correlation length
 y_t - Thermal critical exponent
 y_h - Magnetic critical exponent
 d - The dimensionality of the problem being studied
 σ_x - Standard error associated with a variable x
 ν - Correlation length exponent
 δ - Magnetic critical exponent
 $T(S_I, s_i)$ - Transformation kernel relating coarse grained configurations to original ones
 $H(\{s_i\})$ - The Hamiltonian evaluated for a spin configuration $\{s_i\}$
 Q - The number of orthogonal spin states possible in a Q-state Potts Model
 $\hat{\mathcal{R}}$ - Coarse graining operator
 $\hat{\mathcal{C}}\mathcal{S}$ - Column switch operator

$\hat{R}_S$ - Row switch operator
 $\hat{M}$ - Mirroring operator
 $\hat{P}_{cy}$ - Cyclic permutation operator
 $\hat{R}_x$ - Operator corresponding to x degree rotation

Chapter 2

(Only symbols which are different to, or not present in Chapter 1 are mentioned)

$\mathcal{G}(z_1, z_2; q)$ - Density-density (or spin-spin) correlation function, Fourier Transformed in the transverse plane, as obtained by solving the Ornstein-Zernicke Equation

$G(z_1, z_2; q)$ - Quantity equivalent to $\mathcal{G}(z_1, z_2; q)$ obtained from interfacial Hamiltonian theory

$\sigma(q)$ - Wave vector dependent surface tension characterised by a wave vector q

$m(z)$ - Magnetisation-like order parameter

z - The spatial direction in which translational invariance has been broken

r - Euclidean separation

$f(m)$ - Free energy

H_{LGW} - Landau-Ginzburg-Wilson Hamiltonian

κ - Inverse bulk correlation length

$\delta(x)$ - Dirac Delta function

$S(z; q)$ - Position dependent structure factor

$S(q)$ - Total structure factor

$\kappa_q = \sqrt{\kappa^2 + q^2}$

$G^b(z; q)$ - Correlation function of a bulk liquid/gas/Ising system

H_{CW} - Capillary Wave Hamiltonian

σ - Surface tension of an interface

$\ell(\underline{y})$ - Position of the interface

$m_\pi(z)$ - Planar (equilibrium) profile of a free interface

$m_\Xi(z, \underline{y})$ - Lowest energy profile of a free interface subject to a crossing criterion constraint

m^x - m value chosen as the definition of the interface

z^x - z value for which $m(z) = m^x$

$\Lambda(z; |y - y'|)$ - Function which governs how $m_\Xi(z, \underline{y})$ depends on $\ell(\underline{y}')$

$b(q)$ - Factor introduced by hand to amend crossing criterion
 $G_{\Xi}(|y - y'|)$ - Floating correlation function
 γ - Bending rigidity or 2^{nd} moment of $\sigma(q)$
 g_2 - Coefficient of gradient term in extended LGW Hamiltonian
 g_4 - Coefficient of square gradient term in extended LGW Hamiltonian
 $\gamma_{\kappa} = \sqrt{|\frac{g_2^2}{4g_4^2} - \frac{\kappa^2}{g_4}|}$
 $\Lambda_{\pm} = \frac{g_2}{2g_4} \pm \gamma_{\kappa}$

Chapter 3

a_i - Operator which represents the effect of driving a system at site i and allowing it to fully relax
 a_u - Random/uniform version of a_i
 e_i - Eigenvector of a_i with eigenvalue 1
 L - Linear extent of the system
 $\langle Av \rangle$ - Expected avalanche size
 $r(x, t)$ - Average number of topplings at position x , a (microscopic) time t after system has been driven
 $R(x)$ - Time integrated activity given by $\sum_{t=0}^{\infty} r(x, t)$
 $T_{\alpha\beta}$ - Markov/Transition matrix denoting the probability of the system transitioning to a relaxed state β , given it was in state α before being driven
 $(R_R)_{\alpha\beta}$ - Probability of system being in relaxed state β immediately after a drive, given it was in state α before ("relaxed-relaxed")
 $(R_A)_{\alpha\beta}$ - Probability of system being in active state β immediately after a drive, given it was in state α before ("relaxed-active")
 $P_{\gamma\beta}$ - Probability of active state γ relaxing to state β via any permissible path (only relevant to tree method)
 u_{α} - Fraction of the time a system finds itself in state α once it has reached its steady state
 $(A_R)_{\alpha\beta}$ - Probability that given system is in active state α , it will, after one iteration of microscopic time, be in relaxed state β ("active-relaxed").
 $(A_A)_{\alpha\beta}$ - Probability that given system is in active state α , it will, after one iteration of microscopic time, be in active state β ("active-active").
 $\mathcal{I}$ - Identity matrix
 $P(n)$ - Probability of an avalanche of duration n

$A_{\alpha x}$ - Number of topplings which will occur at site x of an active state α when it updates

F_α - Total number of topplings which occur when state α updates (given by $\sum_{x=1}^{x=L} A_{\alpha x}$)

Thesis Outline

This thesis divides very naturally into three chapters, reflecting the three separate areas I have worked in throughout my PhD studies. During my PhD, I published two papers, one relating to the work in the first chapter, and one to that of the second. At the time of submission, the project which the third chapter relates to was still ongoing, with plans for a future publication.

The first chapter discusses work done on the real space renormalisation group (RG) for Ising and Potts models in 2 dimensions. Taking inspiration from Hasenbusch's work, a new framework for carrying out the RG is developed, its computational implementation discussed in some detail, as well as the results for a variety of systems and the implications of these results. The numerical scaling of the procedure and the consequences of this for future work are also covered.

The results documented in chapter two are purely theoretical and presented in closed form. The research conducted is to do with properties of free interfaces. The second chapter is by and large critical of previous assumptions which have been made about the so-called wave vector dependent, in order to attempt to experimentally measure it and use these measurements to make further predictions. Using some simple toy models, many of these assumptions are shown to be false. In a sense, the goal of the research presented in the chapter two, is not to motivate further research, but to dissuade research in a direction we consider to be misguided, due to the faulty assumptions it is based on.

The third chapter covers a small subset of a project concerned with studying correlations within the so-called Abelian Manna Model. The majority of the project involves (computational) Monte Carlo simulations of the dynamics of such systems, but as these results are not ready to present at the time of writing, the chapter is mainly concerned with some analytical results which were derived in order to validate our models for small systems,

explain certain quirky phenomena arising from our simulations, and help quantify errors.

Finally, there is an appendix which expands upon various topics from the first two chapters.

1. "Exact" Real-Space Renormalisation of the Ising and Potts Models on Small 2-Dimensional Lattices

The work in this chapter presents, expands and extends upon results which were published in *Frontiers in Computational Physics*, 23 June 2015 [92].

Abstract

Hasenbusch's [40] Method of implementing the Real Space RG by calculating the full partition sum for the Ising Model on a 4×4 lattice was extended to include magnetic interactions and be applicable on triangular lattices as well as for the more general Q -State Potts Model. Hasenbusch's remarkable result, that tiny lattices contain information about larger ones which can only be accessed via the RG holds up robustly. For higher Q Potts Models, multiple magnetic exponents are found whose origins are not entirely clear. Likewise (and given certain features of the method unsurprisingly), this procedure fails to capture the transition becoming discontinuous (first order) for $Q > 4$.

1.1. Outline

This Chapter begins by discussing the theoretical background behind the process of coarse graining and using the procedure to calculate critical exponents. All of this theoretical framework has been around for circa 40 years, and thus is presented in a "textbook" style. By this, it is meant that it is not necessarily presented chronologically in terms of when various breakthroughs were made, but simply in the order which makes it easiest to comprehend.

Next, a particular implementation of the position space RG is discussed in quite some detail. I had the good fortune to come across a set of notes by Hasenbusch [40] during the first month of my PhD, and my work builds on some key ideas (one in particular), outlined in Hasenbusch's work. Perhaps even more importantly however, Hasenbusch's successful implementation of the method provided me the inspiration to conduct all of the research contained within this chapter.

After this initial recap, a small extension to Hasenbusch's work is outlined (one which he actually suggested at the end of his notes), and a short analysis of the significance of both Hasenbusch's original results, and my minor extension is provided. Subsequently, I introduce the "categories method", which at first might seem like an arduous reformulation of Hasenbusch's method, but it turns out to be necessary to study systems other than the Ising Model on a 4×4 lattice. As the methods discussed all require computational evaluation, some computational tricks and limitations are also mentioned at this point, in particular an object I refer to as the "god tensor", as without it, it would not have been feasible to study many of the systems I ended up getting results for.

Next, the results of implementing the categories Hamiltonian for the $Q = 2 - 5$ Potts Model on a square lattice are presented in full. This is followed by a section on a rather strange result, related to the categories Hamiltonian, called "combining categories".

After discussing how to "combine categories", a framework for implementing the categories Hamiltonian on triangular lattices is introduced. It is only introduced at this late stage (i.e. after the square lattice results), because the methodology required to "combine categories" is necessary to understand my implementation. The results for the triangular lattice are

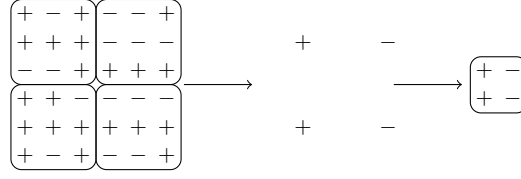


Figure 1.1.: Schematic of the procedure of a Kadanoff Block Spin Transformation based on a majority rule.

also included in this section.

A result common to the square and triangular lattices, is how the results for $Q = 5$ deviate substantially from what is theoretically predicted, and this is subsequently discussed. Before making any final remarks, a short section is included regarding the 4-state clock model. The result is rather nice and backs on the rest of my findings in this chapter, but there was no natural place to slot this is, so I have put it at the end.

Finally, some conclusions/interpretations are provided, and the limitations of the model are discussed further in the context of possible future work.

1.2. General Background Theory

1.2.1. Block Spinning Procedure

Kadanoff [45] proposed that because spins in the Ising Model [44] are correlated over a length scale ξ (known as the correlation length), it may be reasonable to treat regions of spins smaller than this as acting like a single spin. Thus Kadanoff proposed a procedure to systematically decrease the degrees of freedom of a system, referred to as a "Kadanoff Block Spin Transformation" as is outlined in Figure 1.1. The process maps spins s_i on an $N \times N$ lattice (in Figure 1.1 $N = 6$) to spins S_I on a so-called coarse-grained lattice. Blocks of spins of size $B \times B$ are constructed and replaced by a single spin based on a majority rule, that is to say if a $B \times B$ patch contains more positive spins than negative, it is replaced with a single positive spin and vice-versa. After performing the procedure, only $\frac{N}{B} \times \frac{N}{B}$ spins remain. Finally the lattice is rescaled to regain the original lattice spacing. Hence all length scales are rescaled by a factor of B , including the correla-

tion length.

1.2.2. Effect of Coarse Graining

The result of coarse graining is that fluctuations on length scales shorter than the blocking factor B will be averaged out. For Ising systems in which the temperature is well below the critical one, mainly spins of just one species will prevail and successive iterations of the coarse graining procedure will tend to remove the small clusters of remaining minority spins which still exist[94]. Likewise for high temperatures, well above the critical one, the system is highly disordered with only a few small clusters of either spin species present. The coarse graining procedure will tend to break up these small clusters and the system tends to a fully disordered state. It is only if the system is at exactly the critical temperature, that it is self similar and that repeated applications of the process will not affect the temperature. This can best be understood in terms of the correlation length: coarse graining will decrease the correlation length, and thus the typical largest size of spin clusters by a factor of B . Only at the critical temperature is the correlation length infinite and clusters of all sizes exist. Thus after applying the block spin process, the correlation length is still infinite. The critical temperature acts as an unstable fixed point[93], much like the apex of a one-dimensional hill. If a marble sits at exactly the top (equivalent to the stationary point of an upside-down parabola), it will not move. If however, it is placed infinitesimally to the left or the right, it will as time progresses roll further and further from the stationary point.

Working in terms of the reduced temperature $t (= \frac{T-T_c}{T_c})$, note that the transformed temperature t' must be a function of t only, i.e. $t' = t'(t)$. Likewise, $t'(0) = 0$. Thus if $t'(t)$ is analytic, then to first order, $t'(t) = \lambda(B)t$. Furthermore, applying the procedure by a factor B_1 and then B_2 must be commutative and likewise equivalent to performing it in only a single iteration of dilation factor $B_1 B_2$. Thus mathematically:

$$\lambda(B_1)\lambda(B_2) = \lambda(B_2)\lambda(B_1) = \lambda(B_1 B_2) \quad (1.1)$$

whose unique solution is a power law of the form $t' = B^y t$ [18]. A similar argument applies for the magnetic field which is intuitively easier to understand. When the external field is zero (for simplicity's sake, assume

$T > T_c$), there are broadly speaking equal numbers of up and down spin species present and coarse graining should not affect this imbalance. Next however, picture blocking spins by a factor of $B = 3$. It should occur approximately equally frequently that these 3×3 blocks contain 5 up spins and 4 down as the reverse. However, in the presence of a relatively weak external field which creates only a moderate imbalance between one spin species and the other, it will now occur considerably more frequently that there will be five majority spin species in a 3×3 block and thus the imbalance becomes amplified. Thus similarly to temperature, $h(= \frac{H}{k_B T}) = 0$ represents an unstable fixed point and being slightly off the fixed point will result in h becoming amplified by successive applications of the process. Similar mathematical arguments apply and one usually writes

$$\begin{aligned} t' &= B^{y_t} t \\ h' &= B^{y_h} h \end{aligned} \tag{1.2}$$

to describe the evolution of the effective magnetic field and temperature under successive applications of the coarse graining procedure.

1.2.3. Transformation of the Hamiltonian

Let us demand that the process of coarse graining preserves the partition sum, i.e.:

$$Z = Z' \tag{1.3}$$

Note that it is conventional to use primes to denote variables after an iteration of the coarse graining procedure, to use s_i to describe spins on the original lattice and to use S_I to denote spins on the coarse-grained lattice. One way of satisfying condition (1.3) is splitting Z into two sums (using the conventional notation of $\beta = (k_B T)^{-1}$):

$$Z = \sum_{\{S_I\}} \sum_{\{s_i\} \rightarrow S_I} e^{-\beta H(\{s_i\})} = \sum_{\{S_I\}} e^{-\beta H'(\{S_I\})} = Z' \tag{1.4}$$

which is satisfied if:

$$e^{-\beta H'(\{S_I\})} = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} \tag{1.5}$$

In order for (1.5) to be satisfied, it is necessary for the Hamiltonian to be transformed by the process (as denoted by the prime).

Decimation in 1d

While I have used the block spin method outlined in Figure 1.1 throughout my actual research, I will first show how the Hamiltonian transforms using the method of decimation [18] for illustrative purposes.

In 1 dimension, the Ising Model lives on a lattice best visualised as spins in a row with a constant lattice spacing. Each spin s_i interacts with its two nearest neighbours, s_{i-1} and s_{i+1} . Coarse-graining would involve splitting the lattice into clusters of B spins, replacing each of these with one spin based on a majority rule and finally rescaling the lattice to restore the original lattice spacing. Decimation on the other hands involves splitting the lattice into groups of B spins and replacing them with one of the spins in the block, chosen in a consistent way. Consider first the case of grouping the spins into clusters of 2 and replacing these groups with the odd spin (which is an arbitrary choice, it could just as easily be the even spin, so long as this is consistent). Thus spins s_0 and s_1 are replaced by s_1 and so on. The original partition sum is given by:

$$\begin{aligned}
 Z(\beta K) &= \sum_{\{s_i\}} e^{\beta k \sum_{\langle ij \rangle} s_i s_j} = \sum_{s_0=\pm 1} \sum_{s_1=\pm 1} \dots \sum_{s_{N-1}=\pm 1} e^{\beta k (s_0 s_1 + s_1 s_2 + \dots + s_{N-2} s_{N-1} + s_{N-1} s_0)} \\
 &= \sum_{\substack{\text{odd} \\ \text{spins}=\pm 1}} \left(\sum_{s_0=\pm 1} e^{\beta k (s_{N-1} s_0 + s_0 s_1)} \right) \dots \left(\sum_{s_{N-2}=\pm 1} e^{\beta k (s_{N-3} s_{N-2} + s_{N-2} s_{N-1})} \right) \\
 &= \sum_{\substack{\text{odd} \\ \text{spins}=\pm 1}} 2 \cosh [\beta k (s_{N-1} + s_1)] 2 \cosh [\beta k (s_1 + s_3)] \dots 2 \cosh [\beta k (s_{N-3} + s_{N-1})]
 \end{aligned} \tag{1.6}$$

which contains the implicit assumption that there are an even number of spins and makes use of periodic boundary conditions. Now we make the (for now somewhat arbitrary looking) substitution:

$$2 \cosh [\beta k (s_1 + s_3)] = e^{\beta K'_0 + \beta k'_1 s_1 s_3} \tag{1.7}$$

and thus, realising that $\sum_{\substack{\text{odd} \\ \text{spins}=\pm 1}}$ is equivalent to $\sum_{\{S_I\}}$, i.e. the sum over all

decimated configurations, we see that the partition sum before decimation is related to that after:

$$\begin{aligned}
Z &= \sum_{\{S_I\}} e^{\beta(K'_0 + K'_1 s_{N-1} s_1)} e^{\beta(K'_0 + K'_1 s_1 s_3)} \dots e^{\beta(K'_0 + K'_1 s_{N-3} s_{N-1})} \\
&= \sum_{\{S_I\}} e^{\beta \left(N' K'_0 + K'_1 \sum_{\langle IJ \rangle} S_I S_J \right)} \tag{1.8}
\end{aligned}$$

(1.8) is valid if and only if (1.7) holds for all possible values of s_1 and s_3 . The decimation process coupled with the condition of partition sum invariance have transformed the Hamiltonian, albeit to one which looks quite similar to that of the original lattice. It incurs an offset term but more importantly K and K'_1 might be equivalent terms, they describe the strength of nearest neighbour interactions on the original and decimated lattices respectively, but they are not equal. (1.7) can be inverted by realising that $s_1 + s_3$ can only evaluate to $-2, 0$ or 2 (but $\cosh$ is even so the LHS can only take two values) while $s_1 s_3$ will evaluate to -1 or 1 respectively. The result is that:

$$\begin{aligned}
\beta K'_0 &= \ln \left(2 \sqrt{\cosh(2\beta K_1)} \right) \\
\beta K'_1 &= \ln \left[\sqrt{\cosh 2\beta K} \right] \tag{1.9}
\end{aligned}$$

By examining (1.9), it can easily be seen that $K'_1 \leq K_1$ [18] and thus by repeated application of this procedure, the effective nearest-neighbour coupling decreases at each iteration. Note that terms of the form $N' K'_0$ will not affect any expectation values as they don't affect relative probabilities of microstates. Each iteration of this procedure in effect produces a system with a higher temperature. Repeated iterations will cause the effective temperature to increase to infinity if we demand the partition sum must remain constant. This result comes about because the critical temperature of the Ising Model in 1 dimension is exactly 0 [44]. Only if the initial temperature is exactly zero (meaning $\beta K_1 = \infty$), is the temperature still zero after an iteration of the coarse graining procedure and consequently will remain so for any number of iterations.

Likewise, I repeated this argument for decimation by blocks of three, that is to say diving the lattice into blocks of three and keeping only the

central site. The result is similar, one generates an offset term and a nearest neighbour coupling remains but the value is not equal to that of the original system but rather (absorbing the inverse temperature into the couplings):

$$\begin{aligned} K'_0 &= \ln \left[\left(e^{3K_1} + 3e^{-K_1} \right) \left(e^{-3K_1} + 3e^{K_1} \right) \right] \\ K'_1 &= \frac{1}{2} \ln \left[\frac{e^{3K_1} + 3e^{-K_1}}{e^{-3K_1} + 3e^{K_1}} \right] \end{aligned} \quad (1.10)$$

in which again, K'_1 is strictly smaller than K_1 . Note that if we did not know how to calculate the partition sum analytically via a transfer Matrix [44], this would present a convenient way to calculate Z . For example, it is trivial to sum over all configurations on a 2 site lattice in order to calculate the partition sum. It is however an entirely non-trivial task to do so for a 54-site lattice, even with modern computing power. Generating all of the possible configurations on a 162 site lattice is entirely outside of the reach of what modern computers could handle in a human lifetime (note that $54 = 2 \times 3 \times 3 \times 3$ and $162 = 54 \times 3$). Computationally however, it is trivial to calculate K'''_1 from any given K_1 using (1.10) and similarly to calculate K'_0, K''_0 and K'''_0 . It follows that

$$Z_{54}(K_1) = e^{18K'_0} e^{6K''_0} e^{2K'''_0} Z_2(K'''_1) \quad (1.11)$$

in which Z_n denotes the partition sum of an n -site, 1-dimensional lattice as a function of a nearest-neighbour coupling. Similarly:

$$Z_{162}(K_1) = e^{54K'_0} Z_{54}(K'_1) \quad (1.12)$$

Thus once the flow equations ((1.10) and (1.9)) have been determined, the coarse graining procedure can facilitate the explicit calculation of the partition sum of systems which otherwise have far too many degrees of freedom to enumerate.

Decimation in 2d

In 2 dimensions, decimation can be implemented by splitting the lattice (see Figure 1.2) into an even and odd sublattice, removing one or the other all together and then rescaling the lattice. As in 1 dimension, it is instruc-

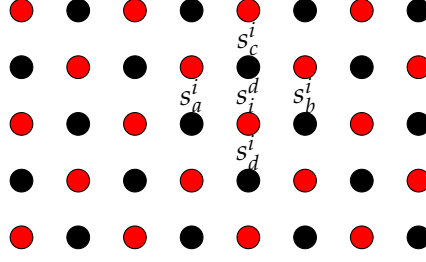


Figure 1.2.: A 2 dimensional lattice split into an even and odd sublattice denoted by shading. Decimation will involve removing either all red or all black sites and then rescaling the lattice. Sites which were previously next-nearest neighbours become nearest neighbours. s_i^d denotes a site which will be removed by decimation, s_j^i are the four nearest neighbours of site s_i^d .

tive to split the partition sum up into sums over the even and odd sublattices:

$$Z(\beta K) = \sum_{\{s_i\}} e^{\beta K_1 \sum_{\langle ij \rangle} s_i s_j} = \sum_{\text{even}=\pm 1} \sum_{\text{odd}=\pm 1} e^{\beta K_1 \sum_{\langle ij \rangle} s_i s_j} \quad (1.13)$$

Next, expand this about every site which is to be decimated, i.e.

$$\begin{aligned} Z(\beta K) &= \sum_{\text{even}=\pm 1} \left(\sum_{s_1^d=\pm 1} \sum_{s_2^d=\pm 1} \dots \right) e^{\beta K s_1^d (s_1^1 + s_2^1 + s_3^1 + s_4^1)} e^{\beta K s_2^d (s_1^2 + s_2^2 + s_3^2 + s_4^2)} \dots \\ &= \sum_{\text{even}=\pm 1} 2 \cosh \left[\beta K (s_1^1 + s_2^1 + s_3^1 + s_4^1) \right] 2 \cosh \left[\beta K (s_1^2 + s_2^2 + s_3^2 + s_4^2) \right] \dots \end{aligned} \quad (1.14)$$

in which $s_1^1, s_2^1, s_3^1, s_4^1$ are the four nearest neighbours of the first site to be removed by decimation. Similarly to the 1 dimensional case, the at first quite arbitrary seeming change of variables will be quite instructive:

$$2 \cosh \left[\beta K (s_1^i + s_2^i + s_3^i + s_4^i) \right] = e^{\beta K'_0 + \frac{\beta K'_1}{2} (s_2^i s_4^i + s_4^i s_3^i + s_3^i s_1^i + s_1^i s_2^i) + \beta K'_2 (s_1^i s_4^i + s_2^i s_3^i) + \beta K'_3 s_1^i s_2^i s_3^i s_4^i} \quad (1.15)$$

This implies (1.14) becomes:

$$Z = e^{N' K'_0} \sum_{\{S_I\}} e^{\beta K'_1 \sum_{\langle IJ \rangle} S_I S_J + \beta K'_2 \sum_{\langle\langle IJ \rangle\rangle} S_I S_J + \beta K'_3 \sum_{\square} S_I S_J S_K S_L} \quad (1.16)$$

Note that K'_1 was multiplied by a factor of $\frac{1}{2}$ in the substitution because any pair of next-nearest neighbours (to become nearest neighbours after decimation) will enter the calculation twice as they will be common nearest neighbours of two different sites which will be removed by decimation. (1.16) implies that the partition sum will be preserved if the Hamiltonian is transformed to include not only an offset term as in 1 dimension, but likewise a next-nearest neighbour ($\langle\langle \rangle\rangle$) interaction and a four point ($\square$) or quadrupole interaction, as well as the original nearest neighbour term. The full details of how to calculate K'_i as a function of K are omitted as the process is related to Hasenbusch's method (see Section 1.3) and can also be found in [18]. Crucially:

$$\beta K'_1 = \frac{1}{4} \ln (\cosh [4\beta K]) \quad (1.17)$$

Similar equations are found for K'_0, K'_2 and K'_3 . It is now not as simple as in 1 dimension in which it became clear that $K'_1 \leq K$, because while this is certainly true for the first iteration, non-zero K'_2 and K'_3 are then generated which upon a second iteration of the process will affect the value of K'_1 .

The purpose of this demonstration however was to introduce that in general, enforcing the condition (1.5) puts constraints on the Hamiltonian which will involve the generation of new interactions. The notation I will adopt throughout is that in general, the Hamiltonian used will contain all possible (and the meaning of "possible" will require further discussion) interactions and their strengths will be given by a set of couplings $\{K_i\}$, for convenience represented as a vector $\underline{K}$. As K_i can be zero and thus interactions can be switched on and off, all information about the Hamiltonian is contained in $\underline{K}$ and consequently, all information about the Hamiltonian after one iteration is contained in $\underline{K}'$, and $\underline{K}''$ parametrises the Hamiltonian after two iterations, etc.

1.2.4. Renormalisation Group Fixed Point

For the Ising Model in the absence of an external field, all information is contained within the dimensionless parameter βK . Applying the block spin procedure and demanding the partition sum remain unchanged provides a new set of couplings $\underline{K}'(\underline{K})$ (this transformation specifically is what

I will henceforth refer to as an RG (renormalisation group) transformation or just renormalisation transformation)[78][27]. Now all information is contained within an ensemble of parameters $\beta K'_i$. $\xi(\underline{K}) = B\xi(\underline{K}')$, i.e. the correlation length depends on the parameters in the Hamiltonian and it decreases by the dilation factor. If however, the correlation length is infinite before the transformation, then it will be infinite afterwards too, thus $\xi(\underline{K}) = \xi(\underline{K}') = \infty$ or $\underline{K} = \underline{K}'$. To express this differently, a diverging correlation length means a stationary point in the transformation $\underline{K}'(\underline{K})$. The same is true when the correlation length is zero which occurs at $T = 0$ and $T = \infty$. Hence we expect the renormalisation transformation to have three stationary points, two of them labelled trivial as they are related to zero and infinite temperature (and in the context of coarse graining, they are the stable attractors) and one of them non-trivial, the unstable fixed point related to a diverging correlation length. The non-trivial fixed point is denoted $\underline{K}^*$ and by definition $\underline{K}'(\underline{K}^*) = \underline{K}^*$.

1.2.5. Critical Exponents

Let $\delta\underline{K}$ denote the distance from the fixed point ($\underline{K} - \underline{K}^*$) and thus when near the fixed point, $\delta\underline{K}$ is a small quantity and $\underline{K}$ can be written as a small perturbation about the fixed point

$$\underline{K} = \underline{K}^* + \delta\underline{K}$$

Upon application of the RG:

$$\underline{K}'(\underline{K}) = \underline{K}'(\underline{K}^* + \delta\underline{K})$$

As $\delta\underline{K}$ is small, one can expand to linear order, making use of the fact that $\underline{K}'(\underline{K}^*) = \underline{K}^*$

$$(\underline{K}'(\underline{K}))_i = (\underline{K}^*)_i + \sum_j \left(\frac{\partial K'_i}{\partial K_j} \right) \bigg|_{\underline{K}=\underline{K}^*} (\delta K)_j$$

or in full:

$$\underline{K}'(\underline{K}) = \underline{K}^* + \underline{M} \cdot \delta\underline{K} \tag{1.18}$$

in which $\underline{M}$ is the Jacobian Matrix evaluated at the fixed point and in general will also depend on the dilation factor B . Next, assume the eigenvectors of the Jacobian Matrix form a complete set (for simplicity, it is sometimes assumed in the literature that they form an orthogonal basis but as this turns out not to be the case for Hasenbusch's implementation, I will not make use of this). Thus the distance from the fixed point can be expressed in terms of these eigenvectors $\underline{e}_i$:

$$\delta \underline{K} = \sum_i u_i(\underline{K}) \underline{e}_i \quad (1.19)$$

and hence:

$$\underline{K}'(\underline{K}) = \underline{K}^* + \underline{M}(B) \sum_i u_i(\underline{K}) \underline{e}_i = \underline{K}^* + \sum_i u_i(\underline{K}) \lambda_i(B) \underline{e}_i \quad (1.20)$$

After one application of the RG, the distance to the fixed point will increase along all directions $\underline{e}_i$ for which $\lambda_i > 1$ and likewise decrease in all direction for which $\lambda_i < 1$. There will be a direction in the multi-dimensional coupling space which corresponds to the temperature direction, as $\underline{K}$ contains all of the information about the system which is intensive. Thus in the absence of an external magnetic field, one expects to find only one eigenvector of $\underline{M}(B)$ with an eigenvalue greater than unity and this direction corresponds directly to varying the temperature. With this in mind, it becomes evident that u_i in (1.20) is equivalent to t , i.e. how far along the temperature direction $\underline{e}_i$ the system is from the fixed point. Similarly, after one iteration of the transformation:

$$t' = \lambda_i(B)(u_i(\delta \underline{K})) = \lambda(B)t \quad (1.21)$$

and thus comparing to (1.2), one can deduce that

$$\lambda_i(B) = B^{y_t} \quad (1.22)$$

Hence finding the fixed point of the transformation, evaluating the Jacobian Matrix there and subsequently finding its eigenvalues facilitates the extraction of y_t , the thermal critical exponent. Furthermore, when introducing an external field, this introduces another unstable direction and for any value of $\underline{K}$ which does not correspond exactly to $h = 0$, $\delta \underline{K}$ will be

amplified upon application of the RG. Thus one expects to find another eigenvector whose eigenvalue is greater than unity.

1.2.6. Connection to Traditional Critical Exponents

Upon application of the RG, the correlation length must contract by a factor of B , i.e.

$$\zeta' = \frac{\zeta}{B} \quad (1.23)$$

Near the fixed point, the reduced temperature will scale as $t' \sim B^{y_t} t$, and by definition, $\zeta \sim |t|^{-\nu}$. It thus follows that

$$|t'|^{-\nu} = |B^{y_t} t|^{-\nu} = \frac{|t|^{-\nu}}{B} \quad (1.24)$$

and consequently, that $\nu = \frac{1}{y_t}$. Thus the critical exponent related to the correlation length [53, 10, 17]

$$\nu = \frac{\ln(B)}{\ln(\lambda)} \quad (1.25)$$

in which λ is the eigenvalue of the eigenvector of the Jacobian matrix at the fixed point which corresponds to the thermal direction (in the absence of a magnetic field, there should only be one relevant direction).

After a magnetic field has been introduced, one would expect to find a second relevant direction corresponding to the magnetic field. The reduced magnetic field scales as $h' \sim h B^{y_h}$. The magnetic exponent δ is defined as

$$m(t=0, h) \sim \text{sgn}(h) |h|^{\frac{1}{\delta}} \quad (1.26)$$

Likewise, due to the invariance of the partition sum (and thus the total free energy F) under renormalisation, the free energy per spin renormalises according to:

$$f(t=0, h) = B^{-d} f'(t=0, h') \quad (1.27)$$

Note that this is only strictly true in the limit $h \rightarrow 0$. In general, a field configuration of the form $(t, h) = (t, 0)$ will renormalise to $(t', 0)$. The reverse however is not true, one finds that $(t, h) = (0, h)$ will renormalise to (t', h') apart from in the limit $h \rightarrow 0^\pm$. This does not pose a problem for the following derivation as δ is defined for $h = 0$. Finally, using the

definition [18] for order parameter (magnetisation):

$$\begin{aligned} m(0, h) &= \frac{\partial}{\partial h} f(0, h) = B^{-d} \frac{\partial}{\partial h} f'(0, h') = B^{-d} \frac{dh'}{dh} \frac{\partial}{\partial h'} f'(0, h') \\ &= B^{-d} B^{y_h} m'(0, h') \sim B^{-d+y_h} h'^{\frac{1}{\delta}} = B^{-d+y_h} (B^{y_h} h)^{\frac{1}{\delta}} \end{aligned} \quad (1.28)$$

and thus, $-d + y_h(1 + \frac{1}{\delta}) = 0$ or:

$$y_h = \frac{d}{1 + \frac{1}{\delta}} \quad (1.29)$$

While it is δ which is most often cited in the literature, it is y_h which is most naturally extracted from the RG. Inverting (1.29):

$$\delta = \frac{y_h}{d - y_h} \quad (1.30)$$

It should however be noted that for the models we will study, extracting δ this way is extremely sensitive to small errors in y_h . To see this, let us examine how a small error in y_h would manifest itself as an error in δ for the Ising Model in 2d in which $\delta = 15$ [96]. Using the formula for propagation of errors[15]:

$$\sigma_\delta = \left| \frac{d\delta}{dy_h} \right| \sigma_{y_h} = \frac{d}{(d - y_h)^2} \sigma_{y_h} \quad (1.31)$$

and thus dividing through by δ as defined in (1.30):

$$\frac{\sigma_\delta}{\delta} = \frac{d}{d - y_h} \frac{\sigma_{y_h}}{y_h} \quad (1.32)$$

which for the aforementioned parameters evaluates to:

$$\frac{\sigma_\delta}{\delta} = 16 \frac{\sigma_{y_h}}{y_h}$$

and thus a relatively small fractional error in y_h propagates through (1.30) rather unfavourably into a relatively large fractional error for δ .

1.3. Hasenbusch's Method

I will now provide a detailed recap of a method provided in a set of notes [40] by Hasenbusch, as it not only provided the motivation for the work

described in this chapter but I built much of my analysis upon his technical insights. Hasenbusch performs an implementation of Kadanoff's [45] block spins on a 4×4 lattice using a blocking factor, B of 2. A 4×4 lattice is sub-divided into four 2×2 lattices, each of which is in turn mapped onto a single spin. As a 2×2 lattice consists of 4 (an even number of) sites, some 2×2 configurations will contain an equal number of up and down spins and thus a suitable rule must be used to deal with such cases. Hasenbusch uses a so-called transformation kernel s.t.

$$e^{-H'(\{S_I\})} = \sum_{\{s_i\}} T(S_I, s_i) e^{-H(\{s_i\})} \quad (1.33)$$

(to be contrasted with (1.5)). Thus the Boltzmann-weighted energy of a 4×4 configuration which renormalises ambiguously will in Hasenbusch's implementation contribute to multiple Boltzmann sums. To clarify, by Boltzmann sum I mean part of the partition sum which contains all of the $N \times N$ configurations which renormalise to a given $\frac{N}{B} \times \frac{N}{B}$ configuration.

We know renormalisation of Ising's original Hamiltonian will generate non-zero next-nearest (and longer range) neighbour interactions. As it is necessary to find the fixed point $\underline{K}^*$ of the transformation, such that $\mathcal{R}(\underline{K}^*) = \underline{K}^*$, it is necessary for the Hamiltonian of the 4×4 configuration to contain the same number of interactions as that of the 2×2 system. This is in fact quite a strong restriction as the only interactions on a 2×2 lattice which respect rotational, translational and parity invariance are a nearest neighbour, a next-nearest neighbour and a four point interaction. A formal way of writing this Hamiltonian on a 2-d lattice is:

$$\begin{aligned} H(\{s_i\}) = K_0 - \sum_i \sum_j [& K_1 s_{i,j} (s_{i+1,j} + s_{i,j+1}) + K_2 s_{i,j} (s_{i+1,j+1} + s_{i+1,j-1}) \\ & + K_3 s_{i,j} s_{i+1,j} s_{i,j+1} s_{i+1,j+1}] \end{aligned} \quad (1.34)$$

however I will use the following intuitive notation throughout to make it clear which coupling corresponds to which type of interaction:

$$H(\{s_i\}) = K_0 - K_1 \sum_{\langle ij \rangle} s_i s_j - K_2 \sum_{\langle\langle ij \rangle\rangle} s_i s_j - K_3 \sum_{\square} s_i s_j s_k s_l \quad (1.35)$$

C_0	$\begin{pmatrix} ++ \\ ++ \end{pmatrix}$	$\begin{pmatrix} -- \\ -- \end{pmatrix}$							$K'_0 + 8K'_1 + 8K'_2 + 4K'_3$
C_1	$\begin{pmatrix} ++ \\ +- \end{pmatrix}$	$\begin{pmatrix} +- \\ +- \end{pmatrix}$	$\begin{pmatrix} +- \\ ++ \end{pmatrix}$	$\begin{pmatrix} +- \\ ++ \end{pmatrix}$	$\begin{pmatrix} -- \\ +- \end{pmatrix}$	$\begin{pmatrix} -- \\ +- \end{pmatrix}$	$\begin{pmatrix} +- \\ -- \end{pmatrix}$	$\begin{pmatrix} +- \\ -- \end{pmatrix}$	$K'_0 - 4K'_3$
C_2	$\begin{pmatrix} ++ \\ -- \end{pmatrix}$	$\begin{pmatrix} +- \\ +- \end{pmatrix}$	$\begin{pmatrix} +- \\ +- \end{pmatrix}$	$\begin{pmatrix} -- \\ ++ \end{pmatrix}$					$K'_0 - 8K'_2 + 4K'_3$
C_3	$\begin{pmatrix} +- \\ +- \end{pmatrix}$	$\begin{pmatrix} +- \\ +- \end{pmatrix}$							$K'_0 - 8K'_1 + 8K'_2 + 4K'_3$

Table 1.1.: The four spin configuration classes. All configurations in the same class have the same energy and thus only four different total energy values (given as a function of $\underline{K}$ in the far right column) are possible on a 2×2 lattice.

Periodic boundary conditions are used throughout the work covered in this chapter.

Clearly on a 4×4 lattice, further, longer range interactions are permitted, for example interactions between two spins separated by a distance of twice the lattice spacing along the vertical or horizontal, or the equivalent diagonal interaction. In order to find a fixed point, it is necessary to ignore these interactions, hoping that the longer range an interaction, the weaker. Only if the transformation were being carried out on an infinite lattice would the resulting coarse-grained configuration also be infinite and thus in order to find a fixed point, it is necessary to perform some such approximation on any lattice of finite size.

In order to calculate the energy of any 4×4 or 2×2 lattice, it is necessary to evaluate (1.35). For all sixteen possible configurations on a 2×2 lattice S_I , one can calculate numerically (for a given $\underline{K}$) the Boltzmann sum

$$\sum_{\{s_i\} \rightarrow S_I} e^{-H(\{s_i\})}$$

which must equal $H'(\{S_I\})$ and this generates sixteen equations for $\underline{K}'$ as a function of $\underline{K}$ (i.e. 16 equations in four variables to be simultaneously satisfied) and thus the problem is over-determined. Hasenbusch however notes that by symmetry, some of these sixteen equations actually impose the exact same constraint and it turns out that only four unique constraints are generated. The most simple way of understanding this is that the LHS of (1.5) can only take four different values or, more specifically, on a 2×2 lattice, the Hamiltonian (1.35) can only evaluate to four different values (which are listed in Table 1.1).

Thus, the choice of (1.5) in order to satisfy (1.3) will only be satisfied if:

$$\sum_{\{s_i\} \rightarrow S_I} e^{-H(\{s_i\})} = \sum_{\{s_i\} \rightarrow S_K} e^{-H(\{s_i\})} \quad (1.36)$$

and $H'(S_I) = H'(S_K)$ are equivalent statements. This realisation will be of fundamental importance when I introduce the categories Hamiltonian (in Section 1.5). It means that one can choose a single spin configuration from each row in Table 1.1 (from here on in referred to as that class' "paradigm") and calculate its Boltzmann sum. Thus for the Ising Model in the absence of an external field, one only has to generate four sums of the form of the RHS of (1.5) numerically or one quarter of the partition sum. Combining this information with the energies of each category stated in Table 1.1, the following matrix equation is obtained:

$$\begin{pmatrix} 1 & 8 & 8 & 4 \\ 1 & 0 & 0 & -4 \\ 1 & 0 & -8 & 4 \\ 1 & -8 & 8 & 4 \end{pmatrix} \begin{pmatrix} K'_0 \\ K'_1 \\ K'_2 \\ K'_3 \end{pmatrix} = \begin{pmatrix} \ln[\sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ ++ \end{pmatrix}} e^{-H(\{s_i\})}] \\ \ln[\sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ +- \end{pmatrix}} e^{-H(\{s_i\})}] \\ \ln[\sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ -+ \end{pmatrix}} e^{-H(\{s_i\})}] \\ \ln[\sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ -- \end{pmatrix}} e^{-H(\{s_i\})}] \end{pmatrix} \quad (1.37)$$

in which the matrix on the LHS consists of the four possible values (1.35) can evaluate to and the four configurations on the RHS are the four arbitrarily chosen paradigms. Note that $\sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ ++ \end{pmatrix}} e^{-H(\{s_i\})}$ could be replaced by

$\sum_{\{s_i\} \rightarrow \begin{pmatrix} -- \\ -- \end{pmatrix}} e^{-H(\{s_i\})}$ etc. Inverting (1.37) yields an equation for $\underline{K}'$ as a function

of $\underline{K}$:

$$\begin{pmatrix} K'_0 \\ K'_1 \\ K'_2 \\ K'_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{8} & \frac{1}{2} & \frac{1}{4} & \frac{1}{8} \\ \frac{1}{16} & 0 & 0 & -\frac{1}{16} \\ \frac{1}{32} & 0 & -\frac{1}{16} & \frac{1}{32} \\ \frac{1}{32} & -\frac{1}{8} & \frac{1}{16} & \frac{1}{32} \end{pmatrix} \begin{pmatrix} \ln[\sum e^{-H(\{s_i\})}] \\ \{s_i\} \rightarrow \begin{pmatrix} ++ \\ ++ \end{pmatrix} \\ \ln[\sum e^{-H(\{s_i\})}] \\ \{s_i\} \rightarrow \begin{pmatrix} ++ \\ +- \end{pmatrix} \\ \ln[\sum e^{-H(\{s_i\})}] \\ \{s_i\} \rightarrow \begin{pmatrix} ++ \\ -- \end{pmatrix} \\ \ln[\sum e^{-H(\{s_i\})}] \\ \{s_i\} \rightarrow \begin{pmatrix} +- \\ -+ \end{pmatrix} \end{pmatrix} \quad (1.38)$$

Thus it is necessary to find the fixed point (see 1.3.1). Hasenbusch finds:

$$\underline{K}^* = (0.2997612004800, 0.087094327205, -0.00125863335)$$

Each sum on the RHS of (1.38), when blocking spins from a $4 \times 4 \rightarrow 2 \times 2$ lattice, will consist of $2^{12} = 4096$ terms and thus must be calculated numerically (we have done this in C/C++ throughout).

Note that because the model described by the Hamiltonian (1.35) belongs to the same universality class as the Ising Model, the critical exponents we extract from the eigenvalues of the Jacobian at the fixed point must be those of the Ising Model. Hasenbusch calculates the derivatives $\frac{\partial K'_i}{\partial K_j}$ by finite differences and finds one eigenvalue greater than unity, $\lambda_1 = 1.928122$ and thus $y_t = \frac{1}{\lambda_1} = 0.947196$.

While two models in the same universality class must have the same critical exponents, their critical temperatures will in general not be equal. In order to extract the critical temperature of the Ising Model, it is necessary to realise that because the transformation preserves the partition sum, the free energy is likewise preserved and thus a 2×2 system with a renormalised set of couplings $\underline{K}'$ will have the same observable properties (e.g. entropy per spin) as the 4×4 system. A further approximation Hasenbusch then makes is to assume that the coupling map from a $4 \times 4 \rightarrow 2 \times 2$ system represents the general $N \times N \rightarrow \frac{N}{2} \times \frac{N}{2}$ mapping. Consequently, the transformation can be applied iteratively by taking $\underline{K}'$ and pretending it represents a set of couplings for a 4×4 system. If one finds K_1 such that when starting at $\underline{K} = (0, K_1, 0, 0)$ and applying the transformation it-

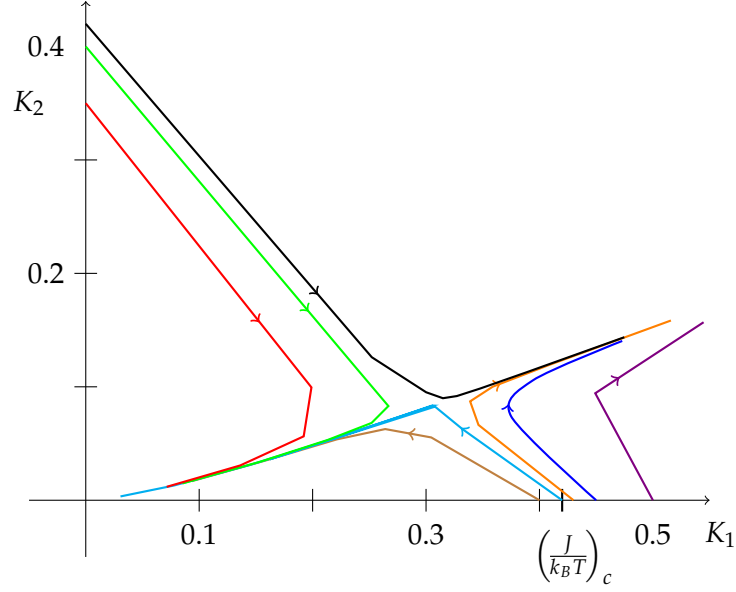


Figure 1.3.: The flow in $K_1 - K_2$ space for the Ising Model in the absence of a magnetic field, after multiple iterations. The high and low temperature attractors are clearly visible as well as the non-trivial fixed point.

eratively, one ends up flowing into the fixed point $\underline{K}^*, \left(\frac{J}{k_B T}\right)_c$ of the Ising Model has been found.

Figure 1.3 shows a cross-section of the flow in the $K_1 - K_2$ plane (with data I have reproduced rather than Hasenbusch's data).

1.3.1. Finding the Fixed Point

Calculating Derivatives

While Hasenbusch calculates $\frac{\partial K'_i}{\partial K_j}$ by finite differences, we quickly realised that this can in fact be done analytically. We first note that it will be necessary to calculate expressions of the form:

$$\frac{\partial}{\partial K_j} \ln \left[\sum_{\{s_i\} \rightarrow S_I} e^{-H(\{s_i\})} \right] = \frac{\sum_{\{s_i\} \rightarrow S_I} \frac{-\partial H(\{s_i\})}{\partial K_j} e^{-H(\{s_i\})}}{\sum_{\{s_i\} \rightarrow S_I} e^{-H(\{s_i\})}} \quad (1.39)$$

Using the example of taking derivatives w.r.t K_2 , this means (by (1.35)), for any given $\{s_i\}$:

$$\frac{\partial H(\{s_i\})}{\partial K_2} = \sum_{\langle ij \rangle} s_i s_j \quad (1.40)$$

and thus:

$$\frac{\partial}{\partial K_2} \ln \left[\sum_{\{s_i\} \rightarrow S_I} e^{-H(\{s_i\})} \right] = \frac{\sum_{\{s_i\} \rightarrow S_I} \left(\sum_{\langle ij \rangle} s_i s_j \right) e^{-H(\{s_i\})}}{\sum_{\{s_i\} \rightarrow S_I} e^{-H(\{s_i\})}} \quad (1.41)$$

and consequently by (1.38), $\frac{\partial K'_i}{\partial K_j}$ can be calculated.

Multi-Dimensional Newton Raphson

In general (overlooking the special status of K_0 momentarily), each renormalised coupling K'_i depends on each initial coupling K_j . For a system with N couplings, finding the fixed point is equivalent to finding $\underline{K}$ such that the system of N equations:

$$\begin{pmatrix} K'_0(K_0, K_1, \dots, K_{N-1}) - K_0 \\ K'_1(K_0, K_1, \dots, K_{N-1}) - K_1 \\ \vdots \\ K'_{N-1}(K_0, K_1, \dots, K_{N-1}) - K_{N-1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (1.42)$$

are satisfied simultaneously.

To find the roots of a function of one variable, Newton's Method is commonly used [73]. If one has a reasonable first estimate of a root x_0 , and it is possible to compute $f(x_0)$ as well as $f'(x_0)$, then

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

will in general be a better estimate of the root. This method can be iterated and will converge relatively quickly if the initial estimate x_0 is good.

A multi-dimensional generalisation of this [69] is that in order to find the simultaneous root of N functions of the same N variables, $\underline{f}(\underline{x})$, one

can iterate from an initial guess $\underline{x}_0$ in an analogous way:

$$\underline{x}_1 = \underline{x}_0 - \underline{J}^{-1}|_{(\underline{x}=\underline{x}_0)} \underline{f}(\underline{x}_0) \quad (1.43)$$

in which $\underline{J}$ represents the Jacobian Matrix i.e. $J_{ab} = \frac{\partial f_a}{\partial x_b}$. As shown in (1.42), the functions whose roots must be found simultaneously are $K'_i(K) - K_i$ and thus crucially, entries in the Jacobian will be given by $J_{ab} = \frac{\partial K'_a}{\partial K_b} - \delta_{ab}$, where δ_{ab} represents the Kroneker-delta function meaning the diagonals contain an extra factor of -1 . Note that but for the offset on the diagonals, the matrix required for root-finding is the same as the Jacobian matrix whose eigenvalues must be computed at the fixed point in order to determine critical exponents.

While the Newton-Raphson procedure has been essentially programmed as outlined by hand in C, the armadillo library [76] was used to invert the Jacobian (and likewise used for computing eigenvalues).

1.3.2. Intelligent Root-Finding

One problem with Newton-Raphson root-finding is its dependence on the accuracy of the initial guess. Furthermore, the transformation has multiple fixed points and it was observed that starting a search without any knowledge of where the fixed point was located would most of the time result in flow toward the (trivial) high or low-temperature fixed points rather than the non-trivial fixed point of interest. Thus rather than generating random starting points until we stumbled upon convergence, it was decided to hybridise the concept of flow from the real line into the fixed point, as shown in Figure 1.3, and Newton's method. This involved initially assigning the couplings values which lie on the real (Ising) line and iterating the transformation until it became clear whether it was converging to the high or low-temperature fixed point. By mapping out the flow landscape and investigating where on the real line the separatrix between the two behaviours lies (as shown in Figure 1.3), not only can the critical temperature of the model being examined be estimated, but starting $\underline{K}$ from near this value will necessarily result in $\underline{K}$ flowing to values near the fixed point after a few iterations of the transformation. Thus it is possible to obtain a good estimate of the fixed point and then subsequently use the aforementioned

multi-dimensional Newton Raphson search to quickly improve numerical accuracy and likewise in so doing evaluate the Jacobian Matrix at the fixed point.

1.3.3. The Role of K_0

Hasenbusch skips over the special role played by the offset term. Specifically, he includes a term of the form K_0 in his Hamiltonian, but then only provides fixed point values for $K_1 - K_3$. For simplicity, consider the example of renormalisation by decimation in 1d. If one includes a term of the form K_0 in the Hamiltonian, it has the following effect on the partition sum:

$$Z = e^{K_0} \sum_{\{s_i\}} e^{\sum_{\langle ij \rangle}^{K_1} s_i s_j} = Z' = e^{K_0} e^{N' K'_0} \sum_{\{S_I\}} e^{\sum_{\langle IJ \rangle}^{K'_1} S_I S_J} \quad (1.44)$$

which is equivalent to defining the renormalised hamiltonian as:

$$H' = -\tilde{K}'_0 - K'_1 \sum_{\langle IJ \rangle} S_I S_J \quad (1.45)$$

in which $\tilde{K}'_0 = K_0 + N' K'_0$ and K'_0 is generated from K_1 according to (1.9). Intuitively, one might then attempt to find a fixed point which includes K_0 in its parameter space but clearly the point $\tilde{K}'_0 = K_0$ is unattainable as neither N' nor $K'_0(K_1)$ can equal zero. This is not strictly a problem, it can be determined from (1.38) that the value of K_0 has no effect on K'_i ($i \neq 0$), even in 2 dimensions and likewise the effect of K_0 cancels out when calculating expectation values of observable quantities. However if K_0 is introduced like this in the Hamiltonian, it must be accepted K_0 has to be excluded from the parameter space in which the fixed point exists. A convenient way to introduce an offset however, and one which I have used throughout as it will make more intuitive sense in the context of the categories Hamiltonian (to follow, see Section 1.5), is to introduce a system size-dependent offset, i.e. a term of the form NK_0 . For 1-dimensional decimation, this implies that:

$$Z = e^{NK_0} \sum_{\{s_i\}} e^{\sum_{\langle ij \rangle}^{K_1} s_i s_j} = Z' = e^{NK_0} e^{N' K'_0} \sum_{\{S_I\}} e^{\sum_{\langle IJ \rangle}^{K'_1} S_I S_J} \quad (1.46)$$

By this definition however, the renormalised Hamiltonian has an offset term of the form $N'\tilde{K}'_0$ which must be equated to $NK_0 + N'K'_0$. Thus the offset term can be included in the parameter space of the fixed point if the condition $K_0 = \tilde{K}'_0$ can be satisfied. This implies that

$$\begin{aligned}\tilde{K}'_0 &= B^2K_0 + K'_0 = K_0 \\ K_0 &= \frac{K'_0}{1 - B^2}\end{aligned}\tag{1.47}$$

Thus the fixed point value for K_0 is linked to the fixed point value of K_1 (because in 1d, K'_0 depends only on K_1) but the reverse is not true. This parametrisation has been used throughout and likewise in 2d, it can be seen that the value of K_0 does not affect the values of any other couplings but the fixed point value of K_0 is a function of all of the other couplings. It also is responsible for the Jacobian Matrix having an additional eigenvalue greater than unity which is equal to B^d (leading to an exponent equal to d). We believe this represents flow in the N direction and is simply telling us our lattice is getting smaller by a factor of B^d at each iteration (this eigenvalue persists away from the fixed point, it is always equal to B^d regardless of the values of any of the couplings).

1.3.4. Ambiguous Cases

Hasenbusch used a blocking kernel to deal with ambiguous cases which arise when renormalising by a factor of $B = 2$. While the following was later revisited, for the majority of what follows (and unless otherwise stated), the rule used for renormalisation of ambiguous cases was a deterministic one, in which a certain spin on the 2×2 lattice is chosen (consistently) to represent the block of spins. The rule used was to use the "top left" spin of every ambiguous 2×2 configuration (see Figure 1.4). Another possible implementation which was experimented with was random number generation, i.e. "flipping a coin" for ambiguous cases. The problem with this is that it introduces a certain (albeit small) amount of stochasticity to the problem and thus the fixed point varies which is somewhat impractical, especially during debugging. Having observed that for the Ising Model with an without external field, it does not change any qualitative results to coarse grain in this manner, it was decided to continue to use the "top left"

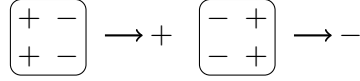


Figure 1.4.: Both 2×2 patches are ambiguous in that they have the same number of up and down spins. In this case, the result of the coarse-graining procedure is to replace the patch with a spin which takes the same value as the "top-left" spin in the original patch.

rule. Furthermore, "flipping a coin" violates parity symmetry, even if it is a "small violation".

1.4. Extending Hasenbusch's Method to Include a Magnetic Field

(1.35) is the most general Hamiltonian possible on a 2×2 lattice which respects both the lattice symmetries, and those of the Ising Model Hamiltonian. A particularly conspicuous absentee in (1.35) is a term of the form $-H \sum_i s_i$, as such a term is present in the Hamiltonian of the original Ising Model. If we include such a term, we are relaxing parity symmetry. Doing so also means that the Hamiltonian can now evaluate to more than four different values. In fact it can now take six different values on a 2×2 lattice leaving the problem under-determined (as the Hamiltonian currently only contains five terms). Fortunately, parity symmetry having been relaxed, a further type of interaction can be introduced (if done so carefully), namely a 'triangular' interaction of the form $\sum_{\triangle} s_i s_j s_k$. In order to not violate rotational invariance, it is important to introduce triangles in all four possible orientations.

Thus the Hamiltonian now reads:

$$\begin{aligned}
 H = (N)K_0 - K_1 \sum_{\langle ij \rangle} s_i s_j - K_2 \sum_{\langle\langle ij \rangle\rangle} s_i s_j - K_3 \sum_{\square} s_i s_j s_k s_l \\
 - K_4 \sum_i s_i - K_5 \sum_{\triangle} s_i s_j s_k
 \end{aligned} \tag{1.48}$$

and as can be seen in Table 1.2, it can evaluate to six different values for any given $\underline{K}$. Now the principle is very similar to Hasenbusch's original one,

C_0	$\begin{pmatrix} ++ \\ ++ \end{pmatrix}$		$K'_0 + 8K'_1 + 4K'_2 + 4K'_3 + 4K'_4 + 8K'_5$
C_1	$\begin{pmatrix} -- \\ -- \end{pmatrix}$		$K'_0 + 8K'_1 + 4K'_2 + 4K'_3 - 4K'_4 - 8K'_5$
C_2	$\begin{pmatrix} ++ \\ +- \end{pmatrix}$	$\begin{pmatrix} +- \\ ++ \end{pmatrix}$	$K'_0 - 4K'_3 + 2K'_4 - 2K'_5$
C_3	$\begin{pmatrix} -- \\ +- \end{pmatrix}$	$\begin{pmatrix} +- \\ -- \end{pmatrix}$	$K'_0 - 4K'_3 - 2K'_4 + 2K'_5$
C_4	$\begin{pmatrix} ++ \\ -- \end{pmatrix}$	$\begin{pmatrix} +- \\ +- \end{pmatrix}$	$K'_0 - 8K'_2 + 4K'_3$
C_5	$\begin{pmatrix} +- \\ -- \end{pmatrix}$	$\begin{pmatrix} +- \\ +- \end{pmatrix}$	$K'_0 - 8K'_1 + 8K'_2 + 4K'_3$

Table 1.2.: When evaluating Equation (1.48), one obtains these six configuration classes, their energies in terms of $\underline{K}$ given by the final column.

except that the Newton-Raphson search must be conducted in a larger parameter space. That said, it is not necessary to carry out a root-finding algorithm at all for physical reasons. I have already discussed how application of the RG will amplify a magnetic field and thus only a magnetic field value of zero will remain as such upon application of the transformation. This means that configurations related by parity symmetry must have equal energies at the fixed point, meaning the fixed point will be found at:

$$\underline{K}^* = ((K_0^*), K_1^*, K_2^*, K_3^*, 0, 0)$$

in which K_{0-3}^* is the fixed point for when parity symmetry was still in place. Just because $K_4 = K_5 = 0$ at the fixed point does not mean this cannot provide us with any extra information. The derivatives $\frac{\partial K'_{4-5}}{\partial K_i} \neq 0 \neq \frac{\partial K'_i}{\partial K_{4-5}}$ and consequently, new directions can be probed in coupling space for a relevant one.

1.4.1. Preliminary Results

The main purpose of this section has been to contextualise and motivate the Categories Hamiltonian which will be introduced in the subsequent section (1.5). When carrying out our own numerics, we found the fixed point to be

$$\underline{K}^* = (K_0, 0.306693, 0.083994, -0.003837)$$

This differs enough from Hasenbusch's result not to be attributable solely to numerical error. In fact we later confirmed that this is due to Hasenbusch's use of a transformation kernel. Likewise we find 3 (or 4 depending on whether K_0 is included in the Jacobian) eigenvalues of which only 1 (or

2, the second being equal to 4) are greater than unity. In terms of the conventionally quoted Ising Model critical exponents, we find $\nu = 0.93659$ (c.f. Onsager's of 1 [62, 96]) and $\delta = 10.669$ (c.f. $\delta = 15$). However, this result could be presented as $y_h = 1.820$ (c.f. $y_h = \frac{15}{8} = 1.875$). As discussed, the propagation of errors for δ is rather unfavourable in 2 dimensions. Furthermore we find that the reduced critical temperature lies on the range:

$$0.419922 < \frac{K}{K_B T_c} < 0.42041$$

(c.f. Onsager's value [62] of $\frac{\ln(1+\sqrt{2})}{2} = 0.440687$).

1.4.2. Preliminary Analysis

The surprising result contained within Hasenbusch's analysis (and likewise apparently confirmed by our extension), is that the RG provides us with a qualitatively correct insight about critical properties of much larger lattices than we have performed the analysis on.

Exact Observable Computation

From a computational point of view, it is possible to calculate expectation values of an observable A by computing the sum:

$$\langle A \rangle = \frac{\sum_{\{s_i\}} A(\{s_i\}) e^{-H(\{s_i\})}}{\sum_{\{s_i\}} e^{-H(\{s_i\})}} \quad (1.49)$$

Computing this exactly requires a number of computational operations of the same order of magnitude as performing one iteration of the RG. It would however have to be done over a range of temperatures to get an understanding of the critical behaviour of the system [94]. This however is not why Hasenbusch's method is of interest, since in practise, the RG transformation must be performed many times in order to find its fixed point (and all of the computational short cuts I will in turn outline could be applied to calculating expectation values). The extremely small, 4×4 lattices we are working with however, are too small to exhibit any meaningful critical behaviour. Figure 1.5 shows the results for calculating (numerically)

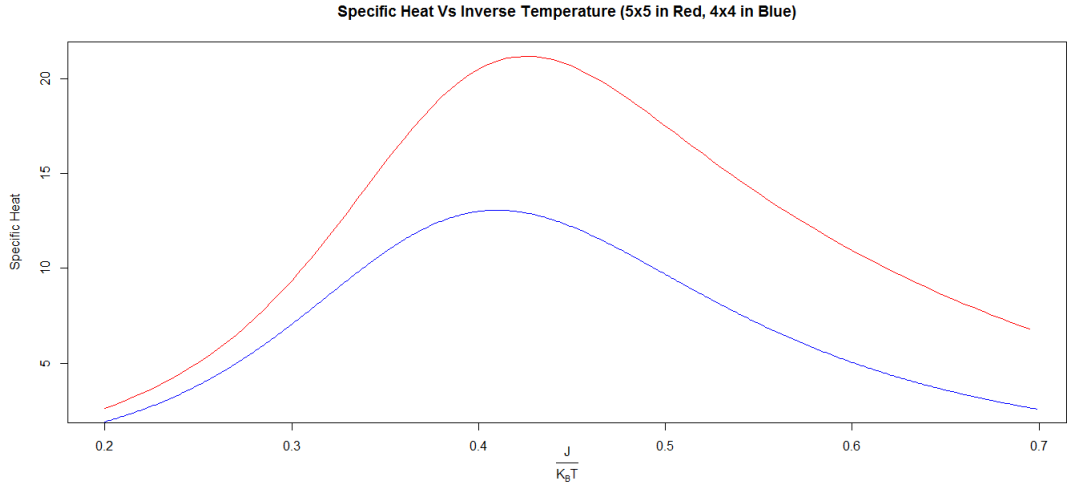


Figure 1.5.: (non-normalised) Specific Heat $\langle E^2 \rangle - \langle E \rangle^2$ as a function of Inverse Temperature $\frac{J}{k_B T}$. A weak peak near the known critical temperature for the infinite system is recognisable.

the quantity $\langle E^2 \rangle - \langle E \rangle^2$, related to the specific heat. While this provides as accurate an estimate for the critical temperature as using Hasenbusch's method (using this method to find the most accurate possible estimate for T_c , I obtained $\left(\frac{J}{k_B T}\right)_c = 0.41002(2)$), the peak is too shallow to extract a meaningful estimate for α , the curve simply flattens off far too far away from the critical temperature for this to be possible. Of course this is a poor example as $\alpha = 0$ in 2 dimensions. Nonetheless, this analysis can be used to estimate the critical temperature, and subsequently Figure 1.6 shows the order parameter m plotted Vs h with the inverse critical temperature set to this best estimate. Clearly the expected magnetisation is not exhibiting the $|h|^{\frac{1}{\delta}}$ behaviour the infinite system is known to show. A back of the envelope analysis of the data shows the behaviour to in fact be close to linear as $h \rightarrow 0$.

Why Continue With Hasenbusch's Method?

The absolute failure of this naive calculation of expectation values should not come as a surprise. Finite size effects can distort critical behaviour for lattice sizes much larger than 4×4 [9]. What however is surprising is that

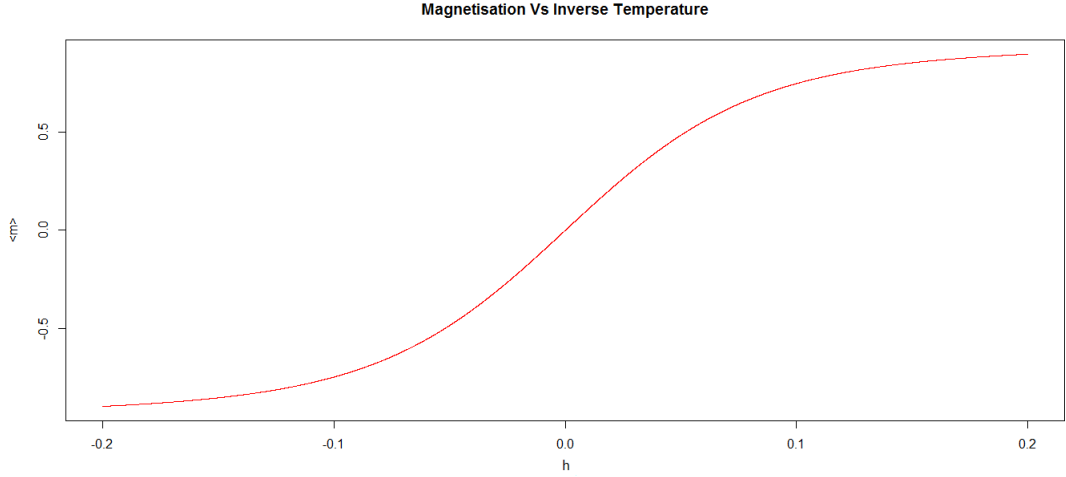


Figure 1.6.: $\langle m \rangle$ Vs h for $\frac{J}{k_B T} = \left(\frac{J}{k_B T} \right)_c$

the RG appears to allow us to extract information from a 4×4 lattice about much larger lattices. In effect, it appears that the qualitative behaviour of much larger systems is somehow encoded in a 4×4 lattice and it is the RG which facilitates the extraction of that information. The critical exponent estimates are certainly far closer to the 2-dimensional results than they are to those of Mean-Field Theory. While no doubt in theory, if one could calculate expectation values of observables exactly in the aforementioned way for much larger lattices, critical behaviour would start to emerge. The numerical scaling is however such, that the number of microstates for an Ising Model on an $N \times N$ lattice is 2^N and thus this very quickly becomes infeasible. Likewise we cannot perform an RG transformation in the way Hasenbusch has on arbitrarily large lattices but by contrast, this method allows us to extract sensible critical exponents for even the smallest of systems.

Due to the small lattices used, we are able to explore the entire phase space of the model. This is novel, as other studies in general have attempted to combine Monte Carlo methods [8] and the RG (MCRG) in order to perform the RG but only use a small, statistically representative sample of the phase space [81]. One early such study by Swendsen[82], performed for the 2-d Ising Model in order to test the validity of the method before

applying it to other systems, found results for ν and δ more accurate than those found by Hasenbusch and ourselves. These however were obtained when coarse graining a 108×108 lattice. It is to be expected, that a considerably larger lattice such as the one investigated by Swendsen would yield a much better estimate for ν than studying 4×4 lattices. Swendsen's triumph is to show that a minute, statistically representative sample of the phase space can be taken into account. Hasenbusch's result however, is of interest precisely because it takes the opposite approach, and manages to obtain (almost as) accurate results by examining the full parameter space of minute systems.

Thus the scene has been set and the remainder of this chapter will be concerned with the necessary amendments required in order to perform this analysis for the Q-state Potts Model and likewise study triangular as well as square lattices.

1.5. The Categories Hamiltonian

1.5.1. $\frac{N}{B} = 3$

While it is certainly not the main focus of this chapter, it is worth mentioning certain aspects of the $6 \times 6 \rightarrow 3 \times 3$ transformation in order to motivate the categories Hamiltonian. The crucial difference to the $4 \times 4 \rightarrow 2 \times 2$ case is that now, more interactions can be added to (1.35), as a 3×3 lattice can support longer range interactions than a 2×2 lattice. As for the 2×2 case, it is necessary to come up with the most general Hamiltonian possible that respects the symmetries of the Ising Model (for simplicity, let us do so in the absence of an external magnetic field). Note that due to periodic boundary conditions, introducing a next-next-nearest neighbour term has no effect as the interaction between any two such neighbours is already covered by a nearest-neighbour interaction (this result only holds on a 3×3 lattice). This is demonstrated in Figure 1.7.

Figures 1.8 and 1.9 demonstrate some of the other interactions which can be included for a 3×3 lattice. It is of course a tedious exercise to think of these, and I have by no means mentioned all of the ones I could think of (thus far I have managed to come up with 11). It is also extremely difficult to decide when all of them have been found. Then, it is necessary to

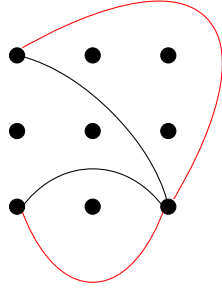


Figure 1.7.: next-nearest horizontal/diagonal neighbour interactions (both shown in black as two horizontal spaces and two diagonal spaces respectively) are equivalent to nearest and next-nearest neighbour interactions (both shown in red) on a 3×3 lattice and thus including them in the Hamiltonian gives no extra information.

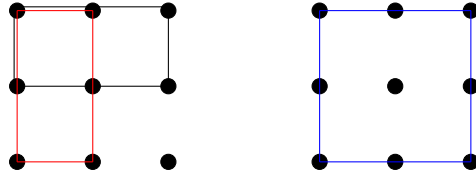


Figure 1.8.: The hectopoles (shown in black and red on the left) and an octopole (blue on the right) originating from the top left site. Similar hecto- and octopoles can be drawn from each of the 9 sites making use of the periodic boundary conditions.

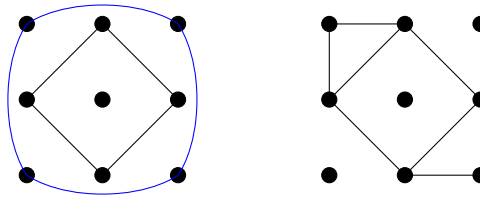


Figure 1.9.: On the left, a rhombic quadrupole and a "next-biggest" quadrupole interaction are denoted in black and blue respectively. On the right another type of hectopole is denoted (its mirror image must be included as well to preserve rotational symmetry).

evaluate which ever new complicated Hamiltonian has been devised for all $2^9 = 512$ configurations which exist on a 3×3 lattice (clearly this is a computational exercise, unlike the 2×2 case which Hasenbusch evaluated by hand and remains tractable) and hope that the number of different outcomes equals the number of couplings in the Hamiltonian for only then is the problem neither over nor under determined. Having carried out this process computationally, an interesting result is that including only the original 4 terms which exist on a 2×2 lattice, as well as the hexapole, 13 different categories are found (they are shown in Appendix C). At this stage, the Hamiltonian contains five terms and the problem is under-determined. Adding an octopole, then a rhombic and then further interactions does not change this. The 13 categories appear to be fundamental. I find it likely that it is possible, for some fundamental reason, to think of 12 interactions (plus the offset term) which obey the symmetries of the Ising Model on a 3×3 lattice but doing so is incredibly tedious. The categories Hamiltonian will remove the need to do this, as well as add credibility to the idea that these thirteen categories are "somehow fundamental" which at this point still seems rather hand waving at best.

1.5.2. The Potts Model

The Q-state Potts[68] (or Ashkin-Teller) Model is a generalisation of the Ising Model in which each site on a lattice can have an integer spin value on the interval $[0, Q - 1]$. In the absence of an external magnetic field, the Hamiltonian reads:

$$H = -J \sum_{\langle ij \rangle} \delta_{s_i, s_j} \quad (1.50)$$

in which J is the strength of nearest neighbour interactions and δ_{s_i, s_j} is the Kroneker-delta function. The spin value should in no way be associated with its magnitude, it is simply a label. A 0-spin interacts with a nearest neighbour 1-spin in exactly the same way as it interacts with a 2-spin. Concentrating first on the Q=3 Potts Model, it behaves in a way entirely analogous to the Ising Model in 2 dimensions [95]. At temperatures above the critical temperature, the system is in a disordered phase but as the temperature is lowered, clusters of aligned spins begin to develop. Below the critical temperature, the system sits in a state of three-phase coexistence

(c.f. the Ising Model in which it is a two-phase coexistence), in each of these states, there is an asymmetry between the number of one of the spin states present and the other two. An infinitesimally weak field which breaks symmetry by energetically favouring spins of one species is required to tip the system into one of these phases.

It should be noted that the Ising Model is simply the $Q=2$ Potts Model. The only difference is that in the Ising Model, the energetic difference between a nearest neighbour bond of two aligned and two mis-aligned spins is $2J$ and in the Potts model it is J . Consequently, the formula (1.51) [95] for the critical temperature in 2 dimensions of the Q -state Potts Model evaluates to twice Onsager's result for the Ising Model when Q is set to 2[51, 50].

$$\left(\frac{J}{K_B T}\right)_c = \ln(1 + \sqrt{Q}) \quad (1.51)$$

From here on in, I will discuss the Ising Model in the context of the two-state Potts model in order to facilitate more simple comparisons between different Q Potts models. Note that increasing Q has the effect of decreasing the critical temperature. This should not come as a surprise, higher Q essentially means more possible fluctuations and thus entropic effects becoming stronger with respect to energetic effects.

Furthermore, as already touched upon, an external field can be introduced which works similarly to that in the Ising Model, that is it energetically favours a given spin state. For $Q=2$, favouring $+$ spins is equivalent to de-favouring $-$ spins, only one magnetic field can exist. For the 3-state Potts model, one can introduce 2 fields (and hence the Q -state Potts model can support up to $Q-1$ fields). The full Potts Hamiltonian for the 3-state Potts Model reads:

$$H = -J \sum_{\langle ij \rangle} \delta_{s_i, s_j} - h_a \sum_i \delta_{a, s_i} - h_b \sum_i \delta_{b, s_i} \quad (1.52)$$

where (a, b) are two arbitrarily chosen spin states from the possible three.

1.5.3. A Generalised Hamiltonian for the Potts Model

One naive approach to constructing a Hamiltonian for the Potts Model on a 2×2 lattice would be as follows:

$$H = -(N)K_0 - K_1 \sum_{\langle ij \rangle} \delta(s_i, s_j) - K_2 \sum_{\langle\langle ij \rangle\rangle} \delta(s_i, s_j) - K_3 \sum_{\square} \delta(s_i, s_j) \delta(s_j, s_k) \delta(s_k, s_l) \quad (1.53)$$

in a notation chosen to correspond to that used by Hasenbusch for the Ising Model. A rather subtle issue with this is that if $s_i = s_j$ and $s_k = s_l$, but $s_i \neq s_l$, in the Ising Model the product $s_i s_j s_k s_l$ is the same as were all spins equal but for the Potts model the combination of delta functions is different to that of all spins equal. This however would not represent a problem (and this interaction certainly respects the symmetries of the Potts Model), if evaluating (1.53) for all $3^4 = 81$ configurations possible for a 3-state Potts Model on a 2×2 lattice could only give four different outcomes. It turns out however, that there are six possible results.

Dasgupta [21] has attempted (although his work significantly pre-dates that of Hasenbusch) to construct a Hamiltonian equivalent to Hasenbusch's (1.35) for the Potts model on a 2×2 lattice. His work is from a time when computational power was considerably behind where it is today, and thus his technique is not "exact" like Hasenbusch's but rather he uses a variational RG technique [46]. In the absence of a magnetic field, he includes six interactions (although they appear to be somewhat arbitrarily chosen). Interestingly however, the number is six. Similarly to the Ising Model for $\frac{N}{B} = 3$, it is rather tedious to determine what the permitted interactions are, and harder yet to know when all of them have been found, but there seems to be a natural number of different values which the Hamiltonian can evaluate to.

1.5.4. Reproducing Hasenbusch's Results using a Categories Hamiltonian

The categories shown in Table 1.1 were derived from Hasenbusch's Hamiltonian (1.35). What if we did not have said Hamiltonian to guide us, but we somehow knew what the categories were anyway? For the 2×2 lattice,

we could then retrospectively introduce our own very simple Hamiltonian:

$$H = -K_0\delta(\{s_i\}, C_0) - K_1\delta(\{s_i\}, C_1) - K_2\delta(\{s_i\}, C_2) - K_3\delta(\{s_i\}, C_3) \quad (1.54)$$

in which $\delta(\{s_i\}, C_j)$ equals 1 if the 2×2 spin configuration $\{s_i\}$ is contained within category C_j and 0 otherwise. By its very design, this Hamiltonian would (re) construct Table 1.1. Likewise, it is simple enough to make reference to Hasenbusch's parametrisation by equating the energies of all configurations in either picture:

$$\begin{pmatrix} 1 & 8 & 8 & 4 \\ 1 & 0 & 0 & -4 \\ 1 & 0 & -4 & 4 \\ 1 & -8 & 4 & 4 \end{pmatrix} \begin{pmatrix} K_0 \\ K_1 \\ K_2 \\ K_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} J_0 \\ J_1 \\ J_2 \\ J_3 \end{pmatrix} \quad (1.55)$$

in which the $\underline{J}$ represents the parametrisation in this new picture. This provides a map between the two pictures.

Patching

The Hamiltonian (1.54) is only of use if it has meaning on a 4×4 lattice (or more generally, can a version of (1.54) which is designed for an $\frac{N}{B} \times \frac{N}{B}$ lattice be implemented on an $N \times N$ lattice?). The way to do this is to visit every site on the lattice in turn and include it within a 2×2 (or $\frac{N}{B} \times \frac{N}{B}$) "patch". For a square lattice, in which $\frac{N}{B} = 2$, a rather formal definition of a patch originating from a given site is a collection of four sites, of which two are nearest neighbours of the original site (themselves next-nearest neighbours of each other), and one next-nearest neighbour (itself nearest neighbours of the other two sites). In short, a patch is an $\frac{N}{B} \times \frac{N}{B}$ square which contains the original site. Four such squares can be drawn from any source site (this is because each site has four next-nearest neighbours and once a next-nearest neighbour has been selected, the choice is unique). However, if a given orientation is chosen (i.e. pair a site with its "down right" next-nearest neighbour) and consistently used, all of the possible squares which fit the formal definition will be generated after visiting every site. Figure 1.10 shows how to perform the patching procedure on a 2×2 lattice, formally taking the periodic boundary conditions into

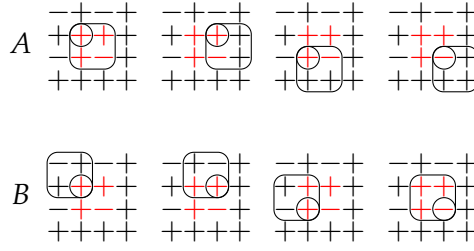


Figure 1.10.: How to patch for a 2×2 lattice configuration. Red sites indicate the original lattice and black sites are the result of periodic boundary conditions. Patches are denoted by the black squares and the site being patched around is circled. Methods A and B differ only by the patching orientation. Method A represents "down right" patching whereas B represents "up left". It is clear that both methods produce the same contributions which are the rotations of the original lattice.

account (which had not been done in (1.54) to avoid confusion). This same procedure can now be applied on any size of lattice.

K_0 Revisited

(1.54) is perhaps the most obvious choice when introducing a categories Hamiltonian but turns out not to be the most convenient. If such a Hamiltonian is to be evaluated on an $N \times N$ lattice using the method of patching, then strictly speaking this process must also be carried out on $\frac{N}{B} \times \frac{N}{B}$ lattices. Thus when evaluating the categories Hamiltonian for the 2×2 lattice configuration $\begin{pmatrix} ++ \\ -+ \end{pmatrix}$, and respecting periodic boundary conditions as in Figure 1.10, four contributions are obtained namely: $\begin{pmatrix} ++ \\ -+ \end{pmatrix}, \begin{pmatrix} ++ \\ +- \end{pmatrix}, \begin{pmatrix} -+ \\ ++ \end{pmatrix}$ and $\begin{pmatrix} +- \\ ++ \end{pmatrix}$. All of these configurations however are in the same category (itself a necessity of the periodic boundary conditions), namely category C_1 and thus the Hamiltonian evaluates to $4K_1$ (see Table 1.1). Note that here we see that the categories Hamiltonian automatically introduces the notion of system size-dependence to the Hamiltonian which is required in order to find a fixed point. This turns out however not to be the most convenient parametrisation. To understand this, it is important to understand the notion of a "relative" and an "absolute" fixed point fixed. Assume a fixed point exists such that $\underline{K}'(\underline{K}^*) = \underline{K}^*$. Next, consider $\underline{K}_\Delta = \underline{K}^* + \underline{\Delta}$ in which

$\underline{\Delta} = \Delta(1, 1, \dots, 1)^T$. It can be shown that

$$K'_i(\underline{K}^* + \underline{\Delta}) = B^2\Delta + K_i^* \quad (1.56)$$

(1.56) shows the effect of adding a constant term to the couplings vector. Crucially, it affects all couplings in the same way and thus the energies of all configurations relative to one and other remain constant. Thus physically, this has no effect, as the concept of an absolute energy has no meaning, as only relative energies can be measured (alternately the relative probability of any two microstates remain unaffected). This means that the quantities $(K_i - K_j)$ are conserved $\forall(i, j)$. Also adding $\underline{\Delta}$ to all couplings does not affect $\frac{\partial K'_i}{\partial K_j}$ and thus has no effect on critical exponents.

It turns out to be more convenient to dump all of the arbitrariness contained within $\underline{\Delta}$ into one of the constants which can then be changed without loss of generality (as opposed to being able to add $\underline{\Delta}$ to all K_i without any loss of information). This is achieved by assigning category C_0 an energy K_0 and all other categories C_i energies $K_0 + K_i$. The high temperature fixed point (HTFP) is the limit in which all couplings have effectively zero strength which means that all configurations have the same energy. Parametrising energies by (1.54), it can be seen that this occurs at the point $\underline{K} = -\ln(Q)(1, 1, \dots, 1)^T$ whereas using the improved parametrisation, the HTFP is at $\underline{K} = (-\ln(Q), 0, 0, \dots, 0)^T$. Finding the non-trivial fixed point is in a sense a two-step process (if done by intelligent root-finding) which involves first finding the relative fixed point and subsequently the absolute one. However finding the relative fixed point using (1.54) is in practise considerably more difficult than doing so using this new parametrisation. The reason for this is that it is necessary, when performing an analysis of the flow, to keep track of the quantities $(K_i - K_j)$ and $(K'_i - K'_j)$ in order to determine whether a fixed point is being approached. This is in contrast to simply keeping track of $(K'_i - K_i)$. Furthermore, while adding $\underline{\Delta}$ to $\underline{K}$ has no effect on $(K'_i - K'_j)$, in general the computation is more simple for small values of $\underline{K}$ and subsequently relatively small values of K'_i and K'_j . While in theory their values are inconsequential and only their difference is of interest, in practise it is in our interests to keep them small and reduce computational time and error. Thus Δ should be chosen as such. One way of doing this would be to choose $\Delta = -K_0$. This is equivalent in

the improved parametrisation to simply resetting $K_0 = 0$ at every iteration of the flow analysis and then when having found $\underline{K}^*$ such that $K'_i = K_i$ for $i \neq 0$, then finding the value of K_0 which insures this relative fixed point is also absolutely fixed.

(1.57) is the matrix equation arising from this parametrisation. From here on in, everything works much like Hasenbusch's method. A paradigm configuration from every category must be chosen, the sums (the RHS of (1.57)) pertaining to each paradigm evaluated and the fixed point of the transformation found. Also, while the Matrix equation in question is not quite as simple as it would be had (1.54) been used (the LHS would simply be the identity matrix), it is considerably simpler than (1.37). Using a categories Hamiltonian also implies that this Matrix has the same form regardless of the number of categories, given by

$$\begin{pmatrix} 4 & 0 & 0 & \dots & 0 \\ 4 & 4 & 0 & \dots & 0 \\ 4 & 0 & 4 & \dots & 0 \\ 4 & . & . & \dots & . \\ 4 & . & . & \dots & . \\ 4 & 0 & 0 & \dots & 4 \end{pmatrix} \begin{pmatrix} J'_0 \\ J'_1 \\ J'_2 \\ . \\ . \\ J'_{N-1} \end{pmatrix} = \begin{pmatrix} \ln \left(\sum_{\{s_i\} \rightarrow C_0} e^{-H'(\{s_i\})} \right) \\ \ln \left(\sum_{\{s_i\} \rightarrow C_1} e^{-H'(\{s_i\})} \right) \\ \ln \left(\sum_{\{s_i\} \rightarrow C_2} e^{-H'(\{s_i\})} \right) \\ . \\ . \\ \ln \left(\sum_{\{s_i\} \rightarrow C_{N-1}} e^{-H'(\{s_i\})} \right) \end{pmatrix} \quad (1.57)$$

(with the factors of 4 replaced by $(\frac{N}{B})^2$ for the general case) whose inverse

(the analogue of (1.38)) reads:

$$\begin{pmatrix} J'_0 \\ J'_1 \\ J'_2 \\ . \\ . \\ J'_{N-1} \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ -1 & 1 & 0 & \dots & 0 \\ -1 & 0 & 1 & \dots & 0 \\ -1 & . & . & \dots & 0 \\ -1 & . & . & \dots & 0 \\ -1 & 0 & 0 & \dots & 1 \end{pmatrix} \begin{pmatrix} \ln \left(\sum_{\{s_i\} \rightarrow C_0} e^{-H'(\{s_i\})} \right) \\ \ln \left(\sum_{\{s_i\} \rightarrow C_1} e^{-H'(\{s_i\})} \right) \\ \ln \left(\sum_{\{s_i\} \rightarrow C_2} e^{-H'(\{s_i\})} \right) \\ . \\ . \\ \ln \left(\sum_{\{s_i\} \rightarrow C_{N-1}} e^{-H'(\{s_i\})} \right) \end{pmatrix} \quad (1.58)$$

Because each term in each sum on the RHS will be multiplied by a factor of $e^{N^2 K_0}$, these could be pulled outside the sum. Furthermore because $\ln(a) - \ln(b) = \ln \frac{a}{b}$, J_0 has no effect at all on J'_i apart from J'_0 .

1.5.5. Equivalence of Critical Exponents

Implementing the categories Hamiltonian method for the $4 \times 4 \rightarrow 2 \times 2$ Ising Model as outlined, as a test before proceeding to the Potts Model, it came as somewhat of a surprise that the critical exponent ν came out to be not just similar, but exactly the same to as high a numerical precision as we could determine. The following proof however will detail why. Firstly, consider the two matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ related by the transformation

$$\underline{\underline{A}} = \underline{\underline{U}}^{-1} \cdot \underline{\underline{B}} \cdot \underline{\underline{U}} \quad (1.59)$$

in which $\underline{\underline{U}}$ is any non-singular matrix. If $\underline{e}_i$ is an eigenvector of $\underline{\underline{A}}$ with eigenvalue λ_i :

$$\begin{aligned} \underline{\underline{U}} \cdot \underline{\underline{A}} &= \underline{\underline{B}} \cdot \underline{\underline{U}} \\ \underline{\underline{U}} \cdot \underline{\underline{A}} \cdot \underline{e}_i &= \underline{\underline{B}} \cdot \underline{\underline{U}} \cdot \underline{e}_i \\ \lambda_i \underline{\underline{U}} \cdot \underline{e}_i &= \underline{\underline{B}} \cdot \underline{v}_i \end{aligned} \quad (1.60)$$

in which $\underline{\underline{U}} \cdot \underline{e}_i = \underline{v}_i$. Thus

$$\lambda_i \underline{v}_i = \underline{\underline{B}} \cdot \underline{v}_i \quad (1.61)$$

Hence if two matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are related by the transformation shown in (1.59), then their eigenvalues are the same, and the eigenvectors of $\underline{\underline{B}}$ are those of $\underline{\underline{A}}$ rotated by $\underline{\underline{U}}$. In (1.55), I introduced the notion that equating the energies of all configurations in two different parametrisations of the Hamiltonian allows us to write down a matrix equation equating the two pictures, which quite generally can be expressed as:

$$\underline{\underline{M}} \cdot \underline{\underline{K}} = \underline{\underline{N}} \cdot \underline{\underline{J}} \quad (1.62)$$

Furthermore the form of the Hamiltonian does not change upon renormalisation, only the coupling values so the same equation is true for $\underline{\underline{K}}'$ and $\underline{\underline{J}}'$. Rearranging (1.62)

$$\begin{aligned} \underline{\underline{K}} &= \underline{\underline{M}}^{-1} \cdot \underline{\underline{N}} \cdot \underline{\underline{J}} \\ \underline{\underline{J}} &= \underline{\underline{N}}^{-1} \cdot \underline{\underline{M}} \cdot \underline{\underline{K}} \end{aligned} \quad (1.63)$$

with the same holding for the primed couplings. Next define the matrices $\underline{\underline{\mathcal{K}}}$ and $\underline{\underline{\mathcal{J}}}$ (not to be confused with $\underline{\underline{K}}$ and $\underline{\underline{J}}$) such that:

$$(\underline{\underline{\mathcal{K}}})_{ij} = \frac{\partial K'_i}{\partial K_j} \quad (\underline{\underline{\mathcal{J}}})_{ij} = \frac{\partial J'_i}{\partial J_j} \quad (1.64)$$

I now calculate the derivative $\frac{\partial K'_i}{\partial K_j}$ explicitly relating it to $\frac{\partial J'_i}{\partial J_j}$. Note that for example, when encountering a term of the form $(MNJ)_i$, the J in question must be $\underline{\underline{J}}$ because the final product is a vector not a matrix.

$$\begin{aligned} \frac{\partial K'_i}{\partial K_j} &= \frac{\partial}{\partial K_j} \left(M^{-1} N J' \right)_i = \frac{\partial}{\partial K_j} \sum_a (M^{-1} N)_{ia} J'_a \\ &= \frac{\partial}{\partial K_j} \sum_a \sum_b M_{ib}^{-1} N_{ba} J'_a = \sum_a \sum_b M_{ib}^{-1} N_{ba} \frac{\partial J'_a}{\partial K_j} \\ &= \sum_a \sum_b M_{ib}^{-1} N_{ba} \sum_c \frac{\partial J_c}{\partial K_j} \frac{\partial J'_a}{\partial J_c} \end{aligned}$$

in which the final step involves invoking the chain rule. Now we have an expression for $\frac{\partial K'_i}{\partial K_j}$ in terms of $\frac{\partial J'_i}{\partial J_j}$ but it needs tidying up. Substituting for

$\frac{\partial J_c}{\partial K_j}$ from (1.62):

$$\frac{\partial J_c}{\partial K_j} = \frac{\partial}{\partial K_j} \sum_d (N^{-1}M)_{cd} K_d = \frac{\partial}{\partial K_j} \sum_d \sum_e N_{ce}^{-1} M_{ed} K_d = \sum_e N_{ce}^{-1} M_{ej} = (N^{-1}M)_{cj}$$

Combining this, we obtain:

$$\frac{\partial K'_i}{\partial K_j} = \sum_a \sum_b M_{ib}^{-1} N_{ba} \sum_c (N^{-1}M)_{cj} \mathcal{J}_{ac} = \sum_a (M^{-1}N)_{ia} (\mathcal{J}N^{-1}M)_{aj} = (M^{-1}N\mathcal{J}N^{-1}M)_{ij}$$

and thus:

$$\underline{\underline{K}} = \underline{\underline{M}}^{-1} \cdot \underline{\underline{N}} \cdot \underline{\underline{J}} \cdot \underline{\underline{N}}^{-1} \cdot \underline{\underline{M}} \quad (1.65)$$

and hence the Jacobian matrices in the two pictures are related by such a transformation and must have the same eigenvalues. This equivalence of parametrisations has a further use. When extending Hasenbusch's method to include a magnetic field, as expected, two critical exponents were found namely the magnetic and the thermal exponents y_h and y_t . What was again not necessarily expected, is that the critical exponent y_t takes exactly the same value as it does in the absence of a magnetic field, that is to say, there is no numerical discrepancy whatsoever. (1.62) holds at the fixed point, as all couplings related to magnetic interactions must take the value of zero. However now, $\underline{\underline{K}}$ is a 4×1 matrix (4 component vector), and $\underline{\underline{J}}$ is 6×1 (using $\underline{\underline{K}}$ to represent the Hamiltonian in the absence of magnetic interactions and $\underline{\underline{J}}$ with them included). The extra complication is that for (1.62) to hold, while $\underline{\underline{M}}$ is still a 4×4 matrix, $\underline{\underline{N}}$ is now 4×6 and thus not invertible. A similar analysis to the case of square $\underline{\underline{N}}$ however can be carried out resulting in:

$$\underline{\underline{T}} \cdot \underline{\underline{J}} = \underline{\underline{K}} \cdot \underline{\underline{T}} \quad (1.66)$$

in which $\underline{\underline{T}} = \underline{\underline{M}}^{-1} \cdot \underline{\underline{N}}$. If $\underline{\underline{e}}_i$ are defined as the eigenvectors of $\underline{\underline{J}}$ with eigenvalues λ_i , and $\underline{\underline{u}}_i$ are defined as $\underline{\underline{T}} \cdot \underline{\underline{e}}_i = \underline{\underline{u}}_i$,

$$\underline{\underline{T}} \cdot \underline{\underline{J}} \cdot \underline{\underline{e}}_i = \lambda_i \underline{\underline{T}} \cdot \underline{\underline{e}}_i = \lambda_i \underline{\underline{u}}_i$$

$$\underline{\underline{K}} \cdot \underline{\underline{T}} \cdot \underline{\underline{e}}_i = \underline{\underline{K}} \cdot \underline{\underline{u}}_i$$

and thus indeed, $\underline{K}$ will share eigenvalues with $\underline{J}$, the eigenvectors having been multiplied by $\underline{T}$. Note that $\underline{K}$ will necessarily have fewer eigenvectors than $\underline{J}$ and thus the latter will have eigenvalues unique to it (including an additional one greater than unity, related to y_h).

Calculating T_c

Calculating T_c is done very similarly to when doing so using Hasenbusch's Hamiltonian. It is necessary to calculate the energy of each category using Ising's Hamiltonian in terms of the nearest neighbour coupling (i.e. $-J \sum_{\langle ij \rangle} s_i s_j$). This generates N simultaneous (N =the number of categories) equations relating each category's (say C_i) coupling value to $-J \sum_{\langle ij \rangle} s_i s_j$ for that particular category. These equations can be solved to find values for K_i in terms of J and then one proceeds as before, varying J , assigning K_i their corresponding values, examining the flow and finding the separatrix. It is convenient to introduce a J_0 into Ising's Hamiltonian and set it such that K_0 can be set to 0 in the categories Hamiltonian. K_0 can then be set to zero at every flow iteration because its value has no effect on K'_i . Having it non-zero however involves the computation of very large exponentials. The final K'_i involve dividing one by the other and the effect cancels out but regardless, it is computationally less expensive and less susceptible to numerical error to not have to do this.

1.5.6. Generating The Categories

To recap, we now know that using a Hamiltonian which is designed to reconstruct Table 1.1 is an equally valid way of implementing an RG transformation from a $4 \times 4 \rightarrow 2 \times 2$ Ising lattice as it results in a transformation which has a fixed point and yields the same critical temperature and exponents. Likewise, coming up with a Hamiltonian analogous to Hasenbusch's for a $Q = 3$ Potts Model or repeating Hasenbusch's procedure for a $6 \times 6 \rightarrow 3 \times 3$ lattice is a non-trivial exercise. Furthermore, having made some attempts to do this, there is strong evidence to suggest that in both cases, there is a "natural" categorisation. For the $Q = 3$ Potts Model on a $4 \times 4 \rightarrow 2 \times 2$ lattice, even without figuring out which interactions must be included in the Hamiltonian, there is strong evidence to suggest there must be six categories, and for the $6 \times 6 \rightarrow 3 \times 3$ Ising Case, there appear

C_0	C_1			C_2			C_3	C_4			C_5		
$\begin{pmatrix} 00 \\ 00 \end{pmatrix}$	$\begin{pmatrix} 00 \\ 01 \end{pmatrix}$	$\begin{pmatrix} 00 \\ 02 \end{pmatrix}$	$\begin{pmatrix} 11 \\ 12 \end{pmatrix}$	$\begin{pmatrix} 00 \\ 11 \end{pmatrix}$	$\begin{pmatrix} 11 \\ 22 \end{pmatrix}$	$\begin{pmatrix} 22 \\ 00 \end{pmatrix}$	$\begin{pmatrix} 01 \\ 10 \end{pmatrix}$	$\begin{pmatrix} 00 \\ 12 \end{pmatrix}$	$\begin{pmatrix} 11 \\ 02 \end{pmatrix}$	$\begin{pmatrix} 22 \\ 01 \end{pmatrix}$	$\begin{pmatrix} 02 \\ 10 \end{pmatrix}$	$\begin{pmatrix} 12 \\ 01 \end{pmatrix}$	$\begin{pmatrix} 21 \\ 02 \end{pmatrix}$
$\begin{pmatrix} 11 \\ 11 \end{pmatrix}$	$\begin{pmatrix} 00 \\ 10 \end{pmatrix}$	$\begin{pmatrix} 00 \\ 20 \end{pmatrix}$	$\begin{pmatrix} 11 \\ 21 \end{pmatrix}$	$\begin{pmatrix} 01 \\ 01 \end{pmatrix}$	$\begin{pmatrix} 12 \\ 12 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 20 \end{pmatrix}$	$\begin{pmatrix} 10 \\ 01 \end{pmatrix}$	$\begin{pmatrix} 00 \\ 21 \end{pmatrix}$	$\begin{pmatrix} 11 \\ 20 \end{pmatrix}$	$\begin{pmatrix} 22 \\ 10 \end{pmatrix}$	$\begin{pmatrix} 01 \\ 20 \end{pmatrix}$	$\begin{pmatrix} 10 \\ 21 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 12 \end{pmatrix}$
$\begin{pmatrix} 22 \\ 22 \end{pmatrix}$	$\begin{pmatrix} 10 \\ 00 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 00 \end{pmatrix}$	$\begin{pmatrix} 21 \\ 11 \end{pmatrix}$	$\begin{pmatrix} 11 \\ 00 \end{pmatrix}$	$\begin{pmatrix} 22 \\ 11 \end{pmatrix}$	$\begin{pmatrix} 00 \\ 22 \end{pmatrix}$	$\begin{pmatrix} 02 \\ 20 \end{pmatrix}$	$\begin{pmatrix} 01 \\ 02 \end{pmatrix}$	$\begin{pmatrix} 10 \\ 12 \end{pmatrix}$	$\begin{pmatrix} 21 \\ 20 \end{pmatrix}$	$\begin{pmatrix} 10 \\ 02 \end{pmatrix}$	$\begin{pmatrix} 21 \\ 10 \end{pmatrix}$	$\begin{pmatrix} 12 \\ 20 \end{pmatrix}$
	$\begin{pmatrix} 01 \\ 00 \end{pmatrix}$	$\begin{pmatrix} 02 \\ 00 \end{pmatrix}$	$\begin{pmatrix} 12 \\ 11 \end{pmatrix}$	$\begin{pmatrix} 10 \\ 10 \end{pmatrix}$	$\begin{pmatrix} 21 \\ 21 \end{pmatrix}$	$\begin{pmatrix} 02 \\ 02 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 02 \end{pmatrix}$	$\begin{pmatrix} 02 \\ 01 \end{pmatrix}$	$\begin{pmatrix} 12 \\ 10 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 21 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 01 \end{pmatrix}$	$\begin{pmatrix} 01 \\ 12 \end{pmatrix}$	$\begin{pmatrix} 02 \\ 21 \end{pmatrix}$
	$\begin{pmatrix} 11 \\ 10 \end{pmatrix}$	$\begin{pmatrix} 22 \\ 20 \end{pmatrix}$	$\begin{pmatrix} 22 \\ 21 \end{pmatrix}$				$\begin{pmatrix} 12 \\ 21 \end{pmatrix}$	$\begin{pmatrix} 12 \\ 00 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 11 \end{pmatrix}$	$\begin{pmatrix} 01 \\ 22 \end{pmatrix}$			
	$\begin{pmatrix} 11 \\ 01 \end{pmatrix}$	$\begin{pmatrix} 22 \\ 02 \end{pmatrix}$	$\begin{pmatrix} 22 \\ 12 \end{pmatrix}$				$\begin{pmatrix} 21 \\ 12 \end{pmatrix}$	$\begin{pmatrix} 21 \\ 00 \end{pmatrix}$	$\begin{pmatrix} 02 \\ 11 \end{pmatrix}$	$\begin{pmatrix} 10 \\ 22 \end{pmatrix}$			
	$\begin{pmatrix} 01 \\ 11 \end{pmatrix}$	$\begin{pmatrix} 02 \\ 22 \end{pmatrix}$	$\begin{pmatrix} 12 \\ 22 \end{pmatrix}$					$\begin{pmatrix} 10 \\ 20 \end{pmatrix}$	$\begin{pmatrix} 01 \\ 21 \end{pmatrix}$	$\begin{pmatrix} 12 \\ 02 \end{pmatrix}$			
	$\begin{pmatrix} 10 \\ 11 \end{pmatrix}$	$\begin{pmatrix} 20 \\ 22 \end{pmatrix}$	$\begin{pmatrix} 21 \\ 22 \end{pmatrix}$					$\begin{pmatrix} 20 \\ 10 \end{pmatrix}$	$\begin{pmatrix} 21 \\ 01 \end{pmatrix}$	$\begin{pmatrix} 02 \\ 12 \end{pmatrix}$			

Table 1.3.: The six configurations of the 3-state Potts model on a 2×2 lattice. 0,1 and 2 are labels for orthogonal states rather than actual spin values

to be 13. Thus in principle it is possible to proceed in exactly this way. The categories obtained for the 3-state Potts Model using (1.53) are shown in Table 1.3.

A Hamiltonian which reconstructs these configurations can be implemented on a 4×4 lattice using the method of patching, six paradigms must be chosen from each category and then according to (1.58) the renormalised couplings can be calculated. Using root finding to find the fixed point of the transformation, the critical exponents of the 3-state Potts model can be found. For this reason, it is necessary to rigorise a method to determine the categories rather than claiming that there is a "natural categorisation which appears to arise as we start adding as many interactions as we can think of".

To understand this, it is important to revisit (1.5). The key piece of information contained here is that if two configurations $\{S_I\}$ and $\{S_J\}$ on the coarse-grained lattice (the categories exist on lattices of the same size as the coarse-grained lattice by necessity) have the same energy, then:

$$\sum_{\{s_i\} \rightarrow \{S_I\}} e^{-H(\{s_i\})} = \sum_{\{s_i\} \rightarrow \{S_J\}} e^{-H(\{s_i\})} \quad (1.67)$$

We can learn a surprising amount from this seemingly innocuous condition. Both the LHS and the RHS of (1.67) consist of a sum of the exponentials of the energies of $Q^{N^2 \left(\frac{B^2-1}{B^2} \right)}$ configurations on an $N \times N$ lattice. The only systematic way to satisfy (1.67) is to insure that each term on the RHS

has a corresponding equal term on the LHS. Thus it is easier to think of (1.67) as $Q^{N^2 \left(\frac{B^2-1}{B^2} \right)}$ different conditions of the form

$$H(\{s_i\}) = H(\{s_j\}) \quad (1.68)$$

that is to say, there exist two groups (groups in the colloquial rather than mathematical meaning of the word) of $Q^{N^2 \left(\frac{B^2-1}{B^2} \right)}$, 4×4 spin configurations, G_i and G_j in which all members of G_i renormalise to $\{S_I\}$ and all members of G_j renormalise to $\{S_J\}$. If each configuration in G_i has a counterpart configuration in G_j of the same energy, then $\{S_I\}$ and $\{S_J\}$ must be in the same category.

Consider an operator $\hat{O}$ which acts on any configuration $\{s_i\}$ on the $N \times N$ lattice and transforms it into another $N \times N$ spin configuration $\{s_j\}$. Furthermore, this operator must respect the symmetries of the original Ising Hamiltonian on the lattice (on the square lattice in the absence of an external field, these symmetries are parity, translational, rotational and mirroring invariance, $\hat{O}$ can contain any combination of these operations). If $\hat{O}G_i = G_j$, then $\{S_I\}$ and $\{S_J\}$ must be in the same category, as this implies that each configuration in G_i has a corresponding configuration in G_j of the same energy.

Furthermore, it has been observed that if $\hat{O}G_i = G_j$, then $\hat{O}'\{S_I\} = \{S_J\}$, that is to say that if we perform some operation to every $N \times N$ configuration in a category G_i , then we generate a new group G_j in which every term renormalises to $\{S_J\}$, which itself is related to $\{S_I\}$ by the equivalent transform $\hat{O}'$ on the $\frac{N}{B} \times \frac{N}{B}$ lattice. If this is the case, then:

$$\begin{aligned} \hat{O}'\{S_I\} &= \hat{O}'\hat{\mathcal{R}}G_i \\ \hat{O}'\{S_I\} &= \{S_J\} = \hat{\mathcal{R}}G_j = \hat{\mathcal{R}}\hat{O}G_i \\ \hat{\mathcal{R}}\hat{O}G_i &= \hat{O}'\hat{\mathcal{R}}G_i \end{aligned} \quad (1.69)$$

and thus but for the fact that $\hat{O}$ and $\hat{O}'$ are not the same operator technically as they operate on different size lattices, $[\hat{O}, \hat{\mathcal{R}}]$, i.e. the operator $\hat{O}$ and the coarse graining operator commute. In practise this means, that if two $\frac{N}{B} \times \frac{N}{B}$ configurations $\{S_I\}$ and $\{S_J\}$ are related by the operator $\hat{O}'$, and the operation represented by $\hat{O}$ commutes with coarse graining, then $\{S_I\}$ and $\{S_J\}$ must be in the same category. While commutation of the operators

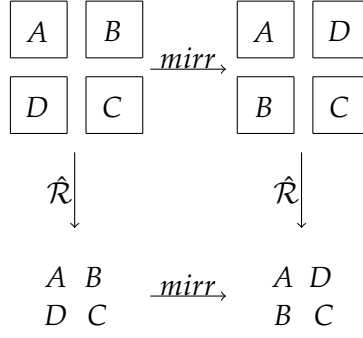


Figure 1.11.: A mirroring operation on an $N \times N$ lattice will keep $B \times B$ blocks together and thus result in a mirroring of the coarse-grained configuration. The mirroring operator commutes with the coarse-graining operator.

implies being in the same category, the reverse is not true, commutation is a stronger restriction. To reiterate, it is sufficient that there exists an operator $\hat{O}$ which respects the symmetries of the Hamiltonian and the lattice, and which when applied to a group of configurations G_i , which renormalise to a given $\{S_I\}$, generates a new group G_j whose members all renormalise to a new configuration $\{S_J\}$. If this is the case, $\{S_I\}$ and $\{S_J\}$ must be in the same category. This is the formal definition of a category, although it will not be the most practical way to actually generate categories.

To make this somewhat less abstract, consider the parity operator $\hat{P}$ which flips the sign of all spins in the Ising Model. Define G_i to be the $2^{12} = 4096$ configurations which renormalise to $\begin{bmatrix} ++ \\ ++ \end{bmatrix}$ and G_j the configurations which renormalise to $\begin{bmatrix} -- \\ -- \end{bmatrix}$. Clearly by its very nature of being based on a majority rule, the coarse-graining procedure commutes with the parity operator, that is to say for any 4×4 configuration which renormalises to $\begin{bmatrix} ++ \\ ++ \end{bmatrix}$, there exists another 4×4 configuration related by a parity exchange which renormalises to $\begin{bmatrix} -- \\ -- \end{bmatrix}$.

Mirroring and Translation as Symmetries

Mirroring has the convenient property that it keeps $B \times B$ blocks together as is shown in Figure 1.11. Translation works similarly but care is needed in interpreting the translation operator. On an $N \times N$ lattice, the operator $\hat{O}$ must translate all columns by B , or all rows by B . This again keeps all $B \times B$

blocks together, that is to say when the coarse-graining procedure is performed, it will involve finding the majority species within the same $(\frac{N}{B})^2$ groups of B^2 spins. If the operator which results in B column switches, $\hat{C}S^B$, is applied to G_i , it will generate G_j , the group of configurations which renormalise to $\hat{C}S'\{S_I\}$, which is a commutation of sorts but care must be taken with this definition as $\hat{O}$ and $\hat{O}'$ involve different numbers of column switches.

Rotation and Ambiguity

The final symmetry which must be taken into account for a square 2d lattice is rotational symmetry. Intuitively, $\begin{pmatrix} + & - \\ + & + \end{pmatrix}$ and $\begin{pmatrix} - & + \\ - & + \end{pmatrix}$ must have the same energy and be in the same category, but can this be rigorised with the current definition? The answer is yes, but ambiguous cases complicate the matter. Rotation likewise has the convenient property that it keeps all blocks together and only moves the blocks within the lattice, like mirroring or multiple column/row shifts. The problem arises when one of the blocks is an ambiguous case such as $\begin{pmatrix} + & + \\ - & - \end{pmatrix}$ which when rotated 90 degrees clockwise becomes $\begin{pmatrix} - & + \\ - & + \end{pmatrix}$. These two configurations renormalise differently using the "top left" rule for disambiguation. Thus the renormalisation operator and the rotation operator do not commute for such configurations. While this is not strictly necessary, they do commute for any configuration with no ambiguities in it and therein lies the problem. Firstly let us examine how to get around the problem using a blocking kernel. Using a blocking kernel, (1.67) becomes:

$$\sum_{\{s_i\} \rightarrow S_I} T(s_i, S_I) e^{-H(s_i)} = \sum_{\{s_i\} \rightarrow S_J} T(s_i, S_J) e^{-H(s_i)} \quad (1.70)$$

Using the particular example of $N = 4, B = 2$, the blocking kernel can take the values 1 (no ambiguous blocks), $\frac{1}{2}$ (one ambiguous block), $\frac{1}{4}$ (two ambiguous blocks), $\frac{1}{8}$ and $\frac{1}{16}$. Thus instead of forming groups G_i , it is necessary within these groups to form sub-groups of configurations $G_{i,a}$ which renormalise to S_I but their contribution to that sum is $(\frac{1}{2})^a$. Then two configurations S_I and S_J are in the same category if and only if:

$$\hat{O}G_{ia} = G_{ja} \quad \forall a \quad (1.71)$$

$\begin{array}{cccc} - & - & + & + \\ - & - & + & + \\ + & + & + & + \\ + & + & + & + \end{array} \longrightarrow \begin{array}{cc} - & + \\ + & + \end{array}$	$\begin{array}{cccc} - & + & + & + \\ + & - & + & + \\ + & + & + & + \\ + & + & + & + \end{array} \longrightarrow \frac{1}{2} \begin{array}{cc} - & + \\ + & + \end{array}$	$\begin{array}{cccc} - & + & + & + \\ + & - & - & - \\ + & + & + & + \\ + & + & + & + \end{array} \longrightarrow \frac{1}{4} \begin{array}{cc} - & + \\ + & + \end{array}$
$\hat{R}_{90} \downarrow$	$\hat{R}_{90} \downarrow$	$\hat{R}_{90} \downarrow$
$\begin{array}{cccc} + & + & - & - \\ + & + & - & - \\ + & + & + & + \\ + & + & + & + \end{array} \longrightarrow \begin{array}{cc} + & - \\ + & + \end{array}$	$\begin{array}{cccc} + & + & + & - \\ + & + & - & + \\ + & + & + & + \\ + & + & + & + \end{array} \longrightarrow \frac{1}{2} \begin{array}{cc} + & - \\ + & + \end{array}$	$\begin{array}{cccc} + & + & + & - \\ + & + & - & + \\ + & + & - & + \\ + & + & - & + \end{array} \longrightarrow \frac{1}{4} \begin{array}{cc} + & - \\ + & + \end{array}$

Figure 1.12.: The top line consists of three configurations in the same group G_i but in different G_{ia} ($a=0,1,2$). The bottom lines shows rotations of these three configurations and shows that they all contribute in the analogous way to their respective G_{ja} after rotation when using a blocking kernel to resolve ambiguous cases in the coarse-graining procedure.

in which $\hat{O}$ has all the same properties as previously. Note that a 4×4 configuration will, if it is in G_{i1} also be in some other G_{j1} . The top line of Figure 1.12 shows three different 4×4 configurations which all belong to the same G_i but into different sub-groups G_{ia} . The bottom line shows three members of G_j which are all in different G_{ja} . The bottom 4×4 configurations all represent 90 degree rotations of the ones above them. Likewise, each G_{ia} on the top line has a contribution to an S_I equal to the S_J contribution on the line below it, in which S_J is a rotation of S_I .

It is preferable from a computational perspective to use the "top left" rule when dealing with ambiguous cases for memory reasons (it allows for a much smaller god tensor (see Section 1.5.8)). Thus it is necessary to show that the definition of a category is not at odds with dealing with ambiguous cases in the coarse graining procedure in this way. While this is certainly a "motivation by example" rather than an entirely rigorous proof, if we imagined that G_i consists of $\{s_i\}$ and its rotation (see Figure 1.13), and similarly G_j consists only of $\{s_j\}$ and its rotation, then because each term in G_i has an energetic counterpart in G_j , we can simply swap configurations in G_i with the relevant ones in G_j without affecting the values of $\sum_{G_i} e^{-H(\{s_i\})}$ or $\sum_{G_j} e^{-H(\{s_j\})}$ but restoring the fact that rotations of all configurations in G_i are also in G_i . Summarising, if a configuration $\{s_i\}$'s rotations do not renor-

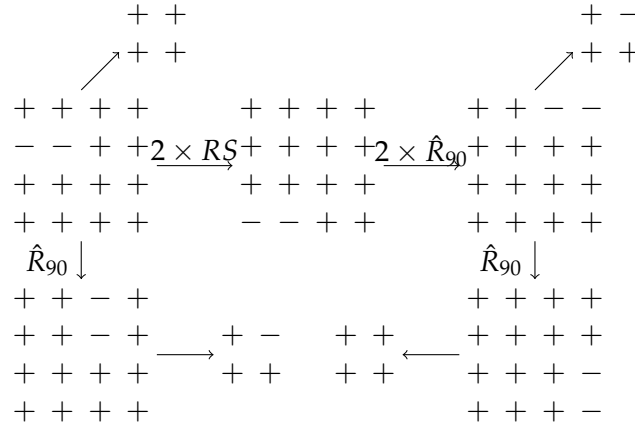


Figure 1.13.: The top left (say $\{s_i\}$) and top right (say $\{s_j\}$) 4×4 configurations are related by a combination of row switches (RS) and rotations which respect the symmetries of the lattice. While both configurations contain an ambiguity and thus upon rotation by 90 degrees, renormalise differently, the rotation of $\{s_i\}$ renormalises like $\{s_j\}$ and vice-versa.

malise to $\{S_I\}$ but rather $\{S_J\}$, but we can find a configuration $\{s_j\}$ whose rotation renormalises to $\{S_I\}$, and if $\{s_i\}$ and $\{s_j\}$ are related by some operation $\hat{O}$ which respects the symmetries of the lattice, then the category generation rule can continue to be used in conjunction with the "top left" rule for dealing with ambiguities. While this is more of a "motivation by example" than rigorous proof, I have yet to come across an example of an $\{s_i\}$ for which I could not find an eligible $\{s_j\}$, although if all of the blocks are ambiguous this does get quite tedious.

1.5.7. The Category Generation Algorithm

While $\hat{O}G_i = G_j$ is the condition required to group $\{S_I\}$ and $\{S_J\}$ in the same category, in practise, it is considerably more simple to implement $\hat{O}'\{S_J\} = \{S_I\}$. It is worth keeping in mind that this is a more strict than necessary imposition but we believe that for the models we have studied, the two rules are equivalent. What this then translates to, is that if two $\frac{N}{B} \times \frac{N}{B}$ configurations are related to one and other by an operation $\hat{O}'$ which satisfies the previously outlined properties, they must be in the same category. The most obvious example is that $\hat{P}\begin{pmatrix} ++ \\ ++ \end{pmatrix} = \begin{pmatrix} -- \\ -- \end{pmatrix}$ and thus in the absence of an external field, these configurations must be in the same

category. A slightly more complicated example (which arises for the $Q > 2$ Potts models) would be:

$$\hat{M}\hat{P}_{cy}\begin{pmatrix} 0 & 2 \\ 1 & 0 \end{pmatrix} = \hat{M}\begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ 2 & 0 \end{pmatrix} \quad (1.72)$$

in which $\hat{P}_{cy}$ is the cyclic parity operator ($0 \rightarrow 1, 1 \rightarrow 2, 2 \rightarrow 0$) and $\hat{M}$ the mirroring operator. All three of the configurations in (1.72) must be in the same category as they are related by operations which respect the symmetry of the Hamiltonian and the lattice. While the following algorithm is certainly overkill in the sense that it will generate each member of a category many times, the number of computational operations required to generate all of the coarse-grained configurations pales into insignificance when compared to the computational time required to generate all of the original configurations. The crux of the algorithm is to generate all of the configurations which can exist on the coarse-grained, $\frac{N}{B} \times \frac{N}{B}$ lattice sequentially (by sequentially, it is meant that any 2d array can be mapped to a 1d array and then the configuration of a state in the Q-state Potts model can be thought of as a number counting in base Q), perform all required symmetry operations on this configuration and group the resulting configurations together. While (1.72) shows how $\begin{pmatrix} 0 & 2 \\ 1 & 0 \end{pmatrix}$ must be grouped with $\begin{pmatrix} 1 & 2 \\ 2 & 0 \end{pmatrix}$ via two symmetry operations, the intermittently generated state is necessarily also in the same category. Thus it is not necessary to think about performing combinations of operations on a single state, and subsequently worrying about whether certain operations commute (incidentally they do not, row and column switches do not commute with rotation). It suffices to generate a configuration, rotate it 4 times (it is now back in its original state), perform $\frac{N}{B}$ column switches, perform a mirroring operation and finally cycle through all permitted parity operations.

Parity

The parity operator $\hat{P}$ for the Ising Model is quite intuitive, it flips the sign of all spins or when considering the Ising Model as the $Q=2$ Potts model, it performs the permutation ($0 \rightarrow 1, 1 \rightarrow 0$) in which (0,1) are now spin labels. One possible symmetry operation alluded to already in the 3-state Potts Model is the cyclic parity operator. Likewise, the anti-cyclic parity operator respects the Z_3 [56] symmetry of the 3-state Potts model in the

absence of any external field. Additionally, it is perfectly valid to perform a parity swap of the form $(0 \rightarrow 0, 1 \rightarrow 2, 2 \rightarrow 1)$, of which there are 3. For the 4 state Potts model however, there are valid parity operations involving 4, 3 or 2 spin states. Furthermore, there is no limitation to cyclic and anti-cyclic permutations when performing operations involving 4 spins, that is to say, it is valid to perform the parity operation $(0 \rightarrow 1, 1 \rightarrow 0, 2 \rightarrow 3, 3 \rightarrow 2)$. Consider the following configuration $\begin{pmatrix} a & a & a \\ b & c & b \\ d & c & d \end{pmatrix}$ on a 3×3 lattice, in which there are four different spin states present. One could for example populate all of the sites labelled "a" with 0,1,2 or 3 spins. Subsequently, one could populate all of the sites labelled "b" with any spin species, other than the one the "a" sites were assigned. Thus for the Q-state Potts Model in the absence of an external field, it is necessary to perform $Q!$ operations to explore all of the configurations allowed by parity symmetry. It has been observed that in order to access all of these permutations, it suffices to nest cyclic permutation loops within each other. That is to say, for the $Q = 4$ Potts Model, one includes a loop which performs four iterations of $(0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 0)$, and within this loop is included a loop which performs three iterations $(0 \rightarrow 1 \rightarrow 2 \rightarrow 0)$ and within this one further loop which performs $(0 \rightarrow 1 \rightarrow 0)$ twice. This will generate the 24 unique parity operations possible for $Q = 4$. For example, for $Q = 4$, there are 24 ($= 4!$) possible 2×2 configurations which contain all four spin states. This algorithm performed on any one of them will generate all of the others. While the process is also carried out 24 times for configurations of the type $\begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}$ for example, over the course of the 24 operations, some states will be visited more than once.

Breaking Symmetry

For the Ising Model, removing the parity operation step from the category generation algorithm reproduces Table 1.2 as found by extending Hasenbusch's Hamiltonian. The situation for the Potts model is similar, except there are more symmetries to break. Up to two fields can be introduced in the 3-state Potts model. Introducing one physically corresponds to introducing a field which couples to one of the spin states, say the 2 states. The

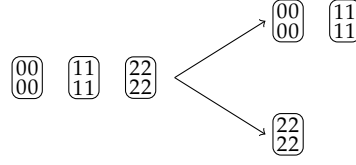


Figure 1.14.: The effect of introducing a field which couples to spins in state 2 on category C_0 in Table 1.3.

	Q				
H		0	1	2	3
	2	4	6	/	/
	3	6	13	21	/
	4	7	16	34	55

Table 1.4.: The number of categories generated for given (Q,H) combinations.

Potts Hamiltonian now reads

$$H = -K \sum_{\langle ij \rangle} \delta(s_i, s_j) - H_2 \sum_i \delta(s_i, 2) \quad (1.73)$$

Intuitively, the effect this will have is to split all of the categories within Table 1.3 based on the number of 2 species present within a configuration. Figure 1.14 shows the effect introducing a single field for the 3-state Potts Model has on the category C_0 . Note that category C_1 in Table 1.3 actually splits three ways as the configurations contained within it can contain 0,1 or 3 spins in state 2. In general, for the Q -state Potts model, introducing the first field will exclude one of the spin states from the Z_Q symmetry. For $Q > 2$, a second field can be introduced. Figure 1.15 shows how upon application of 2 external fields, the original category C_1 of the 3-state Potts Model, which contains 24 of the total 81 configurations, splits into 6 categories each containing 4 spin configurations. The full result of introducing magnetic fields for the 3-state Potts Model can be seen in Appendix A. The number of categories for a given (Q,H) can be seen in Table 1.4. Rather than generate the categories in the absence of a magnetic field using the previously described algorithm and then running a further algorithm on each category to induce additional splitting, the same effect can be achieved as

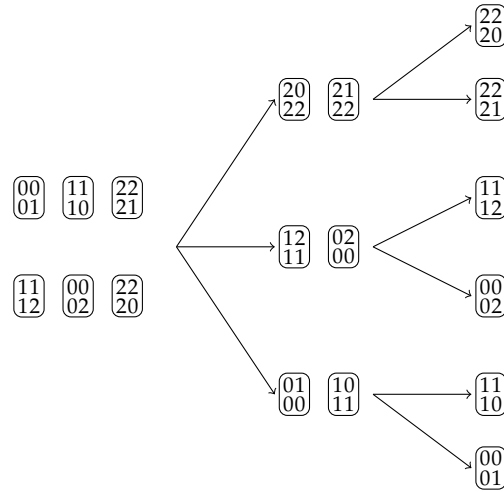


Figure 1.15.: The first set of arrows represent the effect introducing a field which couples to 2-spins has on C_1 in Table 1.3. C_1 splits into three categories. The second set of arrows shows the effect introducing a second field has, in this case the second field could couple to 1-spins or 0-spins and the effect would be equivalent, it would break the still remaining Z_2 symmetry. Each configuration denotes not only itself but also the three states related by rotation.

follows: For the 3-state Potts model, the parity switching algorithm consists of a $3 \times$ repeated cyclic Z_3 permutations operation with a $2 \times$ repeated Z_2 permutations loop nested within it. To break symmetry once, simply do not run the Z_3 cycle at all but allow the Z_2 cycle to run, thus maintaining a Z_2 symmetry. In order to break symmetry a second time, one must omit the Z_2 operation as well, meaning the algorithm only searches for configurations related by rotations, translations and mirroring.

This concludes the discussion of how to generate categories for the 2-dimensional square lattice. Using this method, Hasenbusch's 4 categories for the $(N = 4, B = 2)$ are reproduced, as well as those produced by our extension thereof. Furthermore, it generates the six categories that (1.53) does, confirming our belief that six is somehow the "magic number" and by its very construction it is neither over nor under-determined. Likewise it generates the thirteen categories that appeared to be emerging when attempting to adapt (1.35) for $(N = 6, B = 2)$ without having to worry about having too many or too few couplings. It should also be mentioned that for $(N = 4, B = 2)$, the analysis has been performed for up to $Q = 5$ (for $Q=5$ only in the absence of any symmetry breaking field) and the entire process of generating the categories is computationally inexpensive, that is to say in real time, it is to all intents and purposes negligible.

1.5.8. The God Tensor

The god tensor is a computational detail but the size of the god tensor determines the memory requirements of the entire process and thus what is feasible computationally with the code set up as it currently is.

The entire process of taking a given set of couplings $\underline{K}$ (which are double precision variables in C) and mapping them to a set of renormalised couplings $\underline{K}'$ requires the generation of all Q^{N^2} configurations possible on an $N \times N$ lattice. For $Q = 2$ on a 2×2 lattice, the process takes a fraction of a second, even with little optimisation. The fact that the process might need to be carried out on the order of hundreds of times is of little consequence as the run time pales into insignificance when compared to the coding time. For the 3-state Potts Model on the same lattice however, the same procedure takes on the order of a minute, even after significant optimisation. Thus the runtime of finding the fixed point is by no means

insignificant. For the 4-state Potts Model, the time taken to perform one iteration is on the order of half an hour and consequently finding the fixed point could take on the order of days. It turns out however, that all of the essential information generated during the coarse-graining procedure can be stored in a way that is not dependent on the input parameters $\underline{K}$. Consequently, $\underline{K}'$ can be generated by combining this information and any given $\underline{K}$. This $\underline{K}'$ can then be combined with the very same (and still stored) information to generate $\underline{K}''$, that is to say, the procedure can be iterated indefinitely once this information has been generated. Furthermore, this same information is sufficient to calculate $\frac{\partial K'_i}{\partial K_j}$ and thus after generating this information once, flow iterations can be performed as well as Newton-Raphson iterations (both required for the intelligent Newton-Raphson root finding algorithm used). This information will be stored in a 3-dimensional array (to be thought of as a rank 3 tensor) which was named *god* as it contains all of the information contained within a given RG transformation.

In order to understand how the *god* tensor works (in the context of the Ising Model for simplicity), first it is important to realise that there are 2^{16} possible configurations on the 4×4 lattice and $2^4 = 16$ configurations on a 2×2 lattice. Each renormalised configuration is generated equally frequently and thus each of the sixteen 2×2 coarse-grained configurations will have 2^{12} "parent" configurations.

It is only necessary to store information about a fraction of the coarse-grained configurations, namely one arbitrarily chosen "paradigm" from each category. While clearly the term $H(\{s_i\})$ (see (1.38)) depends on $\underline{K}$, each coarse-grained configuration has the same set of 2^{12} parents at each iteration of the transformation. Furthermore, when evaluating the Hamiltonian of a parent configuration, it will contain the same number of patches belonging to every category, regardless of the input parameters $\underline{K}$, that is to say $\sum_i \delta(s_i, C_i)$ remains unchanged. Finally, the parents are generated in the same order at each iteration of the transformation. The n^{th} parent of a given paradigm is always the same configuration. Thus the *god* tensor is defined such that $god_{ijk} =$ how many contributions to the Hamiltonian from category C_k there are when calculating the energy of the j^{th} $N \times N$ parent of the paradigm configuration of category C_i . Once *god* has been generated, the Boltzmann sums and subsequently the renormalised cou-

Q	God Size
2	61 kB
3	17.8 MB
4	765 MB
5	11.14 GB

Table 1.5.: Memory requirements for $N=4$, $B=2$ in the absence of external fields. God size scales as number of categories squared so if a field doubles the number of categories, the size of god increases by a factor of 4. For simplicity 1 MB is taken to be 1000 kB etc.

plings are generated according to

$$\sum_{\{s_i\} \rightarrow S_I} e^{-H(\{s_i\})} = \sum_{j=1}^{Q^{N^2 \left(\frac{B^2-1}{B^2} \right)}} \left[e^{N^2 K_0 + \sum_{k=1}^{N-1} god_{Ijk} K_k} \right] \quad (1.74)$$

Once the god tensor has been generated and stored in the RAM, the process of accessing it and generating $\underline{K}'$ from a given $\underline{K}$ is (while by no means instant for the large phase spaces associated with higher Q values) an order of magnitude smaller than generation time. Furthermore, differentiating (1.74) gives us:

$$\frac{\partial}{\partial K_m} \sum_{\{s_i\} \rightarrow S_I} e^{-H(\{s_i\})} = \sum_{j=1}^{Q^{N^2 \left(\frac{B^2-1}{B^2} \right)}} \left[(god_{Ijm}) e^{NK_0 + \sum_{k=1}^{N-1} god_{Ijk} K_k} \right] \quad (1.75)$$

and thus by (1.38) the Jacobian can be computed and hence Newton-Raphson iterations performed.

For $Q \geq 4$, the god tensor essentially makes the process feasible from a computational time perspective . It does however have relatively high memory requirements. $god_{ijk} \leq N^2$ and because $N^2 < 512$ for all systems examined, the god tensor can be stored as an (unsigned) char. Nonetheless, the memory requirements become substantial and are estimated in Table 1.5. The computational limits of the process are currently set by memory restrictions, not processing time. For example, performing the process for the Ising Model, with $N = 6$, $B = 2$ should take a similar amount of time

Model	$\left(\frac{J}{k_B T}\right)_c$		y_t		y_h		y_{h2}		y_{h3}	
	me	lit. [62, 95]	me	lit. [62, 22, 61]	me	lit. [62, 61, 11]	me	lit. [84, 61]	me	lit.
2-state Potts	0.840	0.881	0.936	1	1.823	$\frac{15}{8} = 1.875$	-	-	-	-
3-state Potts	0.966	1.005	1.118	$\frac{6}{5} = 1.2$	1.810	$\frac{28}{15} = 1.867$	0.614	$0.55, \frac{2}{3}$	-	-
4-state Potts	1.065	1.099	1.296	$\frac{3}{2} = 1.5$	1.814	$\frac{15}{8} = 1.875$	0.682	$\frac{7}{8} = 0.875$	0.174	-
5-state Potts	1.146	-	1.462	-	-	-	-	-	-	-

Table 1.6.: Theoretical and measured values for all $N = 4, B = 2$ Potts Models on the square lattice. Dashses denote values that are not predicted to theoretically exist, whereas blanks represent values that were not measured, either due to memory restrictions (for $Q = 5$) or for conceptual reasons (e.g. only one magnetic exponent is found for $Q = 2$).

(or at least the same order of magnitude) as the $N = 4, B = 2, Q = 5$ Potts Model. Its memory requirement is $\simeq 21.1\text{GB}$ which is still within feasibility of what some of the most powerful computers in the departmental cluster can handle. From thereon in however, it scales quickly, even the $N = 6, B = 3$ Ising Model would require 64GB of RAM and any sort of $Q > 2$ Potts model for $N = 6$ would require on the order of 10^6 GB of RAM and beyond. While we believe it is certainly possible to only use a subset of the full $Q^{N^2 \left(\frac{B^2-1}{B^2}\right)}$ parents of each paradigm configuration, doing so is certainly no trivial feat, and the saving would certainly be orders of magnitude lower than the rate at which the memory requirements diverge. Thus from a computational perspective, within the framework developed in this chapter, we are operating close to the computational limit.

1.6. Results

The Ising Model

As there is a direct map of the form (1.62), the categories Hamiltonian reproduces the y_t and T_c we see when reproducing Hasenbusch's method and likewise the same y_h obtained when extending it.

Potts Model

All of the results (critical temperatures and exponents) obtained for the square lattice are summarised in Table 1.6. The critical temperature, thermal exponent and first magnetic exponent are all in very good agreement

Model	no fields	1 field	2 fields	3fields
Ising	y_t	y_h	-	-
3-state Potts	y_t	y_h, y_{h2}	y_{h1}, y_{h2}	-
4-state Potts	y_t	y_h, y_{h2}	y_h, y_{h2}, y_{h3}	y_h, y_{h2}, y_{h3}

Table 1.7.: The exponents which are seen when a given number of external fields are introduced. Each entry shows only additional exponents seen when introducing a new field. For example, the 3-state Potts model in the absence of any external field will result in only the thermal exponent y_t being found. When introducing one field, two more exponents y_h and y_{h2} are found as well as y_t and introducing a second field leads to two more exponents being found, which are identical to y_h and y_{h2} . Thus in total, in the presence of two external fields, 5 exponents are found for the 3 state Potts Model: $y_t, y_h \times 2$ and $y_{h2} \times 2$.

with theoretically predicted values, although the thermal exponent value for $Q = 4$ is noticeably worse than for $Q = 2$ and $Q = 3$. The results most at odds with theoretical predictions is that a critical temperature exists for $Q = 5$ which qualitatively simply continues the trend of ever lower critical temperatures (the general formula is $\ln(1 + \sqrt{Q})$) and ever increasing y_t . Furthermore, for $Q = 4$ and presumably for $Q = 5$ if this were computationally feasible, a third magnetic exponent is seen. I am not aware of any reference to a third magnetic exponent anywhere in literature on the subject. Table 1.7 shows how many fields it takes to observe the exponents listed in Table 1.6. This will be crucial to the interpretation of the magnetic exponents.

1.6.1. The $Z_2 \otimes Z_2$ Grouping

There is one type of parity symmetry which is not immediately accessible when using the standard parity algorithm included in the categories generation method. For $Q = 4$, when full parity symmetry is in place, the parity algorithm takes any given configuration and performs 4 cyclic permutation operations, that is to say $0 \rightarrow 1, 1 \rightarrow 2, 2 \rightarrow 3, 3 \rightarrow 0$. Nested within this loop however, that is to say, for every time one of these 4-step cyclic permutations is carried out, another 3-step cyclic permutation is carried out three times. The convention used within my code is that the highest spin species is excluded from this when breaking symmetry, so each of these operations looks like $0 \rightarrow 1, 1 \rightarrow 2, 2 \rightarrow 0, 3 \rightarrow 3$ when introducing a first field

for $Q = 4$. Finally, for each time a 3-step cyclic permutation is carried out, a 2-step cyclic permutation adhering to the same convention is performed. If we examine a category of the $Q = 4$ Potts Model with zero external field which contains the configurations $\begin{pmatrix} 00 \\ 00 \end{pmatrix}, \begin{pmatrix} 11 \\ 11 \end{pmatrix}, \begin{pmatrix} 22 \\ 22 \end{pmatrix}$ and $\begin{pmatrix} 33 \\ 33 \end{pmatrix}$, introducing one field will split this so that $\begin{pmatrix} 00 \\ 00 \end{pmatrix}, \begin{pmatrix} 11 \\ 11 \end{pmatrix}$ and $\begin{pmatrix} 22 \\ 22 \end{pmatrix}$ remain in a single category whereas $\begin{pmatrix} 33 \\ 33 \end{pmatrix}$ now forms a category by itself. Crucially though, introducing a second field will result in $\begin{pmatrix} 00 \\ 00 \end{pmatrix}$ and $\begin{pmatrix} 11 \\ 11 \end{pmatrix}$ remaining in the same category whereas $\begin{pmatrix} 22 \\ 22 \end{pmatrix}$ forms a category of its own and likewise $\begin{pmatrix} 33 \\ 33 \end{pmatrix}$ exists in a category by itself. Nowhere in this process is there an allowance for a symmetry equivalent to introducing a field which couples to two of the four spin species equally. From a symmetry point of view, this is like (for example), having a symmetry between 0 and 2 spin species in place, simultaneously with one between 1 and 3 spin states. It is not excessively difficult to amend existing code and insert a bespoke algorithm which implements such a symmetry. This results in 22 categories (c.f. 16 for 1 "regular" field and 34 for two such fields), see Appendix Figure B.3.

A particularly interesting feature of this grouping is that the configurations $\begin{pmatrix} 01 \\ 23 \end{pmatrix}$ and $\begin{pmatrix} 21 \\ 03 \end{pmatrix}$ are related by such a symmetry operation but $\begin{pmatrix} 10 \\ 23 \end{pmatrix}$ is not and belongs in a different category. For all previously studied external fields, the effect of introducing such a field would be to split the categories present before its introduction based on the number of spin species which couple to the field in each configuration in such a category (see Figure 1.15). In this case however, before introducing such a field, all three of these configurations belong in the same category and contain the same quantity of all types of spin species. The choosing of categories based on symmetry rules however is the correct choice required to keep the partition sum invariant according to (1.5). This demonstrates it being more instructive to think of external fields explicitly as a mechanism of breaking symmetry, rather than a physical entity which couples to a certain spin species, even if the latter definition tends in all cases examined up until this point to have the same effect as the former. The same effect does occur for the 4 state Potts model and higher for two or more external fields.

Performing the transformation and calculating critical exponents according to this grouping yields a fascinating result, namely all three of the magnetic exponents calculated by applying successive fields which couple to single spin species are reproduced exactly, and only once (likewise

of course y_i is exactly reproduced). This result has profound consequences for the interpretation of the magnetic exponents.

As a side note, if we were interested in magnetic exponents for $Q = 5$ (and if memory requirements were not as they are), there are a few more complicated symmetries one could explore such as forming a group of three spin species and another of two, or two groups of two and a solitary one.

1.6.2. Further Fixed Points

For the 3 State Potts Model in the presence of (an) external field(s), numerous other fixed points are found. These must be found, not by intelligent root-finding, which makes use of the physics of the Potts model and searches the "real" Potts line for a separatrix in flow behaviour, but rather by starting our Newton-Raphson search from a wide range of (randomly generated) starting points and recording all (non-trivial) fixed points found. Once the god tensor has been generated, generating $\underline{K}'$ from a given $\underline{K}$ takes approximately 4 or 11 seconds for the 3 state Potts Model, depending on whether there are one or two external fields present. Thus a fixed point can be found in approximately a minute and consequently, the available phase space can be explored fairly comprehensively, although by no means as much so as for the Ising Model. Despite the existence of other fixed points, we can confidently claim the fixed point that has been described thus far is "the" Potts Fixed point, as it is equivalent to the fixed point found in the absence of any symmetry breaking field, whereas the other fixed points require (a) symmetry breaking field(s).

Ising Fixed Point

The folklore of statistical mechanics has it [95], that if an infinitely strong external field is introduced which couples to spins in state 2 only, the 3

state Potts Model essentially reduces to the Ising Model.

$$\begin{aligned}
H\left(\begin{smallmatrix} 00 \\ 00 \end{smallmatrix} / \begin{smallmatrix} 11 \\ 11 \end{smallmatrix}\right) &= H\left(\begin{smallmatrix} ++ \\ ++ \end{smallmatrix} / \begin{smallmatrix} -- \\ -- \end{smallmatrix}\right) \\
H\left(\begin{smallmatrix} 00 \\ 01 \end{smallmatrix} / \begin{smallmatrix} 11 \\ 10 \end{smallmatrix}\right) &= H\left(\begin{smallmatrix} ++ \\ +- \end{smallmatrix} / \begin{smallmatrix} -- \\ -+ \end{smallmatrix}\right) \\
H\left(\begin{smallmatrix} 00 \\ 11 \end{smallmatrix} / \begin{smallmatrix} 11 \\ 00 \end{smallmatrix}\right) &= H\left(\begin{smallmatrix} ++ \\ -- \end{smallmatrix} / \begin{smallmatrix} -- \\ ++ \end{smallmatrix}\right) \\
H\left(\begin{smallmatrix} 01 \\ 10 \end{smallmatrix} / \begin{smallmatrix} 10 \\ 01 \end{smallmatrix}\right) &= H\left(\begin{smallmatrix} +- \\ -+ \end{smallmatrix} / \begin{smallmatrix} -+ \\ +- \end{smallmatrix}\right) \\
H\left(\begin{smallmatrix} 22 \\ 22 \end{smallmatrix}\right) &= H\left(\begin{smallmatrix} 22 \\ 20 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 22 \\ 00 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 20 \\ 00 \end{smallmatrix}\right) = \dots = -\infty
\end{aligned} \tag{1.76}$$

(1.76) shows how to set all of the thirteen or twenty one (depending on whether one or two (respectively) external fields have been introduced) couplings, in order to induce Ising Model-like behaviour in the 3 State Potts Model. Clearly it is not possible computationally to set couplings equal to $-\infty$, and when finite numbers are used, these renormalise to even larger (or more negative in our case) numbers, but the couplings relating to configurations which contain no spins of value 2 remain fixed, and these values are (necessarily) the same as the fixed point values found for the Ising Model. Likewise, the value obtained for y_t is identical.

Clearly, it is equally possible to induce Ising-like behaviour for the $Q = 4$ Potts Model, as well as $Q = 3$ Potts-like behaviour by energetically penalising the appropriate spin species.

1.6.3. First Alternative Fixed Point

$$\begin{aligned}
H\left(\begin{smallmatrix} 00 \\ 00 \end{smallmatrix}\right) &= H\left(\begin{smallmatrix} 11 \\ 11 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 11 \\ 10 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 00 \\ 01 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 11 \\ 00 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 10 \\ 01 \end{smallmatrix}\right) \\
H\left(\begin{smallmatrix} 20 \\ 00 \end{smallmatrix}\right) &= H\left(\begin{smallmatrix} 21 \\ 11 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 21 \\ 10 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 20 \\ 01 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 20 \\ 10 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 21 \\ 01 \end{smallmatrix}\right) \\
H\left(\begin{smallmatrix} 22 \\ 00 \end{smallmatrix}\right) &= H\left(\begin{smallmatrix} 22 \\ 11 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 22 \\ 10 \end{smallmatrix}\right) \\
H\left(\begin{smallmatrix} 22 \\ 20 \end{smallmatrix}\right) &= H\left(\begin{smallmatrix} 22 \\ 21 \end{smallmatrix}\right) \\
H\left(\begin{smallmatrix} 22 \\ 22 \end{smallmatrix}\right) &
\end{aligned} \tag{1.77}$$

A fixed point is found, both in the presence of a single or two external fields which has the properties shown in (1.77). The last line denotes that $H\left(\begin{smallmatrix} 22 \\ 22 \end{smallmatrix}\right)$ is unique. In essence, (1.77) is telling us that 0 and 1 spins do not only interact equivalently with external fields, but also (0,0), (1,0) and (1,1) nearest neighbour bonds are equivalent. The critical exponents found are $y_1 = 0.927$ and $y_2 = 1.837$. This is strangely reminiscent of the Ising Model,

as were the 0 and 1 spins acting as + spins, and 2 as -. Clearly however, such a Model would have very different physics to the Ising Model, the mixed 0/1 ground state would be hugely degenerate whereas the 2 ground state is unique, and thus the system would always find itself in a state dominated by 0 and 1 spins. It turns out however, that at this fixed point, the configuration $\begin{pmatrix} 22 \\ 22 \end{pmatrix}$ is massively energetically favoured compared to $\begin{pmatrix} 00 \\ 00 \end{pmatrix}$ and $\begin{pmatrix} 11 \\ 11 \end{pmatrix}$. Thus hand-wavingly, one could argue that the Ising Model has been recreated, as for any given value of the order parameter, the free energy is conserved, as when the magnetisation is such that there are many more 2 spins than 1 and 0 combined, this is energetically very favourable and entropically penalised, and vice-versa.

It would seem likely that it is possible to induce similar behaviour for the $Q = 4$ Potts Model. That is to say, there in all probability exists a fixed point, when a single magnetic field has been introduced, which treats 0, 1 and 2 spins equivalently, and 3 differently. The fixed point would then involve the coupling related to $\begin{pmatrix} 33 \\ 33 \end{pmatrix}$ being energetically hugely favourable compared to $\begin{pmatrix} 00 \\ 00 \end{pmatrix}$, $\begin{pmatrix} 11 \\ 11 \end{pmatrix}$ and $\begin{pmatrix} 22 \\ 22 \end{pmatrix}$. Furthermore, when introducing a second field, one might expect to find a fixed point which treats 0 and 1 spins equally, as well as treating 2 and 3 spins equally. This would presumably result in the exact same exponents as for the Ising Model, as the phase spaces are greater than for the Ising Model, but equal in size to one and other. That is to say, the ground state is now hugely degenerate, but the GS consisting of 0 and 1 spins has the same multiplicity as that consisting of 2 and 3 spins. It is however rather difficult to probe this for $Q = 4$, as the process of generating $\underline{K}'$ from $\underline{K}$ is considerably more time consuming and thus probing a similar number of randomly generated starting points is trickier.

1.6.4. Second Alternative Fixed Point

The second alternative fixed point is even more mysterious. All thirteen couplings have unique values. The only recognisable trend is that some categories are strongly suppressed, their Boltzmann weightings are orders of magnitude lower than others. All of the strongly suppressed couplings contain (0, 1) nearest neighbour bonds, with the largest suppression coming for the category containing $\begin{pmatrix} 01 \\ 10 \end{pmatrix}$. Even this interpretation is somewhat dubious, as it requires a cut-off to be determined for what constitutes "strong"

suppression and in fact, $\begin{smallmatrix} 12 \\ 20 \end{smallmatrix}$ is the most strongly suppressed configuration which does not contain any $(0, 1)$ bonds, whereas $\begin{smallmatrix} 22 \\ 10 \end{smallmatrix}$, the most weakly suppressed configuration which contains at least one $(0, 1)$ bond has a comparable energy, as shown in (1.78) (the relevant couplings are K_{12} and K_{10} respectively)

$$\begin{aligned}
K_0 &= -0.104620 \\
K_1 &= -0.028077 \\
K_2 &= -3.361740 \\
K_3 &= -0.659700 \\
K_4 &= -0.793527 \\
K_5 &= -3.573974 \\
K_6 &= -0.874945 \\
K_7 &= -5.128792 \\
K_8 &= -1.119716 \\
K_9 &= -2.742928 \\
K_{10} &= -2.292634 \\
K_{11} &= -3.436554 \\
K_{12} &= -2.000711
\end{aligned} \tag{1.78}$$

in which K_0 is the energy of category C_0 and $K_0 + K_i$ is the energy of category C_i ($i \neq 0$) according to the categorisation shown in Appendix A. This is a result which I have yet to explain. It should be noted however, that the 3 state Potts Model in the presence of a single external field has much in common with the BEG model [14]. If instead of using the labels $(0,1,2)$, one used the labels $(-1,0,+1)$, and let the external field couple to 0 spins, by the symmetry of the Hamiltonian (namely a Z_2 permutation of swapping $+1$ and -1 spin states), and those of the lattice, the same 13 categories as shown in Appendix A are generated, with the relabelling $(0 \rightarrow -1, 1 \rightarrow +1, 2 \rightarrow 0)$. Thus it is possible that both this fixed point, and the previous one are related to the rich phase behaviour of the BEG Model which is known to support multiple phase transitions [6].

For $Q = 4$, it is possible there are further fixed points, and it could be speculated that these are related to the $S = \frac{3}{2}$ Ising Model and so forth for

higher Q .

1.6.5. $6 \times 6 \rightarrow 3 \times 3$ Renormalisation

Appendix C shows the 13 categories found by symmetry considerations, or by successively adding further n -point interactions to Hasenbusch's Hamiltonian. In principle, one can perform our RG scheme for $N=6$ for two different values of B , namely $B=2$ and $B=3$. For the former, everything would work in exactly the same way as for $N=4$. Computationally however, each of the four paradigms have $2^{32} \simeq 4.3 \cdot 10^9$ corresponding configurations on the 6×6 lattice. Consequently, the god tensor will contain $2^{32} \cdot 4^2 = 2^{36}$ entries and thus the memory requirement is 64 GB. $B=3$ is considerably less memory intensive, because the number of categories turns out to be 13, but each paradigm configuration only has $2^{27} \simeq 1.34 \cdot 10^8$ parent configurations on the 6×6 lattice. The number of parents per paradigm thus is lower by a factor of 32, while the square of the number of paradigms only increases by a factor of $(\frac{13}{4})^2 \simeq 10.5$ and thus $N = 6, B = 2$ has approximately one third of the memory requirements of $B = 3$. Only the former has been carried out so far. A fixed point is found in the 13 dimensional coupling space, and of the thirteen eigenvalues of the Jacobian matrix found, only two are greater than unity (one trivially equal to $B^d = 4$ as previously). The significant eigenvalue of $\lambda = 1.972$ results in the critical exponent result $y_t = 0.978$.

1.7. Combining Categories

While (1.5) ensures the partition sum remains constant under application of the RG, there are slightly more complicated ways of satisfying this condition. One way of doing this is to construct combined sums of the form

$$e^{-H(\{S_I\})} + e^{-H(\{S_J\})} = \sum_{\{s_i\} \rightarrow \{S_I\}} \left(e^{-H(\{s_i\})} \right) + \sum_{\{s_j\} \rightarrow \{S_J\}} \left(e^{-H(\{s_j\})} \right) \quad (1.79)$$

which is of course satisfied by two separate instances of (1.5). (1.5) however is a stricter restriction than

$$\sum_I e^{\frac{N^2}{B^2} K'_I} = \sum_I \sum_{\{s_i\} \rightarrow S_I} e^{-H(s_i)} \quad (1.80)$$

in which the sums over I could run over just two coarse grained configurations, but likewise could run over all of them, in which case this statement is simply equivalent to demanding the partition sum be conserved. In effect, exploiting symmetry and using only sums corresponding to paradigm coarse-grained configurations is equivalent to using this method. To see this, consider the two conditions:

$$e^{-H'\left(\begin{smallmatrix} \boxed{++} \\ \boxed{++} \end{smallmatrix}\right)} = \sum_{\{s_i\} \rightarrow \begin{smallmatrix} \boxed{++} \\ \boxed{++} \end{smallmatrix}} e^{-H(s_i)}$$

$$e^{-H'\left(\begin{smallmatrix} \boxed{--} \\ \boxed{--} \end{smallmatrix}\right)} = \sum_{\{s_i\} \rightarrow \begin{smallmatrix} \boxed{--} \\ \boxed{--} \end{smallmatrix}} e^{-H(s_i)}$$

which could be combined by (1.80) into a single condition of the form:

$$e^{-H'\left(\begin{smallmatrix} \boxed{++} \\ \boxed{++} \end{smallmatrix}\right)} + e^{-H'\left(\begin{smallmatrix} \boxed{--} \\ \boxed{--} \end{smallmatrix}\right)} = \sum_{\{s_i\} \rightarrow \begin{smallmatrix} \boxed{++} \\ \boxed{++} \end{smallmatrix} \begin{smallmatrix} \boxed{--} \\ \boxed{--} \end{smallmatrix}} e^{-H(s_i)} \quad (1.81)$$

Of course by this point, I have exhaustively shown that in the absence of an external field, the sum on the RHS of (1.81) must split into two numerically equal sums with corresponding terms, thus (1.81) is only satisfied if it is treated as two separate and identical conditions. What if however, it was instead decided to combine the two equations

$$e^{-H'\left(\begin{smallmatrix} \boxed{++} \\ \boxed{+-} \end{smallmatrix}\right)} = \sum_{\{s_i\} \rightarrow \begin{smallmatrix} \boxed{++} \\ \boxed{+-} \end{smallmatrix}} e^{-H(s_i)}$$

$$e^{-H'\left(\begin{smallmatrix} \boxed{++} \\ \boxed{--} \end{smallmatrix}\right)} = \sum_{\{s_i\} \rightarrow \begin{smallmatrix} \boxed{++} \\ \boxed{--} \end{smallmatrix}} e^{-H(s_i)}$$

via (1.80) to make the condition

$$e^{-H'\left(\begin{smallmatrix} \boxed{++} \\ \boxed{+-} \end{smallmatrix}\right)} + e^{-H'\left(\begin{smallmatrix} \boxed{++} \\ \boxed{--} \end{smallmatrix}\right)} = \sum_{\{s_i\} \rightarrow \begin{smallmatrix} \boxed{++} \\ \boxed{+-} \end{smallmatrix} \begin{smallmatrix} \boxed{++} \\ \boxed{--} \end{smallmatrix}} e^{-H(s_i)} \quad (1.82)$$

this would constitute an entirely different condition (although the original solution would still satisfy it). There could however be other ways of satisfying it. This immediately produces two problems, one in the detail, one more fundamental. The problem of detail is that there are eight configurations in the original category C_1 to which $\begin{pmatrix} ++ \\ +- \end{pmatrix}$ belongs, but only four in C_2 (to which $\begin{pmatrix} ++ \\ -- \end{pmatrix}$ belongs) (for a reminder of category labelling see Table 1.1). In order to not violate the lattice symmetries, (1.82) must be amended and its full version reads:

$$8e^{-H'(C_1)} + 4e^{-H'(C_2)} = \sum_{\{s_i\} \rightarrow (S_I \in C_1, S_I \in C_2)} e^{-H(s_i)}$$

which by symmetry can be reduced/simplified to give

$$2e^{-H'(C_1)} + e^{-H'(C_2)} = \sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ +- \end{pmatrix}, \begin{pmatrix} -- \\ +- \end{pmatrix}, \begin{pmatrix} ++ \\ -- \end{pmatrix}} e^{-H(s_i)} \quad (1.83)$$

Thus when constructing combined conditions of the form (1.80) in order to satisfy partition sum invariance, this is a detail which must be kept in mind.

A more fundamental problem however, is that using the example just given, the full constraints required to keep the partition sum invariant under the RG for the 2-d Ising Model on a square lattice in the absence of a magnetic field are now:

$$\begin{aligned} e^{-H'\left(\begin{pmatrix} ++ \\ ++ \end{pmatrix}\right)} &= \sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ ++ \end{pmatrix}} e^{-H(s_i)} \\ 2e^{-H'(C_1)} + e^{-H'(C_2)} &= \sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ +- \end{pmatrix}, \begin{pmatrix} -- \\ +- \end{pmatrix}, \begin{pmatrix} ++ \\ -- \end{pmatrix}} e^{-H(s_i)} \\ e^{-H'\left(\begin{pmatrix} +- \\ +- \end{pmatrix}\right)} &= \sum_{\{s_i\} \rightarrow \begin{pmatrix} +- \\ +- \end{pmatrix}} e^{-H(s_i)} \end{aligned} \quad (1.84)$$

i.e. only three conditions remain, leaving the problem over-determined if there are four couplings. The point of combining categories in this way however is that it allows us to enforce that configurations which are not related by the relevant symmetries have the same energies. The example

chosen is of particular significance because $\begin{pmatrix} ++ \\ +- \end{pmatrix}$ and $\begin{pmatrix} +- \\ -- \end{pmatrix}$ have the same energy in the Ising Model but as they are not related by the lattice symmetries or parity inversion, the categories Hamiltonian assigns them different categories. Furthermore, enforcing that $K_1 = K_2$ and thus assigning the two aforementioned 2×2 configurations the same energy does not imply that $K'_1 = K'_2$ because in general

$$\sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ +- \end{pmatrix}} e^{-H(s_i)} \neq \sum_{\{s_i\} \rightarrow \begin{pmatrix} +- \\ -- \end{pmatrix}} e^{-H(s_i)} \quad (1.85)$$

even if the couplings corresponding to $\begin{pmatrix} ++ \\ +- \end{pmatrix}$ and $\begin{pmatrix} +- \\ -- \end{pmatrix}$ are equal. If we wish to impose that their energies are fundamentally the same, the renormalisation procedure must be defined via (1.83). Now however, because $H\left(\begin{pmatrix} ++ \\ +- \end{pmatrix}\right) = H\left(\begin{pmatrix} +- \\ -- \end{pmatrix}\right)$, this can be rewritten as:

$$-H'\left(\begin{pmatrix} ++ \\ +- \end{pmatrix}\right) = -H'\left(\begin{pmatrix} +- \\ -- \end{pmatrix}\right) = 4(K'_0 + K'_1) = \ln \left[\frac{2}{3} \left(\sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ +- \end{pmatrix}} e^{-H(s_i)} \right) + \frac{1}{3} \left(\sum_{\{s_i\} \rightarrow \begin{pmatrix} +- \\ -- \end{pmatrix}} e^{-H(s_i)} \right) \right] \quad (1.86)$$

in which $\frac{2}{3}$ and $\frac{1}{3}$, the so-called weights, relate to the relative sizes of the two categories that have been combined, i.e. category C_1 has twice as many member configurations as C_2 . While this particular choice of two categories to combine is motivated by the original Ising Model Hamiltonian, and thus the model we are trying to study, mathematically this procedure can be used to combine any two categories for any model. If we wish to lump categories C_2 and C_3 into the same category, it is straight-forward to ensure that any 2×2 patch which belongs to either category has the same energy, and to renormalise this value by constructing a combined constraint based on the relative sizes of the two categories.

Furthermore, in this way, it is possible to not just form one category which combines two of the original four, we could form two categories each containing two of the original two, or likewise one which contains three leaving one of the original categories in tact. (1.86) shows us how these couplings then must renormalise, taking the relative sizes of the categories to be combined into account.

Categories combined	$\left(\frac{J}{k_B T}\right)_c$	y_t
$C_0 \cup C_1$	-	-
$C_1 \cup C_2$	0.432	0.929
$C_2 \cup C_3$	-	0.936
$C_1 \cup C_3$	-	0.997
$C_0 \cup C_2$	-	-
$C_0 \cup C_3$	-	-
$C_1 \cup C_2 \cup C_3$	-	0.9862
$C_0 \cup C_2 \cup C_3$	-	-
$C_0 \cup C_1 \cup C_3$	-	-
$C_0 \cup C_1 \cup C_2$	-	-
$C_0 \cup C_1, C_2 \cup C_3$	-	-
$C_0 \cup C_2, C_1 \cup C_3$	-	-
$C_0 \cup C_3, C_1 \cup C_2$	-	-

Table 1.8.: The thirteen different ways in which the four original Ising Model Categories (as defined in Table 1.1) can be combined and which of these unions result in a fixed point and thus critical exponents.

1.7.1. Combining Categories Results

There are 6 ways of combining two categories as there are 4 original categories in total and $\binom{4}{2} = 6$. Of these six possible unions, three of them do not involve combining category C_0 (in Table 1.1) with any other and these three combinations all result in a fixed point. Of these three unions, only one of them does not involve combining two categories which have different energies by Ising's Hamiltonian and consequently, only this categorisation allows for the estimating of a critical temperature. For this reason though, it is not possible to search the "physical line" and thus carry out intelligent root finding and consequently for any categorisation that combines categories which have different energies according to the original Ising Model Hamiltonian, a more brute force root finding approach must be taken which involves starting Newton-Raphson searches from a wide variety of (randomly generated) starting points. For $Q = 2$ and $N = 4$, the phase space is sufficiently small that the entire process of determining whether a given set of initial conditions converge to a trivial or non-trivial fixed point via the Newton-Raphson scheme is sufficiently fast that thousands of initial conditions have been probed and the non-existence of fixed

points for a given categorisation can be claimed with high confidence.

There are two ways of combining categories such that there are only two final categories. Either three of the original categories can be combined into one combined category, or two combined categories, each containing two of the old ones can be imposed. There are 4 ways of doing the former and 3 ways of doing the latter. Only one however appears to result in a transformation which has a fixed point, namely that which involves keeping $\begin{pmatrix} + & + \\ + & + \end{pmatrix}$ and its parity inversion (i.e. category C_0) in a category of their own and forcing all other coarse-grained configurations into the same category. Table 1.8 can be summarised in the somewhat surprising result that any categorisation which leaves C_0 in a category by itself has a fixed point and sensible critical exponents and any which combines C_0 with any other (pair of) category(ies) does not have a fixed point. This is a peculiar result which I have been unable to explain, but one which I believe not to have a physical origin, but rather to be a mathematical artefact.

1.7.2. Incompatibility with Magnetic Interactions

The particular choice of combining categories C_1 and C_2 (again using the labelling given in Table 1.1) was used for good reason when introducing the methodology of how to combine categories, namely that it makes recourse not just to symmetries but some of the finer details of the model being studied namely the form of the Hamiltonian. Introducing a magnetic field however exposes a fundamental weakness of the method. It would appear that the only sensible way to split the combined category $C_1 \cup C_2$ in a way that reflects the physics of a magnetic field would be to split the category three ways, thus regaining the categorisation obtained using the standard categories Hamiltonian.

Furthermore, combining categories C_1 and C_2 was done based on considering the Ising Model's Hamiltonian. Thus in order to continue in this spirit, it would be necessary to group configurations based on the Ising Model Hamiltonian in the presence of an external field. This Hamiltonian actually reproduces the six categories generated by extending Hasenbusch's method or using the category generation algorithm. We know however, that in this parametrisation, the fixed point is energetically equivalent to that of the 4-category Ising Model, that is to say, all sixteen coarse-

grained configurations have the same energy as they do at the aforementioned fixed point. This means that there are four different allowed energy levels, not three. In order for the 4 category Ising Model to have only three distinct energy levels at the fixed point, it would be necessary for $K_1^* = K_2^*$ and thus:

$$\sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ +- \end{pmatrix}} e^{-H(s_i)} \Big|_{K_1=K_2} = \sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ -- \end{pmatrix}} e^{-H(s_i)} \Big|_{K_1=K_2} \quad (1.87)$$

which is in general NOT the case as the two sums are not related by a symmetry operation.

This means that an expression of the form (1.62) cannot be derived as one side would consist of a 3×1 vector and the other side a 4×1 . Thus the two pictures are not related by a similarity transform and consequently, the thermal critical exponent will be different. From this, it has been learned that while combining categories is possible, it has the rather dis-satisfactory consequence that upon application of an external field, this combining can be undone which has the result of changing the thermal critical exponent. This is due to the fact that lattice configurations with the same energy in the Ising Model in the absence of an external field can interact with a field in a way that is neither equal, nor equal and opposite.

This has a further profound and rather less than satisfactory interpretation. In the absence of a field, we find the constraint (1.86) which determines how the couplings which relate to the energies of $\begin{pmatrix} ++ \\ +- \end{pmatrix}$ and $\begin{pmatrix} ++ \\ -- \end{pmatrix}$ renormalise. In the presence of an external field however, we find that (these are two of the constraints which arise from using the categories Hamiltonian in the presence of a field)

$$\begin{aligned} H' \left(\begin{pmatrix} ++ \\ +- \end{pmatrix} \right) &= \frac{1}{4} \ln \left[\sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ +- \end{pmatrix}} e^{-H(s_i)} \right] \\ H' \left(\begin{pmatrix} ++ \\ -- \end{pmatrix} \right) &= \frac{1}{4} \ln \left[\sum_{\{s_i\} \rightarrow \begin{pmatrix} ++ \\ -- \end{pmatrix}} e^{-H(s_i)} \right] \end{aligned} \quad (1.88)$$

If the limit of $H \left(\begin{pmatrix} ++ \\ +- \end{pmatrix} \right) \rightarrow H \left(\begin{pmatrix} ++ \\ -- \end{pmatrix} \right)$ is taken however, $H' \left(\begin{pmatrix} ++ \\ +- \end{pmatrix} \right) \neq H' \left(\begin{pmatrix} ++ \\ -- \end{pmatrix} \right)$. This can only be achieved if the couplings renormalise according to (1.86)

which is the case only for exactly zero field. Thus in a sense, $h'(h)$ is discontinuous, as a vanishingly small but finite magnetic field will result in a not vanishingly small energy level splitting after renormalisation. This is however problematic, as the relationship between y_h and the eigenvalues of the Jacobian at the fixed point assumes that h' is an analytic function of h .

1.7.3. Discussion of Category Combining

Other than the particular combination of categories based on the original Hamiltonian which was investigated somewhat further (see Section 1.9), it was decided not to further pursue the method of combining categories, for example investigating all possible category combinations possible for the $Q = 3$ Potts Model. There are a number of reasons for this. Firstly, the initial method of generating categories appears to be somehow fundamental. While other categorisations are possible, it is necessary to know about the initial categorisation in order to implement it. By this it is meant, that if it is decided that all coarse-grained configurations should be grouped according to their energy by the Ising Hamiltonian as discussed in the previous section, it is still necessary to know which of these configurations belong to which initial category and thus determine their relative weights. Furthermore, any grouping which forms combined categories which do not split symmetrically upon the application of a magnetic field incur the problem of $h'(h)$ being discontinuous at $h = 0$, or rather $h = 0$ being somewhat of an anomalous point. Finally, it is not clear why some category groupings "work" in the sense that they result in a transformation for which a fixed point is found and others do not. The only robust result, and one which is yet to be explained is that every categorisation which leaves C_0 untouched results in a fixed point being found, and any categorisation which combines C_0 with any other category or pair thereof does not.

This section has come before the section on triangular lattices as the method of combining categories by using weights related to their relative sizes is necessary in order to implement the categories Hamiltonian on triangular lattices.

1.8. Triangular Lattices

By universality [17], the Ising Model on lattices with different topologies in 2 dimensions must exhibit the same critical exponent(s) as on the square lattice and similarly for higher Q-state Potts Models. The following section outlines an implementation of the method on the 2-dimensional triangular lattice for general Q-state Potts Models. The implementation is rather complex and messy and in a sense it cannot provide any new information apart from the critical temperature, which could be estimated simply by calculating the partition sum analytically which as discussed, is similarly computationally expensive to performing the RG and can be done for slightly bigger lattices. It does however serve as a test of the method, to determine whether the exponents obtained for the square lattice hold up robustly.

It would be beneficial to recycle as much of the framework developed for the square lattice as possible. The necessary ingredients are firstly a method of coarse graining spins on a larger lattice in order to generate a map to a smaller lattice. Secondly, the configurations on the coarse-grained lattice must be grouped into categories in which every configuration must be energetically equivalent. Thirdly, a method of implementing this Hamiltonian on the parent lattice must be devised. With this in place, the rest of the method will remain identical.

1.8.1. Triangular Blocking of Spins

In a sense the common names for the triangular lattice, namely triangular or hexagonal are not helpful in determining an RG scheme. The unit cell of the triangular lattice is the parallelogram [39], and the only way of coarse graining to create the same shape of lattice is to start with an $N \times N$ rhombus, block over $B \times B$ rhombuses and thus be left with one of dimensions $\frac{N}{B} \times \frac{N}{B}$ as shown in Figure 1.16. This has the distinct advantage that code which generates 4×4 configurations on the square lattice and renormalises them can be recycled.

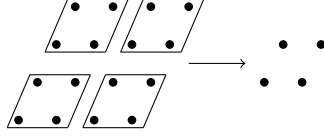


Figure 1.16.: RG transformation scheme for a triangular lattice based closely on the method for a square lattice

1.8.2. Implementing a Categories Hamiltonian

Leaving how to determine the categories aside momentarily, it is more difficult to evaluate the Hamiltonian on a parent lattice given a set of categories on the coarse-grained lattice than it is for square lattices. Figure 1.10 shows two possible methods of implementing the categories Hamiltonian on square lattices of arbitrary size by forming all possible 2×2 "patches". While the definition of a patch on the square lattice is so intuitive it is almost not worth mentioning, the formal definition was introduced because it is somewhat more complex on a triangular lattice. In order to include a given site in a patch, it is sufficient to select one of its next-nearest neighbours. On a square lattice, this then uniquely determines two further sites which are both nearest neighbours of the original site and of its next-nearest neighbour. Each site has four nearest neighbours but due to each patching orientation being a 90 degree rotation of another, which is in itself a lattice symmetry, it is sufficient to consistently use one patching orientation at each point on the lattice. There exist N^2 unique such patches on a square $N \times N$ lattice.

The situation on a triangular lattice is different. Each site has six next-nearest neighbours and likewise, choosing a site and its next-nearest neighbour is sufficient to uniquely determine a patch and thus six patches can be formed from any given site. The six patches are shown in Figure 1.17. Using any one patching orientation however will now not suffice in order to consider every possible rhombic patch it is possible to conceive. It turns out that it is necessary to use three of the six patches. The triangular lattice has three axes of translational symmetry (these are the lines connecting nearest neighbours), and each of the six rhombic patches denoted in Figure 1.17 is the result of a mirroring one of the other patches about one of these axes. It is necessary to use any group of three patches in Figure 1.17 that are

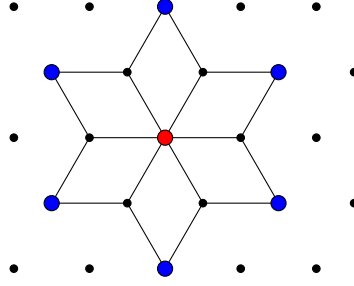


Figure 1.17.: The six next-nearest neighbours (denoted in blue) of a given site (denoted in red) on a triangular lattice and the six resulting rhombic patches.

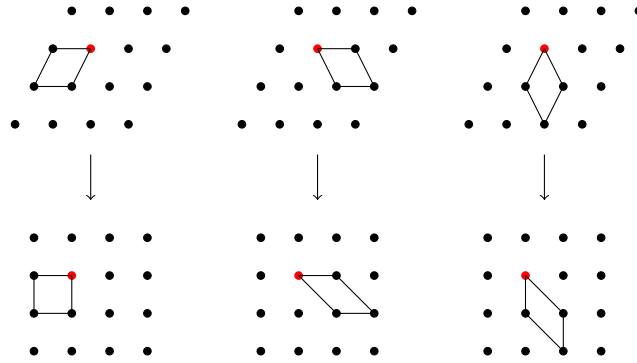


Figure 1.18.: Three of the patching orientations presented in Figure 1.17 and how if mapped back to the square lattice, they do indeed present different interactions.

bordering/touching each other. This is the key computational difference between the process for a square and triangular lattice. The lattice configuration is still stored in a square, 2-dimensional array and renormalised in exactly the same way as for the square lattice. While the categories will be different, as explained subsequently, if this were the only difference, the numerical calculation occurring for the triangular lattice would be equal to that for the square lattice using a different categorisation. This is however not the case, more interactions must be considered. Figure 1.18 shows that in effect, carrying out the transformation on a triangular lattice is equivalent to doing so on a square lattice but including patches of two skewed orientations in the evaluation of the Hamiltonian.

C_0	C_1	C_2	C_3	C_4	C_5
$\begin{array}{cc} + & + \\ + & + \end{array}$	$\begin{array}{cc} + & + \\ + & - \end{array}$	$\begin{array}{cc} + & + \\ - & + \end{array}$	$\begin{array}{cc} + & + \\ - & - \end{array}$	$\begin{array}{cc} + & - \\ + & - \end{array}$	$\begin{array}{cc} + & - \\ - & + \end{array}$
$\begin{array}{cc} - & - \\ - & - \end{array}$	$\begin{array}{cc} - & + \\ + & + \end{array}$	$\begin{array}{cc} + & - \\ + & + \end{array}$	$\begin{array}{cc} - & - \\ + & + \end{array}$	$\begin{array}{cc} - & + \\ - & + \end{array}$	$\begin{array}{cc} - & + \\ + & - \end{array}$
	$\begin{array}{cc} - & - \\ - & + \end{array}$	$\begin{array}{cc} - & - \\ + & - \end{array}$			
	$\begin{array}{cc} + & - \\ + & - \end{array}$	$\begin{array}{cc} - & + \\ - & - \end{array}$			

Table 1.9.: Rotational and Parity invariance generate six categories for the Triangular Ising Model

1.8.3. Determining the Categories

The framework developed for the square lattice must still hold for the triangular lattice. For the Ising Model case, there are sixteen coarse-grained configurations, each of which have $2^{12} = 4096$ "parent" configurations on the 4×4 lattice. Thus there are sixteen groups G_i each containing $2^{12}, 4 \times 4$ configurations which renormalise to the same S_I . If there exists an operator $\hat{O}$ which respects the lattice symmetries as well as those of the Hamiltonian (that is to say $H(\hat{O}s_i) = H(s_i)$), and which has the property $\hat{O}G_i = G_j$, S_I and S_j belong in the same category. The first difference between the square and triangular lattices however is that the operator $\hat{R}$, previously defined as a 90 degree rotation operator can not be applied to the triangular lattice because a triangular lattice cannot be superimposed upon itself after a 90 degree rotation (the resulting lattice would have a different topology). Only a 180 degree rotation allows for this. Thus it might initially seem that the triangular lattice category algorithm is equivalent to that of the square but only allowing for 180 degree rotations. The result of this is shown in Table 1.9. There is however a subtle effect which this does not take into account. It was previously mentioned in the context of the square lattice, that the method of patching should also be used when evaluating the Hamiltonian on an $\frac{N}{B} \times \frac{N}{B}$ lattice. That is to say, even if we did not know about rotational symmetry, $\begin{pmatrix} ++ \\ +- \end{pmatrix}$, $\begin{pmatrix} ++ \\ -+ \end{pmatrix}$, $\begin{pmatrix} +- \\ ++ \end{pmatrix}$ and $\begin{pmatrix} -+ \\ ++ \end{pmatrix}$ are necessarily in the same category. This is because visiting each site in turn in the configuration $\begin{pmatrix} ++ \\ ++ \end{pmatrix}$ and including it in a 2×2 patch originating at this site and respecting the periodic boundary conditions yields all four contributions. If this process is performed on the triangular lattice for any of the members of configurations C_0 in Table 1.9, using the patching method for triangular lattices as detailed in the previous section, twelve contributions from C_0 are found.

If the same analysis is performed for C_1 or C_2 however, this is no longer the case and in fact in either case, 6 contributions from either category are found and thus C_1 and C_2 must be recombined as their analogues were on the square lattice. Surprisingly perhaps and very much not in line with the square lattice, performing the same analysis for categories C_3 , C_4 and C_5 in 1.9 actually results in four contributions from each category in all three cases. So in fact, in the absence of an external field, there are only three categories, as categories C_3 , C_4 and C_5 must constitute a single grouping. It is however still not the case that

$$\sum_{\{s_i\} \rightarrow \left(\begin{smallmatrix} + & - & + & - \end{smallmatrix} \right)} e^{-H(s_i)} = \sum_{\{s_i\} \rightarrow \left(\begin{smallmatrix} + & - & - & + \end{smallmatrix} \right)} e^{-H(s_i)} \quad (1.89)$$

and thus weights need to be used, as was done when combining categories. It should be noted that evaluating Hasenbusch's Hamiltonian (1.35) on a triangular lattice leads to these same three categories. Of course the problem is then over-determined because this Hamiltonian has four couplings but the quadrupole interaction is adding no extra information, including just nearest and next-nearest neighbour interactions will generate these same categories. Thus the problem on a triangular lattice could be solved using a Hasenbusch-like approach but dropping the quadrupole term and taking the weights into account. The same problem as for square lattices however arises for higher-state Potts models and thus we have only proceeded with a categories Hamiltonian approach. It must be the case however, for the Ising Model and the general Q -state Potts model, that while the symmetries of the triangular lattice will always have the effect of combining square lattice categories (at least for $\frac{N}{B} = 2$, the effect has not been studied in depth for larger coarse-grained systems), they will do so in a way that does not cause any problems when introducing a magnetic field. That is to say, it will not group together square categories which have a different magnitude of order parameter.

Now everything is in place to generate constraints of the form (1.58) and turn the crank to obtain critical temperatures and exponents. The process of category generation generalises for higher Q Potts Models, with parity symmetry working exactly as it does on square lattices.

	Q				
H		0	1	2	3
	2	3	5	-	-
	3	4	9	11	-
	4	5	11	22	36

Table 1.10.: The number of categories (after all patching has occurred) for all allowed (Q,H) combinations for the $\frac{N}{B} = 2$ triangular lattice.

Q	$\left(\frac{J}{k_B T}\right)_c$		y_t	y_h	y_{h3}	y_{h3}
	me	lit [95, 30]				
2	0.462	0.549	0.933	1.7535		
3	0.553	0.631	1.158	1.737	0.624	
4	0.626	0.693	1.365	1.756	0.724	0.099
5	0.731	-	1.584			

Table 1.11.: The critical temperature and exponents measured for the triangular lattice. Values from the literature for the critical exponents are listed in Table 1.6

1.8.4. Triangular Results

It must be remembered that by universality, the critical exponents on a triangular lattice must be the same as those on a square lattice. The purpose of performing this analysis is to obtain similar values (to within numerical error) and thus reinforce the results obtained for the square lattice. The critical temperature however is sensitive to lattice details and showing that the value obtained for the critical temperature is in line with expectations for the triangular lattice is thus essential in order to ascertain that the analysis performed does indeed represent the physics of a triangular lattice. The theoretical values for the critical temperatures are calculated from the expression [95]

$$y^3 - 3y + 2 = Q$$

$$y = e^{\left(\frac{J}{k_B T}\right)_c} \quad (1.90)$$

in which y must in general be calculated by Newton's Method or graphically.

1.8.5. Other Fixed Points

For the $Q = 3$ Potts Model, another fixed point is found which resembles that of the Ising Model in its coupling values and exponents, in keeping with our findings for the square lattice. It had been hoped that another non-trivial fixed point might however exist for the Ising Model in the presence of an external field as the categories we generate for this are the same as those generated by the Hamiltonian of the Baxter-Wu Model [4]

$$H = -J_1 \sum_{\langle ij \rangle} s_i s_j - J_2 \sum_{\triangle} s_i s_j s_k - H \sum_i s_i \quad (1.91)$$

in which the triangular interaction runs over trios of common nearest neighbours. The Baxter-Wu model is known to have two non-trivial fixed points. One of these occurs at $J_2 = 0$ and thus this is the standard Ising Model and consequently the two well-known Ising critical exponents are obtained. There exists however a second non-trivial fixed point at which three critical exponents are found. For $Q = 2$, due to the small size of the phase space, we have explored a wide range of starting points for the Newton-Raphson root finding algorithm and have been unable to determine such a fixed point.

1.9. $Q = 5$

A clear trend emerges as Q is increased, the critical temperature decreases and the thermal exponent increases. The physics of the 3-state Potts Model however is rather comparable to the Ising Model [95][79]. Above T_c the system exists in a disordered phase. As the temperature is lowered towards the critical temperature, the correlation length increases and larger and larger clusters of all three spin species are found. Below T_c , in the absence of an external field, there are three possible phases, one in which each spin species is dominant. No phase is energetically favourable and thus for zero external field, the system is in a state of 3-phase coexistence and can be tipped into any phase by an infinitesimal external field. The other extreme is an infinitely large negative field which couples to one spin species, energetically de-favouring it to the point that the system effectively reduces to the Ising Model. The classic phase diagram for the

Ising Model is 2 dimensional as ordered phases can exist below the critical temperature and the temperature axis (or $H = 0$) forms the separatrix between these two phases. The equivalent diagram from the 3-state Potts Model is 3 dimensional as 2 fields can be introduced, and three separatrices exist, lines which represent the fields which couple to two of the three spin species being equal (see [95]). While it is difficult to visualise for $Q > 3$, this rather intuitive generalisation of the Ising Model is relatively easy to understand and there is no obvious reason why it should not continue for arbitrarily large Q . It is however well-known that the Potts Model has a critical, dimension-dependant Q , $Q_c(d)$ above which the system ceases to undergo a second order phase transition. The transition becomes discontinuous (first order)[5]. In the context of the RG, this means we would expect to no longer find a fixed point for $Q > Q_c(d)$. In 2 dimensions, the critical Q is 4 meaning for $Q > 4$, we might expect to no longer find a fixed point. It is also well-known [21][60] however that conventional RG approaches fail to capture this effect and likewise, the categories Hamiltonian method fails. Our method appears to predict the trend continuing ad infinitum, that is to say y_t increasing for increasing Q and the inverse critical temperature increasing according to $\ln(1 + \sqrt{Q})$.

The real space RG in its purest form fails to capture this effect because it is not suited to dealing with so-called effective vacancies. When renormalising a 2×2 block of the form $\begin{pmatrix} 01 \\ 23 \end{pmatrix}$, its most important feature is that it is completely disordered. Such 2×2 blocks have a high multiplicity as Q is increased and are thus favoured entropically. Physically, it is the existence of such patches within the system that causes the transition to become first order[7]. Using the "top-left" rule however, we would simply renormalise the block $\begin{pmatrix} 01 \\ 23 \end{pmatrix}$ to a 0 spin. For the 3-state Potts Model, this is not a problem as such blocks cannot exist, and while blocks of the form $\begin{pmatrix} 00 \\ 11 \end{pmatrix}$ are clearly ambiguous, renormalising them as we have done still captures the essential feature which is that they do not contain any 2 spins. Given the level of accuracy of the method, it is not entirely rigorous to speculate in the following manner, but the result for y_t is considerably worse for $Q = 4$ than it is for $Q = 2$ and $Q = 3$ and this mechanism could be a contributing factor. It has been shown [60] that treating $\begin{pmatrix} 01 \\ 23 \end{pmatrix}$ blocks as vacant states and renormalising them to "holes" on the coarse-grained lattice does capture the effect of the transition being second order for $Q = 4$ and first order for

$Q = 5$ in 2 dimensions.

1.9.1. Including Holes in the Categories Hamiltonian

I have not been able to reconcile the concept of holes within the framework of the categories Hamiltonian. One idea was to renormalise effective vacancies to a Q^{th} spin species. That is to say, the allowed spins on the parent lattice would be $0, 1, 2, \dots (Q - 1)$ for a Q -state Potts Model but the coarse-grained lattice could also have Q spin species. The categories would thus be the same as for a $Q + 1$ state Potts Model in the presence of one external field (as clearly there must be some sort of energetic asymmetry between a vacant and an occupied site). The fundamental problem with this method however, is that for any state $\{S_f\}$ containing at least one vacancy, the associated coupling K'_f would only depend on the set of couplings $\{K_i\}$ which govern the energy of configurations without vacancies, as these are the ones which occur on the parent lattice. Thus if there are N , 2×2 categories containing configurations without holes and M with holes, the set of constraints of the form of (1.5) will generate $(N + M)$ constraints which depend on N couplings and thus be over-determined.

It would be possible to insure the problem is neither over nor under-determined by allowing for holes on the parent lattice too. This means that the Q -state Potts Model must be implemented as the $(Q + 1)$ state Potts Model in the presence of one external field. This however is rather dissatisfactory, as we know that the $(Q + 1)$ Potts Model will have a fixed point in the absence of an external field if the pattern we have observed continues, and thus in the presence of a magnetic field it will have the energetically corresponding fixed point. Furthermore if it were stipulated that this is the "wrong" fixed point, and that there must be a fixed point which energetically distinguishes between hole states and spin states, this would be equivalent to demanding there must be a fixed point in which the magnetic field is non-zero which is physically not possible. Thus if this method were to be carried out, the inescapable and clearly erroneous conclusion would be that there is no fixed point for any Q . Thus there is no obvious way of extending our current framework to include effective vacancies explicitly.

1.9.2. Compensating for Effective Vacancies

Andelman and Berker (A&B) [7] provide further insight on the topic of effective vacancies by means of a Monte Carlo analysis of the Potts Model in 2 dimensions for $Q = 3$ and $Q = 20$. For $Q = 3$, as the critical temperature is approached from above, clusters of aligned spins form as well as long interfaces between clusters of different spins. Regions characterised by non-aligned spins or a general lack of order do persist but they do not dominate the system. For $Q = 20$ however, the system is dominated by regions of complete disorder, with a few clusters of aligned spins. The clusters that do still exist, in general do not border one another to form long interfaces between clusters of different types of spins (the mechanism of such interfaces being a compromise between energy minimisation and entropy maximisation which minimises the free energy can be thought of as causing second order phase transitions), but are separated by regions of complete disorder. It should be noted that A&B do not explicitly show that the system is characterised by large aligned clusters for $Q = 4$ and not for $Q = 5$, presumably because visually, the effect is somewhat continuous (especially when using relatively small lattices as they will have done with the computational power at their disposal in the early 1980s) and thus the critical Q is difficult to determine.

A&B then make a small change to their Hamiltonian, namely they introduce a term which energetically penalises effective vacancies. Explicitly, this involves adding a term of the form:

$$-F \sum_{\langle ijkl \rangle} (1 - \delta(s_i, s_j)) (1 - \delta(s_j, s_k)) (1 - \delta(s_k, s_l)) (1 - \delta(s_l, s_i))$$

in which the sum $\sum_{\langle ijkl \rangle}$ runs over 2×2 squares, equivalent to the "patches" on which we evaluated our categories Hamiltonian on square lattices. This Hamiltonian has the remarkable property that as the temperature is lowered, even for $Q = 20$, large clusters of aligned spins and long interfaces between such clusters begin to form. This analysis, which it should be stated again, uses Monte Carlo methods and does not involve the RG, again highlights that it is effective vacancies which are the mechanism responsible for the transition becoming first order. In light of these results, a few quick fixes to the categories Hamiltonian method were examined in or-

der to see whether treating effective vacancies differently could reproduce the desired effects.

Removing the Penalisation of Effective Vacancies

Currently, effective vacancy states are in a category of their own and thus implicitly are energetically penalised or favoured in general. Note that even if we set the couplings such that $H(\begin{smallmatrix} ab \\ cd \end{smallmatrix}) = H(\begin{smallmatrix} ab \\ ba \end{smallmatrix})$ (this choice is not arbitrary, they have the same energy by the original Potts Hamiltonian),

$$\sum_{\{s_i\} \rightarrow \begin{smallmatrix} ab \\ cd \end{smallmatrix}} e^{-H(s_i)} \neq \sum_{\{s_i\} \rightarrow \begin{smallmatrix} ab \\ ba \end{smallmatrix}} e^{-H(s_i)} \quad (1.92)$$

and thus, $H'(\begin{smallmatrix} ab \\ cd \end{smallmatrix}) \neq H'(\begin{smallmatrix} ab \\ ba \end{smallmatrix})$. This implies that at the fixed point, the couplings relating to the two aforementioned states will not be equal and thus in a sense, $\begin{smallmatrix} ab \\ cd \end{smallmatrix}$ is being energetically favoured or penalised with respect to other configurations which would have the same energy by the original Potts Hamiltonian. Thus perhaps the combination of categories discussed at length for the Ising Model, that is to say combining the original categories such that all states with the same energy by the original Ising Hamiltonian are in the same combined category, is a sensible choice as it removes any such unwanted penalisation. The method works exactly as for the Ising Model, categories are grouped together based on their energies when evaluating the original Hamiltonian, all states in each category are defined to have the same energy and in order to conserve the partition sum, these new couplings must renormalise via weighted sums equivalent to (1.86). Unfortunately, this procedure's results are almost identical to those found using the standard categories Hamiltonian methodology. The results for the inverse critical temperature and y_t are shown in Table 1.12.

Using a Blocking Kernel

The use of a blocking kernel (see (1.70)) has been touched upon already, firstly because Hasenbusch used one and secondly because using one makes it easier to see that the procedure of coarse graining commutes with rotation. In the context of vacancies, it has the advantage that configurations with more disorder contribute less to the sum of their paradigm than they

Model	$\left(\frac{J}{k_B T}\right)_c$	y_t
Ising	0.864	0.929
3-State Potts	0.986	1.121
4-State Potts	1.081	1.311
5-State Potts	1.159	1.485

Table 1.12.: The inverse critical temperature and y_t as obtained by grouping categories based on the original Potts Model Hamiltonian

previously did. That said, while each configuration which renormalises ambiguously contributes less to any given paradigm's Boltzmann sum, it contributes to many different Boltzmann sums including potentially, that of another paradigm. Turning this around, each paradigm's Boltzmann sum will now be receiving many more fractional contributions from ambiguous parent configurations and the total number of such contributions will be the same as when using the top left rule.

Computationally, the downside is that many more parents contribute to the sums ((1.5)) and thus the god tensor must be considerably larger. Of the possible sixteen configurations on a 2×2 Ising lattice, six have zero net magnetisation and are thus ambiguous (see Table 1.1) and the remaining ten renormalise non-ambiguously. Consequently, of the 4096 parent configurations which renormalise to a given paradigm, only $\left(\frac{5}{8}\right)^4 \cdot 4096 = 625$ contained no ambiguities. Conversely, there were $\binom{4}{1} \left(\frac{3}{8}\right) \left(\frac{5}{8}\right)^3 \cdot 4096 = 1500$ parent configurations which contained one ambiguity. There will be 1500 that likewise renormalised ambiguously but, by the "top-left" rule, to a different configuration. If we use a blocking kernel, then information about these 1500 configurations must also be stored. For the Ising model, any block of spins can only be singly ambiguous, that is to say, any ambiguous block of spins can only renormalise to two different spin species, likewise for the 3-State Potts Model (for the 3-State Potts Model, this is only true for $B < 3$). The 4-State Potts Model however allows for spin blocks of the form $\begin{pmatrix} a & a \\ b & b \end{pmatrix}$ and likewise $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$, the former being ambiguous among two spins, the latter among four so the blocking kernel can take the values $0, \frac{1}{4}, \frac{1}{2}$ or 1 (for any given patch, there is a contribution from all $\frac{N^2}{B^2}$ patches which must be multiplied). Thus the general formula for how many more configurations information need to be stored (as a multiple of the number which need to be stored when using the "top left" rule for disambiguation)

for $Q < 4$ is given by

$$\sum_{i=1}^{\frac{N^2}{B^2}} \binom{\frac{N^2}{B^2}}{i} p^i (1-p)^{\frac{N^2}{B^2}-i} \quad (1.93)$$

in which p is the fraction of $B \times B$ configurations which renormalise ambiguously. For the Ising Model, this sum evaluates to 3.57, meaning 3.57 times more information needs to be stored. For the 3-State Potts Model, $\frac{2}{9}$ of the coarse grained configurations contain ambiguities and thus the god tensor's size is multiplied by a factor of 2.23. For $Q > 4$ (and $B = 2$, for larger blocking, patches can have more than 2-way and 4-way ambiguities), the formula is given by

$$\sum_{i=1}^{\frac{N^2}{B^2}} \binom{\frac{N^2}{B^2}}{i} 2^i p^i \sum_{j=0}^{\frac{N^2}{B^2}-i} \binom{\frac{N^2}{B^2}-i}{j} 4^j q^j (1-(p+q))^{\frac{N^2}{B^2}-i-j} \quad (1.94)$$

in which p is the fraction of coarse-grained configurations which are ambiguous between two states and q the fraction which are ambiguous between four. For $Q = 4$, $p = \frac{9}{64}$ and $q = \frac{3}{32}$, thus meaning that we must store approximately 4.09 times more data. For $Q = 5$, $p = \frac{12}{125}$ and $q = \frac{24}{125}$ meaning the god tensor will take up 7.8 times more than the already rather large 11.1 GB.

In terms of the computational resources currently available to us, it was only feasible to repeat the analysis for up to $Q = 4$. Nonetheless for $Q = 2, 3, 4$, results obtained for y_t were close to identical to those obtained without a blocking kernel and thus while it was not possible to probe this for $Q = 5$, we have no reason to suspect that a blocking kernel would be the difference between finding and not finding a fixed point.

1.10. $Q = 4$ Clock Model

In general, the clock Model Hamiltonian is given by

$$H = -J \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \quad (1.95)$$

in which $\theta_i \in [0, \frac{2\pi}{Q}, \frac{4\pi}{Q}, \dots, \frac{2\pi(Q-1)}{Q}]$. For $Q = 2$ and $Q = 3$, the clock and Potts Models are entirely equivalent, as the angles between any s_i and s_j

are the same for all $i \neq j$. For the $Q = 4$ clock model on the other hand, spin species 0 and 2 are anti-parallel, as are 1 and 3 whereas 0 and 1 are perpendicular and so forth. Consequently, if a given spin is in spin state 0, while it is energetically most favourable for its nearest neighbour to be in state 0 as for the Potts Model, it is less favoured for it to be in state 2 than in states 1 or 3. Consequently, its symmetry rules are somewhat different to those of the $Q = 4$ Potts model. For example, $\begin{pmatrix} 00 \\ 01 \end{pmatrix}$ must be energetically favourable compared to $\begin{pmatrix} 00 \\ 02 \end{pmatrix}$ and thus these two configurations must not be in the same category. $\begin{pmatrix} 22 \\ 23 \end{pmatrix}$ however must be in the same category as $\begin{pmatrix} 00 \\ 01 \end{pmatrix}$. In short what must be preserved is the "difference" between all spins. One symmetry which upholds this is to add any n to all spins (cyclically wrapping around when $s_i + n \geq Q$). Devising a general algorithmic framework to preserve all "differences" or angles is considerably more challenging than doing so for $Q = 4$, and thus I have so far only done so for $Q = 4$. The resulting 13 categories are shown in Appendix B.4. A fixed point is found, with only one (aside from the trivial) critical exponent greater than unity, namely $y_t = 0.936$. This is in line with the expectation that the $Q = 4$ Clock Model is equivalent to two decoupled Ising Models [80, 87] and as such must have the same critical exponents. Not only is my value close to the expected value of unity, it is extremely close to the value Hasenbusch and I have found for the Ising Model, and consequently one can speculate, that the (unknown) source of the error, causing systematic underestimation of y_t is the same.

It would be of considerable interest to continue this analysis for increasing Q . By the Mermin-Wagner theorem [58], in the limit $Q \rightarrow \infty$, the model has continuous symmetry and consequently cannot exhibit long range order for any finite temperature in two dimensions. Yet we know that it does for low values of Q , and consequently, there must exist a finite Q above which the system exhibits a Kosterlitz-Thouless [49] transformation. Unlike the case of the Q -state Potts Model however, there remains some uncertainty as to the value of Q at which this occurs [1], with some disagreement about whether it is $Q = 5$ or $Q = 6$. In general, the clock Model will have more categories for a given Q than the Potts Model. As the $Q = 5$ Potts Model was already pushing what was computationally feasible in terms of memory requirements, the $Q = 5$ clock model would be even more of a strain, although in all likelihood still doable. The $Q = 6$ Potts

and consequently clock model however is an order of magnitude beyond what is feasible with current computational resources. Furthermore, due to the failure of the current scheme to determine the critical Q above which the Potts Model's phase transition becomes first order, I have decided not to pursue a general algorithmic framework for determining the categories for the Q -state clock Model.

1.11. Discussion

1.11.1. Magnetic Exponents

The exponent δ in the Ising Model is intuitively easy to understand, it governs how strong the response in order parameter is to a small external field being introduced (when the temperature is equal to the critical temperature, although such a concept likewise is intuitively simple to understand at temperatures greater than the critical temperature as well). Furthermore, it is relatively simple to picture how the process of coarse graining will amplify any imbalance between spin species numbers and thus effectively increase the external magnetic field or mathematically, $h' = b^{y_h} h$. Additionally, it is well understood how these two exponents are related (see (1.29)). The situation for the 3-state Potts Model is not so simple. It is fairly easy to picture the introducing of an external field which energetically favours a single spin species and asking how this affects the order parameter. What if instead, this field de-favoured a single spin species? The resulting response would be a system in which there were two majority spin carriers. Intuitively, it would seem that this might have a different effect on the order parameter.

Considering instead renormalising a system in which one of the three species is slightly dominant, successive applications of the RG would result eventually in this species completely dominating the system. Likewise successively applying the RG to a system in which one species was in a slight minority would wash it out but leave the other two present in equal amounts (i.e. it would look like the an Ising Model). Would these two processes occur at different rates? This seems unlikely as the linearisation of the transformation at the fixed point (1.18) is not sensitive to direction.

While we know of many references in the literature [23, 95, 21, 84, 61]

which calculate a second magnetic exponent for the $Q > 2$ Potts Model, we have yet to find a single interpretation of its physical significance. Table 1.7 also shows the crucial result, that we see two magnetic exponents after introducing a single field for $Q > 2$. This would appear to invalidate any hypothesis that this exponent has anything to do with the presence of two fields.

We have ruled out, that the third magnetic exponent found for the 4-state Potts Model, might be related to the marginal exponent the $Q = 4$ Potts Model is known to exhibit in 2 dimensions, which is due to a logarithmic correction to y_t [83] related to $Q = 4$ being the upper critical Q above which the transition becomes first order. Firstly, we find it highly unlikely, despite the small value of y_{h3} , that this represents a thermal effect, as y_{h3} is only visible after applying two external fields (this point of view is further strengthened by the fact this pattern occurs for both the square and triangular lattice). Furthermore, introducing a third field results in two eigenvectors whose eigenvalues lead to this exponent. This is in keeping with the general trend we have observed, that introducing further fields leads to the magnetic exponents becoming degenerate, which does not happen to the thermal exponent (as there is only one thermal direction, even when multiple magnetic fields have been introduced). Finally, as our scheme fails to capture the transition becoming first order for $Q > 4$, we find it highly unlikely our scheme would be able to observe a marginal exponent related to corrections associated therewith.

To me personally, the most appealing interpretation of the third magnetic exponent, is that it is related to a relevant direction which corresponds to (de)favouring two spin species equally, which is in turn equivalent to the $Z_2 \otimes Z_2$ grouping we experimented with in Section 1.6.1. With such a field in place, one would expect to find the system in a state dominated (ever-increasingly, as the field strength is increased) by two spin species. This would most certainly however have a much weaker effect on the order parameter, than favouring a single spin species, backed up by the considerably smaller value of y_{h3} .

The result presented in Section 1.6.1, namely that a field which (de)favours two spin species equally, is associated with all three magnetic exponents is particularly difficult to reconcile with the notion of y_h representing the effect caused by the introduction of an external field which couples to a

single species.

Thus it can only be concluded that the physical significance of the multiple magnetic exponents found cannot be ascertained from our results alone and the literature on the matter is unclear. We however do not believe this to be a shortcoming of our method as the numerical values we have obtained for the exponents are in good agreement with those calculated by other methods.

1.11.2. Connection to Spin $> \frac{1}{2}$ Models

A natural question which arises, is whether the scheme presented in this chapter might be applicable to models such as the Blume-Emery-Griffiths (BEG) Model[14]. The BEG Hamiltonian is given by

$$H = -J \sum_{\langle ij \rangle} s_i s_j - K \sum_{\langle ij \rangle} s_i^2 s_j^2 - \Delta \sum_i s_i^2 \quad (1.96)$$

in which $s_i \in [-1, 0, 1]$. Clearly (1.96) is invariant under the transformation $s_i \rightarrow -s_i$, i.e. a full parity inversion. Note that if $J \rightarrow 0$, then for example $H\left(\begin{smallmatrix} +1 & +1 \\ -1 & -1 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} +1 & +1 \\ +1 & -1 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} +1 & +1 \\ +1 & +1 \end{smallmatrix}\right)$ and so forth. In fact, when $J = 0$, the lattice and parity symmetries suggest a categorisation along the lines of (1.77), only with a relabelling given by $(-1 \rightarrow 0, 0 \rightarrow 1, +1 \rightarrow 2)$. Thus it seems reasonable to interpret the first alternative fixed point as being related to the behaviour of the BEG model for $J = 0$. Interpreting the second alternative fixed point as related to the BEG Model is for now mere speculation.

1.11.3. Conclusions

In keeping with our preliminary analysis of Hasenbusch's work versus simply calculating the partition sum, we find that the RG does in fact allow us to extract critical properties of general Q -state Potts Models from systems which are too small to exhibit such behaviour themselves. Unfortunately a major shortcoming of the method is that it does not correctly predict the transition becoming first order above a critical Q , but this is a shortcoming of the real-space RG in general and should not be regarded as being due to the small systems being used. Unsurprisingly, the symmetries of the models being studied and the lattices they are being studied

on (and thus grouping configurations into categories) lie at the heart of the method, and thus the fact that categories can be combined is a rather difficult to interpret result. The method outlined becomes computationally very expensive for even the smallest possible increases in system size and thus it would not appear that this process can be applied to a wide variety of other systems. For the Ising Model, it is possible to carry the procedure through for $N=6$, $B=2$, thus increasing the range of interactions included in the Hamiltonian and the value of y_t obtained is likewise very close to Onsager's value, in fact closer than for $N=4$. While one would expect the result to improve for larger values of $\frac{N}{B}$ as this is equivalent to including more (longer range) interactions in the Hamiltonian, as only $\frac{N}{B} = 2$ and $\frac{N}{B} = 3$ are within the realm of what is computationally feasible at this point, it would be premature to claim this to be the case from our results.

1.11.4. Future Work

The problems discussed within this chapter naturally scale very unfavourably, which in turn is why methods such as the aforementioned Monte Carlo RG were developed. It would for example, be interesting to repeat the process in three dimensions, but the size of the phase space is so large, that the computational time and memory requirements would be orders of magnitude above what is currently required, and we have already been operating close to the limit of our computation resources. It is certainly true that it must be possible to get away with considering only a fraction of the parent configurations we currently do, but we estimate this might decrease the memory requirements by roughly an order of magnitude, meaning one might just about be able to bring the $Q = 6$ Potts Model into the realm of what is computationally feasible, but 3 dimensions, or the $Q = 3$ Potts Model on a 6×6 lattice remain out of the question.

A more promising line of enquiry, and one which would certainly be of scientific interest, would be to figure out a way to reconcile the concept of holes with the categories Hamiltonian, in order to hopefully reproduce the first order phase transition for $Q = 5$, and conclusively show that this is not a problem of the categories method per se.

Finally, without a doubt, there are many "alternative fixed points" to be found for the $Q = 4$ Potts model. It would seem like a more sensible

approach however, to first better understand the alternative fixed points found for $Q = 3$ and attempt based upon this, to predict the fixed points one would expect to find for $Q = 4$, before carrying out an exhaustive search of the phase space. These fixed points are of particular interest, because they potentially tell us about the critical behaviour of $S \neq \frac{1}{2}$ Ising Models, which are considerably less well understood than the models discussed in this chapter, which have been studied extensively over many decades.

2. On Spin-Spin Correlations at a Free Interface

The work in this chapter presents, expands upon and extends results which were published in the Journal of Phys.: Condensed Matter, 26, Sept 2014 [64].

Abstract

The density-density correlation function $\mathcal{G}(z_1, z_2; q)$ is studied in the interfacial region of a fluid-gas or Ising like up-down interface, using both square gradient and square Laplacian density functional theory. Within the Double Parabola approximation, the interfacial correlation function splits up cleanly into a bulk and an interfacial contribution and consequently, so does the structure factor. After attempting to reconstruct these density-density correlations by relating them to interfacial height-height fluctuations using an interfacial model characterised by a wave-vector dependent surface tension $\sigma(q)$, it becomes clear that the usual crossing criterion (a key ingredient to an interfacial model) does not correctly explain this separation of the $\mathcal{G}(z_1, z_2; q)$ into bulk and interfacial contributions. Within the Double Parabola approximation, it is possible to define a new definition of the interface, based on correlations between two points which float on the interface which does allow for the correct reconstruction of density-density (magnetisation-magnetisation) fluctuations from the height-height correlation function. Even this new definition of the interface however will result in $\sigma(q)$ not being a quantity which can be experimentally measured. This has profound implications for earlier attempts to extract and interpret $\sigma(q)$. Furthermore, beyond the Double Parabola approximation, $\mathcal{G}(z_1, z_2; q)$ does not split cleanly into bulk and interfacial contributions, meaning that not only can one not reconstruct density-density fluctuations at all positions simultaneously from an interfacial model, but likewise different modifications to the crossing criterion are required in order to correctly reconstruct different quantities.

2.1. Outline

The basic premise of this chapter is that it is not possible to determine the wave vector dependent surface tension, $\sigma(q)$, of a free interface by experimentally measuring the structure factor, as has been assumed time and time again. Before delving into this however, basic concepts from the theory of interfaces are explained, starting from what is meant by a free interface, and moving onto how to calculate the profile, surface tension and interfacial correlation functions using a density functional theory approach.

Next, a simplistic model involving a crossing criterion, namely the Fisher Jin model is introduced, followed by the more sophisticated Parry Boulter method, the latter being discussed in quite some detail. Once the Parry Boulter method has been introduced (this discussion includes a definition of the wave vector dependent surface tension), I discuss and critique earlier approaches to calculate $\sigma(q)$ and how even within a very simplistic toy model, the Double Parabola model, problems arise. In particular, some rather subtle changes to the crossing criterion (part of the definition of the interface) are discussed, and how even after these amendments, the q dependence of the structure factor implies that $\sigma(q)$ cannot be extracted experimentally as had been hoped. Certain assumptions however are shown to hold within the Double Parabola framework, most notably the interfacial correlation function splitting into a bulk and an excess part.

The latter part of the chapter is concerned with applying Parry Boulter theory to a slightly more sophisticated toy model, namely the widely used Landau double well potential. If certain properties of the structure factor observed in Double Parabola were observed within the Landau model too, it could potentially be argued that $\sigma(q)$ could be measured after all (even then, this would be tenuous) but this turns out not to be the case. Furthermore, many of the positive results obtained for the Double Parabola model are shown to break down within Landau theory, most notably the way the interfacial correlation function splits up (or rather fails to do so), and the consequences this has for any amendment to the crossing criterion one might like to make.

Finally, a few comments are made about the Triple Parabola model, and the Extended Landau-Ginzburg-Wilson model, as substantial time was spent carrying out calculations for these models. These results all back up the ba-

sic findings which arise from the Double Parabola and the Landau models.

2.2. Introduction to Free Interfaces

For the interfaces described in this chapter, thermodynamic conditions are assumed to be those which facilitate two-phase coexistence. Mathematically, I will tend to describe this as an Ising system with a magnetisation-like order parameter below T_c . Physically, this is best thought of as a substance such as water, with the temperature between the triple and critical points and the pressure tuned to that of liquid-gas coexistence. In magnetic language, we then introduce an infinitesimally weakly varying magnetic field such that $h(z) \rightarrow +\epsilon$ as $z \rightarrow +\infty$ and $h(z) \rightarrow -\epsilon$ as $z \rightarrow -\infty$ or vice versa. This will enforce that the system will be in its predominantly up phase as $z \rightarrow +\infty$ and in its down phase as $z \rightarrow -\infty$. It is then the goal to study certain features of the spatially dependent magnetisation-like order parameter $m(z)$ in the region of change or the interfacial region. In liquid/gas language, we could introduce an infinitesimally weakly varying pressure gradient such that $P(z \rightarrow -\infty) = P_{coexist} - \epsilon$ and $P(z \rightarrow +\infty) = P_{coexist} + \epsilon$ such that as $z \rightarrow -\infty$, the density will be that of a bulk gas and as $z \rightarrow +\infty$ a bulk liquid. A similar effect could be achieved by a weak symmetry breaking external field such as gravity [29].

A simple model which describes the bulk coexistence of two phases below a critical temperature is a free energy density given by

$$f(m) = f(m = 0) + a(T)m^4 + bm^4 \quad (2.1)$$

in which m is the magnetisation of the system. The parameter $a(T)$ in (2.1) is proportional to $(T - T_c)$ and thus this is a so-called double well potential with two global minima for non-zero m (say $\pm m_0$). While for example, values of $f(m = 0)$, $a(T)$ and b can be derived with relative ease from the mean field free energy of the Ising Model, it is more instructive to think of a double well potential as being the model which causes two-phase coexistence and thus the fundamental model behind the theory of free interfaces. The double well potentials discussed in this chapter will all exhibit Ising symmetry, that is to say that $f(m) = f(-m)$ and consequently, the two global minima will be equidistant from $m = 0$. As we will see, the curva-

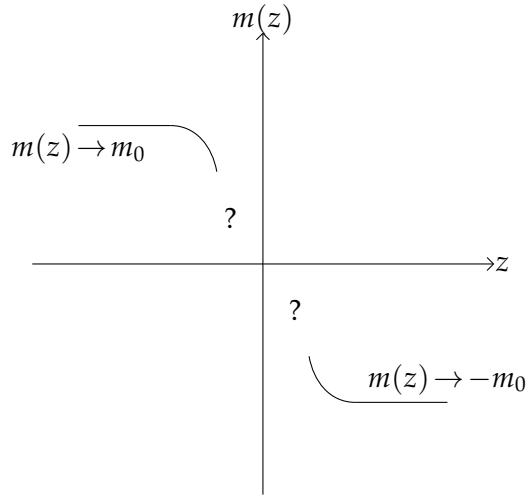


Figure 2.1.: The boundary conditions imposed by the symmetry breaking external field in question. The first question one might ask, is how the density/magnetisation profile looks in the changeover/interfacial region.

ture of $f(m)$ at $m = \pm m_0$ is related to the microscopic correlation length and thus the correlation lengths of the two phases are the same. Clearly this is not the case for a liquid/gas interface as the correlation length of a liquid is much greater than that of a gas. Nonetheless, the effect of using an asymmetric potential is not discussed in this chapter and should be regarded as the next natural progression, and a topic of ongoing research [66, 67].

While (2.1) governs the equilibrium value of the order parameter m , this assumes an infinite, translationally invariant system. Introducing a symmetry breaking external field which breaks this invariance in only one spatial direction (which I will refer to as the z -direction) will have the effect of making the order parameter also vary along this spatial dimension. While I have outlined the boundary conditions, the first question we must ask is how this changeover occurs (see Figure 2.1). (2.1) is only applicable when translational invariance is unbroken. To see this, consider the profile shown in Figure 2.2. Clearly such a profile is completely at odds with the underlying microscopic physics of the Ising Model and likewise there is an infinitum of such solutions. Nonetheless, profiles such as that shown in Figure 2.2 minimise (2.1). Consequently, the so-called Landau-Ginzburg-

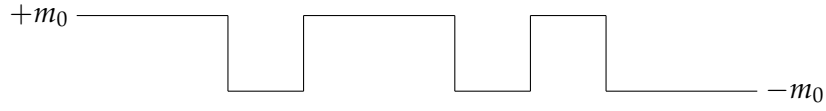


Figure 2.2.: A profile which respects the boundary conditions shown in Figure 2.1 and minimises (2.1)

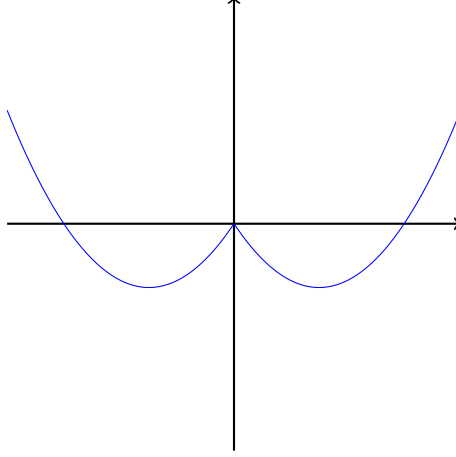


Figure 2.3.: The DP potential. Note the two global minima for non-zero m as well as the discontinuous slope at $m = 0$.

Wilson grand potential functional

$$H_{LW}[m] = \int d\mathbf{r} \left[\frac{g}{2} (\nabla m)^2 + f(m) \right] \quad (2.2)$$

is used to describe interfacial phenomena, as it penalises strong local fluctuations of $m(z)$.

2.3. Microscopic Theory

2.3.1. The Double Parabola Model

The DP potential is a model of two-phase coexistence given by:

$$\Delta f(m) = \frac{\kappa^2}{2} \delta m^2 \quad (2.3)$$

in which Δf is the excess free energy w.r.t the equilibrium value and δm is defined as $(m_0 - |m|)$. A more subtle but essential feature of the DP model is that the first derivative of the potential is discontinuous at $m = 0$ and consequently, the second derivative must contain a delta function. For now, let us simply write $f''(m) = \kappa^2 + a\delta(m)$. I will return to this when discussing the equilibrium magnetisation profile as well as the interfacial correlation function. The reason for introducing the DP potential is that it provides a phenomenological description of two phase coexistence with Ising symmetry, but does not contain terms quartic in the order parameter which in turn simplifies a lot of the mathematics.

Magnetisation Profile of an Interface within DP Theory

For a general free energy such as the DP potential, the functional which must be minimised[29] w.r.t $m(r)$ in order to ascertain the equilibrium profile is:

$$H_{LGW} = \int d\underline{y} \int dz \left[\frac{1}{2} (\nabla m)^2 + \Delta f(m) \right] \quad (2.4)$$

For the case of the DP potential, we note that $\nabla \delta m = \nabla m$ and thus minimise the following functional w.r.t δm instead:

$$H_{LGW} = \int d\underline{y} \int dz \left[\frac{1}{2} (\nabla \delta m)^2 + \frac{\kappa^2}{2} \delta m^2 \right] \quad (2.5)$$

The Euler-Lagrange (EL)[47] equation resulting from (2.4) is $\nabla^2 \delta m = f'(\delta m)$. For now we simply note that $f'(m)$ is discontinuous at $m = 0$ and thus $\nabla^2 \delta m$ will be discontinuous at any $\underline{r}$ for which $m(\underline{r}) = 0$. Noting that in the absence of any field breaking translational invariance in the perpendicular plane, it will always be energetically favourable for the perpendicular gradient terms to be zero (alternately the profile must be translationally invariant), and hence $\nabla^2 \delta m = \frac{d^2 \delta m}{dz^2}$, the resulting EL equation is

$$\frac{d^2 \delta m}{dz^2} = \kappa^2 \delta m \quad (2.6)$$

The general solution to this is $\delta m(z) = Ae^{\kappa z} + Be^{-\kappa z}$. Note however that this does not satisfy either of the boundary conditions as $z \rightarrow \pm\infty$. The key here is that the function $m(z)$ is allowed to change definition at the plane at which $m = 0$ so long as m remains continuous and differentiable. Higher

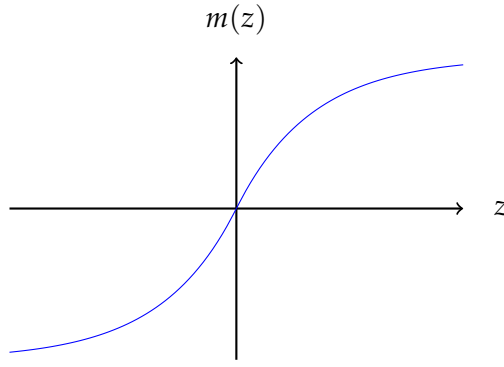


Figure 2.4.: The DP equilibrium profile

derivatives may be discontinuous as the second derivative of the profile is related to the first derivative of the DP potential w.r.t m which contains a δ function. Thus we define

$$\begin{aligned}\delta m_-(z) &= Ae^{\kappa z} \\ \delta m_+(z) &= Be^{-\kappa z}\end{aligned}\tag{2.7}$$

in which the $\pm$ subscripts relate to z being greater or less than 0. Note I have defined $z = 0$ as the plane in which $m = 0$ for simplicity and without loss of generality. Thus the boundary conditions are now satisfied by

$$\begin{aligned}m_-(z) &= -m_0(1 - e^{\kappa z}) \\ m_+(z) &= m_0(1 - e^{-\kappa z})\end{aligned}\tag{2.8}$$

As can be seen in Figure 2.4, the solution looks very much like a tanh profile and indeed, $m(z)$ and its first derivative are continuous at $z=0$ but higher derivatives are not.

Bulk Correlation Function

By translational invariance [43], the Fourier Transform of the bulk correlation function is defined as

$$\tilde{G}(\underline{k}) = \langle |\Delta \tilde{m}(\underline{k})|^2 \rangle\tag{2.9}$$

In which $\Delta m(\underline{r})$ is defined as difference between the local magnetisation and the average, temperature dependent equilibrium magnetisation (below T_c this is equal to $m \pm m_0$ and above T_c simply m). In the context of DP, we can replace Δm with δm and consequently $\Delta \tilde{m}(\underline{k})$ can be replaced with $\delta \tilde{m}(\underline{k})$, the Fourier Transform of δm . Hence

$$\tilde{G}(\underline{k}) = \frac{\sum_{configs} |\delta \tilde{m}(\underline{k})|^2 e^{-\beta \int d^d r \left[\frac{1}{2} (\nabla \delta m)^2 + \frac{\kappa^2}{2} \delta m^2 \right]}}{\sum_{configs} e^{-\beta \int d^d r \left[\frac{1}{2} (\nabla \delta m)^2 + \frac{\kappa^2}{2} \delta m^2 \right]}} \quad (2.10)$$

Note that the δm terms in the integrals within the exponents are expressed in real space. Thus firstly, let us, by writing $\delta m(\underline{r})$ as an inverse Fourier Transform, rewrite the integrals which occur in the exponents of the Boltzmann weighting factors in momentum space

$$\frac{1}{2} \int \frac{d^d q}{(2\pi)^d} (q^2 + \kappa^2) |\delta \tilde{m}(\underline{q})|^2$$

Furthermore, for a finite system with periodic boundary conditions, there exists a discrete set of Fourier coefficients $\delta \tilde{m}(\underline{k})$ and hence the sum over all configurations can be written as the integral over all values of this set, i.e.

$$\sum_{configs} = \int (d\delta \tilde{m}(\underline{k}_1)) (d\delta \tilde{m}(\underline{k}_2)) \dots (d\delta \tilde{m}(\underline{q})) \dots \quad (2.11)$$

Consequently, the Fourier transform of the bulk correlation function is given by

$$\tilde{G}(\underline{k}) = \frac{\int (d\delta \tilde{m}(\underline{k}_1)) (d\delta \tilde{m}(\underline{k}_1)) \dots (d\delta \tilde{m}(\underline{q})) |\delta \tilde{m}(\underline{q})|^2 e^{-\frac{\beta}{2} \int \frac{d^d q}{(2\pi)^d} (q^2 + \kappa^2) |\delta \tilde{m}(\underline{q})|^2} \dots}{\int (d\delta \tilde{m}(\underline{k}_1)) (d\delta \tilde{m}(\underline{k}_2)) \dots (d\delta \tilde{m}(\underline{q})) e^{-\frac{\beta}{2} \int \frac{d^d q}{(2\pi)^d} (q^2 + \kappa^2) |\delta \tilde{m}(\underline{q})|^2}} \quad (2.12)$$

Finally, the integrals in the exponent can be written as sums due to q taking a set of discrete values for any finite system. As a result of this, the exponential separates into a product of exponentials, and the integrals over all modes can be performed independently. All will cancel (as the same integral exists in the denominator and numerator) apart from the q^{th} mode.

Consequently, the problem essentially reduces to

$$\frac{\int x^2 e^{-\alpha x^2} dx}{\int e^{-\alpha x^2} dx}$$

Thus

$$\tilde{G}(\underline{q}) = \frac{k_B T}{\kappa^2 + q^2} \quad (2.13)$$

For the duration of this chapter however, $k_B T$ or β^{-1} will be set to unity. Inverting (2.13) (see Appendix D) in 3 dimensions yields the well-known result for the bulk correlation function

$$G(\underline{r}) \propto \frac{e^{-\kappa|\underline{r}|}}{|\underline{r}|} \quad (2.14)$$

and thus it can be read off that κ is simply the reciprocal of the bulk correlation length. Until this point, κ was simply a parameter in the DP potential which can be tuned but by calculating the bulk correlation function, it becomes evident that it has physical meaning. This should not come as a surprise, we know already from calculating the profile that κ represents a length scale which determines the interfacial width and it would seem reasonable that the interfacial width is on the order of the correlation length.

Surface Tension

As the EL equation for the planar, equilibrium profile is $\frac{d^2 m}{dz^2} = \Delta f'(m)$, we can multiply either side by $\frac{dm}{dz}$. The result is that $\frac{1}{2} \frac{d}{dz} \left(\frac{dm}{dz} \right)^2 = \frac{d}{dz} \Delta f(m)$. Thus up to a constant, $\left(\frac{dm}{dz} \right)^2 = \Delta f(m)$. Hence the excess free energy incurred by an interface within LGW theory reads (up to a constant, which we know must not be associated with the excess free energy)

$$H_{min} = \sigma A = \int d\underline{y} \int dz \left(\frac{dm}{dz} \right)^2 \quad (2.15)$$

i.e. this toy microscopic DFT model re-derives the Triezenburg-Zwanzig formula[88, 42], in which A is the surface area of the interface.

2.4. The Interfacial Correlation Function

In order to determine the interfacial correlation function, it is necessary to solve the Ornstein-Zernicke (OZ) [75, 28] equation which in square-gradient theory reads

$$\left(-\frac{\partial^2}{\partial z_1^2} + f''(m(z_1)) + q^2\right) \mathcal{G}(z_1, z_2; q) = \delta(z_1 - z_2) \quad (2.16)$$

At DP level, the δ function present within $f''(m)$ now becomes important. I have already stated that $f''(m) = \kappa^2 + a\delta(m)$. Integrating over the cusp, it is relatively easy to see that $a = 2m_0\kappa^2$, i.e. the change in slope about $m = 0$. Next, we use the relationship[73]

$$\delta(x - a) = \sum_i \frac{\delta(y - b_i)}{\left|\frac{dy}{dx}\right|_{y=b_i}} \quad (2.17)$$

in which the $\sum_i$ runs over all values of y , for which $x(y) = a$. In this case however, $m(z)$ is a single valued function and thus $f''(m(z)) = \kappa^2 - 2\kappa\delta(z)$. The DP OZ had previously been solved within the context of wetting [63] (in which the calculation is somewhat more cumbersome) by solving the problem in sections and integrating over the δ function to match constants at boundaries. It was however the realisation that we could solve for the entire correlation function that provided much of the motivation for this chapter and our paper [64].

To solve for the interfacial correlation function in DP, we take the Fourier Transform of the OZ (2.16) over all z_1 to obtain

$$\int dz_1 \left[-\frac{\partial^2 \mathcal{G}(z_1, z_2; q)}{\partial z_1^2} + \kappa_q^2 \mathcal{G}(z_1, z_2; q) - 2\kappa\delta(z) \mathcal{G}(z_1, z_2; q) \right] e^{-i\lambda z_1} = e^{-i\lambda z_2} \quad (2.18)$$

in which $\kappa_q = \sqrt{\kappa^2 + q^2}$. Using the notation that $\hat{\mathcal{G}}(\lambda, z_2; q)$ represents the Fourier Transform in z_1 of $\mathcal{G}(z_1, z_2; q)$, and integrating by parts, one obtains

$$\hat{\mathcal{G}}(\lambda, z_2; q) = \frac{2\kappa \mathcal{G}(0, z_2; q)}{\kappa_q^2 + \lambda^2} + \frac{e^{-i\lambda z_2}}{\kappa_q^2 + \lambda^2} \quad (2.19)$$

which can be inverted by contour integral[73] to give

$$\mathcal{G}(z_1, z_2; q) = \frac{\kappa}{\kappa_q} \mathcal{G}(0, z_2; q) e^{-i\kappa_q |z_1|} + \frac{e^{-i\kappa_q |z_1 - z_2|}}{2\kappa_q} \quad (2.20)$$

in which the latter term is easily recognisable as the bulk correlation function. The same process can be carried out for the z_2 OZ PDE resulting in an expression equivalent to (2.20) with z_1 and z_2 relabelled. Making use of the fact that $\mathcal{G}(z_1, z_2; q)$ must equal $\mathcal{G}(z_2, z_1; q)$, one finds that

$$\mathcal{G}(z_1, z_2; q) = \frac{1}{2\kappa_q} e^{-\kappa_q |z_1 - z_2|} + \frac{\kappa}{2\kappa_q} \frac{e^{-\kappa_q |z_1| - \kappa_q |z_2|}}{\kappa_q - \kappa} \quad (2.21)$$

which can be rewritten entirely in terms of the bulk correlation function

$$\mathcal{G}(z_1, z_2; q) = G^b(|z_1 - z_2|; q) + \frac{G^b(z_1; q) G^b(z_2; q)}{G^b(0; 0) - G^b(0; q)} \quad (2.22)$$

and thus the correlation function splits into a bulk contribution and an interfacial contribution as is often assumed in the literature [57, 59]. An obvious consequence of this is that the local structure factor, defined as $S(z; q) = \int_{-\infty}^{+\infty} \mathcal{G}(z_1, z_2; q) dz_2$ and the total structure, defined as $\int_{-L}^{+L} S(z; q) dz$ (in which L is some macroscopic distance) will likewise split into a bulk and an interfacial part given by

$$\begin{aligned} S(z; q) &= \frac{1}{\kappa_q^2} \left(1 + \frac{\kappa}{(\kappa_q - \kappa)} e^{-\kappa_q |z|} \right) \\ S(q) &= \frac{2L}{\kappa_q^2} + \frac{2\kappa}{\kappa_q^3 (\kappa_q - \kappa)} \end{aligned} \quad (2.23)$$

In all three cases (correlation function, local and total structure factors), it can easily be seen that the interfacial term contains a Goldstone Mode (a term proportional to $\frac{1}{q^2}$) [36, 37] related to the continuous symmetry arising from being able to translate the interface without any energetic cost.

2.5. Mesoscopic or Interfacial Hamiltonian Theory

A more simple description of an interface which makes no recourse to the nature of the two bulk phases which the interface separates is one which

simply energetically penalises fluctuations which increase the surface area of the interface

$$H_{cap} = \int \sigma dA \quad (2.24)$$

in which σ represents the surface tension and by its very definition represents how strongly the interface resists such changes. The area element dA refers to the area of the interface. If the height of the interface above some arbitrary surface is defined as $\ell(\underline{y})$, then (working in 2+1 dimensions) the area element can be expanded to give

$$H_{cap} = \int \sigma \left(\sqrt{1 + (\nabla \ell)^2} \right) d\underline{y} = \text{const.} + \int \frac{\sigma}{2} (\nabla \ell)^2 d\underline{y} + O(\nabla \ell)^4 + \dots \quad (2.25)$$

Hence for relatively slowly fluctuating interfaces, the well-known [16, 54] capillary wave (CW) Hamiltonian is given by

$$H_{cap}[\ell(\underline{y})] = \int \frac{\sigma}{2} (\nabla \ell)^2 d\underline{y} \quad (2.26)$$

Writing $\ell(\underline{y})$ as an inverse Fourier Transform leads to the Hamiltonian in wave vector space being expressed as

$$H[\ell(\underline{q})] = \frac{\sigma}{2} \int \frac{d\underline{q}}{(2\pi)^{d-1}} q^2 |\tilde{\ell}(\underline{q})|^2 \quad (2.27)$$

and consequently by equipartition, the interfacial height-height correlation function (in wave-vector space) is given by

$$\langle |\tilde{\ell}(\underline{q})|^2 \rangle = \frac{1}{\sigma q^2} \quad (2.28)$$

in which normally there would also be a factor of $k_B T$, but this has been set to unity.

2.5.1. Extending the Capillary Wave Hamiltonian

In order to invert (2.28) and find the interfacial roughness [77], ad-hoc high and low wavelength cut-offs must be imposed. In a sense, this is perfectly reasonable on physical grounds, the long wavelength cut-off being determined by the finite size of the system and the short wavelength cut-off related to the limited validity of a mesoscopic theory such as a capillary

wave Hamiltonian at microscopic wavelengths. Where the cut-off is applied however is in a sense arbitrary. The interfacial roughness is defined by

$$\langle \ell(0)^2 \rangle - \langle \ell(0) \rangle^2 \quad (2.29)$$

and is thus given by

$$\int \frac{d^{d-1}q}{(2\pi)^{2d-1}} \frac{1}{\sigma q^2} \quad (2.30)$$

Working in 3 dimensions (or 2+1 dimensions), (2.30) can be rewritten in plane polar co-ordinates

$$\int_0^\infty \frac{dq}{(2\pi)^{2d-1}} \frac{2\pi q}{\sigma q^2} = \int_0^\infty \frac{dq}{2\pi\sigma q} \quad (2.31)$$

which contains both an infra red and an ultra violet divergence and hence the need for the high and low wave-vector cut-offs.

Following on from Helfrich's successful mathematical description of Lipid Bilayers [41], Romero-Rochin et.al [74] proposed the Fourier Transform of the height-height correlation function be proportional to

$$\frac{1}{\sigma q^2 + \gamma q^4 + \dots} \quad (2.32)$$

(2.32) has the advantage that it is invertible as it now has poles in the complex plane, so long as γ and σ have the same sign (I shall return to this).

On physical grounds alone, it seems sensible that not only should interfacial fluctuations which increase the surface area of the interface be energetically punished but that the manner in which they do so, for example short or long wavelength undulations, should likewise affect the energetic cost of such a fluctuation. Mathematically, this would involve extending the interfacial Hamiltonian

$$H_{CW}[\ell(\underline{y})] = \int d^{d-1}\underline{y} \left[\frac{\sigma}{2} \left(\nabla \ell(\underline{y}) \right)^2 + \frac{\gamma}{2} \left(\nabla^2 \ell(\underline{y}) \right)^2 \right] \quad (2.33)$$

Re-expressing this in wave-vector space yields

$$H_{CW}[\ell(\underline{q})] = \frac{1}{2} \int \frac{d^{d-1}q}{(2\pi)^{d-1}} \left[(\sigma + \gamma q^2) q^2 |\tilde{\ell}(\underline{q})|^2 \right] \quad (2.34)$$

which re derives Romero-Rochin et. al's expression for the height-height correlation function (2.32). More generally, penalising higher order bending effects (i.e. adding $(\nabla^3 \ell)^2$ etc.) will yield

$$H_{CW}[\ell(\underline{q})] = \frac{1}{2} \int \frac{d^{d-1}q}{(2\pi)^{d-1}} \left[q^2 \sigma(q) |\tilde{\ell}(\underline{q})|^2 \right] \quad (2.35)$$

(2.35) should be regarded as the definition of $\sigma(q)$ which will henceforth be referred to as the wave-vector dependent surface tension, although its thermodynamic status is by no means as straight forward. Clearly as $q \rightarrow 0$, $\sigma(q) \rightarrow \sigma$. Extra information is contained within $\sigma(q)$ such as how strongly the interface resists bending effects and all other higher-order curvature effects. The bending rigidity as defined in (2.33) is the second moment (the coefficient of q^2 in the Taylor expansion) of $\sigma(q)$.

By equipartition,

$$\langle |\ell(\underline{q})|^2 \rangle = \frac{1}{\sigma(q)q^2} \quad (2.36)$$

Thus microscopic features such as the roughness, defined via $\langle \ell(0)\ell(x) \rangle$ can be calculated. Dietrich and Mecke [57] for example, predicted that the wave vector dependent surface tension is not monotonic in q , but that it first decreases until a critical q (say q^*) and subsequently increases and diverges as $q \rightarrow \infty$. Physically, this would mean that for a fluctuation which is known to increase the surface area of the interface (relative to a flat planar profile) by a given amount A , it would be energetically favourable for it to do so, not by stretching the planar interface out, but rather by making it undulate with wave vector q^* . Further comment is passed on this in Figure 2.7.

Should it be possible to measure $\sigma(q)$, the interfacial roughness (an inherently microscopic quantity) could be calculated. This would mean the roughness could be calculated in cases in which the full microscopic solution was not possible. Of course, in a sense this is the reverse of the usual statistical physics approach of explaining the physics of longer length scales in terms of the physics of shorter ones. In the rest of this chapter however, I will discuss some simple microscopic theories which can be solved exactly. It will become clear that even in such simple theories, the structure factor (the experimentally measurable observable) has complex q -dependence which makes the wave-vector dependent surface tension impossible to

measure. Furthermore it will become apparent that a simple crossing criterion definition of the interface leads to interfacial Hamiltonian theory generating an interfacial correlation function at odds with the microscopic theory. For the simplest of models namely double parabola (DP), a new more subtle definition of the interface can overcome this problem but for the full Landau Theory, even this is insufficient.

2.5.2. Fisher Jin Theory

A fundamental goal of statistical physics is to describe macroscopic thermodynamic variables such as pressure or surface tension in terms of microscopic phenomena. Fisher Jin (FJ)[32, 33] theory attempts to do this by introducing the concept of a constrained minimisation w.r.t a crossing criterion. Let us define m_{Ξ} as the profile which minimises the Landau-Ginzburg-Wilson Hamiltonian subject to a constraint or "crossing criterion" defined as a 2-dimensional isomagnetic surface such that $m_{\Xi}(z = \ell(\underline{y}), \underline{y}) = m^x$ (for now we take $m^x = 0$ and exploit Ising symmetry for simplicity). m_{Ξ} will satisfy the EL equation everywhere apart from at the interface. This subtle point is rather critical to understanding the rest of the content in this chapter. Consider calculating the shortest distance between two points using an EL equation, the result being a straight line. If one then adds the constraint that in order to get between these two points, one must pass through another third point (the three points in question not lying on a straight line), then the solution is two straight lines. Clearly both of these solutions satisfy the EL equation separately as they themselves are straight lines. Only at the intermittent point exactly is the EL equation not satisfied.

For a free interface, while the interface can be translated without loss of generality, we must measure interfacial position with regards to a reference position. If we translate the planar (from here on in written as $m_{\pi}(z)$, in which π stands for "planar") equilibrium interfacial profile by a distance ℓ relative to this reference position, the resulting profile will be of the form $m_{\pi}(z - \ell)$. Thus FJ suggested that any profile subject to the constraint $m_{\Xi}(\ell(\underline{y}), \underline{y}) = 0$ is given by $m_{\Xi}(z, \underline{y}) = m_{\pi}(z - \ell(\underline{y}))$. Clearly for any non-planar isomagnetic surface, this will result in a non-zero perpendicular component to the gradient and thus the FJ approximation will not satisfy the Euler Lagrange equation. To see this, note that by FJ's approxi-

mation

$$\nabla^2 m_{\Xi} = \frac{\partial^2 m_{\pi}(z - \ell(\underline{y}))}{\partial z^2} + \frac{\partial^2 m_{\pi}(z - \ell(\underline{y}))}{\partial \ell^2} (\nabla \ell)^2 + \frac{\partial m_{\pi}(z - \ell(\underline{y}))}{\partial \ell} \nabla^2 \ell \quad (2.37)$$

and thus for a sufficiently slowly fluctuating interface, the FJ solution will approximately satisfy the EL equation. As the interface can be translated without changing its shape (which is only true for a free interface), we can make the association $\frac{\partial m_{\pi}}{\partial z} = -\frac{\partial m_{\pi}}{\partial \ell}$. As a result of this, the free energy functional reduces to

$$H[\ell(\underline{y})] = \int d^d \underline{r} \left[\frac{1}{2} \left(\frac{\partial m_{\pi}(z - \ell(\underline{y}))}{\partial z} \right)^2 (1 + (\nabla \ell)^2) + \Delta f(m_{\pi}(z - \ell(\underline{y}))) \right] \quad (2.38)$$

in which the first and third term are simply the energy of the equilibrium profile. Thus the additional energy incurred by the crossing criterion being non-planar (i.e. any fluctuation of the interfacial position which does not only result in a planar translation thereof) is given by

$$\frac{1}{2} \int d\underline{y} (\nabla \ell)^2 \int dz \left(\frac{dm_{\pi}}{dz} \right)^2 \quad (2.39)$$

in which the ℓ -dependence has been dropped as by symmetry, when integrating over all z it will have no effect (and subsequently this means the derivative needs no longer be written as a partial derivative). Comparing this to (2.26) results in the association

$$\sigma = \int \left(\frac{dm_{\pi}}{dz} \right)^2 dz \quad (2.40)$$

i.e. the well-known Triezenberg-Zwanzig formula[88]. Thus FJ succeeded in making a connection between two theories at different length scales, namely the more mesoscopic capillary wave Hamiltonian and the more microscopic full Landau-Ginzburg-Wilson treatment. Their solution however contains a rather crude approximation which does not satisfy the EL equation unless the fluctuations are vanishingly weak. In other words, FJ theory becomes correct for vanishingly small wave vectors (increasingly planar fluctuations).

2.6. Parry-Boulter Theory

Parry and Boulter (PB)[65] improved upon FJ theory by using the same notion of a crossing criterion, but developing a framework to determine the equilibrium profile $m_{\Xi}(z, \underline{y})$ s.t. it satisfies the EL equation (unlike FJ which only does so in the limit of infinitely slowly undulating interfaces). Key to their theory, like FJ is to define an isomagnetic surface. Fluctuations are defined w.r.t to the equilibrium profile, m_{π} (itself not a function of $\underline{y}$). An extra subtlety is that the isomagnetic surface in question does not necessarily need to be the surface $m = 0$ (which for mathematical simplicity I will continue to define as the $z = 0$ plane). It is equally possible to define the interface as the surface $m = m^x$ which is defined to be the plane $z = z^x$. The fluctuation $\delta\ell$ is defined with respect to the plane $z = z^x$, that is to say $m_{\Xi}(\ell(\underline{y}), \underline{y}) = m^x$ where $m_{\pi}(z^x) = m^x$ in which m_{Ξ} is the constrained profile. So far, this is simply a more generalised version of the crossing criterion introduced by FJ. PB however improved on the FJ approximation by allowing $m_{\Xi}(\underline{y}', z)$ to not only depend on $\ell(\underline{y}')$ but rather have a functional (or non-local) dependence on $\ell(\underline{y})$. This is defined by

$$\delta m_{\Xi}(\underline{r}) = m_{\Xi}(\underline{r}) - m_{\pi}(z) = \int d^{d-1} \underline{y}' \Lambda(z, |\underline{y} - \underline{y}'|) \delta\ell(\underline{y}') \quad (2.41)$$

and in Fourier Space

$$\delta \tilde{m}_{\Xi}(\underline{q}) = \tilde{\Lambda}(z; q) \tilde{\delta\ell}(\underline{q}) \quad (2.42)$$

Now, let us expand $\delta\ell(\underline{y}')$:

$$\delta\ell(\underline{y}') = \sum_{N=0}^{\infty} \sum_{k=0}^N \frac{1}{k!} \frac{1}{(N-k)!} \frac{\partial^N \delta\ell}{\partial x^k \partial^{N-k} \underline{y}} \Big|_{\underline{y}} (x' - x)^k (y' - y)^{N-k} \quad (2.43)$$

Substituting this into (2.41) and switching to a plane polar co-ordinate system centred around the point at which we are evaluating δm_{Ξ} gives

$$\delta m_{\Xi}(\underline{r}) = \sum_{N=0}^{\infty} \sum_{k=0}^N \frac{1}{k!} \frac{1}{(N-k)!} \frac{\partial^N \ell}{\partial x^k \partial^{N-k} \underline{y}} \Big|_{\underline{y}} \int_0^{\infty} u \Lambda(z; u) \binom{N}{k} du \int_0^{2\pi} d\theta (u \cos \theta)^k (u \sin \theta)^{N-k} \quad (2.44)$$

It is possible to convince oneself that the integral on the far right is only non-zero if both N and k are even. It evaluates to $\binom{2N}{N} \frac{2\pi}{4^N} \frac{\binom{N}{k}}{\binom{2N}{2k}}$ (see appendix

E) and thus

$$\delta m_{\Xi}(\underline{r}) = \sum_{N=0}^{\infty} \sum_{k=0}^N \frac{1}{(2k)!} \frac{1}{(2(N-k))!} \frac{\partial^{2N} \delta \ell}{\partial^{2k} x \partial^{2(N-k)} y} \Big|_{\underline{y}} \int_0^{\infty} du u^{2N+1} \Lambda(z; u) \binom{2N}{N} \frac{2\pi}{4^N} \frac{\binom{N}{k}}{\binom{2N}{2k}} \quad (2.45)$$

which after rearranging the binomial coefficients and realising that $\nabla^{2N} = (\nabla \cdot \nabla)^N = (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2})^N = \sum_{k=0}^N \binom{N}{k} \frac{\partial^{2N}}{\partial^{2k} x \partial^{2(N-k)} y}$, this becomes

$$\delta m_{\Xi}(\underline{r}) = \sum_{N=0}^{\infty} \frac{2\pi}{4^N} \binom{2N}{N} \frac{1}{(2N)!} (\nabla^{2N} \ell) \Big|_{\underline{y}} \int_0^{\infty} u^{2N+1} \Lambda(z; u) du \quad (2.46)$$

With this in mind, let us now examine the moments of $\tilde{\Lambda}(z; q)$. We start with the definition

$$\tilde{\Lambda}(z; \underline{q}) = \int \Lambda(z; \underline{u}) e^{-i \underline{q} \cdot \underline{u}} d^{d-1} \underline{u} \quad (2.47)$$

Continuing to work in 2-dimensions (as real space is 3 dimensional and thus the transverse plane is 2 dimensional), and using the fact that Λ will only depend on $|u|$ by translation invariance,

$$\tilde{\Lambda}(z; \underline{q}) = \int_0^{2\pi} d\theta \int_0^{\infty} du \left[\Lambda(z; u) e^{-i q u \cos \theta} \right] \quad (2.48)$$

Subsequently, Taylor expand the exponential and note that all integrals which involve odd powers of $\cos \theta$ over all θ will be zero. This yields a general expression for moments of $\tilde{\Lambda}(z; q)$

$$\begin{aligned} \tilde{\Lambda}(z; \underline{q}) &= \tilde{\Lambda}_0 + \tilde{\Lambda}_2 q^2 + \tilde{\Lambda}_4 q^4 + \dots \\ \tilde{\Lambda}_{2N}(z) &= \int_0^{2\pi} (\cos \theta)^{2N} d\theta \int_0^{\infty} (-1)^N \frac{u^{2N+1}}{(2N)!} \Lambda(z; u) du \\ \tilde{\Lambda}_{2N}(z) &= \binom{2N}{N} \frac{(-1)^N 2\pi}{4^N (2N)!} \int_0^{\infty} u^{2N+1} \Lambda(z; u) du \end{aligned} \quad (2.49)$$

and upon re-examination of (2.46), one finds that

$$\delta m_{\Xi}(\underline{r}) = \sum_{N=0}^{\infty} (-1)^N \left(\nabla^{2N} \ell \right) \Big|_{\underline{y}} \tilde{\Lambda}_{2N}(z) \quad (2.50)$$

(2.50) is a generalisation of Eq. 16 in the original PB paper[65] but the derivation is entirely my own rigorisation of this result, particular to $d = 2 + 1$.

2.6.1. Determining $\tilde{\Lambda}(z; q)$

Because (2.41) is a convolution equation, its Fourier Transform is a simple product [73] given by (2.42). Furthermore, by translational invariance, or more precisely the fact that in real space, $\Lambda(z; \underline{y} - \underline{y}')$ can only depend on $(z, |\underline{y} - \underline{y}'|)$, in Fourier space $\tilde{\Lambda}(z; q_x, q_y)$ can in fact only be a function of $\sqrt{q_x^2 + q_y^2}$ which I will in turn write as $\tilde{\Lambda}(z; q)$. Next, PB make use of the fact that $m_\pi(z)$, the equilibrium, planar profile satisfies the EL equation and $m_\Xi(\underline{r})$, the constrained profile likewise satisfies the EL equation everywhere but at the interface. Thus away from the interface

$$\nabla^2 \delta m_\Xi(\underline{r}) = \nabla^2 (m_\Xi(\underline{r}) - m_\pi(z)) = f'(m_\Xi) - f'(m_\pi)$$

and after Taylor expanding $f'(m_\Xi)$ about $f'(m_\pi)$ to 1st order,

$$\nabla^2 \delta m_\Xi(\underline{r}) = f''(m_\pi) \delta m_\Xi(\underline{r}) \quad (2.51)$$

(2.51) is in a sense the EL equation for $\delta m_\Xi(\underline{r})$. Writing $\delta m_\Xi(\underline{r})$ as an inverse Fourier transform of $\delta \tilde{m}_\Xi(z; \underline{q})$, the q-space EL equation reads:

$$\left[\frac{d^2}{dz^2} - q^2 - f''(m_\pi) \right] \delta \tilde{m}(z; q) = 0 \quad (2.52)$$

and when re-writing via (2.42), we have an expression for $\tilde{\Lambda}(z; q)$:

$$\left[\frac{\partial^2}{\partial z^2} - q^2 - f''(m_\pi(z)) \right] \tilde{\Lambda}(z; q) = 0 \quad (2.53)$$

Note that (2.53) is based on $m_\Xi(\underline{r})$ satisfying the EL equation and thus it does not hold at the interface itself. The meaning of this, is that there are two Λ functions, one which holds "below" the interface and one "above". Because (2.53) is a second order PDE, we expect to find two linearly-independent solutions. Without (yet) making recourse to the form of $f(m)$ and thus the exact form of Λ , we expect $\Lambda(z, y - y')$ to decay both for large $|z|$ and large

$|y - y'|$. The large $|z|$ behaviour is due to the fact that far from the interface, the profile must tend to the bulk value. Pre-empting that the two linearly-independent solutions to (2.53) will contain exponentials, potentially multiplied by functions, we will be able to throw one solution away "below" the interface and the other "above" so as to avoid $\Lambda(z, y)$ diverging. It has already been discussed that while m_Ξ does not obey the EL equation, it is continuous at the interface (and everywhere else) in order to keep the (free) energy finite. Thus by (2.42), and the fact that $\ell(y)$ is continuous by definition, $\Lambda(z, y)$ is also continuous at the interface.

PB Crossing Criterion

Due to the continuity requirement on $\Lambda(z, y)$ at the interface, if we can derive a boundary condition for $\tilde{\Lambda}(z; q)$ exactly at the interface, this will be sufficient to determine $\tilde{\Lambda}(z; q)$ from (2.53). The crossing criterion demands of any constrained profile $m_\Xi(\underline{y}, z)$

$$m_\Xi(\underline{y}, \ell(\underline{y}))[\ell(\underline{y})] = m^x \quad (2.54)$$

in which the positional dependence on $(z = \ell(\underline{y}))$ and the functional dependence on $\ell(\underline{y})$ have been explicitly emphasised. If the interfacial shape is perturbed from $\ell(\underline{y})$ by an arbitrary $\delta\ell(\underline{y})$

$$m_\Xi(\underline{y}, \ell(\underline{y}) + \delta\ell(\underline{y}))[\ell(\underline{y}) + \delta\ell(\underline{y})] - m_\Xi(\underline{y}, \ell(\underline{y}))[\ell(\underline{y})] = m^x - m^x = 0$$

Now the chain rule can be used to compute the LHS to first order in $\delta\ell(\underline{y})$

$$\frac{\partial m_\Xi(\underline{y}, \ell(\underline{y}))[\ell(\underline{y})]}{\partial z} \delta\ell(\underline{y}) + \int \frac{\delta m_\Xi(\underline{y}, \ell(\underline{y}))[\ell(\underline{y})]}{\delta\ell(\underline{y}')} \delta\ell(\underline{y}') d^{d-1}\underline{y}' = O(\delta\ell^2) \dots \quad (2.55)$$

in which $\frac{\delta a}{\delta b(x)}$ represents the functional derivative of the functional $a[b(x)]$ w.r.t $b(x)$ [35, 10].

Instead of perturbing about an arbitrary interfacial shape, let us perturb about the equilibrium shape, namely $\ell(\underline{y}) = z^x$. In this case, the first term in (2.55) becomes $\frac{\partial m_\Xi(\underline{y}, z^x)[z^x]}{\partial z} \delta\ell(\underline{y})$. Note that $m_\Xi(\underline{y}, z)[z^x] = m_\pi(z)$ i.e. the m_Ξ which minimises the EL equation subject to a planar constraint, is sim-

ply the equilibrium profile. Hence

$$\frac{dm_\pi(z^x)}{dz}\delta\ell(\underline{y}) = - \int \frac{\delta m_\Xi(\underline{y}, z^x)[z^x]}{\delta\ell(\underline{y}')} \delta\ell(\underline{y}') d^{d-1}\underline{y}' \quad (2.56)$$

Next, consider a functional Taylor of expansion of $\delta m_\Xi(\underline{y}, z^x)[z^x]$ (physically this asks the question, if we are sitting at $z = z^x$ for a planar profile, what happens to the magnetisation at this point for a given interfacial fluctuation about this particular isomagnetic plane) to first order in $\delta\ell$

$$\delta m_\Xi(\underline{y}, z^x)[\ell(\underline{y})] = m_\pi(z^x) + \int \frac{\delta m_\Xi(\underline{y}, z^x)[z^x]}{\delta\ell(\underline{y}')} \delta\ell(\underline{y}') d^{d-1}\underline{y}' + O(\delta\ell)^2 + \dots - m_\pi(z) \quad (2.57)$$

and hence

$$\delta m_\Xi(\underline{y}, z^x)[\ell(\underline{y})] = -m'_\pi(z^x)\delta\ell(\underline{y}) \quad (2.58)$$

which after Fourier Transforming, gives a boundary condition for $\tilde{\Lambda}(z; q)$.

$$\tilde{\Lambda}(z^x; q) = -m'_\pi(z^x) \quad (2.59)$$

(2.59) looks at first glance, a lot like FJ in which, $\delta m_\Xi(z; q) = -m'_\pi(z)\delta\ell(\underline{y})$ and thus

$$\tilde{\Lambda}(z; q) = -m'_\pi(z) \quad (2.60)$$

(2.60) however, holds for all z , not only z^x which in turn means that $\tilde{\Lambda}(z; q)$ is not in fact a function of q , again highlighting the fact that in FJ theory, interfacial fluctuations only affect the profile locally. For the derivation of (2.59) however, the non-local influence of fluctuations on the profile was taken into account when functionally Taylor expanding δm_Ξ to first order in $\delta\ell$.

(2.59) is a direct consequence of defining the crossing criterion as constraining the profile m_Ξ to take a certain (constant) value everywhere on a 2d surface given by $\ell(\underline{y})$ so long as $\ell(\underline{y})$ is a relatively small fluctuation w.r.t the equilibrium profile and thus a first order functional Taylor expansion of the non-local dependence of m_Ξ on $\ell(\underline{y})$ is sufficient. Likewise (2.59) provides the first hint that the functional form of $\tilde{\Lambda}$ will depend on the definition of the interface (see also [86, 85]). Depending on where we define the interface to be, or which cross sectional surface of the equilibrium pro-

file we define fluctuations with respect to, the boundary condition on $\tilde{\Lambda}$ changes. Consider two different but both entirely valid definitions of the interface, say one as the interface being located at z^x and the other z^y . For the case of the interface being located at $z = z^x$, we know that both of the $\tilde{\Lambda}$ functions will satisfy $\tilde{\Lambda}_{\pm}(z^x; q) = -m_{\pi}(z^x)$ in which $\tilde{\Lambda}_{\pm}$ represent the $\tilde{\Lambda}$ valid "above/below the interface" respectively. Consequently, if $z^y > z^x$, it is impossible for $\tilde{\Lambda}_{-}(z^y; q) = -m'_{\pi}(z^y)$ as $\tilde{\Lambda}_{-}$ is not defined for $z > z^x$. Furthermore, it is unlikely that $\tilde{\Lambda}_{+}(z^y; q) = -m'_{\pi}(z^y)$ will be satisfied, and impossible for it to be satisfied for all z^y , unless in fact, (2.60) holds true. To summarise this point, the definition of the interface via a crossing criterion implies that the $\tilde{\Lambda}$ functions, as defined by (2.41), are themselves functions of the interface definition and consequently, any observables which depend on $\tilde{\Lambda}(z; q)$ are themselves functions of the definition of the interface.

If we define $\delta\ell(\underline{y}) = \ell$, i.e. we wish to shift the interface by a constant distance, then (2.50) tells us the profile will be given by

$$\delta m_{\Xi}(\underline{r}) = \delta\ell(\underline{y})\tilde{\Lambda}_0(z) = \delta\ell(\underline{y})\tilde{\Lambda}(z; 0) \quad (2.61)$$

Likewise however we know the solution will be $m_{\pi}(z - \ell)$, i.e. a rigid shift of the interface thus $\tilde{\Lambda}(z; 0) = \tilde{\Lambda}_0(z) = -m'_{\pi}(z)$. Combining this with the crossing criterion (2.59), it becomes clear that

$$\tilde{\Lambda}(z^x; q) = \tilde{\Lambda}_0(z^x) \quad (2.62)$$

and thus all higher moments of $\tilde{\Lambda}$ must vanish at the interface.

2.6.2. Calculating $\sigma(q)$

If we substitute the convolution (2.41) into the LGW Hamiltonian (2.5), and expand about m_{π} in small δm_{Ξ}

$$H[m_{\pi} + \delta m_{\Xi}] = \int d^d \underline{r} \left[\frac{1}{2} (\nabla(m_{\pi}(z) + \delta m_{\Xi}(\underline{r})))^2 + f(m_{\pi}) + f'(m_{\pi})\delta m_{\Xi}(\underline{r}) + f''(m_{\pi})\frac{\delta m_{\Xi}^2}{2!} \right] \quad (2.63)$$

which, after expanding out the square gradient term and noting that $m_{\pi}(z)$ obeys the EL equation $\frac{d^2 m_{\pi}(z)}{dz^2} = f'(m_{\pi})$ at all points including at the inter-

face, becomes

$$H[m_\pi + \delta m_\Xi] - H[m_\pi] = \int d^d \underline{r} \left[\frac{dm_\pi}{dz} \frac{\partial \delta m_\Xi}{\partial z} + f'(m_\pi) \delta m_\Xi + \frac{1}{2} (\nabla \delta m_\Xi)^2 + f''(m_\pi) \frac{\delta m_\Xi^2}{2!} \right] \quad (2.64)$$

As will become clear, because δm_Ξ does not obey the EL equation at the interface, its derivatives will in general be discontinuous at $z = 0$ (for mathematical tractability, the following calculation is carried out with the interface defined to be at $m^x = 0$). For this reason, care must be taken when integrating any term containing δm_Ξ by parts. Consider first, the part of (2.64) given by

$$\int_{-\infty}^{+\infty} \left[\frac{dm_\pi}{dz} \frac{\partial \delta m_\Xi}{\partial z} + \frac{d^2 m_\pi}{dz^2} \delta m_\Xi \right] dz$$

in which a substitution has been made using the EL equation for m_π . Examining the second term, it contains no δ functions and more generally is continuous everywhere. Consequently, integrating by parts, this integral cancels entirely and we are left with

$$\delta H = \frac{1}{2} \int d^d \underline{r} \left[(\nabla \delta m_\Xi(\underline{r}))^2 + \delta m_\Xi(\underline{r})^2 f''(m_\pi) \right] \quad (2.65)$$

in which for brevity, I have defined δH as the excess energy incurred by the magnetisation profile $m_\Xi(\underline{r})$ over of $m_\pi(z)$. In interfacial terms, this is the excess energy incurred by a fluctuation $\delta \ell(\underline{y})$ over that of a planar interface for which $\ell(\underline{y}) = c$. Next, I write δm_Ξ as the Inverse Fourier Transform of $\tilde{\delta m}_\Xi$, itself a product as given in (2.42):

$$\delta m_\Xi(\underline{r}) = \int \frac{d^{d-1} \underline{q}}{(2\pi)^{d-1}} \tilde{\delta m}_\Xi(\underline{q}) e^{i \underline{q} \cdot \underline{y}} \quad (2.66)$$

Consequently

$$\begin{aligned} \delta H = \frac{1}{2} \int \frac{d^{d-1} \underline{p} d^{d-1} \underline{q}}{(2\pi)^{2d-2}} \tilde{\delta \ell}(\underline{p}) \tilde{\delta \ell}(\underline{q}) \int d^{d-1} \underline{y} dz \\ \left[-\underline{p} \cdot \underline{q} \tilde{\Lambda}(z; q) \tilde{\Lambda}(z; p) + \frac{\partial \tilde{\Lambda}(z; q)}{\partial z} \frac{\partial \tilde{\Lambda}(z; p)}{\partial z} + f''(m_\pi) \tilde{\Lambda}(z; q) \tilde{\Lambda}(z; p) \right] e^{i \underline{y} \cdot (\underline{p} + \underline{q})} \end{aligned} \quad (2.67)$$

which after performing the integral in the transverse plane and then integrating over the resulting δ function, and noting that because $\Lambda(z; \underline{y})$ is only a function of $|\underline{y}|$ by translational invariance and thus $\tilde{\Lambda}(z; q) = \tilde{\Lambda}(z; -q)$, leaves the expression

$$\delta H = \frac{1}{2} \int \frac{d^{d-1}q}{(2\pi)^{d-1}} |\tilde{\ell}(\underline{q})|^2 \int_{-\infty}^{\infty} dz \left[\left(\frac{\partial \tilde{\Lambda}(z; q)}{\partial z} \right)^2 + (q^2 + f''(m_\pi)(z)) (\tilde{\Lambda}(z; q))^2 \right] \quad (2.68)$$

which, by (2.35), can be seen to give us a relation for the wave-vector dependent surface tension of

$$\sigma(q)q^2 = \int_{-\infty}^{\infty} dz \left[\left(\frac{\partial \tilde{\Lambda}(z; q)}{\partial z} \right)^2 + (q^2 + f''(m_\pi)(z)) (\tilde{\Lambda}(z; q))^2 \right] \quad (2.69)$$

While $\tilde{\Lambda}(z; q)$ is continuous at the interface, $\frac{\partial \tilde{\Lambda}}{\partial z}$ is not and consequently is ill-defined at the interface. Because $\tilde{\Lambda}(z; q)$ is continuous however, we know that $\frac{\partial \tilde{\Lambda}}{\partial z}$ remains finite, that is to say, it will not contain any δ functions. Thus

$$\int_{-\infty}^{\infty} dz \left(\frac{\partial \tilde{\Lambda}(z; q)}{\partial z} \right)^2 = \lim_{\epsilon \rightarrow 0} \left[\int_{-\infty}^{-\epsilon} dz \left(\frac{\partial \tilde{\Lambda}(z; q)}{\partial z} \right)^2 + \int_{\epsilon}^{\infty} dz \left(\frac{\partial \tilde{\Lambda}(z; q)}{\partial z} \right)^2 \right] \quad (2.70)$$

which can be integrated by parts to obtain

$$\lim_{\epsilon \rightarrow 0} \left[\tilde{\Lambda}(0; q) \left[\frac{\partial \tilde{\Lambda}(-\epsilon; q)}{\partial z} - \frac{\partial \tilde{\Lambda}(\epsilon; q)}{\partial z} \right] - \int_{-\infty}^{-\epsilon} dz \frac{\partial^2 \tilde{\Lambda}(z; q)}{\partial z^2} \tilde{\Lambda}(z; q) - \int_{\epsilon}^{\infty} dz \frac{\partial^2 \tilde{\Lambda}(z; q)}{\partial z^2} \tilde{\Lambda}(z; q) \right] \quad (2.71)$$

Thus the full expression for the wave-vector dependent surface tension now becomes

$$\begin{aligned} \sigma(q)q^2 = & \lim_{\epsilon \rightarrow 0} \left[\tilde{\Lambda}(0; q) \left[\frac{\partial \tilde{\Lambda}(-\epsilon; q)}{\partial z} - \frac{\partial \tilde{\Lambda}(\epsilon; q)}{\partial z} \right] + \int_{-\epsilon}^{+\epsilon} dz (q^2 + f''(m)) (\tilde{\Lambda}(z; q))^2 \right] \\ & + \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{-\epsilon} dz \left[-\frac{\partial^2 \tilde{\Lambda}(z; q)}{\partial z^2} + (q^2 + f''(m_\pi)) \tilde{\Lambda}(z; q) \right] \tilde{\Lambda}(z; q) \\ & + \lim_{\epsilon \rightarrow 0} \int_{\epsilon}^{\infty} dz \left[-\frac{\partial^2 \tilde{\Lambda}(z; q)}{\partial z^2} + (q^2 + f''(m_\pi)) \tilde{\Lambda}(z; q) \right] \tilde{\Lambda}(z; q) \end{aligned} \quad (2.72)$$

By (2.53) however, the second and third line are simply equal to zero as the integrand is equal to zero everywhere apart from exactly at the interface (i.e. $\epsilon = 0$). Thus the full (again, because $\tilde{\Lambda}(z; q)$ is continuous at the interface and also making use of (2.59)) expression for the wave-vector dependent surface tension becomes:

$$\sigma(q)q^2 = m'_\pi(0)\Delta\frac{\partial\tilde{\Lambda}(z;q)}{\partial z} + \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} f''(m_\pi(z)) (\tilde{\Lambda}(z;q))^2 dz \quad (2.73)$$

in which $\Delta\frac{\partial\tilde{\Lambda}(z;q)}{\partial z}$ represents the step, or difference in the derivatives of $\tilde{\Lambda}(z;q)$ at $\pm\epsilon$. Note that unless the potential itself has a cusp (as it does in DP), then the expression reduces to the first term only, an entirely local expression, not requiring the evaluation of an integral to calculate. Even if the potential has a cusp, the second term will be a very simple integral to calculate as it will contain a δ function.

Next I will derive an alternative expression for (2.73) which is in fact the result we published (see Eq.38 in [64]). Following the PB approach, examine (2.53) in terms of moments, that is to say

$$\left[\frac{d^2}{dz^2} - f''(m_\pi) \right] \tilde{\Lambda}_2(z) = \tilde{\Lambda}_{2N-2}(z) \quad (2.74)$$

in which $N \neq 0$ because $\tilde{\Lambda}_{-2}$ does not exist, as $\tilde{\Lambda}$ is analytic (other than at the interface). PB made the Ansatz $\tilde{\Lambda}_2(z) = m'_\pi(z)f(z)$ but I will make the more general Ansatz $\tilde{\Lambda}_{2N}(z) = m'_\pi(z)f_{2N}(z)$. Inserting this into (2.74), and noting that $m'''_\pi(z) - f''(m_\pi)m'_\pi(z) = 0$, one finds that

$$2m''_\pi(z)f'_{2N}(z) + m'_\pi(z)f''_{2N}(z) = \tilde{\Lambda}_{2N-2}(z) \quad (2.75)$$

which, after multiplying both sides by $m'(z)$ gives the relation

$$\frac{d}{dz} ((m'_\pi(z))^2 f'_{2N}(z)) = m'_\pi(z) \tilde{\Lambda}_{2N-2} \quad (2.76)$$

Integrating both sides and noting that $m'_\pi(z) \rightarrow 0$ as $z \rightarrow \pm\infty$ yields

$$(m'_\pi(z))^2 f'_{2N}(z) = \int_{\pm\infty}^z m'_\pi(z') \tilde{\Lambda}_{2N-2}(z') dz' \quad (2.77)$$

Finally, because $\tilde{\Lambda}(0; q) = -m'_\pi(0)$ (i.e. the crossing criterion (2.59)), and

thus $\tilde{\Lambda}_{2N}(0) = 0$ for $N \neq 0$, and because $m'_\pi(0) \neq 0$, we know that $f_{2N}(0) = 0$ and thus we can integrate (2.77) from $0 \rightarrow z$ to find $f_{2N}(z)$ and subsequently $\tilde{\Lambda}_{2N}(z)$:

$$\tilde{\Lambda}_{2N}(z) = m'_\pi(z) \int_0^z (m'_\pi(z'))^{-2} dz' \int_{\pm\infty}^{z'} m'_\pi(z'') \tilde{\Lambda}_{2N-2}(z'') dz'' \quad (2.78)$$

Using the product rule, we now have an expression for the derivative of any given moment of $\tilde{\Lambda}(z; q)$:

$$\begin{aligned} \frac{d\tilde{\Lambda}_{2N}}{dz} &= m''_\pi(z) \int_0^z (m'_\pi(z'))^{-2} dz' \int_{\pm\infty}^{z'} m'_\pi(z'') \tilde{\Lambda}_{2N-2}(z'') dz'' \\ &\quad + \frac{1}{m'_\pi(z)} \int_{\pm\infty}^z m'_\pi(z') \tilde{\Lambda}_{2N-2}(z') dz' \end{aligned} \quad (2.79)$$

In order to evaluate (2.73), it is necessary to calculate $\lim_{\epsilon \rightarrow 0} \left[\frac{\partial \tilde{\Lambda}(z; q)}{\partial z} \right]_{-\epsilon}^{+\epsilon}$ or, by Ising symmetry, $2 \cdot \lim_{\epsilon \rightarrow 0} \frac{\partial \tilde{\Lambda}(\epsilon; q)}{\partial z}$ given by

$$2 \frac{d\tilde{\Lambda}_0(\epsilon)}{dz} + 2 \sum_{N=1}^{\infty} \frac{d\tilde{\Lambda}_{2N}(\epsilon)}{dz} q^{2N} \quad (2.80)$$

in which

$$\frac{d\tilde{\Lambda}_{2N}(\pm\epsilon)}{dz} = \frac{1}{m'_\pi(0)} \int_{\pm\infty}^{\pm\epsilon} m'_\pi(z') \tilde{\Lambda}_{2N-2}(z') dz' \quad (2.81)$$

because the first term in (2.79) will go to zero as the first integral's interval becomes squeezed to zero. Consequently, (2.73) can be rewritten as

$$\sigma(q)q^2 = 2m'_\pi(0) \frac{d\tilde{\Lambda}_0(\epsilon)}{dz} \pm 2 \sum_{N=1}^{\infty} q^{2N} \int_{\pm\infty}^{\pm\epsilon} m'_\pi(z) \tilde{\Lambda}_{2N-2}(z) dz + \int_{-\epsilon}^{\epsilon} f''(m_\pi) (\tilde{\Lambda}(z; q))^2 dz \quad (2.82)$$

in which the middle term can be recognised to equal

$$-q^2 \int_{-\infty}^{\infty} m'_\pi(z) \tilde{\Lambda}(z; q) \quad (2.83)$$

Finally, I will shown that the first and third terms in (2.82) cancel. In m^4 theory, by symmetry, $m''(0) = 0$ and thus $\frac{d\tilde{\Lambda}_0(0)}{dz} = 0$, the first term in (2.82) is zero and likewise the third term is, because there is no cusp in $f'(m)$. In DP theory however, $m''_\pi(z)$ is discontinuous at $z = 0$ because $f'(m)$ is discontinuous at $m = 0$. Nonetheless, we can take the limit $\epsilon \rightarrow 0$

and in this limit, $m''(\epsilon) = f'(0^+)$. Thus the first term in (2.82) becomes $-2m'_\pi(0)f'(0^+)$. The third term quite simply evaluates to $c(m'_\pi(0))^2$ in which c is the coefficient of the δ function in $f''(m)$. In m co-ordinates, this term is simply given by the jump in derivative $f'(0^+) - f'(0^-) = 2f'(0^+)$ (again by Ising symmetry) and making use of (2.17), $c = \frac{2f'(0^+)}{m'_\pi(0)}$. Thus the third term in (2.82) is given by $2f'(0^+)m'_\pi(0)$ and consequently the first and third term cancel in (2.82), even if there is a cusp in the potential and thus it has been shown that for the crossing criterion being defined for $m^x = 0$, (2.73) is equivalent to

$$\sigma(q) = \int_{-\infty}^{\infty} \tilde{\Lambda}_0(z) \tilde{\Lambda}(z; q) dz \quad (2.84)$$

in square gradient theory. Note that this has made heavy use of Ising symmetry to replace expressions of the form $\lim_{\epsilon \rightarrow 0} \left[\partial \frac{\tilde{\Lambda}(z; q)}{\partial z} \right]_{-\epsilon}^{\epsilon}$ with $2 \cdot \lim_{\epsilon \rightarrow 0} \frac{\partial \tilde{\Lambda}(\epsilon; q)}{\partial z}$.

2.6.3. Parry Boulter Results for the Double Parabola Approximation

Let us first examine the most simple case, namely defining fluctuations about the plane $z = 0$ with m_π defined as the planar solution for which $m_\pi(0) = 0$. Examining (2.8), it can be seen that $m'_\pi(0) = m_0\kappa$ or $\tilde{\Lambda}(0, q) = -m_0\kappa$. As we are solving for $\tilde{\Lambda}(z; q)$ everywhere but at the interface exactly, within DP we can write $f''(m_\pi) = \kappa^2$ as the δ function in the second derivative of f w.r.t m only plays a part at $m = 0$ which is exactly at the interface. We will not be able to make use of this simplification once the interface is not defined as the point at which $m = 0$. (2.53) becomes

$$\left[\frac{\partial^2}{\partial z^2} - \kappa_q^2 + 2\kappa\delta(z) \right] \tilde{\Lambda}(z; q) = 0 \quad (2.85)$$

with κ_q defined as before. The general solution to (2.85) is rather simple

$$Ae^{\kappa_q z} + Be^{-\kappa_q z} \quad (2.86)$$

and thus as postulated, "below" the interface, $\tilde{\Lambda}(z; q) = Ae^{\kappa_q z}$ and "above" $\tilde{\Lambda}(z; q) = Be^{-\kappa_q z}$ to satisfy the boundary condition of non-divergence as

$z \rightarrow \pm\infty$. In this case, evaluating the boundary condition is particularly simple resulting in

$$\tilde{\Lambda}(z; q) = -m_0 \kappa e^{-\kappa_q |z|} \quad (2.87)$$

Next let us examine the more complicated case of $m^x \neq 0$. Without loss of generality, let us assume $m^x > 0$. (2.85) must now be satisfied at $z = 0$ where there is a δ function. As (2.85) is a second order PDE, the first derivative of $\tilde{\Lambda}$ must be discontinuous as $z = 0$. $\tilde{\Lambda}$ itself however must be continuous in order that (2.85) does not include a derivative of a δ function and likewise because (2.42) now holds at $z = 0$ and m_{Ξ} must be continuous. Consequently, $\tilde{\Lambda}$ has three regions of solution namely $]-\infty, 0[$, $]0, z^x[$ and $]z^x, \infty[$. We know that the non-divergence boundary condition will enforce that

$$\begin{aligned} \tilde{\Lambda}_B(z; q) &= A e^{\kappa_q z} \\ \tilde{\Lambda}_C(z; q) &= B e^{-\kappa_q z} + C e^{\kappa_q z} \\ \tilde{\Lambda}_A(z; q) &= D e^{-\kappa_q z} \end{aligned} \quad (2.88)$$

in which the subscripts (B,C,A) stand for below, centre and above, referring to the three aforementioned regions of solution. Continuity of $\tilde{\Lambda}$ at both $z = 0$ and $z = z^x$ provide two boundary conditions and the crossing criterion (2.59) a further one. The fourth boundary condition is a so-called cusp condition. Integrating (2.85) from $z = -\epsilon \rightarrow z = +\epsilon$ and taking the limit $\epsilon \rightarrow 0$, one finds

$$\left[\frac{\partial \tilde{\Lambda}(z; q)}{\partial z} \right]_{z=-\epsilon}^{z=\epsilon} + 2\kappa \tilde{\Lambda}(0; q) = 0 \quad (2.89)$$

which provides the necessary fourth boundary condition. Solving the four aforementioned conditions simultaneously yields the result

$$\begin{aligned} A &= \frac{m_0 \kappa \kappa_q e^{-\kappa z^x}}{(\kappa - \kappa_q) e^{\kappa_q z^x} - \kappa e^{-\kappa_q z^x}} \\ B &= \frac{m_0 \kappa^2 e^{-\kappa z^x}}{(\kappa - \kappa_q) e^{\kappa_q z^x} - \kappa e^{-\kappa_q z^x}} \\ C &= \frac{m_0 \kappa (\kappa_q - \kappa) e^{-\kappa z^x}}{(\kappa - \kappa_q) e^{\kappa_q z^x} - \kappa e^{-\kappa_q z^x}} \\ D &= -m_0 \kappa e^{(\kappa_q - \kappa) z^x} \end{aligned} \quad (2.90)$$

2.7. Connecting Interfacial Hamiltonian Theory to Microscopic DFT via PB Theory

PB theory allows us to calculate m_{Ξ} subject to a constraint, i.e. the shape of the interface. In general the partition sum is given by

$$Z = \int (\mathcal{D}_{\text{configs}}) e^{-H[m]} \quad (2.91)$$

The process of performing an integral over all configurations could be broken into a two-stage process namely

$$Z = \int (\mathcal{D}\ell) \int (\mathcal{D}m_{\Xi}) e^{-H[m_{\Xi}]} \quad (2.92)$$

i.e. considering every possible interfacial configuration and then integrating over every possible profile which respects this configuration. The m_{Ξ} profile we have calculated is the profile which will contribute most to the integral for every configuration $\ell(\underline{y})$. We know however that for any finite temperature, thermal fluctuations will allow the system to fluctuate to microstates which do not minimise the energy. From our microscopic theory, we know how to describe such thermal fluctuations, namely via the correlation function $\mathcal{G}(\underline{r}_1, \underline{r}_2)$ which tells us the strength of such fluctuations and the length scale over which they decay. The equivalent quantity in PB theory, namely

$$G(\underline{r}_1, \underline{r}_2; q) = \langle \delta m_{\Xi}(\underline{r}_1) \delta m_{\Xi}(\underline{r}_2) \rangle = \int d^{d-1}\underline{y}' d^{d-1}\underline{y}'' \Lambda(z_1; |\underline{y}_1 - \underline{y}'|) \Lambda(z_2; |\underline{y}_2 - \underline{y}''|) \langle \delta \ell(\underline{y}') \delta \ell(\underline{y}'') \rangle \quad (2.93)$$

describes fluctuations in the profile which do not minimise the energy outright, but do so w.r.t to a given constraint $\ell(\underline{y})$. It will however not capture fluctuations which do not minimise their energy w.r.t to such a constraint. In a sense, $G(z_1, z_2; q)$ correctly captures fluctuations in the order parameter in as far as the partition sum is well approximated by

$$\int (\mathcal{D}\ell) e^{-H[m_{\Xi}]} \quad (2.94)$$

In the bulk however, far away from the interface, all fluctuations must be of the type which do not minimise the energy w.r.t to a given constraint as fluctuations in the interfacial position do not affect the magnetisation value

far from the interface. Thus we would expect $G(\underline{r}_1, \underline{r}_2)$ as defined in (2.93) not to capture these effects and for it to decay to zero far from the interface. As we now know that at DP level, our microscopic theory predicts the split of the correlation function into a bulk and an interfacial part, we might hope that (2.93) would produce the interfacial part of $\mathcal{G}(z_1, z_2; q)$ only. The [59, 57, 26] assumption made in the literature is that this is the case, and that fluctuations in the profile are related to capillary wave fluctuations via

$$\langle \delta m_{\Xi}(z_1; q) \delta m_{\Xi}(z_2; q) \rangle = m'_{\pi}(z_1) m'_{\pi}(z_2) \langle |\delta \ell(q)|^2 \rangle \quad (2.95)$$

This is however only the case if $q = 0$, i.e. FJ theory. As soon as one allows for a non-local relationship between m_{Ξ} and $\delta \ell$, it is necessary to make recourse to the convolution given by (2.41). By translational invariance in the transverse plane, (2.93) can be Fourier Transformed to obtain

$$G(z_1, z_2; q) = \langle \delta \tilde{m}(z_1, \underline{q}) \delta \tilde{m}(z_2, \underline{q}) \rangle = \tilde{\Lambda}(z_1; q) \tilde{\Lambda}(z_2; q) \langle |\delta \tilde{\ell}(q)|^2 \rangle \quad (2.96)$$

Both (2.95) and (2.96) inherently describe fluctuations in m which are related to capillary waves, as both equal 0 if the interface is held flat and $\langle |\delta \tilde{\ell}(q)|^2 \rangle = 0$.

Using the definition of $\sigma(q)$ (2.35),

$$G(z_1, z_2; q) = \frac{\tilde{\Lambda}(z_1; q) \tilde{\Lambda}(z_2; q)}{q^2 \sigma(q)} \quad (2.97)$$

which within DP, with m^x set to 0, evaluates to

$$G(z_1, z_2; q) = \frac{e^{-\kappa_q(|z_1| + |z_2|)}}{2(\kappa_q - \kappa)} \quad (2.98)$$

with

$$\sigma(q) = \frac{2m_0^2 \kappa^2}{\kappa + \kappa_q} \quad (2.99)$$

By inspection, we can see that (2.98) is not the same as (2.21). As discussed, this is not to be expected as the reconstructed correlation function does not know about fluctuations in the order parameter that are not due to a fluctuating interface, i.e. the bulk term. It might however seem reasonable to expect (2.98) to reproduce the interfacial term in (2.21) but as we can see,

this is not the case either, the dependence on (z_1, z_2) is the same but the pre-factor is not. A further peculiar result is that for $z_1 = 0$, (2.98) does in fact reconstruct (2.21) in its entirety, an undesirable consequence. Furthermore and even more strangely, if $z_1 z_2 < 0$, then $|z_1 - z_2| = |z_1| + |z_2|$ and thus if calculating the density-density correlation between two points on different sides of the interface, the reconstructed correlation function also correctly reconstructs the entire one. Thus the reconstructed function only differs from the exact result when z_1 and z_2 are both non-zero and are on the same side of the interface. This is not what we desire from the reconstructed correlation function and we believe this to be somewhat of a coincidence.

A further consequence of the reconstructed correlation function having the same dependence on (z_1, z_2) and thus being proportional to the interfacial part of the microscopic correlation function is that the reconstructed position-dependent and total structure factors will likewise be proportional to the interfacial parts of the equivalent quantities as determined from the microscopic theory with the constant of proportionality the same in each case. This begs the question of whether a small amendment to PB theory could reproduce this constant of proportionality and if so, what its interpretation would be.

A further point worth making, is that $\sigma(q)$, as given by (2.99) can be Taylor expanded to second order in order to determine the bending rigidity. One finds that it is given by $-\frac{\sigma}{4\kappa^2}$ and consequently, the rigidity and surface tension have opposite signs. In the context of Romero-Rochin et.al's reasoning behind introducing the rigidity in the first place, this does not result in poles in the complex plane when calculating the interfacial height-height correlation function, but rather less mathematically convenient poles on the real axis.

2.8. The Amended Crossing Criterion

While (2.59) was rigorously derived from the FJ isomagnetic surface crossing criterion which seems physically reasonable, let us by hand change (2.59) so that it reads

$$\tilde{\Lambda}(z^x; q) = -b(q)m'(z^x) \quad (2.100)$$

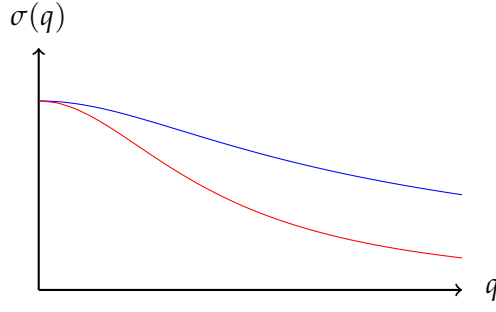


Figure 2.5.: $\sigma_{cc}(q)$ (blue) and $\sigma(q)$ according to a new crossing criterion (red) plotted as a function of q . Qualitatively they look similar but $\sigma(q) \leq \sigma_{cc}(q)$.

As I will discuss in Section 2.8.2 the following can only be done when considering interfacial fluctuations about the plane $z^x = 0$ when the cusp due to the interface and the cusp in the DP potential occur at the same point in space. Changing the crossing criterion to (2.100) has the effect

$$\begin{aligned}\tilde{\Lambda}(z; q) &= b(q)\tilde{\Lambda}_{cc}(z; q) \\ \sigma(q) &= b(q)\sigma_{cc}(q) \\ G(z_1, z_2; q) &= b(q)G_{cc}(z_1, z_2; q)\end{aligned}\tag{2.101}$$

in which quantities with the subscript "cc" refer to those previously derived according to (2.59) and those without are those acquired using (2.100). Thus the new reconstructed correlation function is multiplied by a constant of proportionality $b(q)$, the same one which was added to the crossing criterion and this can be tuned so that the reconstructed correlation function equals the interfacial one, and consequently the reconstructed structure factors likewise match those derived from the microscopic theory. $\sigma(q)$ using both the FJ and new crossing criterion are plotted in Figure 2.5.

2.8.1. Interpreting $b(q)$

Let us examine the effect of introducing a more subtle definition of the interface than the FJ crossing criterion. We shall continue to impose $\langle m_{\Xi}(\ell(\underline{y}), \underline{y}) \rangle = 0$. The FJ crossing criterion however defines the position of the interface up to an arbitrary precision when perhaps it is only sensible to do so with pre-

cision up to a bulk correlation length. The FJ crossing criterion would also enforce that

$$\langle \delta m_{\Xi}(\ell(\underline{y}_1), \underline{y}_1) \delta m_{\Xi}(\ell(\underline{y}_2), \underline{y}_2) \rangle = 0$$

If we relax this restriction and define the interface as a surface on which the magnetisation is on average zero, but allow for fluctuations of the order parameter on this surface, what are the consequences? To this end, let us define the floating correlation function which measures correlations between two points on the interface separated by a spatial transverse distance $|\underline{y} - \underline{y}'|$.

$$G_{\Xi}(|\underline{y} - \underline{y}'|) = \langle \delta m_{\Xi}(\ell(\underline{y}), \underline{y}) \delta m_{\Xi}(\ell(\underline{y}'), \underline{y}') \rangle \quad (2.102)$$

Just as was done when deriving the crossing criterion (2.59) from the FJ condition, $m_{\Xi}(\ell(\underline{y}), \underline{y})$ can be expanded about $m_{\pi}(0)$ to obtain

$$\delta m_{\Xi}(\ell(\underline{y}), \underline{y}) = m'_{\pi}(0) \delta \ell(\underline{y}) + \int \Lambda(0; |\underline{y} - \underline{y}'|) \delta \ell(\underline{y}') d^{d-1} \underline{y}'$$

or in Fourier Space

$$\tilde{\delta m}_{\Xi}(\underline{q}) = m'_{\pi}(0) \tilde{\delta \ell}(\underline{q}) + \tilde{\Lambda}(0; q) \tilde{\delta \ell}(\underline{q}) \quad (2.103)$$

(note the difference between $\tilde{\delta m}_{\Xi}(z; \underline{q})$ and $\tilde{\delta m}_{\Xi}(\underline{q})$) and thus by translational invariance

$$\tilde{G}_{\Xi}(\underline{q}) = (m'_{\pi}(0) + \tilde{\Lambda}(0; q))^2 \langle |\tilde{\delta \ell}(\underline{q})|^2 \rangle \quad (2.104)$$

This is a rather profound result as it shows that not only does the crossing criterion (2.59) immediately imply that $\tilde{G}_{\Xi}(\underline{q}) = 0$, but also that other choices of $b(q)$ will make this no longer be the case. Thus $b(q)$ is related to the floating correlation function. Rewriting (2.104) in terms of $b(q)$ yields

$$\tilde{G}_{\Xi}(\underline{q}) = \frac{m_{\pi}^{\prime 2}(0) (1 - b(q))^2}{b(q) \sigma_{cc}(q) q^2} \quad (2.105)$$

This can be rewritten by noting that $\frac{m_{\pi}^{\prime 2}(0)}{\sigma_{cc}(q) q^2}$ is simply $\mathcal{G}(0, 0; q)$ and using the $b(q)$ which results in the reconstructed correlation function correctly

reproducing the interfacial part of the DFT correlation function

$$\tilde{G}_{\Xi}(q) = \frac{G^b(0; q)G^b(0; q)}{\mathcal{G}(0, 0; q) - G^b(0; q)} \quad (2.106)$$

which in itself is not hugely instructive. Rearranging however, one finds

$$\mathcal{G}(0, 0; q) = G^b(0; q) + \frac{G^b(0; q)G^b(0; q)}{\tilde{G}_{\Xi}(q)} \quad (2.107)$$

By comparison with (2.21), it becomes clear that

$$\tilde{G}_{\Xi} = G^b(0; 0) - G^b(0, 0; q) \quad (2.108)$$

and thus by inverse Fourier Transform

$$G_{\Xi}(\underline{y}) = \frac{(2\pi)^{d-1}}{2\kappa} \delta(\underline{y}) - G^b(|\underline{y}|) \quad (2.109)$$

in which the G^b in question on the RHS is in fact the full (i.e. not partially Fourier Transformed) bulk correlation function. The significance of this result has not been fully comprehended. Clearly (2.109) appears to be saying that order parameter values on the floating interface are anti-correlated (with this decaying over transverse separation). Anti-ferromagnetic lattices [31] exhibit anti correlation and one possible interpretation of (2.109) is that an interface for which $\langle m_{\Xi}(\ell(\underline{y}), \underline{y}) \rangle = 0$ will at a microscopic level look rather like an anti-ferromagnetic ground state, i.e. the surface attempts to maximise its entropy.

2.8.2. Reconstructing Correlations for non-zero m^x

The expression for the wave-vector dependent surface tension turns out to be more simple for $m^x \neq 0$. There are now two points at which $\frac{\tilde{\Lambda}(z; q)}{\partial z}$ is discontinuous, namely at $z = 0$ and at the interface, $z = z^x$. Carrying out the same analysis as for $z^x = 0$, one finds that

$$\sigma(q)q^2 = \lim_{\epsilon \rightarrow 0} \left[\tilde{\Lambda}(0; q) \left[\frac{\partial \tilde{\Lambda}(z; q)}{\partial z} \right]_{\epsilon}^{-\epsilon} + \tilde{\Lambda}(z^x; q) \left[\frac{\partial \tilde{\Lambda}(z; q)}{\partial z} \right]_{z^x - \epsilon}^{z^x + \epsilon} + \int_{-\epsilon}^{+\epsilon} f''(m_{\pi}(z)) (\tilde{\Lambda}(z; q))^2 \right] \quad (2.110)$$

Now however, because the EL equation must be satisfied at $z = 0$ as this is no longer the interface, one can integrate the OZ over this cusp and generate the cusp condition (2.89) which implies that the first and third terms cancel leaving

$$\sigma(q)q^2 = m'(z^x)\Delta_{z^x}\left(\frac{\partial\tilde{\Lambda}(z;q)}{\partial z}\right) \quad (2.111)$$

in which the subscript on the Δ denotes that it is the discontinuity in the derivative at the point $z = z^x$ which must be taken. The cusp condition does not apply if $z^x = 0$ because the EL equation is not satisfied at the interface and thus the two terms in (2.73) do not cancel. This applies equally to DP and m^4 theory and the result in DP is

$$\sigma(q)q^2 = \frac{2m_0^2\kappa^2\kappa_q(\kappa - \kappa_q)e^{\kappa_q z^x}e^{-2\kappa z^x}}{(\kappa - \kappa_q)e^{\kappa_q z^x} - \kappa e^{-\kappa_q z^x}} \quad (2.112)$$

which recovers (2.99) in the limit $z^x \rightarrow 0$. Thus we recover the PB result that the interface's resistance to bending effects depends on the definition of the interface.

The reconstructed correlation function splits up into six different regimes, namely $(z_1, z_2 < 0)$, $(z_1 < 0 < z_2 < z^x)$, $(z_1 < 0 < z^x < z_2)$, $(0 < z_1, z_2 < z^x)$ and $(z^x < z_1, z_2)$ according to the three different regions of solution of $\tilde{\Lambda}(z;q)$ as given in (2.88). We found that for $z^x = 0$, the reconstructed correlation function was a function of distance to the interface only, that is to say of $|z_1|$ and $|z_2|$. This is now only true if neither z_1 nor z_2 lies on the interval $]0, z^x[$. We then found that for $z_1 z_2 < 0$, the reconstructed correlation function matched the analytic one exactly. Clearly if $z_1 < 0, 0 < z_2 < z^x$, the reconstructed correlation function will also contain an exponential of the form $e^{-\kappa_q|z_2| + \kappa_q|z_2|}$ and thus it has a different functional form to that of the interfacial part of $\mathcal{G}$. If we however ignore this "central" region and examine $z_1 < 0 < z^x < z_2$, we find, rather remarkably that all z^x dependence cancels and the reconstructed correlation function exactly matches the full correlation function, including the (unwanted) bulk contribution. The same is true for $G(0, z; q)$ for $z > z^x$ but not for $z < z^x$. What this means is that there is no single $b(q)$ which correctly reconstructs $\mathcal{G}$. For the special case of neither of z_1, z_2 in the central region, it is the same $b(q)$ which correctly reconstructs $\mathcal{G}(z_1, z_2)$ and otherwise, every other region will require a different $b(q; z^x)$.

To determine the bending rigidity for non-zero m^x , (2.112) can be expanded to second order and the result is

$$\gamma(z^x) = \sigma \left(\frac{z^x}{\kappa} - \frac{1}{4\kappa^2} (2e^{2\kappa|z^x|} - 1) \right) \quad (2.113)$$

in disagreement with PB Eq. (35). This discrepancy appears to originate from PB not correctly accounting for both cusps in the PDE which describes $\tilde{\Lambda}(z; q)$.

2.8.3. Analysis of DP Results

The DP findings can be broken into four statements of good and bad news as we did in [64]

1) **Good news:** Within the DP approximation, the correlation function splits up into a bulk and an excess contribution, meaning that the position dependent and total structure factor likewise do so. This does not allow us to identify $\sigma(q)$ but it raises the possibility that this might be possible to do using an interfacial Hamiltonian and reconstructing the structure factor.

2) **Bad news:** Using a crossing criterion definition of the interface, the reconstructed correlation function and structure factor have the same z dependence as the equivalent quantities calculated using our toy DFT model, but they differ by a (wave-vector dependent) constant of proportionality. Thus while $\sigma(q)$ can be defined in an extended CW Hamiltonian, we cannot make any claims about its structure.

3) **Good news:** Using a rather subtle definition of the interface which goes beyond the FJ crossing criterion and rejects the notion that the interface can be defined to arbitrary precision, it is possible to reconstruct the correlation function and thus the structure factors using an interfacial Hamiltonian and consequently, $\sigma(q)$ can be calculated in terms of microscopic parameters.

4) **Very bad news:** The (experimentally measured) total structure factor is given by

$$S(q) = 2LS^B(q) + \left(\frac{2m_0b(q)\kappa}{\kappa_q} \right)^2 \frac{1}{\sigma(q)q^2} = 2LS^b(q) + \frac{4m_0^2}{\sigma(q)q^2} \left(\frac{S^b(q)}{S^b(0)} \right)^2 \quad (2.114)$$

meaning that the q dependence is not restricted to $\sigma(q)q^2$. This is because

the correlation function's q dependence arises not only from the wave-vector dependent surface tension but likewise the q dependence of the $\tilde{\Lambda}$ functions. Unless that q dependence of the pre-factor of $\frac{1}{\sigma(q)q^2}$ is known a priori, the wave-vector dependent surface tension cannot be experimentally measured. Note that in the FJ crossing criterion for which $b(q) = 1$, (2.114) still contains q dependence outside of the $\frac{1}{\sigma(q)q^2}$ term. It is of course possible to choose [26] $\sigma(q)$ such that

$$S(q) = 2LS^B(q) + \frac{4m_0^2}{\sigma_{eff}(q)q^2} \quad (2.115)$$

but this $\sigma_{eff}(q)$ does not contain the desired information, namely the physical information supposedly contained within the wave-vector dependent surface tension as defined by (2.35). (2.115) is of course asymptotically correct in the long wavelength limit[91, 90], i.e. in the local, FJ limit.

Furthermore, if interfacial fluctuations are not defined w.r.t the $z = 0$ plane, it is impossible to define $\sigma(q, z^x)$ such that the reconstructed correlation function matches $\mathcal{G}$ due to the $\tilde{\Lambda}(z; q)$ functions changing definition twice. This is of course an artifact of the DP model having a cusp at $m = 0$ regardless of how the interface is defined. It is however that cusp which allows $\mathcal{G}$ to separate so cleanly into a bulk and interfacial contribution, as will become clear when studying the m^4 double well potential or Landau theory.

2.9. Full Landau Theory

If it is possible to determine a $b(q)$ for the full Landau theory which reconstructs the interfacial correlation function and structure factors, and likewise the result gives identical q dependence of the total interfacial structure factor to that obtained in DP according to (2.114), this could go some way to negating the "very bad news" in our analysis of the DP results as there might then be some actual physics in this pre-factor.

2.9.1. Bulk Correlation Function

The bulk correlation calculation follows a very similar route to that of the DP potential. $\delta m = m - m_0$ is defined in which m_0 is the value of m which

minimises $f(m)$, i.e. the bulk equilibrium magnetisation value. Taylor expanding to second order, one finds

$$\delta H_{LGW}[\delta m] = \int d^d \underline{r} \left[\frac{1}{2} (\nabla \delta m)^2 + f''(m_0) \frac{\delta m^2}{2!} \right] \quad (2.116)$$

Note that the bulk correlation function will be equal to $\langle \delta m(\underline{r}_1) \delta m(\underline{r}_2) \rangle$ and thus in wave-vector space

$$\delta H_{LGW}[\delta m] = \int \frac{1}{2} (q^2 + f''(m_0)) |\delta \tilde{m}(\underline{q})|^2 \frac{d^d q}{(2\pi)^d} \quad (2.117)$$

And thus by the same path integral calculation as for the DP bulk correlation function,

$$\tilde{G}(\underline{q}) = \langle |\delta \tilde{m}(\underline{q})|^2 \rangle = \frac{k_B T}{q^2 + f''(m_0)} \quad (2.118)$$

Hence we make the association that $f''(m_0) = \xi_b^2$, i.e. the curvature of the potential about the bulk equilibrium value m_0 is related to the bulk correlation length. Thus the bulk correlation function for the full Landau model is also given by

$$G^b(z_1, z_2; q) = \frac{1}{2\kappa_q} e^{-\kappa_q |z_1 - z_2|} \quad (2.119)$$

in which κ is again defined as the bulk inverse correlation length.

2.9.2. Magnetisation Profile

The EL equation is the same for the full Landau Theory but the potential is different. To see this, it is instructive to first re-write the potential $f(m)$ as given in (2.1) making use of the fact that $m_0 = -\frac{a}{2b}$ and $f''(m_0) = -4a = \kappa^2$:

$$f(m) = -\frac{\kappa^2}{4} m^2 + \frac{\kappa^2}{8m_0^2} m^4 \quad (2.120)$$

Clearly this only holds for non-zero m_0 , i.e. below the critical temperature, when two-phase coexistence and thus an interface can exist. Next, multiply either side of the EL equation by $\frac{dm_\pi}{dz}$ [77] to obtain

$$\frac{1}{2} \frac{d}{dz} \left(\frac{dm_\pi}{dz} \right)^2 = \frac{df(m_\pi)}{dz} \quad (2.121)$$

and making use of the boundary conditions for $z \rightarrow \pm\infty$

$$\left(\frac{dm_\pi}{dz}\right)^2 = \frac{\kappa^2}{8m_0^2} (m^2 - m_0^2) \quad (2.122)$$

Taking the square root and integrating by partial fractions [15] gives

$$\frac{1}{m_0} \operatorname{arctanh}\left(\frac{m}{m_0}\right) = \pm \frac{\kappa z}{2m_0} + c \quad (2.123)$$

in which the $\pm$ tells us we can have an interface for which $m(-\infty) = -m_0$ and $m(\infty) = m_0$ or vice versa. Choosing the former, one finds the family of solutions

$$m(z) = m_0 \tanh\left(\frac{\kappa(z - \ell)}{2}\right) \quad (2.124)$$

and in keeping with the results presented for the DP model, I set $\ell = 0$. This is equivalent to setting the zero of the infinitesimally weak magnetic field, which breaks translational invariance and causes the interface to exist, to occur at $z = 0$ and does not constitute a loss of generality. Comparing this to Figure 2.4 and (2.8), it is evident that qualitatively, the profile is very similar to that of the DP model. It is however analytic, that is to say its second derivative (or any derivative for that matter) is not discontinuous at $z = 0$. This is because the Landau potential is analytic everywhere and as a result, its second derivative does not generate a δ function at the interface.

2.9.3. Interfacial Correlation Function

Because $f''(m)$ is not a constant but rather a function of m for the Landau potential, the OZ equation becomes a rather messy, non-linear PDE (in contrast to the DP model) given by

$$\frac{\partial^2 \mathcal{G}(z_1, z_2; q)}{\partial z^2} + \left(\kappa_q^2 + \frac{3\kappa^2}{2} \operatorname{sech}^2\left(\frac{\kappa z}{2}\right) \right) \mathcal{G}(z_1, z_2; q) = \delta(z_1 - z_2) \quad (2.125)$$

Note that as $z \rightarrow \pm\infty$, this equation becomes $\frac{\partial^2 \mathcal{G}(z_1, z_2; q)}{\partial z^2} + \kappa_q^2 \mathcal{G}(z_1, z_2; q) = \delta(z_1 - z_2)$ and thus reassuringly, the solution must look like the bulk correlation function far from the interface. Along the lines of Zittartz [97] we proceed by using the trial solution $G(z_1, z_2; q) = A_\pm(z_2) f_{\pm z_1} e^{\pm \kappa_q z_1}$ to solve the z_1 PDE and similarly for the z_2 equation by symmetry. Solving for f ,

we find

$$f_{\pm}(z_1) = \frac{9\kappa^4}{8\kappa_q q^2 (3\kappa_q^2 + q^2)} \left[1 + \frac{4q^2}{3\kappa^2} \mp \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa z_1}{2}\right) + \tanh^2\left(\frac{\kappa z_1}{2}\right) \right] \quad (2.126)$$

and thus for $z_1 > z_2$

$$\mathcal{G}(z_1, z_2; q) = \frac{9\kappa^4}{8\kappa_q q^2 (3\kappa_q^2 + q^2)} \left[1 + \frac{4q^2}{3\kappa^2} - \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa z_1}{2}\right) + \tanh^2\left(\frac{\kappa z_2}{2}\right) \right] \cdot \left[1 + \frac{4q^2}{3\kappa^2} + \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa z_2}{2}\right) + \tanh^2\left(\frac{\kappa z_2}{2}\right) \right] e^{-\kappa_q(z_1 - z_2)} \quad (2.127)$$

in which the pre-factor was determined by integrating over the cusp $z_1 = z_2$. (z_1, z_2) are relabelled for $z_2 > z_1$ in (2.127). Unlike the DP interfacial correlation function, this does not split into an obvious bulk and interfacial contribution. (2.85) does have a term of the form $c(q)e^{-\kappa_q|z_1 - z_2|}$ and thus it is possible to subtract $\frac{1}{2\kappa_q}$ from $c(q)$ yielding the rather messy

$$\begin{aligned} \mathcal{G} &= G^b(|z_1 - z_2|; q) \\ &+ \frac{9\kappa^4 e^{-\kappa_q|z_1 - z_2|}}{8\kappa_q q^2 (3\kappa_q^2 + q^2)} \left[\left(\tanh^2\left(\frac{\kappa z_1}{2}\right) - \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa z_1}{2}\right) \right) \left(\tanh^2\left(\frac{\kappa z_2}{2}\right) + \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa z_2}{2}\right) \right) \right] \\ &+ \left(1 + \frac{4q^2}{3\kappa^2} \right) \left(1 + \frac{2\kappa_q}{\kappa} \left(\tanh\left(\frac{\kappa z_2}{2}\right) - \tanh\left(\frac{\kappa z_1}{2}\right) \right) + \tanh^2\left(\frac{\kappa z_1}{2}\right) + \tanh^2\left(\frac{\kappa z_2}{2}\right) \right) e^{-\kappa_q|z_1 - z_2|} \end{aligned} \quad (2.128)$$

which unlike the DP model, does not have the property that the interfacial parts of $\mathcal{G}(z, z; q) = \mathcal{G}(z, -z; q)$.

Position Dependent and Total Structure Factors

While it is possible to integrate (2.127) to obtain the position dependent structure factor, a nice trick is to integrate the OZ equation w.r.t z_2

$$\int dz_2 \left[-\frac{\partial^2 \mathcal{G}(z_1, z_2; q)}{\partial^2 z_1^2} + \left(\kappa_q^2 + \frac{3\kappa m'(z_1)}{m_0} \right) \mathcal{G}(z_1, z_2; q) \right] = \int \delta(z_1 - z_2) dz_2 \quad (2.129)$$

and thus

$$\left[-\frac{\partial^2}{\partial z^2} + \kappa_q^2 + \frac{3m'(z)}{m_0} \right] S(z; q) = 1 \quad (2.130)$$

If we make the Ansatz, that the structure factor does in fact consist of a bulk contribution plus an interfacial one, we trial the solution

$$S(z; q) = \frac{1}{\kappa_q^2} + \frac{c(q)}{\kappa_q^2} m'(z) \quad (2.131)$$

which satisfies (2.130) if and only if $c(q) = \frac{3\kappa}{m_0 q^2}$ and thus

$$S(z; q) = \frac{1}{\kappa_q^2} + \frac{3\kappa^2}{2q^2 \kappa_q^2} \text{sech}^2 \left(\frac{\kappa z}{2} \right) \quad (2.132)$$

Perhaps surprisingly, the structure factor splits up quite cleanly into a bulk and an interfacial contribution. (2.131) can be integrated again to give

$$S(q) = 2LS^b(q) + \frac{6}{\kappa q^2} \frac{S^b(q)}{S^b(0)} \quad (2.133)$$

in which L is some macroscopic distance and $S^b(q) = \frac{1}{\kappa_q^2}$ is the bulk structure factor. Unsurprisingly, as the position dependent structure factor breaks up neatly, so must the total one.

2.9.4. PB Theory for the Landau Potential

Calculating the $\tilde{\Lambda}$ functions is the main ingredient of PB theory from which all follows. Recall (by comparing (2.53) and (2.16)) that the equation for $\tilde{\Lambda}(z; q)$ is the same as the OZ equation for $\mathcal{G}(z^x, z; q)$ up to a δ function which only comes into effect at $z = z^x$ and thus

$$\tilde{\Lambda}(z; q) = \frac{\tilde{\Lambda}(z^x; q)}{\mathcal{G}(z^x, z^x; q)} \mathcal{G}(z^x, z; q) \quad (2.134)$$

a fact which could also have been used to determine $\tilde{\Lambda}(z; q)$ for the DP model. Sticking with the original crossing criterion (2.59), the $\tilde{\Lambda}$ functions

are given by

$$\tilde{\Lambda}(z; q) = -\frac{m_0 \kappa}{2} \frac{3\kappa^2}{3\kappa^2 + 4q^2} \left[\frac{3\kappa^2 + 4q^2}{3\kappa^2} - \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa|z|}{2}\right) + \tanh^2\left(\frac{\kappa z}{2}\right) \right] e^{-\kappa_q |z|} \quad (2.135)$$

Now that we know the form of the $\tilde{\Lambda}(z; q)$ functions in the full Landau theory, the wave-vector dependent surface tension can be determined by evaluating the first term in (2.73), as the potential is now continuous at the interface. The result is given by:

$$\sigma(q) = \frac{2m_0^2 \kappa_q}{3 \left(1 + \frac{4q^2}{3\kappa^2}\right)} \quad (2.136)$$

from which both the surface tension and the bending rigidity can be extracted

$$\begin{aligned} \sigma &= \frac{2m_0^2 \kappa}{3} \\ \gamma(z^x = 0) &= -\frac{5}{6} \frac{\sigma}{\kappa^2} \end{aligned} \quad (2.137)$$

in which again, the bending rigidity and surface tension have opposite signs.

Note that (2.135) enforced the crossing criterion (2.59) at $z = 0$, the result for arbitrary z^x is considerably more complicated:

$$\begin{aligned} \tilde{\Lambda}(z; q) &= A_{\pm} \left[1 + \frac{4q^2}{3\kappa^2} \pm \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa z}{2}\right) + \tanh^2\left(\frac{\kappa z}{2}\right) \right] e^{\mp \kappa_q z} \\ A_{\pm} &= \frac{\frac{m_0 \kappa}{2} \operatorname{sech}^2\left(\frac{\kappa z}{2}\right) e^{\pm \kappa_q z^2}}{1 + \frac{4q^2}{3\kappa^2} \pm \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa z^x}{2}\right) + \tanh^2\left(\frac{\kappa z^x}{2}\right)} \end{aligned} \quad (2.138)$$

in which $\pm$ refers to $z > z^x$ and $z < z^x$ respectively, and the sign of z^x plays no role.

Reconstructing Correlations

Now we are in a position to examine the reconstructed correlation function for the Landau potential and to investigate whether the crossing criterion, or a minimally amended one allows us to reconstruct the interfacial part of the correlation function from interfacial fluctuations and thus assign mean-

ing to $\sigma(q)$. Substituting (2.136) and (2.135) into (2.97), one obtains

$$G(z_1, z_2; q) = \frac{9\kappa^4}{8\kappa_q q^2 (3\kappa^2 + 4q^2)} \left[\frac{3\kappa^2 + 4q^2}{3\kappa^2} - \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa|z_1|}{2}\right) + \tanh^2\left(\frac{\kappa z_1}{2}\right) \right] \left[\frac{3\kappa^2 + 4q^2}{3\kappa^2} - \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa|z_2|}{2}\right) + \tanh^2\left(\frac{\kappa z_2}{2}\right) \right] e^{-\kappa_q(|z_1| + |z_2|)} \quad (2.139)$$

which clearly has neither the same z dependence as the interfacial part of the DFT correlation function (2.128) nor the full correlation function (2.127). Rather surprisingly however, $G(0, 0; q) = \mathcal{G}(0, 0; q)$, which should be seen as somewhat equivalent to the result we found for the DP, namely that the reconstructed correlation function equals the full $\mathcal{G}$, not just the interfacial part. While we know that we will not be able to reconstruct the full interfacial correlation function as the $\tilde{\Lambda}$ functions have the wrong z -dependence for this, it is possible to at least amend the crossing criterion such that correlations are correctly reconstructed at the interface. This is done in the same way as for the DP model, i.e. by introducing $b(q)$ as in (2.100) with

$$b(q) = 1 - \frac{G^b(0; q)}{\mathcal{G}(0, 0; q)} = \frac{3\kappa^2}{3\kappa^2 + 4q^2} \quad (2.140)$$

Because the dependence of (z_1, z_2) of $\mathcal{G}$ and G differ however, they will behave differently when the first integral is performed to obtain the position dependent structure factor. Integrating (2.139) (this is not as difficult as it looks, doing so repeatedly by parts results in all hyperbolic terms cancelling), the reconstructed structure factor is obtained

$$S^{rec}(z; q) = \frac{9\kappa^4 \left(2 + \frac{4q^2}{3\kappa^2}\right)}{4\kappa_q^2 q^2 (3\kappa^2 + 4q^2)} \left[\frac{3\kappa^2 + 4q^2}{3\kappa^2} - \frac{2\kappa_q}{\kappa} \tanh\left(\frac{\kappa|z|}{2}\right) + \tanh^2\left(\frac{\kappa|z|}{2}\right) \right] e^{-\kappa_q|z|} \quad (2.141)$$

which clearly does not have the same functional form as either the full or the interfacial part of the position dependent structure factor as determined by integrating the OZ equation and solving the resulting equation (2.130). Remarkably, once again, the reconstructed position dependent structure factor at $z = 0$ is given by $\frac{3\kappa + 2q^2}{2\kappa_q^2 q^2}$ which is the same result obtained when evaluating the full DFT result, again, an undesired property. Because introducing a new crossing criterion (2.100) affects $G(z_1, z_2; q)$ by multiplying it

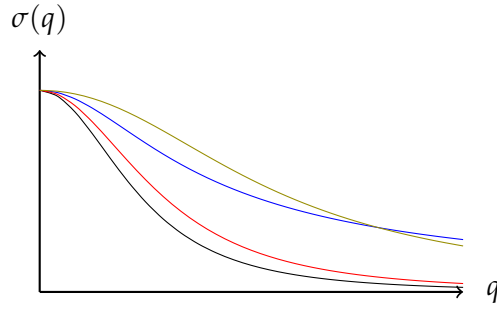


Figure 2.6.: $\sigma(q)$ according to the original crossing criterion (2.59) (blue) and $\sigma(q)$ as given by (2.100) when reconstructing the interfacial correlation function (black), position dependent structure factor (red) and total structure factor (green).

by $b(q)$, it has the same effect on the structure factor. Thus if we wish the reconstructed structure factor to produce only the interfacial part of the full solution, we perform a process very similar to that which we performed for the correlation function and enforce

$$b(q) = 1 - \frac{S^b(q)}{S(0;q)} = \frac{3\kappa^2}{3\kappa^2 + 2q^2} \quad (2.142)$$

in contrast to (2.140). Thus while in DP theory, any single $b(q)$ correctly reconstructs the interfacial part of the correlation function and structure factors for all positions, in Landau theory not only can we only reconstruct the aforementioned quantities at any given position, but it requires a different $b(q)$ for different quantities. This is also true for the total structure factor, and a third and distinct $b(q)$ is required in (2.100) in order to correctly reconstruct the interfacial contribution to the total structure factor

$$b(q) = 3\kappa\kappa_q \frac{3\kappa^2 + 4q^2}{(3\kappa^2 + 2q^2)^2} \quad (2.143)$$

Figure 2.6 shows the different wave-vector dependent surface tensions which are obtained depending on how one defines the crossing criterion. While as $q \rightarrow 0$, all tend to the same value namely the surface tension, for finite q , $\sigma(q)$ has different possible definitions leaving us unable to come up with sensible expressions for (say) the bending rigidity in terms of the

correlation length.

Comparison of DP and Landau Model Results

Both the DP and Landau models' interfacial correlation functions can be written as the sum of the bulk correlation function and an excess part, but the DP model's interfacial part has the simple property that it depends on $(|z_1|, |z_2|)$ only. This is however possibly somewhat of an artefact of the DP model, as it is the cusp at $m = 0$ which causes this behaviour. The Landau correlation function changes definition (has a cusp) only at $z_1 = z_2$ and thus is inherently not a function of distance to the interface. $m_{\Xi}(z, y)$ however does not obey the EL equation at the interface and consequently the equation which governs $\tilde{\Lambda}(z; q)$ continues to have a cusp at the interface and thus $\tilde{\Lambda}(z; q)$ is a function of $|z - z^x|$, i.e. distance to the interface only. Thus the reconstructed correlation function and structure factors can only ever match the exact ones at any given (z_1, z_2) or z respectively. In a way analogous to the DP model, the FJ crossing criterion reconstructs the correlation function and position dependent structure factors at the interface, which is not a desirable result as we would not expect an interfacial Hamiltonian to reconstruct bulk fluctuations. A new crossing criterion involving $b(q)$ can easily solve this, but unlike for the DP model, because the positional dependence of the reconstructed quantities also differs from the exact values, there are in effect three different $b(q)$ and nothing to suggest any is more valid than any other. Nonetheless, different $b(q)$ values will result in different $\sigma(q)$. Furthermore, the integrals

$$\int_{-\infty}^{+\infty} \tilde{\Lambda}(z; q) dz = \frac{2m_0\kappa}{\kappa_q} \left(\frac{3\kappa^2 + 2q^2}{3\kappa^2 + 4q^2} \right)$$

If one wishes to introduce a new crossing criterion such that $\sigma(q) = b(q)\sigma_{cc}(q)$, the total structure factor becomes

$$S(q) = \frac{(b(q))^2 4m_0^2 \kappa^2 (3\kappa^2 + 2q^2)^2}{\sigma(q) q^2 \kappa_q^2 (3\kappa^2 + 4q^2)^2} \quad (2.144)$$

which has considerable q dependence outside of the $\frac{1}{\sigma(q)q^2}$ term, unless $b(q)$ were to be chosen to exactly cancel this. This (complicated) $b(q)$ though is a different $b(q)$ to any of those shown in Figure 2.6, and likewise that of

the DP model and one to which we have not assigned any physical significance.

Using instead the $b(q)$ which correctly reconstructs the total structure factor found using our microscopic theory, it is found that

$$S(q) = \frac{36m_0^2\kappa^4}{(3\kappa^2 + 2q^2)^2} \frac{1}{\sigma(q)q^2} \quad (2.145)$$

which crucially has q dependence beyond the $\frac{1}{\sigma(q)q^2}$ term and it is not that seen in (2.114). If it makes sense to use any of the three discussed $b(q)$, it is perhaps the third, firstly because the total structure factor is not position dependent so the reconstructed and analytically determined structure factors do not only match at the interface and secondly because this is the experimentally determinable quantity. If however we were to choose $b(q)$ such that the correlation functions or position dependent structure factors matched, equivalent expressions to (2.145) can be derived, all turn out to have complicated q dependence on top of $\frac{1}{\sigma(q)q^2}$ and none of which agree with that seen in (2.114). Thus the Landau theory results further back up the "very bad news" obtained when examining the DP model, that is to say, if we define the crossing criterion along the lines of (2.100), $\sigma(q)$ will not be experimentally measurable.

Furthermore, studying the Landau potential brings into question how seriously any of the "good news" we found within the DP approximation can be taken. The correlation function $G(z_1, z_2; q)$, derived by reconstructing correlations from an interfacial model must have the strange property that $G(z, z^x + a; q) = G(z, z^x - a; q)$ when using a crossing criterion, even if it has been amended by $b(q)$. In a sense, this is a physically ridiculous equality, as correlations must decay over distance. It shows that inherently, any interfacial model assumes that all thermally induced fluctuations must be bulk-like, that is to say, the existence of an interface can not incur any stronger (or weaker) thermally induced fluctuations. In DP theory, the correlation function derived from the OZ equation does split into a bulk term, plus a term which does have this unique property of $\mathcal{G}(z, z^x + a; q) = \mathcal{G}(z, z^x - a; q)$, but this completely breaks down in Landau theory, in which one can write $\mathcal{G}(z_1, z_2; q)$ as a bulk + excess part, as is physically reasonable, but the excess part also decays as the distance be-

tween z_1 and z_2 increases and must therefore be interpreted as having an extra contribution from thermally induced fluctuations.

It is however my personal view, that the correlation function $\mathcal{G}(z_1, z_2; q)$ splitting cleanly into a bulk part, and a part that has no inherently thermal contributions to it, is an artefact of the DP model, not a shortcoming of the Landau model. The δ function in the DP potential does seem rather artificial and while one might hope that it only affects an infinitely small range of the values m can take, the discontinuity in the slope of the DP potential has a huge (even if it is rather convenient) effect on the physics.

Without going into the messy mathematics, it is worth mentioning that I have gone through the calculation of $\mathcal{G}(z_1, z_2; q)$ for a Triple Parabola (TP) [3, 38] model, to investigate whether a quadratic potential without a cusp exhibits such behaviour and it becomes clear that $\mathcal{G}(z_1, z_2; q) \neq \mathcal{G}(z_1, -z_2; q)$, especially not in the interfacial region (as in the region between the two inflection points) where the spatial dependence is particularly complicated.

The fact that it appears that correlations in an interface do not, in general, separate into a bulk and an interfacial contribution does not necessarily in my opinion mean, that $\sigma(q)$ does not exist. It still seems reasonable to suggest the free energy cost of a fluctuating interface can be written in terms of energetically penalising increases to the surface area as well as bending effects, and it might be possible to characterise the strength of these penalisations in terms of microscopic variables such as the correlation length. It does however mean that a crossing criterion picture of an interface is insufficient to capture the idea. Likewise the more sophisticated floating interface definition and the new boundary condition this generates for $\tilde{\Lambda}(z; q)$ is not sufficient either. Also, within our current definition of the interface, we cannot experimentally measure $\sigma(q)$, or worse yet, try to subsequently use $\sigma(q)$ to make predictions about certain microscopic variables.

2.10. The Extended Landau Ginzburg Wilson Hamiltonian (ELGW)

I have studied the ELGW Hamiltonian in depth, initially to investigate the validity of a result published by Blokhuis [12, 13] for the rigidity of an

ELGW Hamiltonian which suggested the rigidity vanishes with the same exponent as the surface tension as the critical point is approached. The "extension" in the ELGW Hamiltonian is to include a $(\nabla^2 m)^2$ term in the Hamiltonian. For a full discussion of how the coefficients of gradient terms are related to moments of the direct correlation function, see [28].

$$H_{ELGW}[m] = \int d^d r \left[\frac{g_4}{2} (\nabla^2 m(r))^2 + \frac{g_2}{2} (\nabla m(r))^2 + f(m(r)) \right] \quad (2.146)$$

While I quote some of my results in Appendix F, the purpose of mentioning the ELGW Model in the context of the wave vector dependent surface tension is to show that the value obtained for $b(q)$ results in qualitatively very different behaviour of $\sigma(q)$. As I have discussed in Appendix F, the result that $\mathcal{G}(0, 0; q)$ and the reconstructed correlation function (using the FJ crossing criterion) are equal at the interface, appears to hold in the ELGW too. This is in fact the only robust result that holds up for DP in both square gradient and ELGW models as well as for the square gradient theory with a Landau potential, as regards reconstructing order parameter fluctuations from interfacial ones.

The result for calculating the wave-vector dependent surface tension holds up in an ELGW Model as well. The only difference to square-gradient theory is that the OZ and the equation which describes the $\tilde{\Lambda}(z; q)$ functions is a fourth order PDE and consequently, the first and second derivatives of $\tilde{\Lambda}(z; q)$ must be continuous, the third derivative is discontinuous and thus the fourth derivative contains a δ function. The result is:

$$\sigma(q)q^2 = \gamma m'_\pi(0) \Delta \frac{\partial^3 \tilde{\Lambda}(z; q)}{\partial z^3} + \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} dz f''(m_\pi(z)) (\tilde{\Lambda}(0; q))^2 \quad (2.147)$$

in which $\Delta \frac{\partial^3 \tilde{\Lambda}(z; q)}{\partial z^3}$ denotes the difference between the third gradient of $\tilde{\Lambda}(z; q)$ either side of the interface. If $z^x \neq 0$, the first term must be evaluated either side of $z = z^x$ and the second term omitted, analogous to DP.

Finally, I return to $b(q)$ in the ELGW model, by showing $\sigma(q)$ and $b(q)\sigma(q)$ for three different values of γ in Figure 2.7. $b(q)$ in this case is defined such that $G(0, 0; q) = \mathcal{G}(0, 0; q) - G^b(0; q)$. The original crossing criterion does in fact result in a $\sigma(q)$ somewhat reminiscent of Dietrich and Mecke [57] in that there does exist a q^* , or global minimum for $\sigma(q)$ for non-zero q . The amended crossing criterion however completely changes the qualita-

tive behaviour of $\sigma(q)$ and it becomes a monotonically decreasing function. While I personally do not believe that even the amended crossing criterion provides a good description of the interface, due to its failure to give a meaningful way of extracting $\sigma(q)$ beyond DP, it is certainly an improvement upon FJ as it relaxes the over-precise definition of the interface. Thus it is not my intention to champion the monotonically decreasing $b(q)\sigma(q)$ (shown in red in) in Figure 2.7, but certainly to state that I do not believe there to be any physics contained within the crossing criterion $\sigma(q)$ (shown in black in Figure 2.7), and thus not to lend credence to the idea, that there exists a critical, non-zero q^* which minimises $\sigma(q)$.

2.10.1. Concluding Remarks

To end this chapter, I bring together its key conclusions in one place. The main findings which arise from the simplest of models, namely the DP model, are summarised in some detail in Section 2.8.3. Here I provide a succinct recap:

- At Double Parabola level, the interfacial correlation function, as calculated from the OZ equation, splits cleanly into a bulk and an interfacial part.
- Reconstructing correlations from an interfacial model which makes use of a crossing criterion does not reproduce the interfacial correlation function one gets by solving the OZ equation.
- The crossing criterion can be amended in a way that perhaps has physical meaning, in order to rectify this mismatch.
- Regardless of the crossing criterion, the structure factor has q -dependence outside of the wave vector dependent surface tension meaning $\sigma(q)$ still cannot be calculated in the way that is often assumed.

After redoing the analysis for the Landau Model, the situation becomes worse:

- At Landau level, the interfacial correlation function, as calculated from the OZ equation, does not cleanly split into a bulk and an excess part.

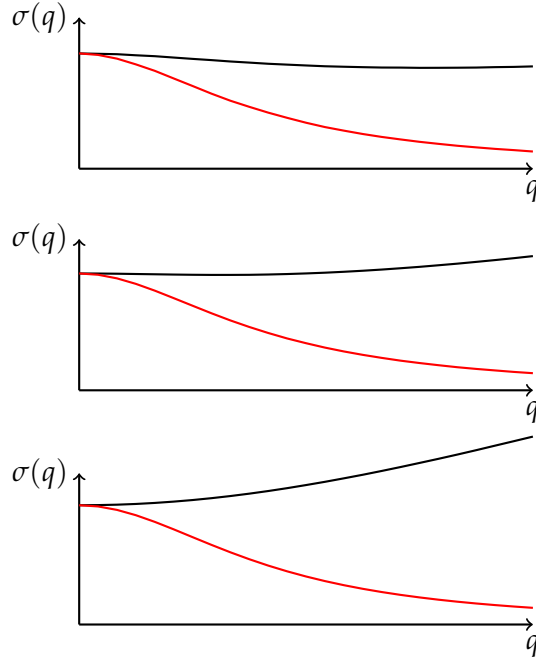


Figure 2.7.: $\sigma(q)$ (black) and $b(q)\sigma(q)$ (red) vs q in an Extended LGW DP model for successively larger γ values. The standard crossing criterion will cause $\sigma(q)$ to diverge for large q , although it dips first and as $\gamma \rightarrow 0$, and the standard square gradient theory is approached, this divergence must occur for larger and larger q . Introducing a new a new crossing criterion as in (2.100) changes this behaviour entirely and causes $\sigma(q)$ to be monotonically decreasing as was the case in square gradient theory. Before introducing an amended crossing criterion, there exists a (γ dependent) q^* along the lines of Mecke and Dietrich [57]. I do not encourage this result to be interpreted with any particular physical significance.

- The reconstructed correlation function, as calculated from an interfacial model, has an entirely different functional form to the DFT correlation function, rather than just being wrong by a multiplicative factor as was the case in the DP model.
- Due to this mismatch, the crossing criterion can only be amended to match correlation functions at the interface rather than for all (z_1, z_2) . Likewise, a different tweak is needed depending on whether one wishes to match the correlation function, position dependent structure factor, or total structure factor.
- Regardless of which amendment one makes (or does not make), the structure factor contains complex q dependence outside of $\sigma(q)$, and this is not the same dependence as is found at DP level. This makes our underlying conclusion even more resolute: the approach of calculating the wave vector dependent surface tension from the experimentally measured structure factor is fundamentally flawed and neglects q -dependence which arises from the non-local dependence of the magnetisation profile on the interfacial configuration.

2.10.2. Further Work

Firstly, it must be stated that the goal of the paper we published on this research [64] was not to motivate further research, but to dissuade further efforts to measure the wave vector dependent surface tension. Nonetheless, a recurring concept within this chapter has been there being a "background/bulk contribution" to the interfacial correlation function. For interfaces with Ising symmetry, there is less ambiguity as to what this should be. For a liquid/gas interface which separates two phases with different correlation lengths and thus different bulk correlation functions, this background contribution is less obvious. Should it simply be a linear superposition of the two correlation functions, each weighted equally? This topic has been addressed in two papers [66, 67] since I completed the research contained within this chapter and moved to a different field of research.

3. On Analytic Methods for Solving the Manna Model for Small Systems

Abstract

Some results are presented which form part of an ongoing project which looks into characteristic correlations which are traditionally at the centre of critical phenomena, but have been widely ignored in the field of self-organised criticality, as they are difficult to measure due to separate time scales and the presence of boundary conditions. The results I will present are for systems too small to provide insight into asymptotic behaviour, hence the need for numerical simulations. Nevertheless, they are useful as a reference to ascertain the validity of such numerical approaches.

3.1. Outline

The final chapter opens with a brief and rather non-quantitative introduction to the types of models that are frequently studied in self-organised criticality. This is of particular importance within a thesis such as my own, in light of how different such systems are to for example, the Ising Model, seeing as such models were at the heart of the first two chapters. After setting the scene, the rules/dynamics of the Abelian Manna Model, the model studied within this chapter are outlined in quite some detail, as well as the definitions of the properties which are to be investigated. Important concepts such as the separation of time scales into micro- and macroscopic time are likewise introduced. Subsequently, the two analytical methods which have been devised to tackle the problem are introduced.

Firstly, I discuss the tree method, a diagrammatic method which can be used to determine the steady state of the Manna Model by deriving the transition matrix. The method is somewhat intuitive as it can be described through diagrams (many are provided), but the equations it generates quickly become intractable. By the end of the discussion of the tree method, it will have been made clear, how it can be used to calculate some but not all of the properties discussed in the introduction, in particular only the ones resolved at macroscopic time. Results for systems of size $L = 2$ and $L = 3$ are presented in this section.

Secondly, the matrix method, a computational but closed form (this apparent paradox is explained) method which facilitates the calculation of the transition matrix, is introduced. Because the method is computational, it facilitates such calculations for systems larger than the tree method does, but in systems that both methods can be applied to, the results are identical. The ability to study larger systems is however not the only reason the matrix method is of interest however. It turns out, that it can be used to make predictions about the variables discussed in the introduction, which are resolved at microscopic time, something the tree method cannot. Results for systems of size $L = 4$ and $L = 5$ are presented in this section, as these were not covered in the tree method section. Finally, numerical limitations are discussed.

Unlike the first two chapters, the material presented in this one is very much a work in progress. The results in this chapter reflect the state of my

research on the day of my original submission, 29th May 2015. Substantial progress was made between the original and final submissions. In particular, a lot of effort has gone into discussing how the matrix method was carried out not using the even-odd sublattice dynamics, as I ideally would have liked to. I had used a more simple dynamics, as this was a computationally much easier task, and substantial effort towards the end of this chapter goes into discussing what information this more simple dynamics can provide, and what its limitations are. In light of the fact, that I have successfully developed a method to generate transition matrices for the even-odd sublattice dynamics in the meantime, much of this later content is no longer of relevance.

3.2. Introduction

The field of self-organised criticality [70] has been an extremely active field of research since Bak, Tang and Wiesenfeld (BTW) [2] published their pioneering paper which provided a mechanism by which a dynamical system can organise itself into a critical state. This is in stark contrast to the Ising, Potts, BEG etc models which have been discussed in the two previous chapters, as these models only exhibit critical behaviour at one (or more) critical points, which are reached by tuning an external parameter such as the temperature. The Manna Model is one within the field of self-organised criticality (SOC) and it is the goal of this chapter to present some analytic results which I have developed alongside a longer, numerical project which is still very much ongoing. For that reason, it is most certainly not the goal, to present these findings within the wider context of SOC, or comment on the applicability of these methods to other problems in the field, as this has not yet been investigated. In what follows, I will introduce the dynamics of the Manna Model, introduce some key prior analytic results and then present my own.

3.2.1. The Driven Sandpile

The sand pile metaphor is commonly used [18] in SOC and provides a good starting point for introducing the Manna Model. Consider a small 2 dimensional surface (e.g. a coffee table), and slowly dropping a fine pow-

der such as sand onto this surface from above. Assuming all of the sand falls exactly onto the same part of the surface or within a sufficiently small region, one would expect a pile to develop, that is to say, the height of the sand will be highest at the point where the sand is being dropped and there will exist a height gradient. If enough sand were dropped, one would expect the base of the pile to reach the edges of the surface and some sand would begin to fall off the edges. If sand continued to be dropped onto the surface indefinitely, the amount of sand on the table would not increase ad infinitum. The system would organise itself into a state in which on average, for every grain of sand added to it, one would fall off of the edge. The underlying mechanism that BTW suggested for this, is that there is a certain natural height gradient that the pile will support. If a single grain of sand is added, and it lands on top of another grain, such that the height of the pile where it has fallen is sufficiently higher than at neighbour sites, it will topple. Clearly nature does not work quite like this, but this idealised model certainly captures some of our physical intuition of what is going on. There is an inherent "steepness" that a pile of sand can support and anything above this will result in a toppling event. Furthermore, this natural steepness must not be an average over the entire pile, as a toppling near the top can trigger an entire avalanche. Likewise, if particles are added slowly enough that the system is in a stable state each time a new particle is added, intuitively, the system will not always respond to such an addition. Sometimes when a sand particle is added to the pile, it will stay in place. Sometimes however, the addition of a single grain will trigger a relatively large avalanche. On average however, the process of adding a single sand particle will result in one leaving the system, otherwise it would not be in a steady state.

3.2.2. The Manna Model

The aforementioned thought experiment was quantified and idealised first by BTW, but I will continue directly to the dynamics of the model which will be studied in this chapter, namely the Manna Model [55]. Manna first introduced a model which evolves according to the following rules. Particles are added to a d -dimensional (usually hypercubic) lattice until there is a site which contains more than a threshold value of particles, usually

taken to be one. As soon as a single site contains more than this threshold value of particles, it redistributes those particles independently and with uniform probability amongst its nearest neighbours. Thus in the absence of any directional bias (see [72, 20]), the probability of a particle hopping to any of its nearest neighbours is $\frac{1}{z}$ in which z is the coordination number, usually $2d$ in which d is the dimensionality of the lattice. Once these particles (if the threshold value is one, once this pair of particles) have been redistributed, it is possible that they hopped to sites which already contained the threshold value, or all (both) hopped to the same site, which in either case will contain more than the threshold number of particles, thus triggering a further redistribution event. The system has open boundaries meaning particles located at sites on the edge of the system can hop off the edge and be lost. The addition of a single particle to the system can in turn trigger a long series of such redistribution events. This so-called “avalanche” will eventually end, when all sites contain a number of particles less than or equal to the threshold value. The system is studied in its steady state, that is to say, while avalanches of a huge range of sizes can occur, the addition of one particle to the system will result in the system losing a particle at a boundary, when averaged over many drives.

If two particles hop to a site which is already populated, this site will contain three particles. In the original Manna Model, with the threshold value set to 1, all three of these particles must then be redistributed. Dhar [25, 24] however introduced the concept of an Abelian sand pile model, in which the order of drives does not affect the distribution of resultant states. That is to say, driving the system by adding a particle at site n , waiting for it to relax, driving it at site m , and waiting for it to relax again will result in the same possible final states with the same probabilities as driving in the reverse order. In order to achieve this, particles must always be redistributed in pairs. If a site contains three particles, only two are redistributed, if it contains four, all four must be redistributed, and so forth.

A key imposition on such a model, regardless of how active states are updated, is the absolute separation of time scales. The system is driven at a rate of 1 drive per iteration of “macroscopic” time. While the definition of microscopic time depends somewhat on update dynamics (see Section 3.2.4), roughly speaking, the more redistribution events occur, the more “microscopic” time has elapsed. It is possible, for the system to require

a vast number of topplings until it relaxes, but regardless of how much microscopic time elapses, the system is not driven again (i.e. macroscopic time is not incremented) until it has relaxed.

Note that these dynamics differ somewhat from the physical intuition of how a driven sand pile remains more or less stable, namely that there is a critical gradient which the system supports. The Manna Model is a so-called stochastic sand pile and clearly a level of abstraction away from the sand pile metaphor.

3.2.3. Driving

The system can either be driven at the same site over and over again, referred to as "deterministic" driving, or the site at which particles are added can be randomly selected for each drive. In principle of course, other rules for selecting the drive site such as randomly selecting it from a subset could be used. Here I consider only deterministic and uniform (random) driving.

3.2.4. Update Dynamics

A key feature of the Abelian Manna Model, is that the order in which active sites are updated does not affect the final distribution of states. Clearly however, it will affect the path by which an active state relaxes, that is to say, the sequence of transient active states the system passes through before successfully relaxing. A consequence of this is that any quantities which are a function of microscopic time, e.g. the response function (see Section 3.2.7) will be sensitive to the order in which updates are implemented. Quantities resolved at macroscopic time only (i.e. the value they take after the system has fully relaxed, averaged over many drives), such as the density profile, will be insensitive to such dynamics. I now in detail describe two ways in which one might choose to update active sites, and a further method which is useful as it makes the generation of transition matrices particularly simple (see Section 3.4).

Even-Odd Sublattice Dynamics

The even-odd sublattice dynamics requires all sites which are active to be updated simultaneously. In such a case, all sites which were active will

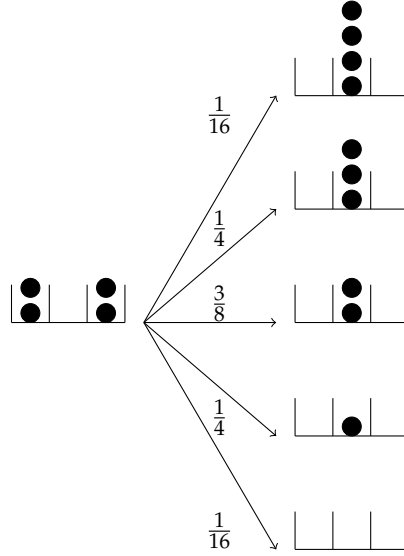


Figure 3.1.: The distribution of states after one iteration of microscopic time after the system was originally in the state $|2|0|2|$ using the even-odd sublattice dynamics.

not be active at the next iteration of microscopic time. Initially, only the site which was driven can be active. After the drive site redistributes the two particles present there, the two (in 1 dimensions) sites either side of it can be active. After these sites have redistributed their particles simultaneously, the initial drive site can be active again, as well as the sites two to the left (again in 1 dimension) and two to the right. Thus at even microscopic times (as well at $t=0$), sites an even distance away from the drive site can be active whereas at odd times, sites an odd distance from the drive site can be active. This has profound implications for the response function in particular (see Section 3.2.7). The numerics I am running which form the main part of our ongoing project on the Manna Model implement these dynamics. It turns out that for systems small enough to implement the tree method (to follow, see Section 3.3), such dynamics remain tractable but when generating transition matrices for the matrix method (to follow, see Section 3.4), it is particularly cumbersome to implement a dynamics which allows for a variable number of sites to be simultaneously active.

Poissonian Dynamics

A process is Poissonian [48] if the event of interest can only occur once in a sufficiently small time interval (defined here as one iteration of microscopic time). Thus a Poissonian update rule is one in which only one site can ever be updated at once. Likewise, making an analogy for example with radioactivity [52], the probability of an active site redistributing its particles at any given time is in no way dependent on how long the site has been active for (the probability of an unstable radioactive particle decaying is not a function of how long it has existed for). One way to (computationally) implement this is to store the addresses of all active particles but rather than looping over all these addresses as would be done for even-odd sublattice dynamics, select a site at random to update. This particular update can generate active sites at its neighbour sites. It is equally likely that these newly generated active sites will decay before a site that has been active for a long time does. Even within Poissonian dynamics, there is an ambiguity as to how to treat sites that are multiply-active (i.e. have a population greater than 3). If such a site is randomly selected for an update, it can be fully relaxed and subsequently removed from the list of active particles, or only two particles can be redistributed and the site in question would then continue to be stored as active. The first update of $|2|0|2|$ according to Poissonian dynamics is shown in Figure 3.2 (to be compared with Figure 3.1).

Other Dynamics

As long as dynamics are used which uphold the Abelian property, more obscure rules to update active states can be used and the distribution of final relaxed states for a given drive will remain unchanged. Likewise, this will not affect the average number of topplings required to relax a given active state and consequently has no effect on the average avalanche size (to be defined in section 3.2.6). In principle, if we are only interested in such quantities, any rule which distributes particles in pairs only can be used. The "scan from the left" (or right) dynamics might seem rather nonsensical / non-physical but when generating transition matrices (see Section 3.4), it will become clear why it is the easiest to implement. It involves scanning an active state from one side until an active site is found, updating this

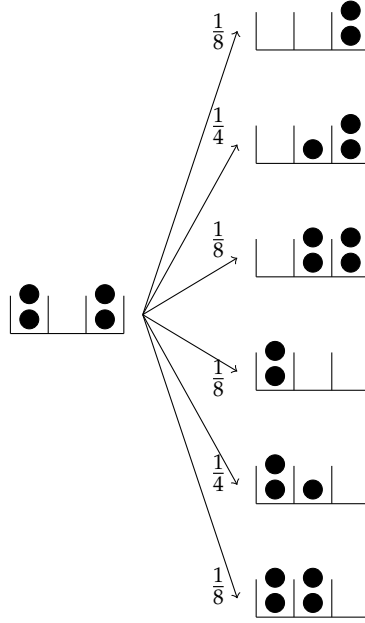


Figure 3.2.: The distribution of states resulting from $|2|0|2|$ after one iteration of microscopic time if Poissonian dynamics are used.

site (and only allowing for one re distribution should it be a doubly-active site) and repeating the process. Figure 3.3 demonstrates how this particular dynamics determines the distribution of states which the active state $|2|0|2|$ can transition into (to be compared with Figures 3.1 and 3.2).

3.2.5. Density Profile

The density is defined for every given site, by the probability it will be occupied after the system has fully relaxed. This chapter will provide meth-

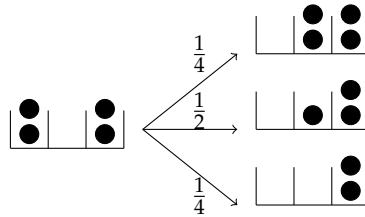


Figure 3.3.: The way in which the state $|2|0|2|$ is updated when using dynamics which scan the lattice from the left to find the first active site.

ods for determining this analytically for small systems but in general, for large systems, this will be defined at each site x_i , as the population of site i (which can be zero or unity) after the system has relaxed, averaged over many drives.

Intuitively, as particles are lost at the boundary, one would expect the density to decrease towards the boundaries. In fact, one would expect the density to be highest at the centre of the system and decrease monotonically towards either boundary. One might however also expect the density to be higher near the drive site for deterministic driving. While our initial numerical models in one dimension showed a clear drop in average density in the vicinity of the boundary, the density profile exhibited no discernible sensitivity to drive site for systems of any size. Our following proof confirms this.

Firstly consider the operator a_n , which evolves the system by driving it at site n and then allowing it to fully relax. If the system finds itself in a state or statistical distribution of states given by v , then $a_n \cdot v$ will describe the distribution of states after a drive at site n and subsequent relaxation. Next, we make use of Dhar's conjecture [25, 24]

$$a_n^2 = \frac{1}{4} (a_{n-1}^2 + a_{n+1}^2 + a_{n+1}a_{n-1} + a_{n-1}a_{n+1}) = \frac{1}{4} (a_{n+1}^2 + a_{n-1}^2)^2 \quad (3.1)$$

which makes use of the Abelian property of the Manna model, namely that $[a_{n-1}a_{n+1}, a_{n+1}a_{n-1}] = 0$. Also note that $a_0 = \mathcal{I} = a_{L+1}$, i.e. adding a particle to a site outside of the boundary has no effect. Consequently

$$a_1^2 = \frac{1}{4}a_2^2 + \frac{1}{2}a_2 + \frac{1}{4}\mathcal{I} \quad (3.2)$$

Assuming a_1 has a steady state vector s.t. $a_1 \cdot e_1 = e_1$,

$$(a_2^2 + 2a_2) \cdot e_1 = 3e_1 \quad (3.3)$$

By inspection, $a_2 \cdot e_1 = e_1$ is a solution to (3.3), but can there be others? By the Frobenius Perron theorem [34], if a_2 were a positive matrix, it would follow that all other eigenvalues were negative, or had an imaginary component. Consequently, one could claim that if the steady state of a_1 is given by e_1 , then the steady state of a_2 is given by e_1 as well. If both a_{n-1} and a_n

have the same steady state e_1 , then (3.1) implies

$$(a_{n+1}^2 + 2a_{n+1}) \cdot e_1 = 3e_1 \quad (3.4)$$

and hence the system has the same steady state for all deterministic driving. A caveat here is that if for example, a_2 is not positive but rather non-negative, it can in fact have degenerate eigenvectors and it could be the case that for $e_1 = \alpha e_2 + \beta e_3$

$$a_2 (\alpha e_2 + \beta e_3) = \alpha e_2 + \beta e_3 = e_1 \quad (3.5)$$

When driving at a given site, it may well be impossible to reach certain relaxed states (an example of this will be given in Section 3.3) and thus a_n will in fact be non-negative but contain zero entries. When driving uniformly however, it will always be possible to reach every relaxed state. To see this, the following path allows any relaxed state α to transition to any other relaxed state β . First, drive the system at all sites which are populated in state α but not β , and consider the path which involves the resultant pair of particles hopping in the same direction repeatedly until they are lost at a boundary. Once all of the relevant sites have been depopulated in this way, driving the system at all sites which are depopulated in state α but populated in state β will complete one possible path for the transition $\alpha \rightarrow \beta$ (there will in all likelihood be many others). Thus the operator a_u^N in which N is the number of drives required (whose upper bound must be L , the system size), will have all positive entries. Consequently, a_u^N must have a unique steady state, and thus so must a_u . As a_u represents uniform driving, it can be written as

$$a_u = \frac{1}{L} \sum_{i=1}^L a_i \quad (3.6)$$

and consequently, if there exists a deterministic driving operator a_i such that all relaxed states are reachable, the unique steady state e_i will also be the unique steady state of a_u . Furthermore, there might (can) exist forms of deterministic driving governed by an operator a_i , which result in the system not being able to relax to certain relaxed states. In such cases, the system can have multiple steady states, but it must be possible to construct

a linear superposition of these states to form the unique steady state of the uniform driving operator.

3.2.6. Avalanche Size

The average size of an avalanche is defined to be the average number of topplings required for the system to transition from the state it is in directly after being driven, to a relaxed state, in which a toppling is defined as the redistribution of two particles. Thus if a given site has a population of 4, it will decay via two separate redistributions of two particles and consequently contribute two to the size of the avalanche it is involved in. The average avalanche size, like the density profile, is averaged over macroscopic time only and thus if update rules resulting in Abelian dynamics are used, the average avalanche size is not sensitive to how active sites are updated (e.g. even-odd sublattice or Poissonian dynamics). This is non-trivial because which (transient) active states the system finds itself in is very much a function of the dynamics used to evolve active states.

Pruessner has shown [71] that in 1 dimension, the average avalanche size $\langle Av \rangle$, for a given system size L and drive site n is given by

$$\langle Av \rangle(L, n) = \frac{n}{2} (L + 1 - n) \quad (3.7)$$

which can be averaged over all n (for random driving) to obtain

$$\langle Av \rangle = \frac{1}{12} (L + 1) (L + 2) \quad (3.8)$$

3.2.7. Activity

The activity or response function, $r(x, t)$ is defined as the average number of topplings at site x , t microscopic time iterations after a drive. Clearly $r(x, t)$ will tend to zero as $t \rightarrow \infty$ as the system must eventually relax. At $t = 0$, the only site active will be the drive site and the activity will propagate out towards the boundaries. For a site x a distance y away from the drive site, $r(x, t) = 0$ for $t < y$ as it will take y iterations of microscopic time for any particles to hop this far from the drive site. When using an even-odd sublattice dynamics, half of the entries in $r(x, t)$ will by necessity be equal to zero. If a site x can be active at a time t (i.e. $r(x, t) \neq 0$), then

$r(x, t+1) = r(x+2n, t+1) = 0$ for any integer n and likewise $r(x \pm n, t) = 0$ for any odd number n .

Consider a single particle sitting at a site, say i , as the system is in the process of relaxing. Until another particle arrives at site i , this particle cannot move. As soon as another particle hops onto this site however, the original particle behaves like a random walker in one dimension (with no hopping bias). It will continue to behave like a random walker until it hops onto an unoccupied site. Thus in a sense, any particle in the Manna Model behaves like a random walker, except while the latter hops at every iteration of microscopic time, the former each have their own personal "clock" which only "ticks" at every iteration of global microscopic time, if they are active. For this reason, we do not expect the response function to obey a diffusion equation of the form

$$\frac{\partial \phi(x, t)}{\partial t} = D \frac{\partial^2 \phi(x, t)}{\partial x^2} \quad (3.9)$$

but rather have a more complicated time dependence, something we wish to study.

3.2.8. Time Integrated Activity

The time integrated activity, $R(x)$ is the average number of topplings which occur at site x over the course of the system relaxing. Clearly, this is equivalent to $\sum_{t=0}^{\infty} r(x, t)$. Furthermore, summing the time integrated activity over all positions will recover the average total number of topplings per drive, or average avalanche size. While the activity itself will not obey the diffusion equation, we expect the time integrated activity to do so, because integrating $r(x, t)$ over all time will compensate for the effect that there are microscopic time iterations at which a given particle will not move, as it is inactive. To motivate this somewhat further, consider the response function in continuum space, such that one can integrate the diffusion equation over all time

$$\int_0^{\infty} \frac{\partial r(x, t)}{\partial t} dt = D \frac{\partial^2}{\partial x^2} \int_0^{\infty} r(x, t) dt = D \frac{d^2 R(x)}{dx^2} \quad (3.10)$$

In the continuum limit, when driving at $x = x_0$, $r(x, t = 0) = \frac{1}{2}\delta(x - x_0)$ in which the factor of $\frac{1}{2}$ originates from the fact that particles are added one at a time, but a response of unity is defined as a single toppling which involves two particles. Hence we have an ODE for $R(x)$

$$D \frac{d^2 R(x)}{dx^2} = -\frac{1}{2}\delta(x - x_0) \quad (3.11)$$

The complementary function is simply $ax + b$ and the cusp condition will allow $R(x)$ to change definition at $x = x_0$. Integrating (3.11)

$$-2D = \lim_{\epsilon \rightarrow 0} \left[\frac{dR(x_0 + \epsilon)}{dx} - \frac{dR(x_0 - \epsilon)}{dx} \right] \quad (3.12)$$

Furthermore, in the slight abstraction that is the continuum limit, $\lim_{x \rightarrow 0} R(x) = 0 = \lim_{x \rightarrow L} R(x)$. Finally, of course, one must impose continuity at $x = x_0$. Solving the aforementioned four conditions simultaneously, it is found that

$$\begin{aligned} R(x) &= \frac{L - x_0}{2DL}x & (x \leq x_0) \\ R(x) &= \frac{L - x}{2DL}x_0 & (x > x_0) \end{aligned} \quad (3.13)$$

Upon examining the results of my numerical simulations, it has become clear that (3.13) describes $R(x)$, if every instance of L is replaced by $(L + 1)$, and $D = \frac{1}{2}$. Clearly the continuum limit is only valid as $L \rightarrow \infty$ in which $\frac{L+1}{L} \rightarrow 1$. Furthermore, summing this expression over all (discrete) positions gives Pruessner's result (3.7) for the average avalanche size.

3.3. The Tree Method

The technique I will present in this section, is a graphical method for calculating the density profile of the Manna Model, which has some similarities to a technique developed by Corral [19] for studying transition probabilities in the Oslo Model. It also leads directly to the density-density correlation profile, and an extension to the method leads to the average avalanche size. While in theory the method can be extended indefinitely, for system sizes greater than $L = 3$, I have found it to be entirely intractable. Nonetheless, it explains some of the interesting features found in our simulations

for $L = 3$ as well as providing a benchmark to reference the effectiveness of the Matrix Method (see Section 3.4) which can be applied for slightly larger systems.

The goal of both the tree method and the matrix method is to calculate the Markovian matrix [89] which describes the probability of the system transitioning from any given relaxed state α to every other relaxed state β via an external drive, denoted as $T_{\alpha\beta}$ (T for transition matrix). Once the matrix T has been determined, its ("normalised") eigenvector will give the steady state of the system. That is to say, if T has the eigenvector u with eigenvalue 1, then $\frac{u_\alpha}{\sum_\alpha u_\alpha}$ gives the steady state (or statistical average) probability of the system being in a state α after it has fully relaxed, i.e. immediately before a subsequent drive. The word "normalised" has been put in inverted commas as it is not normalised in the conventional Euclidean sense of $\sum_\alpha u_\alpha^2 = 1$ but rather $\sum_\alpha u_\alpha = 1$.

If the system is being deterministically driven, then if it is in a state α before a particle is added, it can instantly be deduced, whether it will be in another relaxed state β after a drive, or whether it will be in an active state. Thus the two matrices R_R (for relaxed-relaxed) and R_A (for relaxed-active) can be instantly deduced, and will consist of 0 and 1 entries only. Considering the case of driving a two site Manna system from the left only, relaxed state $|0|0\rangle$ for example, will always after a drive be in relaxed state $|1|0\rangle$. The latter however, will after a drive, be in the active state $|2|0\rangle$. Going through this procedure for the four relaxed states yields (in which "bef" for "before a drive" and "aft" for "after a drive" have been added for clarity):

$$R_R = \begin{pmatrix} \text{aft} \rightarrow & \text{bef} \\ & \downarrow & |0|0\rangle & |1|0\rangle & |0|1\rangle & |1|1\rangle \\ |0|0\rangle & 0 & 1 & 0 & 0 \\ |1|0\rangle & 0 & 0 & 0 & 0 \\ |0|1\rangle & 0 & 0 & 0 & 1 \\ |1|1\rangle & 0 & 0 & 0 & 0 \end{pmatrix} \quad R_A = \begin{pmatrix} \text{aft} \rightarrow & \text{bef} \\ & \downarrow & |2|0\rangle & |2|1\rangle & |0|2\rangle & |1|2\rangle \\ |0|0\rangle & 0 & 0 & 0 & 0 \\ |1|0\rangle & 1 & 0 & 0 & 0 \\ |0|1\rangle & 0 & 0 & 0 & 0 \\ |1|1\rangle & 0 & 1 & 0 & 0 \end{pmatrix} \quad (3.14)$$

The probability of the system transitioning from state $\alpha \rightarrow \beta$ via a drive and possibly a subsequent relaxation is given by $(R_R)_{\alpha\beta} + \sum_\gamma (R_A)_{\alpha\gamma} P_{\gamma\beta}$ in which $P_{\gamma\beta}$ denotes the probability of an active state γ relaxing to a re-

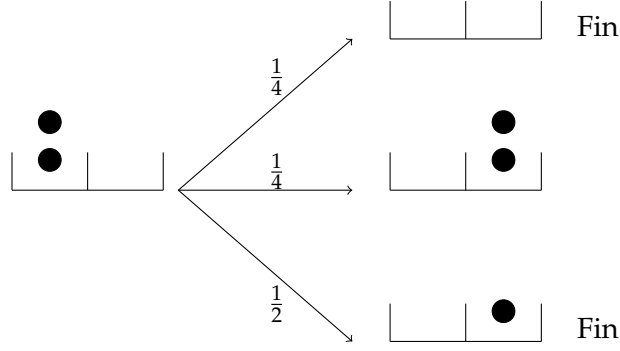


Figure 3.4.: The probability tree for the first microscopic time step after the system is in active state $|2|0|$. States denoted Fin (finished) are relaxed states.

laxed state β via any possible path, that is to say, summed over all possible trajectories of transient active states. In matrix form

$$T_{\alpha\beta} = (R_R + R_A \cdot P)_{\alpha\beta} \quad (3.15)$$

I will now show how to calculate $P_{\gamma\beta}$ using a graphical method.

To clarify the notation, the quantity $\delta(|1|1|, x)$ is equal to 1 if x denotes the relaxed state $|1|1|$ and zero if it denotes any other relaxed state. Thus, as there are four relaxed states of the $L = 2$ Manna Model, namely $|0|0|$, $|1|0|$, $|0|1|$ and $|1|1|$, we know that

$$P(|2|0| \rightarrow x) = a\delta(|0|0|, x) + b\delta(|1|0|, x) + c\delta(|0|1|, x) + d\delta(|1|1|, x) \quad (3.16)$$

with a, b, c, d yet to be determined, but $a + b + c + d = 1$.

To proceed, consider the first iteration of microscopic time after the system finds itself in the active state $|2|0|$ shown in Figure 3.4. From Figure 3.4, it is the case that

$$P(|2|0| \rightarrow x) = \frac{1}{4}\delta(|0|0|, x) + \frac{1}{2}\delta(|0|1|, x) + \frac{1}{4}P(|0|2| \rightarrow x) \quad (3.17)$$

The diagram for $P(|0|2| \rightarrow x)$ looks almost identical (see Figure 3.5).

Thus we can likewise conclude (as we could have done by symmetry in

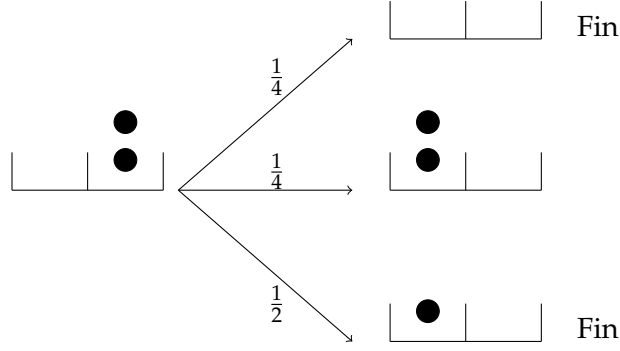


Figure 3.5.: The probability tree for the first microscopic time step after the system is in active state $|0|2|$. States denoted Fin (finished) are relaxed states.

this case) that

$$P(|0|2| \rightarrow x) = \frac{1}{4}\delta(|0|0|, x) + \frac{1}{2}\delta(|1|0|, x) + \frac{1}{4}P(|2|0| \rightarrow x) \quad (3.18)$$

and thus substituting (3.18) into (3.17):

$$\frac{15}{16}P(|2|0| \rightarrow x) = \frac{5}{16}\delta(|0|0|, x) + \frac{1}{2}\delta(|0|1|, x) + \frac{1}{8}\delta(|1|0|) \quad (3.19)$$

Figure 3.6 shows the next two tree diagrams, from which $P(|2|1| \rightarrow x)$ can be calculated, as well as $P(|0|3| \rightarrow x)$. The latter is however only required as an intermittent active state which can be reached from $|2|1|$. $|0|3|$ can never be reached directly from a drive and thus if the system finds itself in the state $|0|3|$, we know that after the most recent drive, it must have found itself in the state $|2|1|$. From Figure 3.6 we can ascertain that

$$\begin{aligned} P(|2|1| \rightarrow x) &= \frac{1}{4}\delta(|0|1|, x) + \frac{1}{2} \left(\frac{1}{3}\delta(|0|0|, x) + \frac{8}{15}\delta(|1|0|, x) + \frac{2}{15}\delta(|0|1|, x) \right) + \frac{1}{4}P(|0|3| \rightarrow x) \\ P(|0|3| \rightarrow x) &= \frac{1}{4}\delta(|0|1|, x) + \frac{1}{2}\delta(|1|1|, x) + \frac{1}{4}P(|2|1| \rightarrow x) \end{aligned} \quad (3.20)$$

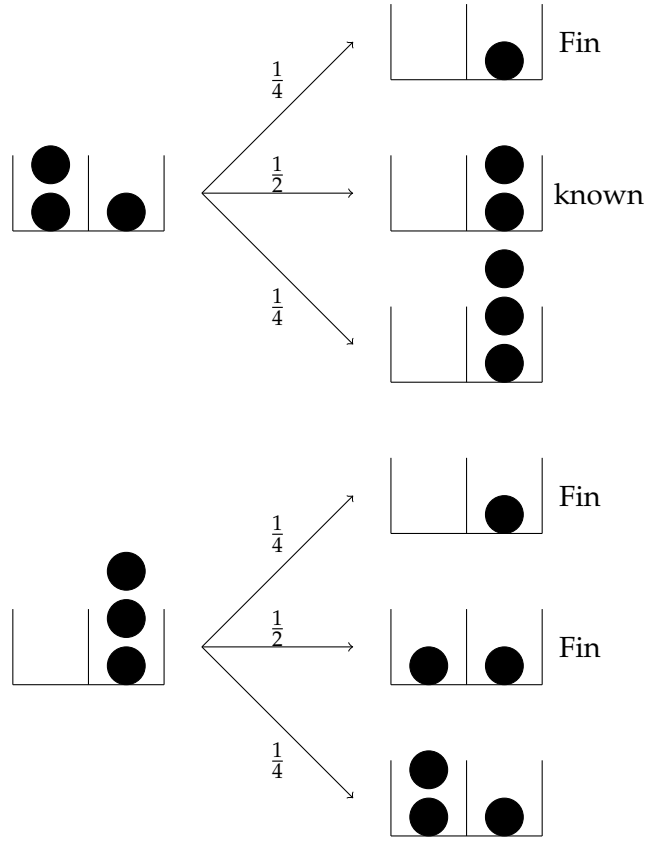


Figure 3.6.: A single iteration of microscopic time starting from $|2|1|$ and $|0|3|$ respectively. These two tree diagrams are quite clearly linked by the fact that each active state can transition into the other one. As in Figures 3.4 and 3.5, Fin denotes a relaxed state and "known" denotes a value we already know, as the tree diagram for the state $|0|2|$ has already been calculated.

Solving (3.20) simultaneously, one finds that

$$P(|2|1| \rightarrow x) = \frac{91}{225}\delta(|0|1|, x) + \frac{8}{45}\delta(|0|0|, x) + \frac{64}{225}\delta(|1|0|, x) + \frac{2}{15}\delta(|1|1|, x) \quad (3.21)$$

i.e., if after a drive, the system finds itself in the active state $|2|1|$, all four of the possible relaxed states are possible outcomes with their probabilities given by (3.21) (and reassuringly, they sum to unity). The expression for $P(|1|2| \rightarrow x)$ can be obtained similarly, or simply read off by symmetry.

As $P_{\alpha\beta}$ is defined as the probability of the system relaxing to state β given it is in state α immediately after a drive, we do not need to include any information about the states $|3|0|$ and $|0|3|$ in P , as these cannot be reached directly from a drive (we do however need to calculate their properties in order to determine those of, for example, $|2|1|$). There are four active states which can be reached by driving relaxed states, namely $|2|0|$, $|2|1|$, $|0|2|$ and $|1|2|$. A systematic way of labelling these states and thus determining their positions within transition matrices is required. This has already been used when presenting the information contained within (3.14). The relaxed states are ordered by their hash numbers in base 2, and the active states by their hash numbers in base 3 (for larger systems, a higher base will be required to label the active states).

Combining the information obtained from the tree diagrams, we see that

$$P = \begin{pmatrix} \frac{1}{3} & \frac{2}{15} & \frac{8}{15} & 0 \\ \frac{8}{45} & \frac{64}{225} & \frac{91}{225} & \frac{2}{15} \\ \frac{1}{3} & \frac{8}{15} & \frac{2}{15} & 0 \\ \frac{8}{45} & \frac{91}{225} & \frac{64}{225} & \frac{2}{15} \end{pmatrix} \quad (3.22)$$

Combining this with R_A and R_R , one finds the transition matrix

$$T = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \frac{1}{3} & \frac{2}{5} & \frac{8}{15} & 0 \\ 0 & 0 & 0 & 1 \\ \frac{8}{45} & \frac{64}{225} & \frac{91}{225} & \frac{2}{15} \end{pmatrix} \quad (3.23)$$

A slight subtlety is that it is the transpose (with all transposes henceforth denoted by the superscript "T") of T whose eigenvectors must be found. We want to find the state vector u , such that the probability of being in a

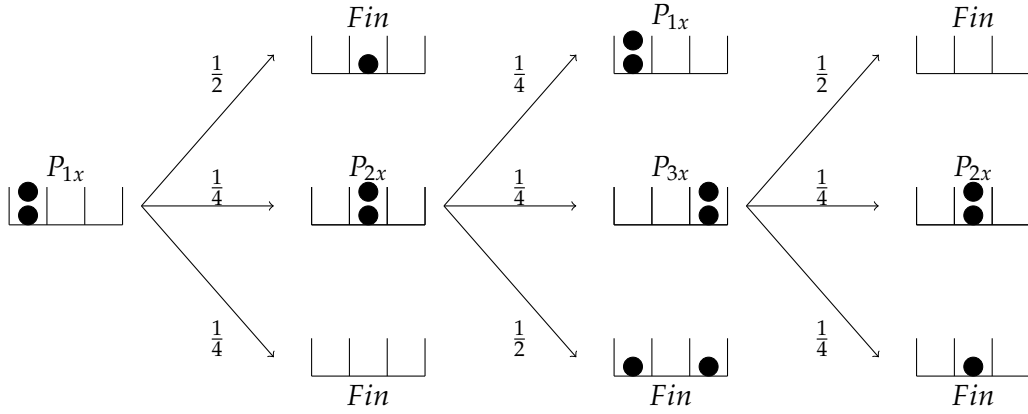


Figure 3.7.: The complete tree needed to calculate the row of the matrix P which gives the distribution of resulting relaxed states given the system finds itself in the active state $|2|0|0\rangle$ immediately after a drive.

state α after a drive, is the same as being in that same state before the drive. The probability of being in state α after a drive is given by

$$\sum_{\beta} u_{\beta} T_{\beta\alpha} \quad (3.24)$$

i.e. the sum over the probabilities of all of the possible states β the system could have been in before the drive multiplied by the probability of transitioning to state α . (3.24) however represents the matrix operation $T^T u$. This notational inconvenience arises due to the notion that $T_{\alpha\beta}$ should represent the probability of state α transitioning to state β and not vice versa, being for our purposes at odds with how matrix multiplication is defined.

Using MapleTM, the eigenvector with unity eigenvalue, normalised such that the sum of its entries equals unity, is given by

$$u = \begin{pmatrix} |0|0| \\ |1|0| \\ |0|1| \\ |1|1| \end{pmatrix} = \begin{pmatrix} \frac{7}{48} \\ \frac{13}{48} \\ \frac{13}{48} \\ \frac{15}{48} \end{pmatrix} \quad (3.25)$$

For a 3 site system however, the evaluation of such a tree diagram is already considerably more complex. Figure 3.7 contains all of the information required to generate the first (first because the hash of the active state

$|2|0|0|$ will be the lowest of any active state) row of the matrix P . Figure 3.7 generates the set of equations

$$\begin{aligned} P_{1x} &= \frac{1}{2}\delta(|0|1|0|, x) + \frac{1}{4}\delta(|0|0|0|, x) + \frac{1}{4}P_{2x} \\ P_{2x} &= \frac{1}{2}\delta(|1|0|1|, x) + \frac{1}{4}P_{1x} + \frac{1}{4}P_{3x} \\ P_{3x} &= \frac{1}{2}\delta(|0|0|0|, x) + \frac{1}{4}\delta(|0|1|0|, x) + \frac{1}{4}P_{2x} \end{aligned} \quad (3.26)$$

which can easily solved to give the statistical distribution of relaxed states based on the system being in the active state $|2|0|0|$ after a drive. Similar diagrams exist for other active states however the larger the number of active states that can be accessed from a given starting active state, the larger the set of linear equations which must be solved. For a 3 site system, when driving in the middle, the active state $|1|2|1|$ can be accessed by driving the system when in state $|1|1|1|$ and subsequently, the state $|2|0|2|$ can be accessed which is doubly active, making the evaluating of such a tree all the more difficult. Nonetheless, when driving from the left or right, the final result for the steady state is given by

$$u = \begin{pmatrix} |0|0|0| \\ |1|0|0| \\ |0|1|0| \\ |1|1|0| \\ |0|0|1| \\ |1|0|1| \\ |0|1|1| \\ |1|1|1| \end{pmatrix} = \begin{pmatrix} \frac{13}{392} \\ \frac{1}{16} \\ \frac{47}{392} \\ \frac{3}{16} \\ \frac{1}{16} \\ \frac{13}{98} \\ \frac{3}{16} \\ \frac{3}{14} \end{pmatrix} \quad (3.27)$$

and thus the result that the average density at either ends are equal holds, despite the fact we are driving on the left. The density at either end is equal to $\frac{117}{196}$. The average density in the centre is higher and equal to $\frac{139}{196}$. By symmetry the same result is obtained when driving from the right. An interesting result however is obtained when driving from the centre. The transition matrix T 's transpose has two eigenvectors with eigenvalues equal to

1.

$$u_1 = \begin{pmatrix} |0|0|0| \\ |1|0|0| \\ |0|1|0| \\ |1|1|0| \\ |0|0|1| \\ |1|0|1| \\ |0|1|1| \\ |1|1|1| \end{pmatrix} = \begin{pmatrix} \frac{13}{196} \\ 0 \\ \frac{47}{196} \\ 0 \\ 0 \\ \frac{13}{49} \\ 0 \\ \frac{3}{7} \end{pmatrix} \quad u_2 = \begin{pmatrix} 0 \\ \frac{1}{8} \\ 0 \\ \frac{3}{8} \\ \frac{1}{8} \\ 0 \\ \frac{3}{8} \\ 0 \end{pmatrix} \quad (3.28)$$

And consequently, either the density profile is $|\frac{34}{49}|\frac{131}{196}|\frac{34}{49}|$ or $|\frac{1}{2}|\frac{3}{4}|\frac{1}{2}|$, the former explaining the rather peculiar result we first observed in computational simulations that for the 3 site Manna Model, driving the centre results in a lower average density at the central site than at the edge sites, when starting from a completely empty or completely fully populated lattice. The two eigenvectors show that the system has two steady states, each inaccessible from the other and which one the system is in is based on initial conditions. By inspecting Figure 3.7, it can be seen that if the system is in active state $|0|2|0|$ after a drive, the final states it can relax to are all "even" in the sense that they are invariant under reflection about the middle site. Driving these resulting "even" relaxed states will eventually result in either the active state $|0|2|0|$ or $|1|2|1|$ being reached. A similar analysis to that of Figure 3.7 can be carried out for $|1|2|1|$ and it is found that likewise only even relaxed states can be reached from the active state $|1|2|1|$. If conversely, the system were in the relaxed state $|1|0|0|$, after two drives, it would be in the "odd" or "asymmetric" state $|1|2|0|$. A further tree diagram would show that the relaxed states that can be reached from the active state $|1|2|0|$ are themselves all odd or asymmetric.

Random Driving

The matrix P does not depend on where one drives the system, but the matrices R_R and R_A do. Consequently, three different matrices T are generated for the three site Manna Model. The T for deterministic driving is found by simply taking the sum $\frac{1}{3}(T_1 + T_2 + T_3)$. As driving from either edge site results in a steady state in which all relaxed states are accessible, we can conclude that the operator a_1 as previously defined, is a positive

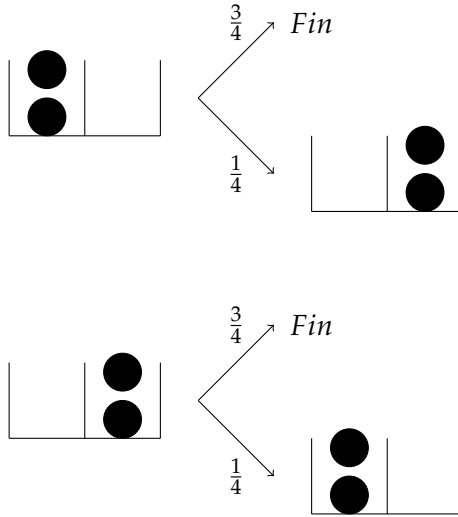


Figure 3.8.: The ways in which the active states $|2|0|$ and $|0|2|$ can relax via a single toppling or transition into another active state via such a toppling.

matrix. Consequently, as we have shown earlier, the steady state of the uniform driving operator a_u must be the same as that of a_1 and a_3 . Furthermore, note that this steady state is given by a linear combination of the two steady states of a_2 in which the coefficient of both is $\frac{1}{2}$.

3.3.1. Calculating Avalanche Size via the Tree Method

Using the notation that $A(|2|0|)$ represents the average number of topplings required for active state $|2|0|$ to fully relax, we see from Figure 3.8 that

$$\begin{aligned} A(|2|0|) &= \frac{3}{4} + \frac{1}{4} (1 + A(|0|2|)) \\ A(|0|2|) &= \frac{3}{4} + \frac{1}{4} (1 + A(|2|0|)) \end{aligned} \tag{3.29}$$

In words, (3.29) says that the average number of topplings required to fully relax state $|2|0|$ is $\frac{3}{4}$, i.e. the contribution of it relaxing directly, plus $\frac{1}{4}$ times $1 +$ the number of further topplings it will require to relax, should it transition to the active state $|0|2|$. Solving (3.29) simultaneously, one finds that

$A(|2|0|) = \frac{4}{3}$. A similar diagram to Figure 3.8 yields the equations

$$\begin{aligned} A(|2|1|) &= \frac{1}{4} + \frac{1}{2} (1 + A(|0|2|)) + \frac{1}{4} (1 + A(|0|3|)) \\ A(|0|3|) &= \frac{3}{4} + \frac{1}{4} (1 + A(|2|1|)) \end{aligned} \quad (3.30)$$

which after inserting the result for $A(|2|0|) = A(|0|2|)$ and solving simultaneously yields $A(|2|1|) = \frac{92}{45}$. For driving from the left, the steady state is given by (3.25). Thus the probability of an avalanche of size zero is $\frac{20}{48}$, i.e. the sum of the probabilities of the system being in states which remain relaxed when driven. If the system is in the state $|1|0|$ before driving, it will be in the active state $|2|0|$ afterwards and similarly $|1|1|$ will become $|2|1|$. Thus combining the steady state probabilities with the size of avalanches they will invoke upon driving, one finds the average avalanche size is given by

$$\langle Av \rangle = \frac{13}{48} \frac{4}{3} + \frac{5}{16} \frac{92}{45} = 1 \quad (3.31)$$

in agreement with Pruessner's result [71] of $\frac{1}{2} (2 + 1 - 1) = \frac{2}{2} (2 + 1 - 2) = 1$ for driving from the left and right respectively.

Similarly to when calculating the steady state of the 3 site Manna Model, the tree diagrams become considerably more complex. When driving at the centre, it becomes even more difficult as doubly active states can exist leading to considerably more branches in the tree diagram. For 3 sites, the result is just about tractable but beyond, more sophisticated techniques are needed. Thus the tree method, while appealing as it provides an intuitive graphical solution of the Manna Model, is of limited help beyond $L=3$. Furthermore, so far I have only been able to use it to calculate density profiles and avalanche sizes (and given the steady states, density-density correlations can easily be calculated as well). These are quantities evaluated after the system has fully relaxed and are insensitive to the details of the path taken to get there (in the case of avalanche size, it is the size of the avalanche, but not the nature of it which is calculated). To calculate properties resolved at microscopic time, it will be necessary to invoke the matrix method.

3.3.2. Sensitivity to Dynamics

When driving from the centre for $L=3$, the state $|1|2|1|$ can occur, which after one iteration of microscopic time can transition to $|2|0|2|$. In an even-odd sublattice dynamics, two sites are active at once, meaning in theory there are $3^2 = 9$ possible outcomes and thus 9 branches on our tree diagram. Some of these are degenerate, and it turns out there are only five, namely $|0|0|0|$, $|0|1|0|$, $|0|2|0|$, $|0|3|0|$ and $|0|4|0|$. Messy as this is, it does not fundamentally change how the tree method works as regards calculating the steady state and average avalanche size. Figure 3.1 shows the tree diagram of the active state $|2|0|2|$. The equation it generates (making use of symmetry to ascertain that $A(|4|0|0|) = A(|0|0|4|)$ etc.) is

$$A(|2|0|2|) = \frac{1}{16} (2 + A(|0|4|0|)) + \frac{1}{4} (2 + A(|0|3|0|)) + \frac{3}{8} (2 + A(|0|2|0|)) + 2 \cdot \frac{5}{16} \quad (3.32)$$

Drawing similar diagrams starting at $|0|4|0|$, $|0|3|0|$ and $|0|2|0|$ will generate a set of simultaneous equations facilitating the calculation of $\langle Av \rangle$. The difference between this calculation and that outlined in Figure 3.8 is the factors of 2 which need to be added to each branch calculation as each branch represents two topplings. As soon as states can be triply-active, as becomes the case for $L=5$, such states will incur considerably more complicated branching. If instead random sequential (Poissonian) dynamics are used, a different tree diagram (shown in Figure 3.2) is generated, which implies the equation (again making heavy use of symmetry)

$$A(|2|0|2|) = \frac{1}{4} (1 + A(|2|0|0|)) + \frac{1}{2} (1 + A(|2|1|0|)) + \frac{1}{4} (1 + A(|2|2|0|)) \quad (3.33)$$

Nonetheless, the final average avalanche size must remain insensitive to dynamics.

3.3.3. An Example of the Abelian Property

The tree method can be adapted to any dynamics including the type in which sites containing more than the threshold number of particles redistribute all of their particles, rather than redistributing only multiples of 2 (which is an Abelian dynamics [24]). Figure 3.9 shows how the active state $|3|0|$ can evolve during a single iteration of microscopic time in both

Abelian and non-Abelian dynamics. This provides a good example of the Abelian property. Consider an initially empty 2 site lattice, subsequently driven three times, twice at site 2 and once at site 1. Consider however, two different orders of driving, namely driving the second site twice, followed by the first $(2, 2, 1)$ and driving the first site, followed by the second site twice $(1, 2, 2)$. For the driving sequence $(2, 2, 1)$, the system will, after the first two drives find itself in state $|0|2\rangle$ which we know (in both Abelian and non-Abelian dynamics) can relax to $|0|0\rangle$, $|1|0\rangle$ or $|0|1\rangle$ with respective probabilities $\frac{1}{3}$, $\frac{8}{15}$ and $\frac{2}{15}$ (see Figures 3.4 and 3.5 for the relevant tree diagrams). After the final drive at site 1, the system can either be in relaxed states $|1|0\rangle$ or $|1|1\rangle$ with probabilities $\frac{1}{3}$ and $\frac{2}{15}$ respectively, or in the active state $|2|0\rangle$, whose relaxation probabilities are the mirror of those of $|0|2\rangle$. Combining this information, one finds that the driving sequence $(2, 2, 1)$ can result in the final states $|0|0\rangle, |1|0\rangle, |0|1\rangle, |1|1\rangle$ with respective probabilities $\frac{8}{45}, \frac{91}{225}, \frac{64}{225}$ and $\frac{2}{15}$. This distribution might look familiar to the reader, as up to a mirroring, these are the transition probabilities found in (3.21) for the active state $|2|1\rangle$ and thus represent the transition probabilities for the active state $|1|2\rangle$.

Considering instead the drive sequence $(1, 2, 2)$, the system only finds itself in an active state after the third and final drive, namely in the state $|1|2\rangle$ and thus the two drive sequences result in the same probability distribution of final relaxed states. (3.21) however was derived using Abelian dynamics. It can be seen however from Figure 3.9, that the active state $|3|0\rangle$, whose tree diagram is connected to that of $|1|2\rangle$, must be different in non-Abelian dynamics. The state $|3|0\rangle$ can in non-Abelian dynamics, only update to two relaxed states in one single update, namely $|0|0\rangle$ and $|0|1\rangle$. It can also update to the active states $|0|2\rangle$ and $|0|3\rangle$. States whose active sites all contain a number of particles divisible by two update in the same way in both Abelian and non-Abelian dynamics. Hence we already know the relaxation probabilities of $|0|2\rangle$ from Figure 3.5 and from here we can see that it cannot relax to $|1|1\rangle$. Thus by symmetry, $|0|3\rangle$ cannot relax to $|1|1\rangle$ and consequently, we know the active state $|1|2\rangle$ must have a different relaxation probability in Abelian and non-Abelian dynamics. In non-Abelian dynamics, the tree diagram gives the resulting possible states $|0|0\rangle, |1|0\rangle$ and $|0|1\rangle$ with probabilities $\frac{5}{21}, \frac{8}{21}$ and $\frac{8}{21}$ respectively, which in turn represents the possible outcomes of the drive sequence $(2, 2, 1)$ in non-Abelian

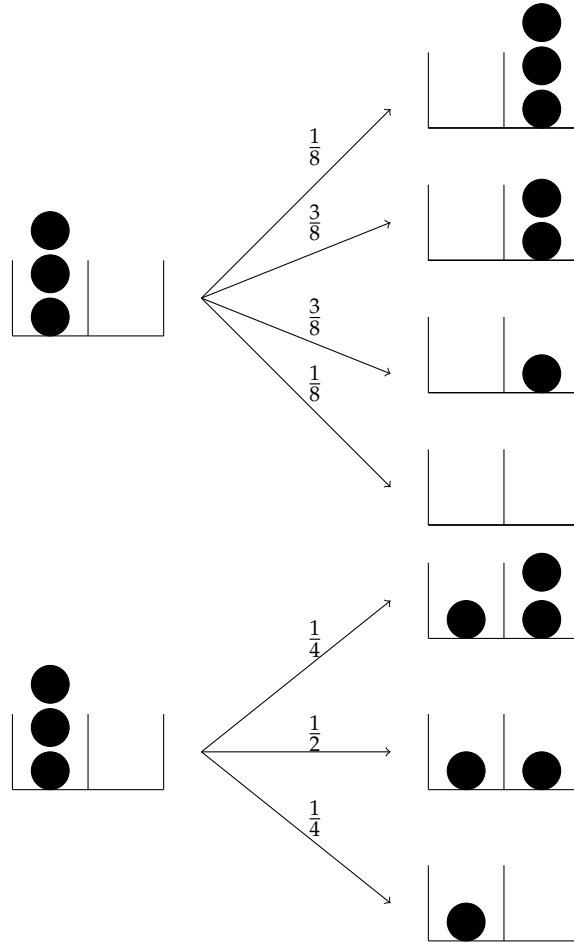


Figure 3.9.: The first branching of the relaxation of state $|3|0|$ for both non-Abelian (top) and Abelian (bottom) update dynamics.

dynamics.

Thus it has been demonstrated for a relatively simple example, that the so-called non-Abelian dynamics are indeed non-Abelian and that the order of driving will result in different final distributions of states.

3.4. The Matrix Method

The Matrix Method will allow us to calculate the steady state for, in principle, much larger systems although in practise it is also very limited by computational resources. As will become evident, despite making use of computational techniques, the method is inherently exact, provided libraries (in this case those used by MapleTM) are used which perform matrix manipulations in closed form, that is to say results are given in rational $\frac{p}{q}$ representation rather than floating point form. The matrix method relies heavily on the steady state of the system as well as the average avalanche size being insensitive to update dynamics. The matrix method can also be used to determine analytically, quantities resolved at microscopic time such as the activity. These results however will be sensitive to the dynamics used to update active states.

As was the case for the tree method, the matrix method will provide a way of determining the transition matrix T for which $T_{\alpha\beta}$ describes the probability of the system being in relaxed state β given it was in the relaxed state α before the most recent drive. Consider the four matrices: R_R , R_A , A_R and A_A which stand for relaxed-relaxed, relaxed-active, active-relaxed and active-active respectively. $(R_R)_{\alpha\beta}$ and $(R_A)_{\alpha\gamma}$ give the probability that if the system is initially in a relaxed state α , it is in a relaxed state β or an active state γ immediately after the drive, respectively (and are the same matrices discussed in Section 3.3). $(A_R)_{\alpha\beta}$ and $(A_A)_{\alpha\gamma}$ describe the probabilities that given the system is in a certain active state α at a microscopic time t , it will be in either the relaxed state β after one further iteration of microscopic time, or another active state γ respectively. In order to calculate the probability that the system ends up in a relaxed state β after a drive, having been in state α before it, one must take into account the possibility that this occurred via a drive directly, via the system having been excited and then having relaxed immediately into state β , the system having been excited, having transitioned into another active state and then relaxed to

state β and so forth. The system could in principle have relaxed to state β via any number of transient active states. Mathematically,

$$\begin{aligned} T_{\alpha\beta} = & (R_R)_{\alpha\beta} + \sum_{\gamma} (R_A)_{\alpha\gamma} (A_R)_{\gamma\beta} + \sum_{\gamma} (R_A)_{\alpha\gamma} \sum_{\delta} (A_A)_{\gamma\delta} (A_R)_{\delta\beta} \\ & + \sum_{\gamma} (R_A)_{\alpha\gamma} \sum_{\delta} (A_A)_{\gamma\delta} \sum_{\phi} (A_A)_{\delta\phi} (A_R)_{\phi\beta} \dots \end{aligned} \quad (3.34)$$

and thus

$$\begin{aligned} T &= R_R + R_A \cdot A_R + R_A \cdot A_A \cdot A_R + R_A \cdot A_A \cdot A_A \cdot A_R + \dots \\ T &= R_R + R_A \cdot \left(\sum_{n=0}^{\infty} A_A^n \right) \cdot A_R \end{aligned} \quad (3.35)$$

If one makes the assumption that sum on the RHS of (3.35) converges on the physical grounds that each consecutive term in this sum essentially represents the system relaxing via an increasing number of microscopic time iterations, and thus becomes eventually less and less probable due to particle loss at the boundaries, then this infinite geometric sum can be evaluated (in which $\mathcal{I}$ represents the identity matrix)

$$\begin{aligned} S &= \sum_{n=0}^{\infty} A_A^n \\ (\mathcal{I} - A_A) \sum_{n=0}^{\infty} A_A^n &= \lim_{N \rightarrow \infty} (\mathcal{I} - A_A^N) \\ \sum_{n=0}^{\infty} A_A^n &= (\mathcal{I} - A_A)^{-1} \end{aligned} \quad (3.36)$$

And thus

$$T = R_R + R_A \cdot (\mathcal{I} - A_A)^{-1} \cdot A_R \quad (3.37)$$

and as already seen, it is the eigenvector(s) of the transpose of T with eigenvalue unity which are of interest.

Avalanche Size

The following method of computing the average avalanche size is a relatively straight forward extension of the matrix method of calculating the steady state, if done so using a dynamics in which only one update ever

occurs simultaneously. To be precise, the following calculation is only feasible if an active state of the form $|0|4|0|$, i.e. one with a doubly active site also only updates one toppling at a time (and thus has possible outcomes $|2|2|0|$, $|1|2|1|$ and $|0|2|2|$ for this particular example). The reason for this is that it is convenient to write the average avalanche size $\langle Av \rangle$ as

$$\langle Av \rangle = \sum_{n=0}^{\infty} nP(n) \quad (3.38)$$

in which $P(n)$ is the probability of an avalanche of size n . If each iteration of microscopic time can involve multiple numbers of topplings however, calculating $P(n)$ becomes considerably more difficult. For example, for a system of size $L=5$, there exist states which are singly, doubly and triply active. Thus an avalanche of size three can occur as a series of three single topplings, a double toppling followed by a single and vice versa, or three simultaneous toppling events. Let us for now assume that each active state is only singly active (i.e. A_A describes the probabilities of transitions between active states subject to the restriction they involve a single toppling only). In that case, what is the probability of an avalanche of size n ? The probability of an avalanche of size zero is given by the probability of the system still being in a relaxed state after a drive, i.e.

$$P(0) = \sum_{\alpha} \sum_{\beta} u_{\alpha} (R_R)_{\alpha\beta} \quad (3.39)$$

in which the two sums run over all initial (α) and final (β) relaxed states the system can be in. The probability of the system relaxing after a single iteration of microscopic time is given by

$$P(1) = \sum_{\alpha} \sum_{\beta} u_{\alpha} \sum_{\gamma} (R_A)_{\alpha\gamma} (A_R)_{\gamma\beta} = \sum_{\alpha} \sum_{\beta} u_{\alpha} (R_A \cdot A_R)_{\alpha\beta} \quad (3.40)$$

in which γ is the label of the state the system is in immediately after the drive, and thus the sum over γ will only sum over one non-zero value for deterministic driving.

The probability of the system relaxing via one transient active state is

given by

$$P(2) = \sum_{\alpha} \sum_{\beta} u_{\alpha} \sum_{\gamma} (R_A)_{\alpha\gamma} \sum_{\delta} (A_A)_{\gamma\delta} (A_R)_{\delta\beta} = \sum_{\alpha} \sum_{\beta} u_{\alpha} (R_A \cdot A_A \cdot A_R)_{\alpha\beta} \quad (3.41)$$

and so forth, yielding the general expression for the n^{th} term

$$P(n) = \sum_{\alpha} \sum_{\beta} u_{\alpha} \left(R_A \cdot A_A^{n-1} \cdot A_R \right)_{\alpha\beta} = \sum_{\beta} \left(u^T \cdot R_A \cdot A_A^{n-1} \cdot A_R \right)_{\beta} \quad (3.42)$$

Hence evaluating (3.38),

$$\langle Av \rangle = \sum_{\beta} \left(u^T \cdot R_A \cdot \left(\sum_{n=0}^{\infty} (n+1) A_A^n \right) \cdot A_R \right)_{\beta} \quad (3.43)$$

The sum can be easily evaluated, if one assumes the solution I derived for $\sum_{n=0}^{\infty} A_A^n$ based on the fact that $\lim_{n \rightarrow \infty} A_A^n = 0$

$$\begin{aligned} S &= \sum_{n=0}^{\infty} (n+1) A_A^n \\ A_A \cdot S &= \sum_{n=0}^{\infty} (n+1) A_A^{n+1} = \sum_{n=0}^{\infty} n A_A^n \\ (\mathcal{I} - A_A) \cdot S &= \sum_{n=0}^{\infty} A_A^n = (\mathcal{I} - A_A)^{-1} \\ S &= (\mathcal{I} - A_A)^{-2} \end{aligned} \quad (3.44)$$

And thus the average avalanche size, $\langle Av \rangle$ is given by

$$\langle Av \rangle = \sum_{\beta} \left(u^T \cdot R_A \cdot (\mathcal{I} - A_A)^{-2} \cdot A_R \right)_{\beta} \quad (3.45)$$

While the average avalanche size is not sensitive to the dynamics used to update active states within the Abelian Manna Model, this derivation certainly is, in that it is only valid when the matrices A_A and A_R describe the probabilities of transitions which involve only one toppling at a time. The simplest such dynamics to implement computationally is to "scan an active state from the left" (or equivalently from the right) until the first active site is found, and update this site only. If this site is doubly-active, it must still be updated only once. Of course such a dynamics will yield asymmet-

ric results when calculating properties resolved at microscopic time such as the activity profile. Scanning from the left will cause for a left/right asymmetry, i.e. for the activity in general to be higher towards to the left for lower microscopic times as these updates tend to happen first, and for the activity towards the right of the system to pick up (relatively speaking) at a later microscopic time. One way to get around this is to scan from the left and the right, and find the site closest to a boundary (or equivalently furthest from a boundary) and use this to systematically decide which of the active sites to update. This will still however not result in the same response function as it will boost activity closer to the boundaries at earlier times and essentially accelerate the avalanche (although it will last longer as microscopic time now updates once per toppling).

Generating A_A and A_R computationally has proved considerably more challenging when allowing for multiply-active states. I have thus also implemented a variation on random sequential updates, in which the rule used to update an active state with more than one active site, is to choose a site at random to update. Crucially though, if this site is multiply active, it only redistributes two particles at each iteration of microscopic time. These dynamics will however still yield subtly different results to standard Poissonian dynamics in which if a site is selected to update, it fully relaxes. This difference will become greater for larger systems as states with multiply active sites begin to occur with a higher frequency.

The derivation of (3.45) is sensitive to dynamics, in that unlike the derivation for the response function (see Section 3.4.2 to follow), it does not only depend on the dynamics implicitly as A_A and A_R are determined by the dynamics, the actual derivation of (3.45) is limited to the case of allowing states to only be singly-active. An expression for the average avalanche size, which does not depend on the dynamics explicitly will be derived in Section 3.4.2.

3.4.1. Results Beyond $L=3$

Reassuringly, the matrix method reproduces the results found using the tree method for $L = 2$ and $L = 3$. With the current computational resources available to me, I have calculated the steady state for $L=4$ and $L=5$. Maple routines do facilitate the calculation of the aforementioned quantities of

interest as rational numbers, although the expressions are so cumbersome (the most simple fractions quickly become 10 digit numerators and denominators but the floating point representations are necessarily between 0 and 1) so I will quote the results in floating point form. Nonetheless, the only numerical approximation in this is my presentation of the results, there has been no further approximation in their calculation and thus the results should be regarded as "exact" .

The steady state result for L=4, like for L=2 does not depend on how the system is driven and is given by

$$u = \begin{pmatrix} |0|0|0|0| \\ |1|0|0|0| \\ |0|1|0|0| \\ |1|1|0|0| \\ |0|0|1|0| \\ |1|0|1|0| \\ |0|1|1|0| \\ |1|1|1|0| \\ |0|0|0|1| \\ |1|0|0|1| \\ |0|1|0|1| \\ |1|1|0|1| \\ |0|0|1|1| \\ |1|0|1|1| \\ |0|1|1|1| \\ |1|1|1|1| \end{pmatrix} = \begin{pmatrix} 0.005864224 \\ 0.011367798 \\ 0.026479042 \\ 0.043067961 \\ 0.026479042 \\ 0.052432017 \\ 0.098216025 \\ 0.134570678 \\ 0.011367798 \\ 0.01953125 \\ 0.052432017 \\ 0.092890368 \\ 0.043067961 \\ 0.092890368 \\ 0.134570678 \\ 0.154773312 \end{pmatrix} \quad (3.46)$$

Which results in the density profile $|0.60152348|0.7369981|0.7369981|0.60152348|$.

For the five site Manna Model, the density profile when driving from the far left, far right or centre is given by $|0.60287521|0.75029651|0.76970457|0.75029651|0.60287521|$.

When driving at the site directly left or right of centre however, the system has two stable modes, again depending on initial conditions. The density profiles are $|0.640804579|0.737242858|0.789128472|0.737242858|0.640804579|$ and $|0.564945842|0.763350165|0.750280663|0.763350165|0.564945842|$, again in line with the L=3 Manna Model in that it has two stable modes, one of which has a lower density at the central site than immediately to the left

or right. Likewise, the steady state vector when driving at the edges or the centre is equal to the superposition of the two steady states resulting from driving at sites 2 or 4, again with coefficients of $\frac{1}{2}$. Our numerics for larger systems appear to indicate that this trend continues, although the difference in density profiles between the two steady states (which only occur for odd system sizes) become negligible as the system size increases and thus we do not believe it is an effect we need to consider when modelling large systems.

Density-density correlations can be calculated exactly from the steady state as well. For example, to calculate $\langle \rho(1)\rho(2) \rangle - \langle \rho(1) \rangle \langle \rho(2) \rangle$, one must simply add up the probabilities of all relaxed states in which both sites 1 and 2 are simultaneously occupied which will give $\langle \rho(1)\rho(2) \rangle$ and then subtract off the already calculated $\langle \rho(1) \rangle$ and $\langle \rho(2) \rangle$. The correlations matrix DD in which $DD_{ij} = \langle \rho(i)\rho(j) \rangle - \langle \rho(i) \rangle \langle \rho(j) \rangle$, for $L=5$, driving from the extremities or the centre is given by

$$\begin{pmatrix} 0.239417 & -0.015852 & -0.008781 & -0.001563 & -0.000871 \\ -0.015852 & 0.1873517 & -0.019189 & -0.007335 & -0.001563 \\ -0.008781 & -0.019189 & 0.1772594 & -0.019189 & -0.008781 \\ -0.001563 & -0.007335 & -0.019189 & 0.187352 & -0.015852 \\ -0.000871 & -0.001563 & -0.008781 & -0.015852 & 0.239417 \end{pmatrix}$$

Using the same method, the correlation matrix can be found for driving off centre for both stable modes. The correlation matrices serve as a useful test of the code we have developed to investigate much larger systems and in particular is being used for an ongoing investigation of whether we are estimating our errors correctly.

3.4.2. Extending to Microscopic Time

Consider a further matrix, A , in which $A_{\alpha\beta}$ denotes the activity of the β^{th} site in active state α . Clearly the matrix A will depend on the dynamics used to update active states. Using the even-odd sublattice dynamics, for example $|2|0|2|$ will be doubly active and thus if the aforementioned state is labelled α , $A_{\alpha 1} = A_{\alpha 3} = 1$, $A_{\alpha 2} = 0$. Using the simplest dynamics to implement, i.e. scanning the lattice from the left to find the first active site, $A_{\alpha 1} = 1$, $A_{\alpha 2} = A_{\alpha 3} = 0$. Within the simplified random-sequential

dynamics, in which a given site can only be singly active, $A_{\alpha 1} = \frac{1}{2} = A_{\alpha 3}$, $A_{\alpha 2} = 0$. Note that in this dynamics, if the state $|0|4|0|$ is labelled β , $A_{\beta 2} = 1$.

Regardless of the form of A , the following method for calculating the response function $r(x, t)$ is valid, but the rules for updating an active state must be taken into account when generating the matrices A_A and A .

If $P_\beta(t)$ denotes the probability of the system being in an active state β , t microscopic time iterations after a drive, let us examine this for the first few iterations of microscopic time. For all of what follows, I denote the number of relaxed states by N and the number of active states by M . The number of relaxed states is simply 2^L as all L sites can either be occupied or unoccupied. In theory, M has an upper bound of $(L + 2)^L$ as the system's maximum population is $(L+1)$ and in theory, each site can contain anywhere from 0 to all $L + 1$ particles. This is however clearly a vast overestimate as if all $(L + 1)$ particles are on a given site, this uniquely determines the state. With this in mind, one could perform a complex analysis of the combinatorics to find a (smaller) theoretical upper bound by finding the number of states which have a population between 2 and $(L + 1)$ and have at least one active site, but this is in all probability also an overestimate of M as not all states can in general be reached. For this reason, we accept there will be some number of active states M , which we find by evolving all active states, finding which new active states can be reached and iterating the process until no further active states are generated. In the following derivation(s), I will denote whether a sum runs over all active states, or all relaxed states by explicitly adding the upper limit on the summations (with N implying relaxed and M implying active)

$$\begin{aligned}
P_\beta(0) &= \sum_{\alpha}^N u_{\alpha} (R_A)_{\alpha\beta} \\
P_\beta(1) &= \sum_{\alpha}^N u_{\alpha} \sum_{\gamma}^M (R_A)_{\alpha\gamma} (A_A)_{\gamma\beta} = \sum_{\alpha}^N (R_A \cdot A_A)_{\alpha\beta} \\
P_\beta(t) &= \sum_{\alpha}^N u_{\alpha} (R_A \cdot A_A^t)_{\alpha\beta}
\end{aligned} \tag{3.47}$$

Now that we know the probability of a state being in all of the allowed active states t time iterations after a drive, we sum these multiplied by the

activity of each state at a given position

$$r(x, t) = \sum_{\beta}^M P_{\beta}(t) A_{\beta x} = \sum_{\alpha}^N \sum_{\beta}^M u_{\alpha} (R_A \cdot A_A^t)_{\alpha\beta} A_{\beta x} \quad (3.48)$$

or in matrix form ¹

$$r(x, t) = \sum_{\beta}^M \left(u^T \cdot R_A \cdot A_A^t \right)_{\beta} A_{\beta x} = \left(u^T \cdot R_A \cdot A_A^t \cdot A \right)_x \quad (3.49)$$

In order to find the time integrated activity defined as in Section 3.2.8, it is necessary to sum the response function $r(x, t)$ over all times, i.e. $R(x) = \sum_{t=0}^{\infty} r(x, t)$.

$$R(x) = \sum_{t=0}^{\infty} \left(u^T \cdot R_A \cdot A_A^t \cdot A \right)_x = \left(u^T \cdot R_A \cdot (\mathcal{I} - A_A)^{-1} \cdot A \right)_x \quad (3.50)$$

By its very definition, if we sum over all positions, then $\sum_{x=1}^L R(x) = \langle Av \rangle$, i.e. we obtain the avalanche size. The sum over all positions x only affects A in (3.50) and thus if we define F , or the "full activity" of a state such that $F_{\beta} = \sum_x A_{\beta x}$, then

$$\langle Av \rangle = \sum_{\alpha}^M \left(u^T \cdot R_A \cdot (\mathcal{I} - A_A)^{-1} \right)_{\alpha} F_{\alpha} \quad (3.51)$$

For singly active states however, $F_{\alpha} = 1$ and consequently, the average avalanche size is simply the sum over the entries in the (transposed) vector

$$u^T \cdot R_A \cdot (\mathcal{I} - A_A)^{-1}$$

At first glance, it is in no way obvious that (3.51) and (3.45) are equivalent for any dynamics which only allows for singly active sites. Equating the

¹As an aside to clarify the following notation, the inconvenience can be traced back to the discussion in Section 3.3 of how the definition of matrix multiplication is at odds with how I have defined $T_{\alpha\beta}$. Rather than express the sum $\sum_{\gamma} \sum_{\delta} A_{\delta\gamma} B_{\gamma\alpha} u_{\delta}$ as $\sum_{\delta} (A \cdot B)_{\delta\alpha} u_{\delta} = \left[(A \cdot B)^T \cdot u \right]_{\alpha} = (B^T \cdot A^T \cdot u)_{\alpha}$ I will express this as $(u^T \cdot A \cdot B)_{\alpha}$

expressions, one obtains

$$\sum_{\beta}^M \left(u^T \cdot R_A \cdot (\mathcal{I} - A_A)^{-1} \right)_{\beta} = \sum_{\alpha}^N \left(u^T \cdot R_A \cdot (\mathcal{I} - A_A)^{-2} \cdot A_R \right)_{\alpha} \quad (3.52)$$

Rewriting the RHS as

$$\sum_{\alpha}^N \sum_{\beta}^M \left(u^T \cdot R_A \cdot (\mathcal{I} - A_A)^{-1} \right)_{\beta} \left((\mathcal{I} - A_A)^{-1} \cdot A_R \right)_{\beta\alpha}$$

it can be seen that in order for (3.52) to hold

$$\sum_{\alpha}^N \left((\mathcal{I} - A_A)^{-1} \cdot A_R \right)_{\beta\alpha} = 1 \quad (3.53)$$

It turns out however, that (3.53) is necessarily true, that is to say it does not provide us with any extra information. To see this, we follow a very similar procedure to that used to derive (3.45). The probability of the system relaxing to a state α , given that it is in a state β immediately after a drive, and doing so via a single iteration of microscopic time is given by $(A_R)_{\beta\alpha}$. As shown when deriving (3.45), the probability of a system transitioning from active state β to relaxed state α in n iterations of microscopic time is given by $(A_A^{n-1} \cdot A_R)_{\beta\alpha}$ and consequently, given the system finds itself in an active state β before a drive, the probability of it relaxing to a state α (via any path allowed) is given by $\left((\mathcal{I} - A_A)^{-1} \cdot A_R \right)_{\beta\alpha}$. Summing over all resulting relaxed states, and noting that the system must eventually find itself in one of the N relaxed states, we see indeed that (3.53) is in a sense almost trivial, it simply says that an active state must eventually relax.

Thus equating (3.45) and (3.51) does not provide us with any extra information, and as already stated, its validity is limited to certain dynamics. The two different forms of $\langle Av \rangle$ as given in (3.51), can be juxtaposed however, namely for dynamics which limit states to being singly active, and thus $F_{\alpha} = 1 \forall \alpha$, and those in which it is not. Let us label the two dynamics-dependent matrices A_A and R_A for the case of singly-active states, and A'_A and R'_A for a dynamics without this restriction (say even-odd sublattice). One then finds that (making use of the fact that the steady states must be

equal)

$$\sum_{\alpha}^M \sum_{\gamma}^N \left[R_A \cdot (\mathcal{I} - A_A)^{-1} \right]_{\gamma\alpha} = \sum_{\alpha}^{M'} \sum_{\gamma}^N \left[R'_A \cdot (\mathcal{I} - A'_A)^{-1} \right]_{\gamma\alpha} F_{\alpha} \quad (3.54)$$

in which the sums over active states in all probability run over different sets of active states as some states will be reachable via some dynamics and not by others. It is trivial to determine F_{α} for all active states, regardless of the dynamics but unfortunately, it is still not possible to rearrange (3.54) to give us expressions for A'_A and A'_R in terms of A_A , A_R and F . Thus it is not possible to generate A_A and A_R for simple dynamics and use the Abelian property to determine the equivalent matrices for more complicated dynamics.

3.5. Numerical Limitations of the Matrix Method

As already discussed, the number of relaxed states which in theory can exist scales as 2^L . Predicting the number of active states the system can find itself in, or even estimating a reasonable upper bound is no simple task. Consequently, this has been done by brute force, computationally. Figure 3.10 shows the result using a dynamics which involves scanning from the left. The result for simplified random-sequential dynamics does not differ substantially. When generating the transition matrices R_A and A_A , the active states are sorted by order of their hash number in base $L + 2$, for example for a system of size 5, it is necessary to count in base 7. Consequently the active state $|1|1|2|1|1|$ has a hash number of 2863. Note that it is necessary to invert a matrix of size $M \times M$. The process has so far been found to be hugely sensitive to numerical error when using floating point methods and thus using closed form methods has been necessary. Such routines (such as the ones used by Maple) are extremely computationally expensive and thus in practise, the procedure becomes infeasible very quickly. As M increases, A_A becomes increasingly sparse, especially when only one site is allowed to be updated per iteration of microscopic time. Using sparse matrix libraries in C/C++ is one avenue which has yet to be explored.

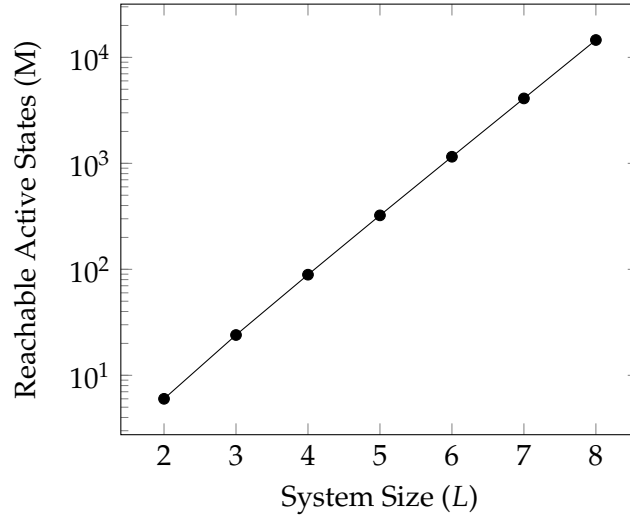


Figure 3.10.: The number of active states (M) reachable using dynamics which involve scanning the lattice from the left (and thus by symmetry equivalently from the right) and only updating the first active site found. The line connecting the data points is aesthetic only.

3.6. Concluding Remarks

3.6.1. Ongoing Work

Since the thesis was originally submitted, the algorithm used to generate transition matrices has been substantially improved and now supports the even-odd sublattice dynamics. This has resulted in accurate predictions for the response function, in particular the even-odd structure is observed, and our numerical simulations agree with with it. Furthermore, we have been pushing the matrix method to run for up to $L = 7$ to further investigate the multiple steady states of systems of sizes $L = 3, 5, 7$, especially to determine whether there are only 2, or whether in general, larger systems have more steady states.

The numerical studies which form the main body of the project have almost been completed in 1 dimension, and we are focussing our attention to higher dimensions, for which we currently have no analytic methods.

3.6.2. Key Findings

- Both the tree and matrix methods are powerful techniques for calculating the steady state and average avalanche size for the 1d Manna Model.
- Both methods quickly become intractable but computational techniques which use closed form methods can be applied to the matrix method, allowing somewhat larger systems to be studied.
- The matrix method can be extended to calculate quantities resolved at microscopic time, in particular the response function.
- The results from this section agree with our numerical simulations thus far, and explain some counter-intuitive results which emerged for small systems. Likewise it has been of use when estimating errors.
- $L = 7$ appears to be roughly the point at which even the matrix method stretches the limits of our computational resources (see Figure 3.10). Thus while a 2×2 lattice in 2 dimensions should still be within the realms of feasibility, the matrix method is going to be of limited use in dimensions higher than 1, limiting future applications of the techniques discussed within this chapter.

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A. $Q=3$ Categories

The following two pages show how the original 6 categories of the 3 state Potts model split into first 13 and subsequently 21 categories upon applying one and then two symmetry breaking external fields. The convention I have used (for algorithmic simplicity) is that the first field couples to spins in state $Q - 1$ and removes it from the Z_Q symmetry, leaving a Z_{Q-1} symmetry in place. The next field couples to spin species $Q - 2$ and so forth.

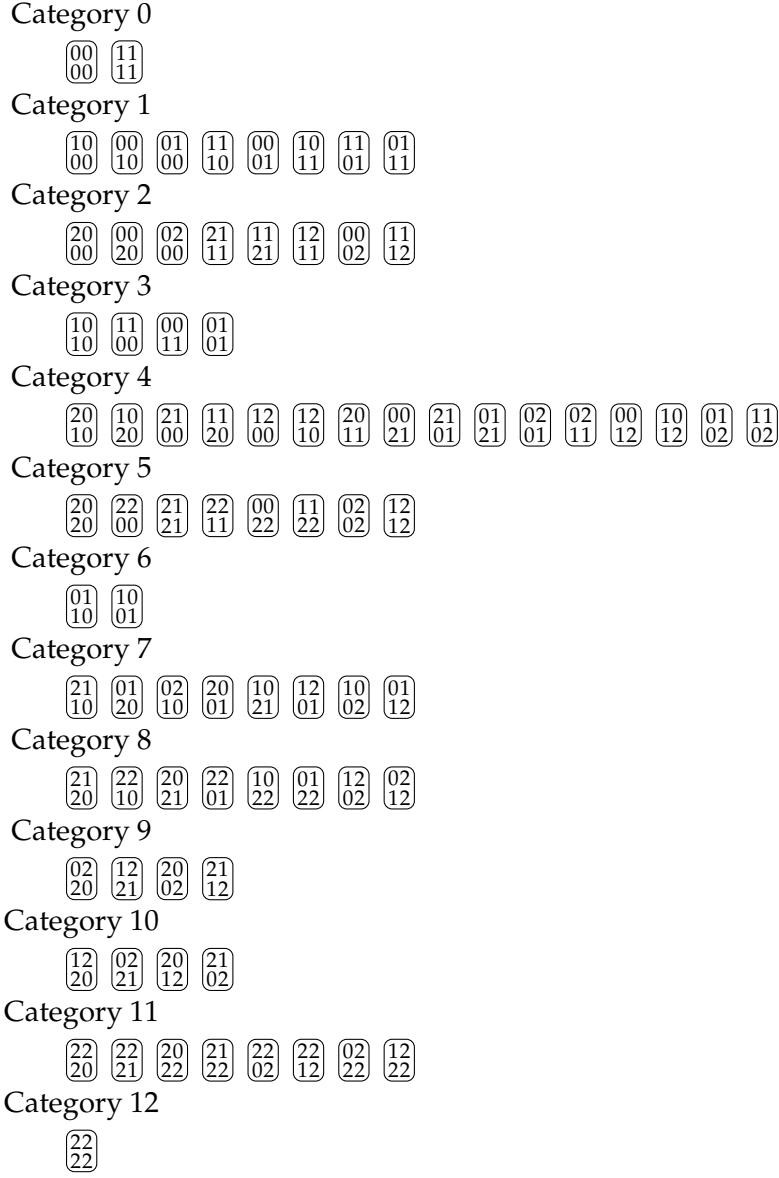


Figure A.1.: The 13 categories of the $Q = 3$ Potts Model in the presence of a single external field which couples to 2 spins. These (after a relabelling of $2 \rightarrow 0, 0 \rightarrow -1$) are also necessarily the categories of the BEG model.

Category 0	$\begin{pmatrix} 00 \\ 00 \end{pmatrix}$
Category 1	$\begin{pmatrix} 10 & 00 & 01 & 00 \\ 00 & 10 & 00 & 01 \end{pmatrix}$
Category 2	$\begin{pmatrix} 20 & 00 & 02 & 00 \\ 00 & 20 & 00 & 02 \end{pmatrix}$
Category 3	$\begin{pmatrix} 10 & 11 & 00 & 01 \\ 10 & 00 & 11 & 01 \end{pmatrix}$
Category 4	$\begin{pmatrix} 20 & 10 & 21 & 12 & 00 & 02 & 00 & 01 \\ 10 & 20 & 00 & 00 & 21 & 01 & 12 & 02 \end{pmatrix}$
Category 5	$\begin{pmatrix} 20 & 22 & 00 & 02 \\ 20 & 00 & 22 & 02 \end{pmatrix}$
Category 6	$\begin{pmatrix} 01 & 10 \\ 10 & 01 \end{pmatrix}$
Category 7	$\begin{pmatrix} 11 & 10 & 11 & 01 \\ 10 & 11 & 01 & 11 \end{pmatrix}$
Category 8	$\begin{pmatrix} 21 & 10 & 12 & 01 \\ 10 & 21 & 01 & 12 \end{pmatrix}$
Category 9	$\begin{pmatrix} 01 & 02 & 20 & 10 \\ 20 & 10 & 01 & 02 \end{pmatrix}$
Category 10	$\begin{pmatrix} 11 & 12 & 20 & 21 & 01 & 02 & 10 & 11 \\ 20 & 10 & 11 & 01 & 21 & 11 & 12 & 02 \end{pmatrix}$
Category 11	$\begin{pmatrix} 21 & 22 & 20 & 22 & 10 & 01 & 12 & 02 \\ 20 & 10 & 21 & 01 & 22 & 22 & 02 & 12 \end{pmatrix}$
Category 12	$\begin{pmatrix} 02 & 20 \\ 20 & 02 \end{pmatrix}$
Category 13	$\begin{pmatrix} 12 & 02 & 20 & 21 \\ 20 & 21 & 12 & 02 \end{pmatrix}$
Category 14	$\begin{pmatrix} 22 & 20 & 22 & 02 \\ 20 & 22 & 02 & 22 \end{pmatrix}$
Category 15	$\begin{pmatrix} 11 \\ 11 \end{pmatrix}$
Category 16	$\begin{pmatrix} 21 & 11 & 12 & 11 \\ 11 & 21 & 11 & 12 \end{pmatrix}$
Category 17	$\begin{pmatrix} 21 & 22 & 11 & 12 \\ 21 & 11 & 22 & 12 \end{pmatrix}$
Category 18	$\begin{pmatrix} 12 & 21 \\ 21 & 12 \end{pmatrix}$
Category 19	$\begin{pmatrix} 22 & 21 & 22 & 12 \\ 21 & 22 & 12 & 22 \end{pmatrix}$
Category 20	$\begin{pmatrix} 22 \\ 22 \end{pmatrix}$

Figure A.2.: The 21 Categories obtained when running the category generating algorithm for the 3 state Potts Model in the presence of two symmetry breaking fields.

B. 4-state Potts Model Categories

Here I show the original 7 categories of the 4-state Potts model, the split to 16 categories under the application of a single field, the 22 categories resulting from introducing a field which couples to 0 and 2 spins simultaneously, and finally the 13 categories of the $Q = 4$ clock model.

Category 0

00	11	22	33
00	11	22	33

Category 1

10	20	30	00	00	00	01	11	02	22	03	33	00	10	11	01
00	00	00	10	20	30	00	10	00	20	00	30	01	11	01	11
21	31	11	11	12	22	13	33	00	20	11	21	22	22	02	12
11	11	21	31	11	21	11	31	02	22	12	22	02	12	22	22
32	22	23	33	00	30	11	31	22	32	33	33	33	03	13	23
22	32	22	32	03	33	13	33	23	33	03	13	23	33	33	33

Category 2

10	20	30	11	22	33	00	01	21	31	22	33	00	11	02	12
10	20	30	00	00	00	11	01	21	31	11	11	22	22	02	12
32	33	00	11	22	03	13	23								
32	22	33	33	33	03	13	23								

Category 3

20	30	10	30	10	20	21	31	11	21	11	31	12	32	12	22
10	10	20	20	30	30	00	00	11	20	20	30	00	00	10	10
22	32	13	23	13	33	23	33	20	11	30	11	20	31	21	31
30	30	00	00	10	10	20	20	11	20	11	21	21	31	01	01
01	31	01	21	02	22	02	32	22	32	03	33	03	23	23	33
21	21	31	31	01	01	11	11	31	31	01	01	11	11	21	21
00	10	10	30	00	30	01	11	01	31	11	31	12	32	02	32
12	12	22	22	32	32	02	02	22	22	32	32	02	02	12	12
02	12	03	33	13	33	03	13	00	10	00	20	10	20	01	11
32	32	02	02	12	12	22	22	13	13	23	23	33	33	03	03
11	21	01	21	02	22	12	22	02	12	13	23	03	23	03	13
23	23	33	33	03	03	13	13	33	33	03	03	13	13	23	23

Category 4

01	02	03	10	12	13	20	21	23	30	31	32
10	20	30	01	21	31	02	12	32	03	13	23

Category 5

21	31	01	01	02	12	32	02	03	03	13	23	20	30	10	10
10	10	20	30	10	20	20	30	10	20	30	30	01	01	21	31
12	02	32	12	13	13	03	23	10	30	20	20	21	01	31	21
01	21	21	31	01	21	31	31	02	02	12	32	02	12	12	32
23	23	03	13	10	20	30	30	31	01	21	31	32	32	02	12
02	12	32	32	03	03	13	23	03	13	13	23	03	13	23	23

Category 6

31	21	32	12	23	13	30	20	32	02	23	03	30	10	31	01
20	30	10	30	10	20	21	31	01	31	01	21	12	32	02	32
13	03	20	10	21	01	12	02								
02	12	13	23	03	23	03	13								

Figure B.1.: How the 256 configurations split into 7 categories for the 4-state Potts Model in the absence of an external field.

Category 0

00	11	22
00	11	22

Category 1

10	20	00	00	01	11	02	22	00	10	11	01	21	11	12	22
00	00	10	20	00	11	00	20	01	11	01	11	21	11	12	22
00	20	11	21	22	22	02	12	02	12	02	12	02	12	02	12

Category 2

30	00	03	31	11	13	32	22	23	00	11	22
00	30	00	11	31	11	22	32	22	03	13	23

Category 3

10	20	11	22	00	01	21	22	00	11	02	12
10	20	00	00	11	01	21	21	22	11	02	12

Category 4

20	10	21	11	21	12	12	22	20	00	20	21	01	02	22	02
10	20	00	20	20	00	10	10	11	21	21	01	21	01	01	11
00	10	10	01	11	01	12	02	00	12	02	12	02	12	02	12

Category 5

30	30	10	20	31	11	32	22	13	23	13	23	30	00	31	31
10	20	30	30	00	30	00	30	00	00	10	20	11	31	01	21
01	21	32	22	03	03	23	23	30	00	31	11	32	32	02	12
31	31	11	31	01	11	21	21	22	32	22	32	02	12	32	32
03	13	03	13	00	10	00	20	01	11	11	21	02	22	12	22
02	12	22	22	13	13	23	23	03	03	23	23	03	03	13	13

Category 6

30	33	31	33	32	33	00	11	22	03	13	23
30	00	31	11	32	22	33	33	33	03	13	23

Category 7

01	02	10	12	20	21
10	20	01	21	02	12

Category 8

21	01	02	12	20	10	12	02	10	20	21	01
10	20	01	20	01	21	01	21	02	12	02	12

Category 9

31	01	32	02	03	03	30	10	32	12	13	13	30	20	31	21
10	30	20	30	10	20	01	31	21	31	01	21	02	32	12	32
23	23	10	20	01	21	02	12	02	12	02	12	02	12	02	12
02	12	03	03	13	13	23	23	03	03	23	23	03	03	13	13

Category 10

31	21	32	12	23	13	20	31	20	32	02	23	03	30	10	31	01
20	30	10	30	20	10	21	31	21	01	31	01	21	12	32	02	32
13	03	20	10	21	01	12	02	02	12	02	12	02	12	02	12	02
02	12	13	23	03	23	03	03	13	13	23	23	03	03	13	13	23

Category 11

31	32	33	33	30	32	33	33	30	31	33	33	10	20	01	21
30	30	10	20	31	31	01	21	32	32	02	12	33	33	33	33
02	12	13	23	03	23	03	23	03	03	23	23	03	03	13	13
33	33	03	03	13	13	23	23	03	03	23	23	03	03	13	13

Category 12

03	13	23	30	31	32
30	31	32	03	13	23

Category 13

13	23	03	23	03	13	30	30	31	31	32	32
30	30	31	31	32	32	13	23	03	23	03	13

Category 14

33	33	33	30	31	32	33	33	33	33	03	13	23
30	31	32	33	33	33	03	13	23	33	33	33	33

Category 15

33
33

Figure B.2.: The resultant 16 categories (c.f. 13 for the 3 state Potts model) when introducing one external field which couples to 2 spins.

Category 0

00	11	22	33
00	11	22	33

Category 1

10	30	00	00	01	11	03	33	00	10	11	01	21	11	12	22
00	00	10	30	00	11	00	30	01	11	01	11	21	11	12	22
11	21	22	12	32	22	23	33	00	30	22	32	33	33	03	23
12	22	12	22	22	32	22	32	03	33	23	33	03	23	33	33

Category 2

20	00	02	22	31	11	13	33	00	20	22	02	11	31	33	13
00	20	00	20	11	31	11	31	02	22	02	22	13	33	13	33

Category 3

10	30	11	33	00	01	21	22	11	12	32	33	00	22	03	23
10	30	00	00	11	01	21	11	22	12	32	32	00	33	03	23

Category 4

20	10	30	20	21	21	11	31	12	32	22	22	23	13	33	23
10	20	20	30	00	20	11	30	00	00	22	10	30	00	13	10
30	00	20	30	31	31	01	21	02	22	32	32	33	03	23	33
11	21	21	31	01	21	31	31	01	01	11	31	01	11	11	21
00	10	30	00	01	01	11	31	12	32	02	02	03	13	33	03
12	22	22	32	02	22	32	32	02	02	12	32	02	12	12	22
10	00	20	10	11	11	01	21	02	22	12	12	13	03	23	13
13	23	23	33	03	23	03	33	03	03	13	33	03	13	13	23

Category 5

30	10	31	11	12	32	13	33	20	00	21	01	02	22	03	23
10	30	00	20	10	30	00	20	11	31	01	21	11	31	01	21
10	30	11	31	32	12	33	13	00	20	01	21	22	02	23	03
12	32	02	22	12	32	02	22	13	33	03	23	13	33	03	23

Category 6

20	22	31	33	00	02	11	13
20	00	31	11	22	02	33	13

Category 7

01	03	10	12	21	23	30	32
10	30	01	21	12	32	03	23

Category 8

21	01	03	23	30	10	12	32	01	21	23	03	10	30	32	12
10	30	10	30	01	21	01	21	12	32	12	32	03	23	03	23

Category 9

31	01	02	12	32	02	03	13	20	10	02	12	13	13	03	23
10	20	10	20	20	30	20	30	01	31	21	31	01	21	31	31
10	30	20	20	21	31	23	13	20	30	31	01	21	31	32	02
02	02	12	32	02	12	02	32	03	13	03	13	13	23	13	23

Category 10

31	32	12	13	20	02	23	03	30	10	31	13	20	21	01	02
20	10	30	20	31	31	01	21	12	32	02	02	13	03	23	13

Category 11

21	23	30	32	01	03	10	12
30	10	21	01	32	12	23	03

Category 12

02	13	20	31
20	31	02	13

Figure B.4.: How the 256 configurations on a $Q=4$, 2×2 lattice split into 13 categories for the case of the 4-state clock model in the absence of any external field.

C. $\frac{N}{B} = 3$ Ising Model Categories

Category 0 :

000	111
000	111
000	111

Category 1 :

100 000 000	010 000 000	001 000 000	000 100 000	000 010 000	000 001 000	000 000 100	000 000 010	111 111 110	000 000 001
111 111 101	111 111 011	111 110 111	111 101 111	111 011 111	110 111 111	101 111 111	011 111 111		

Category 2 :

110 000 000	101 000 000	011 000 000	100 100 000	010 010 000	000 110 000	001 001 000	000 101 000	000 011 000	100 000 100
000 100 100	111 111 100	010 000 010	000 010 010	111 111 010	000 000 110	111 110 110	110 111 110	001 000 001	000 001 001
111 111 001	000 000 101	111 101 101	101 111 101	000 000 011	111 011 011	011 111 011	111 100 111	111 010 111	110 110 111
111 001 111	101 101 111	011 011 111	100 111 111	010 111 111	001 111 111				

Category 3 :

Figure 1 shows a 2x10 grid of boxes, each containing a 3x3 binary matrix. The matrices are arranged in two rows of five. The first row contains matrices with columns (111, 000, 111, 100, 010), (110, 001, 101, 011, 000), and (000, 001, 001, 011, 111). The second row contains matrices with columns (111, 000, 111, 111, 111) and (000, 111, 111, 111, 111).

Category 4 :

010 100 000	001 100 000	100 010 000	001 010 000	100 001 000	010 001 000	010 000 100	001 000 100	000 010 100	000 001 100
100 000 010	001 000 010	000 100 010	000 001 010	111 101 110	111 011 110	101 111 110	011 111 110	100 000 001	010 000 001
000 100 001	000 010 001	111 110 101	111 011 101	110 111 101	011 111 101	111 110 011	111 101 011	110 111 011	101 111 011
101 110 111	011 110 111	110 101 111	011 101 111	110 011 111	101 011 111				

Category 5 :

110 100 000	101 100 000	110 010 000	011 010 000	100 110 000	010 110 000	101 001 000	011 001 000	100 101 000	001 101 000
010 011 000	001 011 000	110 000 100	101 000 100	000 110 100	111 110 100	000 101 100	111 101 100	110 111 100	101 111 100
110 000 010	011 000 010	000 110 010	111 110 010	000 011 010	111 011 010	110 111 010	011 111 010	100 000 110	010 000 110
000 100 110	111 100 110	000 010 110	111 010 110	100 111 110	010 111 110	101 000 001	011 000 001	000 101 001	111 101 001
000 011 001	111 011 001	101 111 001	011 111 001	100 000 101	001 000 101	000 100 101	111 100 101	000 001 101	111 001 101
100 111 101	001 111 101	010 000 011	001 000 011	000 010 011	111 010 011	000 001 011	111 001 011	010 111 011	001 111 011
110 100 111	101 100 111	110 010 111	011 010 111	100 110 111	010 110 111	101 001 111	011 001 111	100 101 111	001 101 111
010 011 111	001 011 111								

Category 6 :

011 100 000	101 010 000	001 110 000	110 001 000	010 101 000	100 011 000	011 000 100	010 100 100	001 100 100	100 010 100
010 010 100	100 001 100	001 001 100	000 011 100	111 011 100	011 111 100	101 000 010	100 100 010	010 100 010	100 010 010
001 010 010	010 001 010	001 001 010	000 101 010	111 101 010	101 111 010	001 000 110	101 110 110	011 110 110	000 001 110
111 001 110	110 101 110	101 101 110	110 011 110	011 011 110	001 111 110	110 000 001	100 100 001	001 100 001	010 010 001
001 010 001	000 110 001	111 110 001	100 001 001	010 001 001	110 111 001	010 000 101	000 010 101	111 010 101	110 110 101
101 110 101	110 101 101	011 101 101	101 011 101	011 011 101	010 111 101	100 000 011	000 100 011	111 100 011	110 110 011
011 110 011	101 101 011	011 101 011	110 011 011	101 011 011	100 111 011	011 100 111	101 010 111	001 110 111	110 001 111
010 101 111	100 011 111								

Category 7 :

111 100 000	111 010 000	111 110 000	111 001 000	111 101 000	111 011 000	100 111 000	010 111 000	110 111 000	001 111 000
101 111 000	011 111 000	111 000 100	110 100 100	101 100 100	100 110 100	110 110 100	100 101 100	101 101 100	000 111 100
111 000 010	110 010 010	011 010 010	010 110 010	110 110 010	010 011 010	011 011 010	000 111 010	111 000 110	100 100 110
110 100 110	010 010 110	110 010 110	100 110 110	010 110 110	000 111 110	111 000 001	101 001 001	011 001 001	001 101 001
101 101 001	001 011 001	011 011 001	000 111 001	111 000 101	100 100 101	101 100 101	001 001 101	101 001 101	100 101 101
001 101 101	000 111 101	111 000 011	010 010 011	011 010 011	001 001 011	011 001 011	010 011 011	001 011 011	000 111 011
100 000 111	010 000 111	110 000 111	001 000 111	101 000 111	011 000 111	000 100 111	000 010 111	000 110 111	000 001 111
000 101 111	000 011 111								

Category 8 :

110 110 000	101 101 000	011 011 000	111 100 100	100 111 100	111 010 010	010 111 010	110 000 110	000 110 110	111 001 001
001 111 001	101 000 101	000 101 101	011 000 011	000 011 011	100 100 111	010 010 111	001 001 111		

Category 9 :

101 110 000	011 110 000	110 101 000	011 101 000	110 011 000	101 011 000	110 010 100	111 010 100	010 110 100	101 110 100
101 001 100	111 001 100	110 101 100	001 101 100	010 111 100	001 111 100	110 100 010	111 100 010	100 110 010	011 110 010
011 001 010	111 001 010	110 011 010	001 011 010	100 111 010	001 111 010	101 000 110	011 000 110	010 100 110	101 100 110
100 010 110	011 010 110	000 101 110	100 101 110	000 011 110	010 011 110	101 100 001	111 100 001	011 010 001	111 010 001
100 101 001	011 101 001	010 011 001	101 011 001	100 111 001	010 111 001	110 000 101	011 000 101	110 100 101	001 100 101
000 110 101	100 110 101	100 001 101	011 001 101	000 011 101	001 011 101	110 000 011	101 000 011	110 010 011	001 010 011
000 110 011	010 110 011	010 001 011	101 001 011	000 101 011	001 101 011	010 100 111	001 100 111	100 010 111	001 010 111
100 001 111	010 001 111								

Category 10 :

$\begin{pmatrix} 011 \\ 100 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 011 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 011 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 010 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 101 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 101 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 110 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 001 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 001 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 110 \\ 001 \end{pmatrix}$
$\begin{pmatrix} 001 \\ 110 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 001 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 010 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 010 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 101 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 100 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 100 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 011 \\ 011 \end{pmatrix}$		

Category 11 :

$\begin{pmatrix} 001 \\ 010 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 001 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 100 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 001 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 101 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 011 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 100 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 010 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 110 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 011 \\ 101 \end{pmatrix}$
$\begin{pmatrix} 101 \\ 110 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 101 \\ 011 \end{pmatrix}$								

Category 12 :

$\begin{pmatrix} 101 \\ 010 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 010 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 110 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 110 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 001 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 001 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 101 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 101 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 011 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 011 \\ 100 \end{pmatrix}$
$\begin{pmatrix} 001 \\ 011 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 011 \\ 100 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 100 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 100 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 110 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 110 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 001 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 001 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 101 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 101 \\ 010 \end{pmatrix}$
$\begin{pmatrix} 001 \\ 101 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 101 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 011 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 011 \\ 010 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 100 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 100 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 010 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 010 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 001 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 001 \\ 110 \end{pmatrix}$
$\begin{pmatrix} 101 \\ 001 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 001 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 101 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 101 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 011 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 011 \\ 110 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 100 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 100 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 010 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 010 \\ 001 \end{pmatrix}$
$\begin{pmatrix} 100 \\ 110 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 110 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 110 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 110 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 101 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 101 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 011 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 011 \\ 001 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 100 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 100 \\ 101 \end{pmatrix}$
$\begin{pmatrix} 100 \\ 010 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 010 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 010 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 011 \\ 010 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 110 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 110 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 001 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 001 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 011 \\ 101 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 011 \\ 101 \end{pmatrix}$
$\begin{pmatrix} 010 \\ 100 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 100 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 100 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 100 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 010 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 101 \\ 010 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 110 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 001 \\ 110 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 100 \\ 001 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 110 \\ 001 \\ 011 \end{pmatrix}$
$\begin{pmatrix} 100 \\ 101 \\ 011 \end{pmatrix}$	$\begin{pmatrix} 010 \\ 101 \\ 011 \end{pmatrix}$								

Figure C.1.: How the $2^9 = 512$ possible configurations of the Ising Model on a 3×3 lattice group into 13 categories based on parity, rotational, translational and mirroring symmetries. The same categorisation appears to arise by successively adding n-point interaction terms to (1.35).

D. A Commonly-Used Integral

The following integral is required to carry out the inverse Fourier Transform of the bulk correlation length and is not entirely trivial to evaluate

$$\int_{-\infty}^{\infty} \frac{e^{i\mathbf{k} \cdot \mathbf{r}}}{k^2 + q^2} d^3k \quad (\text{D.1})$$

This is best performed in spherical polar co-ordinates in which the volume element is $k^2 \sin \theta$ [73]. Furthermore the dot product in the exponential is given by $k|r| \cos \theta$ in which k is defined as $\sqrt{k_x^2 + k_y^2 + k_z^2}$. Thus the integral now reads

$$2\pi \int_0^{\infty} \frac{k^2}{k^2 + q^2} dk \int_0^{\pi} e^{ik|r| \cos \theta} \sin \theta d\theta \quad (\text{D.2})$$

which evaluates to

$$\frac{2\pi i}{|r|} \int_0^{\infty} dk \frac{k^2}{k^2 + q^2} \left(e^{-ik|r|} - e^{ik|r|} \right) \quad (\text{D.3})$$

which upon performing the substitution $k \rightarrow -k$ for the second term becomes

$$\frac{2\pi i}{|r|} \int_{-\infty}^{\infty} \frac{k}{k^2 + q^2} e^{-ik|r|} dk \quad (\text{D.4})$$

which is relatively straight-forward to solve by contour integral in the complex plane as it has two simple poles at $k = \pm iq$. The result is $-i\pi e^{-q|r|}$ and thus the original integral evaluates to

$$\frac{2\pi^2}{|r|} e^{-q|r|} \quad (\text{D.5})$$

E. A Further Integral

The following integral was used when deriving a rigorous generalisation of PB Eq 16:

$$\int_0^{2\pi} d\theta \sin^{2(N-k)} \theta \cos^{2k} \theta \quad (\text{E.1})$$

To evaluate this integral, I first evaluate

$$I_{2N} = \int_0^{2\pi} \sin^{2N} \theta d\theta \quad (\text{E.2})$$

by parts to obtain:

$$I_{2N} = \frac{2N-1}{2N} I_{2N-2} = \frac{(2N-1)!!}{(2N)!!} I_0 \quad (\text{E.3})$$

in which $(2a)!!$ is defined as $2 \cdot 4 \cdot 6 \dots (2a-2) \cdot 2a = (2 \cdot 1) \cdot (2 \cdot 2) \cdot (2 \cdot 3) \dots 2 \cdot (a-1) \cdot 2 \cdot a = 2^a a!$.

$(2N-1)$ however is odd so this trick will not work. Note that

$$(2N-1)!! = \frac{2N(2N-1)(2N-2)(2N-3)\dots}{(2N)(2N-2)(2N-4)} = \frac{(2N)!}{(2N)!!} \quad (\text{E.4})$$

and thus

$$I_{2N} = \frac{(2N)!}{N!!N!!} I_0 = \frac{(2N)!}{4^N N!N!} 2\pi = \binom{2N}{N} \frac{2\pi}{4^N} \quad (\text{E.5})$$

Thus we now tackle

$$J_k = \int_0^{2\pi} \sin^{2(N-k)} \theta \cos^{2k} \theta d\theta \quad (\text{E.6})$$

also integrating by parts to obtain

$$J_k = \frac{(2k-1)(2k-3)}{(2(N-k)+1)(2(N-k)+3)} J_{k-2} \quad (\text{E.7})$$

iterating this formula leads to the expression

$$J_k = \left(\frac{(2k)!(2(N-k))!}{(2N)!} \right) \left(\frac{N!}{k!(N-k)!} \right) J_0 \quad (\text{E.8})$$

Finally, inserting the expression already derived for J_0 , i.e. that for I_N , we obtain

$$\int_0^{2\pi} \sin^{2(N-k)} \theta \cos^{2k} \theta d\theta = \frac{\binom{N}{k}}{\binom{2N}{2k}} \binom{2N}{N} \frac{2\pi}{4^N} \quad (\text{E.9})$$

F. ELGW Results within the DP Model

I have a substantial amount of results for the ELGW model, the calculation of which constituted a substantial part of my PhD but which do not fit in well with the discussion of the wave-vector dependent surface tension. To reiterate, I have defined the ELGW Hamiltonian as

$$H[m] = \int d^d r \left[\frac{g_4}{2} (\nabla^2)^2 + \frac{g_2}{2} (\nabla m)^2 + f(m) \right] \quad (\text{F.1})$$

in which the constant g_2 can be set to unity for easier comparison with results from square gradient theory.

A key feature of the ELGW model is that it splits up into two regimes of solution, one in which the bulk correlation function is monotonically decaying as in the LGW model, and one in which it is of the form of an oscillation modulated by an exponential decay. This is summed up by the Fourier Transform of the bulk correlation function being given by

$$\tilde{g}(q) = \frac{k_B T}{g_4} \frac{1}{(q^2 + a_1)(q^2 + a_2)} \quad (\text{F.2})$$

in which

$$a_{1,2} = \frac{g_2}{2g_4} \pm \sqrt{\frac{g_2^2}{4g_4^2} - \frac{\kappa^2}{g_4}} \quad (\text{F.3})$$

and thus, $a_{1,2}$ become complex depending on whether $g_4 > \frac{g_2^2}{4\kappa^2} = g_{4,crit}$. For values of g_4 smaller than $g_{4,crit}$, $a_{1,2}$ are purely real (and it turns out, positive) and thus the bulk correlation function is simply the sum of two exponentials, each with a different characteristic length. For $g_4 > g_{4,crit}$, there are also two characteristic length scales, one of them the length over which the modulating exponential decays and one the wave-vector of the oscillations. When $g_4 = g_{4,crit}$, the two length scales in either regime be-

come the same and (F.2) incurs a double pole. In general, the quantities calculated for $g_4 = g_{4,crit}$ are remarkably similar to those of square gradient theory with an effective inverse bulk correlation length proportional to κ . In ELGW theory, the bulk correlation function does not diverge as $|r| \rightarrow 0$, a result which should not be taken too seriously as continuum models cease to make sense at length scales below the lattice spacing. It will be more useful to quote the partially Fourier Transformed bulk correlation functions

$$\begin{aligned}
G^{g_4 < g_{4,crit}}(z_1, z_2; q) &= \frac{1}{4g_4\gamma_\kappa} \left[\frac{e^{-\sqrt{q^2 + \frac{g_2^2}{2g_4} - \gamma_\kappa}|z_1 - z_2|}}{\sqrt{q^2 + \frac{g_2^2}{2g_4} - \gamma_\kappa}} - \frac{e^{-\sqrt{q^2 + \frac{g_2^2}{2g_4} + \gamma_\kappa}|z_1 - z_2|}}{\sqrt{q^2 + \frac{g_2^2}{2g_4} + \gamma_\kappa}} \right] \\
G^{g_4 = g_{4,crit}}(z_1, z_2; q) &= \frac{\kappa^2}{g_2^2 \left(q^2 + \frac{2\kappa^2}{g_2} \right)} \left(\sqrt{\frac{2\kappa^2}{g_2} + q^2|z_1 - z_2| + 1} \right) e^{-\sqrt{\frac{2\kappa^2}{g_2} + q^2}|z_1 - z_2|} \\
G^{g_4 > g_{4,crit}}(z_1, z_2; q) &= \frac{1}{4g_4\gamma_\kappa} \frac{e^{-\beta_+|z_1 - z_2|}}{\sqrt{\left(\frac{g_2^2}{2g_4} + q^2 \right)^2 + \gamma_\kappa^2}} (\beta_+ \sin(\beta_-|z_1 - z_2|) + \beta_- \cos(\beta_-|z_1 - z_2|)) \\
\beta_\pm &= \frac{\sqrt{\sqrt{\left(\frac{g_2^2}{2g_4} + q^2 \right)^2 + \gamma_\kappa^2} \pm \left(\frac{g_2^2}{2g_4} + q^2 \right)}}{2}
\end{aligned} \tag{F.4}$$

in which $k_B T$ has been set to unity and γ_κ is defined as $\sqrt{\frac{g_2^2}{4g_4^2} - \frac{\kappa^2}{g_4}}$ for $g_4 < g_{4,crit}$ and $\sqrt{\frac{\kappa^2}{g_4} - \frac{g_2^2}{4g_4^2}}$ otherwise. The quantity γ_κ was introduced as it tends to zero as $g_4 \rightarrow g_{4,crit}^\pm$ and thus one can expand in small γ_κ to probe the effect of approaching $g_{4,crit}$ from above or below. It should be noted that in general however, it is systems near the critical point which are of interest and thus κ will be small. Consequently, it seems safe to assume we are generally in the regime $g_4 < g_{4,crit}$ although all results will be included for academic completeness.

F.1. Magnetisation Profile

The magnetisation profile breaks into the same three regimes of solution as the bulk correlation function. For $g_4 < g_{4,crit}$, δm decays monotonically

either side of $m = 0$, as the sum of two exponentials with different characteristic lengths (the same ones as found in the bulk correlation function). For $g_4 > g_{4,crit}$, δm decays away from the interface as a trigonometric oscillation modulated by an exponential function. The profile is given by

$$\begin{aligned}
\delta m^{g_4 < g_{4,crit}}(z) &= -\frac{m_0}{2\gamma_\kappa} \left(\left(\frac{g_2}{2g_4} + \gamma_\kappa \right) e^{-\sqrt{\frac{g_2}{2g_4} - \gamma_\kappa} z} - \left(\frac{g_2}{2g_4} - \gamma_\kappa \right) e^{-\sqrt{\frac{g_2}{2g_4} + \gamma_\kappa} z} \right) \\
\delta m^{g_4 > g_{4,crit}}(z) &= -\frac{m_0}{2} \sqrt{\frac{g_2}{2g_4}} z e^{-\sqrt{\frac{g_2}{2g_4}} z} + m_0 e^{-\sqrt{\frac{g_2}{2g_4}} z} \\
\delta m^{g_4 = g_{4,crit}}(z) &= -m_0 e^{-Az} \left(\cos(Bz) + \frac{A^2 - B^2}{2AB} \sin(Bz) \right) \\
A, B &= \left(\frac{\kappa^2}{g_4} \right)^{\frac{1}{4}} \sqrt{\frac{1 \pm \frac{g_2}{2\kappa\sqrt{g_4}}}{2}}
\end{aligned} \tag{F.5}$$

for $z > 0$ and similarly for $z < 0$. To calculate the $\tilde{\Lambda}(z; q)$ functions, it is only the derivatives one needs, and they are given by

$$\begin{aligned}
(\delta m^{g_4 < g_{4,crit}})' &= \frac{m_0}{2\gamma_\kappa} \sqrt{\frac{\kappa^2}{g_4}} \left(\sqrt{\frac{g_2}{2g_4} - \gamma_\kappa} e^{-\sqrt{\frac{g_2}{2g_4} + \gamma_\kappa} |z|} - \sqrt{\frac{g_2}{2g_4} + \gamma_\kappa} e^{-\sqrt{\frac{g_2}{2g_4} - \gamma_\kappa} |z|} \right) \\
(\delta m^{g_4 = g_{4,crit}})' &= \frac{m_0}{2} \sqrt{\frac{g_2}{2g_4}} e^{-\sqrt{\frac{g_2}{2g_4}} |z|} \left(1 + |z| \sqrt{\frac{g_2}{2g_4}} \right) \\
(\delta m^{g_4 > g_{4,crit}})' &= \frac{m_0}{2AB} \sqrt{\frac{\kappa^2}{g_4}} e^{-A|z|} [B \cos(Bz) + A \sin(Bz)]
\end{aligned} \tag{F.6}$$

F.2. Calculating $\tilde{\Lambda}(z; q)$

$m_\Xi(\underline{r})$ is defined as in square gradient theory, and thus the equivalent equation to (2.53) reads

$$\left[g_4 \frac{\partial^4}{\partial z^4} - 2g_4 q^2 \frac{\partial^2}{\partial z^2} + g_4 q^4 - g_2 \frac{\partial^2}{\partial z^2} + g_2 q^2 + f''(m_\pi) \right] \tilde{\Lambda}(z; q) = 0 \tag{F.7}$$

Unsurprisingly, (F.7) likewise splits into three regimes of solution, that of monotonic exponential decay, that of oscillation modulated by an exponential and the critical value of g_4 at which the behaviour switches. The algebra gets over more messy from here on in and consequently more ab-

breviations will be used. For $g_4 < g_{4,crit}$, I found

$$\tilde{\Lambda}(z; q) = \frac{\sqrt{\Lambda_+} - \sqrt{\Lambda_-}}{\sqrt{\Lambda_- + q^2} - \sqrt{\Lambda_+ + q^2}} \sqrt{\frac{\kappa^2}{g_4} \frac{m_0}{2\gamma_\kappa}} \left(\sqrt{\Lambda_+ + q^2} e^{-\sqrt{\Lambda_- + q^2}|z|} - \sqrt{\Lambda_- + q^2} e^{-\sqrt{\Lambda_+ + q^2}|z|} \right) \quad (\text{F.8})$$

in which $\Lambda_\pm = \frac{g_2}{2g_4} \pm \gamma_\kappa$.

When $g_4 = g_{4,crit}$,

$$\tilde{\Lambda}(z; q) = -\frac{m_0}{2} \sqrt{\frac{g_2}{2g_4}} e^{-\sqrt{\frac{g_2}{2g_4} + q^2}|z|} \left(1 + \sqrt{\frac{g_2}{2g_4} + q^2}|z| \right) \quad (\text{F.9})$$

and for completeness' sake, when $g_4 > g_{4,crit}$

$$\tilde{\Lambda}(z; q) = -\frac{m_0}{2} \sqrt{\frac{\kappa^2}{g_4} \frac{1}{A}} \left(\cos(\beta_- z) + \frac{\beta_+}{\beta_-} \sin(\beta_- |z|) \right) e^{-\beta_+ |z|} \quad (\text{F.10})$$

in which A and $\beta_\pm$ have been defined in (F.5) and (F.4).

F.3. Calculating the Bending Rigidity

The purpose of this project initially was simply to show that the bending rigidity does in fact vanish as the critical point is approached. This was initially done using a moments approach as presented originally in PB [65]. I showed that in an ELGW model, the rigidity is given by

$$\gamma = \int_{-\infty}^{+\infty} dz \left[g_4 m'^2(z) - g_2 m'(z) \tilde{\Lambda}_2(z) + 2g_4 \Lambda_2(z) m'''(z) \right] \quad (\text{F.11})$$

More recently, I showed (2.147) and thus that the rigidity can be calculated without performing any integrals. I have however not yet evaluated (2.147)

so I will quote the result I obtained using (F.11) for $g_4 < g_{4,crit}$

$$\begin{aligned} \gamma = & \frac{m_0^2 \kappa^2}{2\gamma_\kappa^2} \left[\frac{\Lambda_+^{\frac{3}{2}} + \Lambda_-^{\frac{3}{2}}}{2\sqrt{\frac{\kappa^2}{g_4}}} - 2\sqrt{\frac{\kappa^2}{g_4}} \frac{1}{\sqrt{\Lambda_+} + \sqrt{\Lambda_-}} \right] \\ & - \frac{g_2 m_0^2}{4\gamma_\kappa^2} \left((\sqrt{\Lambda_+} + \sqrt{\Lambda_-}) \sqrt{\frac{\kappa^2}{g_4}} \left(1 - \frac{g_2}{2\kappa\sqrt{g_4}} \right) - \frac{\kappa^2}{2g_4\gamma_\kappa} (\sqrt{\Lambda_+} - \sqrt{\Lambda_-}) + \frac{\Lambda_+^{\frac{5}{2}} + \Lambda_-^{\frac{5}{2}}}{4\sqrt{\frac{\kappa^2}{g_4}}} \right) \\ & + \frac{m_0^2 \kappa^2}{2\gamma_\kappa^2} \left(\Lambda_+^{\frac{3}{2}} + \Lambda_-^{\frac{3}{2}} \right) \left(\frac{1}{4\sqrt{\frac{\kappa^2}{g_4}}} - \frac{1}{(\sqrt{\Lambda_+} + \sqrt{\Lambda_-})^2} \right) \end{aligned} \quad (F.12)$$

It should come as no surprise, that in the limit $g_4 \rightarrow 0$, one regains the square gradient theory result $\gamma = -\frac{m_0^2 g_2^{\frac{3}{2}}}{4\kappa}$. A less obvious result is that in the limit of $\kappa \rightarrow 0$, all g_4 dependence drops out of (F.12) and exactly the same expression is regained. Thus as the critical point is approached, the Laplacian-squared term in the Hamiltonian has no effect on the rigidity and the rigidity goes as $\frac{\sigma}{\kappa^2}$. Clearly this invalidates Blokhuis' result [12, 13] that the rigidity vanishes with the same critical exponent as the surface tension.

When $g_4 = g_{4,crit}$, the rigidity becomes

$$\gamma = \frac{3}{16\sqrt{2}} \frac{m_0^2 g_2^{\frac{3}{2}}}{\kappa} \quad (F.13)$$

which has the expected behaviour of being similar to square gradient theory with an effective inverse bulk correlation length proportional to κ . Interestingly however, the bending rigidity has become positive. In square gradient theory it is constrained to be negative, because setting $g_4 = 0$ in (F.11) yields an inherently negative quantity. A result of this, is that there must exist a special (κ , and thus temperature dependent) g_4 , say g_4^* for which the bending rigidity vanishes. g_4^* is apparently not related to $g_{4,crit}$. Figure F.1 shows this transition for units in which $m_0 = \kappa = g_2 = 1$, in which $g_{4,crit} = \frac{1}{4}$. While it may appear from the plot that $g_4^* = \frac{g_{4,crit}}{2}$, this is not the case. Similar plots are obtained when varying κ that show g_4^* is roughly on the middle of the range for $0 \leq g_4 \leq g_{4,crit}$ although not exactly.

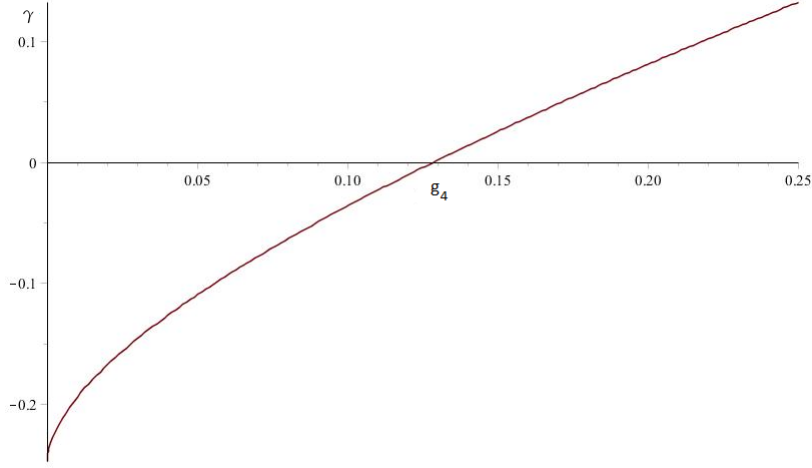


Figure F.1.: The rigidity (in units of $m_0 = \kappa = g_2 = 1$) in the region $g_4 < g_{4,crit}$. Note that for $g_4 \rightarrow 0$, the rigidity approaches $-\frac{1}{4}$, the square gradient theory result and likewise as $g_4 \rightarrow g_{4,crit}^-$, the rigidity tends to $\frac{3}{16\sqrt{2}}$, the result derived in (F.13).

F.4. Wave-Vector Dependent Surface Tension

As mentioned in Section F.3, the calculations for the ELGW model were done before I had proved that $\sigma(q)$ is a local property of the interface not requiring the evaluation of integrals. I had previously calculated it as follows.

Firstly, I showed that $G(0,0;q) = \mathcal{G}(0,0;q)$ as has held up robustly before and thus

$$\sigma(q) = \frac{\tilde{\Lambda}(0;q)\tilde{\Lambda}(0;q)}{\mathcal{G}(0,0;q)q^2} = \frac{(m'_\pi(0))^2}{q^2\mathcal{G}(0,0;q)} \quad (\text{F.14})$$

Next, it is possible to show, by multiplying the OZ by $m'_\pi(z)$ and integrating over all z , that

$$q^2 \int_{-\infty}^{+\infty} dz [g_2 m'_\pi(z) - 2g_4 m'''_\pi(z) + g_4 q^2 m'_\pi(z)] \mathcal{G}(0,z;q) = m'(0)$$

and thus, using $\mathcal{G}(0, z; q) = -\frac{\mathcal{G}(0, 0; q)}{m'_\pi(0)} \tilde{\Lambda}(z; q)$:

$$q^2 \int_{-\infty}^{+\infty} dz [g_2 m'_\pi(z) - 2g_4 m'''_\pi(z) + g_4 q^2 m'_\pi(z)] \mathcal{G}(0, 0; q) \tilde{\Lambda}(z; q) = - (m'_\pi(0))^2 \quad (\text{F.15})$$

or

$$\mathcal{G}(0, 0; q) = \frac{-(m'_\pi(0))^2}{q^2 \int_{-\infty}^{+\infty} dz [g_2 m'_\pi(z) - 2g_4 m'''_\pi(z) + g_4 q^2 m'_\pi(z)] \tilde{\Lambda}(z; q)} \quad (\text{F.16})$$

And hence it can be read off that

$$\sigma(q) = \int_{-\infty}^{+\infty} [g_2 \tilde{\Lambda}_0(z) - 2g_4 \tilde{\Lambda}_0''(z) + g_4 q^2 \tilde{\Lambda}_0(z)] \tilde{\Lambda}(z; q) \quad (\text{F.17})$$

(F.17) is a non-local expression for the wave-vector dependent surface tension, which I believe to be equivalent to the local expression (2.147), in which the equality could be shown by a similar proof to that which I used to show the equivalence of the non-local (2.84) and local (2.73) expressions in square-gradient theory. To do this however, it would first be necessary to derive a recursive relationship for the moments of $\tilde{\Lambda}(z; q)$.