Quantum Entanglement in Random Antiferromagnetic Spin Chains

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A SENIOR THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF
Bachelor of Arts in Physics
at Princeton University

2003

Honor Code Pledge
This paper represents my own work in accordance with University regulations.
Abstract

Classical continuous phase transitions are in a sense “driven” by the emergence of long-ranged correlations in the order parameter field at the critical point. It seems logical that phase transitions which are uniquely quantum mechanical in nature would be driven by a uniquely quantum mechanical extension of the classical correlation function, and in the past few years several researchers, thinking along these lines, have investigated the role quantum mechanical entanglement might play in quantum phase transitions.

In this thesis, we calculate the behavior of an entanglement measure for an infinite family of quantum critical points in random Heisenberg spin chains. The randomness works to our advantage both in simplifying the entanglement structure of the ground state (though not to a trivial extent) and in simplifying the mathematical apparatus necessary for performing the calculation (unfortunately, also not to a trivial extent. Connections are made to a recent conjecture about the behavior of entanglement under renormalization group flows.
Acknowledgements

First off, I’d like to thank my parents for supporting and encouraging me throughout my college career. Next in line is my advisor, professor Huse, who exercised what must surely be the patience of a saint when I continued to miss some glaringly obvious point several weeks in a row. Finally, I’d like to thank Natalie Deffenbaugh, Adrienne Erickcek, Dan Grin, Catherine Kealhofer and Ziggy Kermish for their enthusiasm and mutual encouragement. Every so often I remember that only four years ago the complete extent of my knowledge of physics was blocks sliding down ramps and resistors in parallel — it’s been an incredible time.
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Chapter 1

Introduction

1.1 Introduction

The modern understanding of classical continuous phase transitions is that all the critical point behavior is “driven” by the divergence of the correlation length: a critical system has a scale invariant distribution of its order parameter. This symmetry is harnessed by renormalization group methods, a set of mathematical techniques which have transformed the way theoretical physics is done in the thirty years since their introduction.

We can turn from the familiar situation of classical statistical mechanics carried out in thermodynamic ensembles and instead look for nonanalytic behavior in the limit of zero temperature — in other words, we look for phase transitions in the ground state of a system. This is the starting point for the theory of quantum phase transitions [42], a rapidly growing area of physics.

There exists a general sentiment that, because quantum mechanical phase transitions exhibit behavior that fundamentally differs from classical phase transitions, there must be a uniquely quantum-mechanical extension to the classical notion of the correlation function. In particular, in the last few years a number of researchers have begun to investigate the possible role of entanglement in quantum phase transitions [24, 1, 36, 38]. In one sentence or less, a quantum state of two objects is entangled if it isn’t a tensor product of states of the two objects considered individually. This seeming innocuous definition has far reaching consequences which we explore in the text.

Therefore, one interesting question is to investigate how entanglement behaves during
a quantum phase transition. This is easier said than done, since for many cases there is currently no consensus on how one should quantify entanglement. In this thesis we calculate a particular measure of entanglement for an infinite family of critical points of random quantum systems, and we can give a substantial argument that the measure we use is the most logical choice. The addition of randomness to the system actually makes our life much easier, both in the sense of simplifying the form the entanglement of the ground state takes and in simplifying the mathematics we use to calculate it — we can employ an elegant energy-space renormalization group technique developed by Fisher [21].

In a nutshell, we view this work as an investigation of what is perhaps the simplest nontrivial manifestation of entanglement at a quantum critical point. Physics usually progresses in uncertain areas by coming to a thorough understanding of the simplest models first, and so we think that the results presented here will offer a worthwhile perspective for future investigations.

In chapter 2 we give a quick review of general concepts in the statistical mechanics of quantum systems that occupy a prominent role in the discussion to follow — the material of this thesis has been written on the level of an advanced undergraduate without special training. Chapter 3 summarizes directly relevant background material (most importantly, references [21, 15, 32]) that we make detailed use of in chapter 4, which presents the original work done for the thesis.

Finally, a note on notation — in order to avoid ambiguity, we use the standard convention for the Pauli spin matrices:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

When we refer to the “$\sigma^z$” basis of a spin system, we mean the basis formed from the tensor products of the $\sigma^z$ eigenstates of the individual spins. For a spin-1/2, we denote the +1 eigenstate of $\sigma^z$ by $|\uparrow\rangle$ and the −1 eigenstate by $|\downarrow\rangle$. We extend the conventional use of the term “singlet state” somewhat to refer to any collection of spins in a pure state of total spin 0.
Chapter 2

General considerations

2.1 Introduction: phase transitions

We begin by a brief overview of the current picture of phase transitions, beginning with
the most general aspects and adding more detail in the area of the specific systems we
investigate further on. This material was gleaned from the opening chapters of [3, 29, 12].

2.1.1 Phase transitions, criticality and scale invariance

In problems of condensed matter, one considers systems described by some hamiltonian
which is a functional of certain variables specifying the state of the system (which become
promoted to operators when we consider quantum-mechanical problems) and parameters,
which are taken to consist of everything else. These parameters may be experimentally
controllable variables (e.g. temperature, pressure, volume, density) or quantities further
removed from our everyday experience (ratios of interaction strengths); from the point of
view of the mathematics there is no distinction.

Perhaps the first fact of life in condensed matter physics is the distinction that while
our “inputs” (the degrees of freedom and interactions of a system) are described on micro-
scopic length scales, the desired “outputs” (correlation functions, susceptibilities, ...) are
macroscopic averages. What makes life interesting is the fact that the road from the high
energy interaction to the low energy observable theory is almost never trivial.

In particular, consider the common scenario of measuring some macroscopic quantity as
a function of a microscopic one; for example, the magnetic susceptibility of a ferromagnet as a function of temperature.

measuring some macroscopic quantity of the system as a function of some parameter. It may happen that as we sweep the parameter set across a given value, various observable quantities will suddenly vanish, blow up to infinity\textsuperscript{1} or exhibit a discontinuous jump. We call this phenomenon a phase transition and refer to the set of parameters that produce the singular behavior as the critical point.

We can make a distinction between first-order and continuous phase transitions, which are distinguished by the existence of a discontinuity in the first derivative of the free energy. First order transitions\textsuperscript{2} are relatively straightforward: locally, one has two competing macroscopically different phases of the system which have different free energies as a function of the parameter values. As we change our parameter, the phase which was previously higher energy becomes lower in energy.

Continuous phase transitions, on the other hand, exhibit phenomena of much greater theoretical interest. The fact that the first derivative of the free energy is continuous means that at a certain parameter value (the critical point) the two competing phases will be energetically indistinguishable. This has far-reaching consequences: on either side of the transition the two-point correlation function decays with some scale length $\xi$, and at the critical point this correlation length diverges — the system is scale-invariant. A concrete illustration of this is provided by magnetic ordering in the familiar classical Ising model: below the critical point we have well-defined domains (thanks to the discrete nature of the symmetry) of spin-up and spin-down whose size is of order $\xi$. At the critical point, the size of these domains diverges, and we produce domains within domain with domains... and the pattern of domain walls has a fractal structure.

\subsection{2.1.2 The renormalization group}

The presence of symmetries in any physical system always makes our calculations easier. The emergence of scale invariance makes a powerful theoretical tool called the renormaliza-

\textsuperscript{1}Strictly speaking, divergences can only happen in the limit of a system of infinite size.

\textsuperscript{2}A familiar example is the boiling of water to form steam.
The essential concept behind the renormalization group is that scale invariance permits one to solve a system iteratively: one takes the Hamiltonian for a system, integrates out the least important degrees of freedom and find a way to express the new Hamiltonian as a transformation of the parameters of the old. By iterating this process in the limit of infinitesimal transformations, one can write down differential equations that describe how the Hamiltonian describing a system moves through its parameter space as we integrate our way down to a low energy limit.

The real action starts when we find the fixed points of these RG flow equations, which by definition correspond to parameter values that produce scale invariant systems. This may mean include scale invariance of a trivial nature: for example, the completely ordered or disordered phases of a ferromagnet obviously look the same on all scales. The phases of the system are described by stable fixed points of the flow equations which have various basins of attraction in the parameter space. The saddle points on the boundaries between basins of attraction describe the scale-invariant critical points.

Figure 2.1: Generic RG flow behavior during a second-order phase transition. As we tune one parameter (the temperature in this case) across its critical value, we switch from one fixed point to another.

---

3Despite the fact that the name is always used in the singular, there is no unique renormalization group: rather, the name is given to any mathematical technique that operates on the qualitative level as we describe. Moreover, to the extent that RG techniques can be formalized mathematically their structure is not that of a group.

4Here “least important” means shortest range/highest wavenumber/highest energy, since we’re interested in macroscopic/low energy behavior.

5Qualitatively one can thinks of “looking at the system on larger scales” by integrating out the high energy behavior: the small details become progressively more “fuzzy” as they are averaged out.

6A somewhat confusing conflict of terminology is that in discussions of the renormalization group, “stable” fixed points are taken to be any fixed point with at least one stable eigenvector, in contrast to the definition usually used in the study of differential equations.
Already this is a powerful simplification: this picture tells us that no matter where we start the Hamiltonian in parameter space, many important aspects of its macroscopic behavior will be described by one of the fixed points. By linearizing the RG equations in the neighborhood of a given fixed point, we can learn much about its low energy physics.

It may seem odd that such a drastic compression of information takes place: why shouldn’t a larger subset of the parameter space produce unique behavior? To answer this question we consider the RG equations linearized around the fixed point: we obtain a set of eigenvectors corresponding to a basis for perturbations from the fixed point in parameter space and a set of eigenvalues associated with them.

Consider what happens if a renormalization group eigenvalue is negative. This means as the RG is run, the rescaled value of the reduced parameter asymptotically approaches zero, regardless of where we start from in some neighborhood of the fixed point. When this happens, we say that the operator conjugate to this parameter is irrelevant: its effect on low-energy behavior of the system is very small compared to operators with positive eigenvalues. Consequently, if two systems have the same set of relevant operators, they will have the same fixed points and the same phase diagram structure, even if the models in question arise in drastically different physical scenarios. This idea is called universality. In practice, it means that if the questions one asks are framed in terms of universal quantities (i.e., independent of microscopic details), they can be answered using any model in the same universality class.

We make extensive use of the renormalization group ideas discussed here to perform the calculations of chapter 4. We go into greater detail on the specific methods we use later (section 3.4), but right now we describe the object of our study: quantum critical points of (various generalizations of) the antiferromagnetic Heisenberg spin chain.

2.2 Quantum phase transitions

Since all matter is ultimately quantum mechanical in nature and these quantum phenomena become ever more apparent on the microscopic level, why do we draw a line between

---

7 This is an oversimplification; it’s not uncommon to have lines of fixed points or “crossover effects” combining features of two fixed points, but the statement is qualitatively correct.

8 The reason why RG fixed points don’t provide a complete description of a physical system is an issue of universality, which we discuss below.
“classical” and “quantum” phase transitions? The distinction is not between the nature of the interactions included in the Hamiltonian but in the properties of the system as a whole that are being studied. By definition one describes a classical system as a probability distribution over many quantum states, and classical phase transitions occur when the shape of that distribution changes discontinuously — there’s nothing intrinsically quantum mechanical about a distribution changing.

Quantum phase transitions, on the other hand, describe discontinuous changes in the nature of a single quantum state: the ground state [42]; in this way it can be though of as statistical mechanics at zero temperature but nonzero $\hbar$. Since the physical world generally remains at finite temperature, these phenomena would appear to be irrelevant — however, from our discussion of the renormalization group, we know that the zero temperature fixed points will control the behavior of the system at low but nonzero temperature. Aside from this point, the idea is the same: as we change a parameter in the Hamiltonian, the properties of the ground state may change abruptly as the result of a level crossing — what was once an excited state is now the ground state and vice versa.

2.2.1 Quantum spin systems

In condensed matter physics, we commonly study Hamiltonians describing a collection of many quantum mechanical spins. These types of systems are meant to model the spin degrees of freedom of valence electrons in magnetic crystals: the dominant interaction between electron spins comes not from dipolar alignment but from the Pauli exclusion principle, which requires that the wavefunction of all the electrons be antisymmetric under the exchange of any two of them. In introductory solid state physics courses one considers this as a perturbation to the independent electron approximation and writes down the exchange integral describing the level splitting between parallel and antiparallel spin states.

In this thesis we concern ourselves specifically with one of the oldest and most throughly studied quantum spin systems (and several of its generalizations), the Heisenberg antiferromagnet:

$$H = J \sum_i \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z$$

with $J > 0$; for now we take the degrees of freedom to be spin-1/2. We restrict ourselves to the case of a one-dimensional lattice (a “chain”). The classical limit of this model is a
collection of compass needles free to rotate in three dimensions with a dipolar interaction; we can clearly minimize the energy in this limit by making adjacent spins antiparallel. Equivalently, we can define two sublattices of even and odd-numbered spins; all the spins on one sublattice are ferromagnetically aligned in the direction opposite to those on the other lattice. This is known as the Néel-ordered ground state [42], and when we return to the quantum system it provides the correct description in two dimensions and higher [31]. We describe the nature of the antiferromagnetic ground state in one dimension below.

(WHAT’s The real GS?)

2.2.2 Why one dimension?

The class of one-dimensional spin systems appears to be highly artificial at first glance — solutions of the spin Hamiltonian don’t constitute a complete description of the electronic wavefunction and the real world is, after all, three dimensional. The short answer to this question is that what one dimensional systems lack in realism they make up in solubility. Frequently one can gain at least some qualitative understanding of three dimensional behavior from a low dimensional solution.

Although we won’t be concerning ourselves with connections to experimental results, we note that good approximations to one dimensional systems are physically realizable. One can manufacture anisotropic crystals (such as Mn(HCOO)$_2$·2H$_2$O; see [33]) with extremely weak couplings along two axes, so that the magnetic properties of the material are well approximated by an independent collection of spin chains.

We finally recall that one-dimensional quantum systems are described by field theories in $(1 + 1)$ dimension, which is something of a special situation. We can consider extending the scale-invariant symmetry we found at the critical point by considering all transformations that leave the metric invariant up to a spatially variable scale factor: invariance under this group of transformations defines conformal symmetry [29], and field theories in two$^9$ dimensions possessing this symmetry acquire a rich additional structure. The Heisenberg antiferromagnet is described by a conformally invariant field theory; however, we do not make use of this result and deeper discussion of conformal invariance is beyond the scope.

$^9$Specifically two dimensions; in that case conformal transformations are generated by any analytic map on the complex plane which provides a more extensive set of constraints.
of the current work.

2.2.3 Higher spin

One might think that as we increase the spin \( J \) of the degrees of freedom in the Heisenberg chain, the behavior would interpolate smoothly between the \( J = 1/2 \) and \( J \to \infty \) limits. It turns out that this is not the case: heisenberg chains with integer spin have drastically different properties than those with half-integer spin. Most notably, half-integer chains have excited states at arbitrarily low energies while for integer spin one always finds a finite energy gap between the ground and first excited states. The latter phenomenon was quite unexpected when it was first predicted by Haldane [26, 27]. His demonstration requires concepts from field theory too advanced to develop here; instead, we develop a qualitative argument based on the valence bond solid picture of [31, 2]. Our discussion will in no way be a rigorous demonstration, but we hope to give an intuitive feel for why this should be the case.

One way to deal with chains of higher spin is to treat each spin-\( J \) degree of freedom as a collection of \( 2J \) spin-1/2 objects in a completely symmetrized state\(^{10} \). In order to obtain a ground state with total spin 0, we form singlet between the spin-1/2 components of different lattice sites — these are the valence bonds.

For half-integer spin at least some of the valence bonds can’t be symmetrically paired up, and the lattice symmetry is broken: instead of states that are translationally invariant with period \( a \), we obtain dimerized states with period \( 2a \):

![Dimerized states](image)

For integer spin, on the other hand, we can draw a valence bond state that preserves the lattice symmetry and has no dimerization. This is called the valence bond solid state.

![Valence bond solid state](image)

In their presentation, Affleck et. al. [31] first wrote down these states and then created

\(^{10}\)Otherwise they would add up to less than spin \( J \)
Hamiltonians that had these states as ground states\textsuperscript{11}. These hamiltonians have the Heisenberg interaction plus additional isotropic couplings between spins.

We're only interested in the ground state of the regular Heisenberg model, though. As we adjust couplings in the Hamiltonian to get rid of the special interactions we've introduced, the ground state will no longer be a single valence bond solid state; instead it will be a superposition of these states with additional contributions from states that have bonds of longer length. This is sometimes referred to as a “resonating valence bond solid” model.

In a topological sense however, the valence bond solid picture is still accurate: one can define a “string correlation” order parameter corresponding to the number of different continuous paths one can take along the lattice\textsuperscript{12}. Moving away from the valence bond hamiltonian makes the valence bond states themselves unstable, but since this topological order parameter is quantized it’s stable against these perturbations. Therefore, on this qualitative level, we can expect the valence bond picture to be relevant for the Heisenberg chain.

We can select between the different dimerization states by including explicit dimerization in our interaction; i.e. we take $J_i = J(1 + \delta(-1)^i)$. By changing dimerization $\delta$, we expect some dimerized bonds to form on the favored sublattice which will have the effect of “screening out” the dimerization in the interaction [14], and we recover the picture shown in figure 2.2.3.

How does this discussion relate to the differences in the excitation spectrum we alluded to above? In [31] it was shown that the spin-1 valence bond solid state has an energy gap; in fact, as pointed out in [2], this is really the default behavior for valence bond states. In integer spin chains, the valence bond solid state is mixed with similar states having longer bonds such that the probability of obtaining a bond with a given length falls off exponentially. On the other hand, in the half-integer spin case at zero dimerization the resonance mixes states to a sufficient degree to go from the two degenerate dimerized ground states to a single translationally invariant ground state; Affleck and Lieb have proved [2] that given this condition the half-integer spin ground state must be gapless.

\textsuperscript{11}They start with a general isotropic spin-spin interaction and then project out the subspace pertaining to the valence bond states.

\textsuperscript{12}The correlation function in this case is a nonlocal product of operators on many lattice sites; a similar object appears in the definition of the Jordan-Wigner transformation.
As we tune the dimerization $\delta$, we switch from states where $n$ bonds are dimerized to states where $n - 1$ bonds are dimerized. We have a critical point in between these phases where the bonds “can’t decide” which sublattice to be on, while all the other spin-1/2 objects are “frozen in” to their configuration — in other words, the critical point separating two valence bond phases of different dimerization is simply the (gapless) spin-1/2 Heisenberg critical point discussed above.

### 2.3 Correspondences

Having given a brief introduction to the major one-dimensional spin chain models, we now present the main techniques for solving them. This isn’t simply mathematical footwork, though: the two techniques we present in this section are actually very general mappings from quantum mechanical systems to classical systems on one hand and continuum field theory on the other. These correspondences lie at the heart of much of the modern work in condensed matter, which is why we present them in significant depth.

#### 2.3.1 Suzuki-Trotter formalism

There exists a very general mathematical connection between quantum mechanical spin systems in $d$ dimensions and classical spin systems in $d + 1$ dimensions. We emphasize that
this a purely formal result which doesn’t arise from physical considerations — see [44, 5] or [10, 42] for an overview.

The first step is Trotter’s formula, which lets us expand exponentials of sums of quantum mechanical operators $O_i$ which need not commute with each other:

$$\exp\left(\sum_i O_i\right) = \lim_{M \to \infty} \left[ \prod_i \exp\left(\frac{O_i}{M}\right) \right]^M$$ (2.2)

More concretely, once we’ve chosen a definite basis this means that matrix elements of the left-hand side of equation 2.2 can be expanded as

$$\langle \psi | \exp \sum_i^{K} O_i | \psi' \rangle = \lim_{M \to \infty} \sum_{\{\phi_{i,j}\}} \langle \psi | O_1 | \phi_{1,1} \rangle \langle \phi_{1,1} | O_2 | \phi_{1,2} \rangle \times \cdots \times \langle \phi_{1,K-1} | O_K | \phi_{1,K} \rangle$$

$$\times \langle \phi_{1,K} | O_1 | \phi_{2,1} \rangle \langle \phi_{2,1} | O_2 | \phi_{2,2} \rangle \times \cdots \times \langle \phi_{M,K-1} | O_K | \psi' \rangle$$ (2.3)

Formally, this bears a resemblance to a path integral formulation of quantum mechanics in a new dimension (parameterized by $i$ in the above equation). It was Suzuki’s insight to use this to simplify the evaluation of the partition function of any quantum system, since

$$Z = \text{Tr} \exp -\beta H \equiv \sum_{\psi} \langle \psi | e^{-\beta H} | \psi \rangle.$$ The fact that we’re taking a trace imposes periodic boundary conditions on the Trotter dimension.

We apply this result to the specific case of the partition function for the Heisenberg antiferromagnet:

$$Z = \text{Tr} \exp \beta J \left[ \sum_{i=1}^N \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z \right]$$

where for convenience we work in the $\sigma^z$ basis, which makes the factors involving $\exp(\sigma^z)$ in equation 2.3 trivial. In order to handle $\sigma^x$ and $\sigma^y$, we first expand

$$e^{a\sigma^x} = 1 + a\sigma^x + \frac{a^2}{2} + \frac{a^3}{6}\sigma^y + \cdots = \cosh a + \sigma^y \sinh a$$

with an analogous result for $\sigma^y$. Therefore, introducing $s, s' = \pm 1$ as the eigenstates of $\sigma^z$,

$$\langle s | e^{a\sigma^x} | s' \rangle = \begin{cases} \cosh a & \text{if } s = s', \\ \sinh a & \text{if } s \neq s'. \end{cases} = \sqrt{\sinh a \cosh a \exp \left( \frac{ss'}{2} \log \coth a \right)}$$

\footnote{Recall that $(\sigma^x)^2 = (\sigma^y)^2 = 1.$}
\[ \langle s | e^{\alpha y} | s' \rangle = \begin{cases} \cosh a & \text{if } s = s', \\ is' \sinh a & \text{if } s \neq s'. \end{cases} = \sqrt{\frac{1}{2}} \sinh 2a \exp \left( \frac{ss'}{2} \log \coth a \right) \exp \left( i\pi \frac{2 - s}{2} \right) \]

where the final forms on the right-hand side are merely a more convenient way to write the case specification in a closed form. This lets us rewrite our original partition function only making reference to the discrete eigenvalues \( s_i \):

\[
Z = \lim_{M \to \infty} C^{MN} \text{Tr} \exp \beta \left[ \sum_{j=1}^{N} \sum_{k=1}^{M} c'_{z} s_{j,k} s_{j+1,k} + c'_{x} s_{j,k} s_{j+1,k+1} \right]
\]

where \( C \) is an unimportant normalization constant. In other words, the periodic transverse-field quantum Ising system is equivalent to a classical spin system (with four-spin “plaquette” interactions) defined on a \( M \times N \) toroidal lattice. The new couplings are

\[
c'_{z} = \frac{c_z}{M}
\]

and

\[
c'_{x} = \frac{1}{2M} \log \coth \frac{c_x}{M}
\]

The former vanishes while the latter has a logarithmic divergence as \( M \to \infty \), which is rather awkward behavior: for this reason the \( M \to \infty \) limit is sometimes called the extreme anisotropic limit. We can deal with this by simultaneously taking the \( \beta \to \infty \) limit; \( M \) only enters our expression for \( Z \) in the form \( \beta/M \), so by working in the \( T \to 0 \) limit we obtain a non-degenerate result. In the quantum system we obtain a phase transition by varying \( c_z/c_x \) at \( T = 0 \); in

Although the Suzuki-Trotter result can be useful if the quantum system maps onto a well-studied classical system\(^{14}\), its primary utility is in numerical simulations, since one can apply all the techniques of Monte Carlo sampling to the classical system in a straightforward way no matter how complicated the interaction becomes.

### 2.3.2 Jordan-Wigner fermions

The basis states of a spin-1/2 object form a hilbert space of size 2. Another obvious example of a two-level quantum system is any single fermion mode: it can be occupied by either one

\(^{14}\)For example, the quantum transverse field Ising Hamiltonian \( \sum_i \sigma_i^z \sigma_{i+1}^z + c \sigma_i^x \) maps onto a (strongly anisotropic) two-dimensional classical Ising model.
or zero fermions, with no other possibilities. In the case of a single spin it’s easy to make this identification: we simply call the spin raising operator a fermion creation operator and vice-versa. When we have more than one spin, things get more complicated, though: through a unitary transformation we can switch the roles of the raising and lowering operators on any one site. The solution to this problem is to effectively pick one spin out as a reference, and define all other spin states in terms of it. In the language of fermions, the problem is that fermion operators at different locations must anticommute while spin raising and lowering operators that act on different sites commute. Our creation and annihilation operators become [10]:

\[
c_i = \prod_{j=1}^{i-1} \exp \left( i \pi \sigma_j^+ \sigma_j^- \right) \sigma_i^-; \quad c_i^\dagger = \sigma_i^+ \prod_{j=1}^{i-1} \exp \left( -i \pi \sigma_j^- \sigma_j^+ \right)
\]

Note that these are nonlocal: the product of exponentials provides the sign necessary to make the commutation relations work out. In both cases the exponentials simply evaluate to \(-\sigma_i^z\). These operators have all the properties you’d expect of fermions on a lattice; in other words, \(\{c_i, c_j^\dagger\} = \delta_{ij}\) and \(\{c_i, c_i\} = 0\). Although they arose from treating spin-1/2 objects, the fermions themselves are spinless: there’s only one type of excitation possible and no spin index on the creation/annihilation operators.

Obtaining the fermionic theory is just a simple matter of substitution — starting from

\[
H = -J \sum_i g \sigma_i^x + \sigma_i^z \sigma_{i+1}^z
\]

from the definition of the creation and annihilation operators we can obtain

\[
\sigma_i^x = (-1)^i \prod_{j<i} (c_j c_j^\dagger - c_j^\dagger c_j)(c_i + c_i^\dagger); \quad \sigma_i^y = (-1)^i \prod_{j<i} (c_j c_j^\dagger - c_j^\dagger c_j)(c_i - c_i^\dagger); \quad \sigma_i^z = c_i c_i^\dagger - c_i^\dagger c_i
\]

and substitute these into the hamiltonian. We note that \((c_j c_j^\dagger - c_j^\dagger c_j)^2 = 1\), so the factors in the products drop out for \(j < i\). Using the anticommutator relations to simplify things, we see that the operators on the \(i\)th site resulting from \(\sigma^x\) are \((c_i + c_i^\dagger)(c_i c_i^\dagger - c_i^\dagger c_i) = (c_i^\dagger - c_i)\). We therefore obtain

\[
H = -J \sum_i 2 \left( c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}^\dagger \right) + \left( 2c_i^\dagger c_i - 1 \right) \left( 2c_{i+1}^\dagger c_{i+1} - 1 \right)
\]

So far we’ve only described fermions on a lattice. In order to take the limit of a continuum field theory, we must make sure the operators \(c_i, c_i^\dagger\) scale correctly [42]: they need to be
multiplied by the appropriate power of the lattice spacing $a$ (which is the only microscopic length scale available in the lattice problem). One can go much deeper into the subject along these lines (bosonization etc.) but because the field theoretic methods aren’t really relevant to our calculation we stop here and refer to [33, 42].

2.3.3 Interpretation

In this section we’ve seen that a general one-dimensional quantum spin chain can be mapped on to an equivalent two-dimensional classical spin system or one-dimensional field theory. It would be perhaps most accurate to call these mappings mathematical formalisms; after all, we certainly can’t “crack open” our quantum spin and find classical spins or spinless fermions inside. However, this description trivializes the importance of the results above — the point is that the statement “this model describes that physical system” is by no means exclusive. In light of the phenomenon of universality, life is made easier for all concerned if we first decide what questions we’re going to ask and then decide which model makes those calculations easiest. In fact, later on we’ll switch descriptions of this model in mid-sentence.

2.4 Randomness in quantum systems

2.4.1 Why randomness?

The real world isn’t perfect, and neither are the materials in it — any macroscopic crystal will have a nonzero amount of lattice defects (impurity atoms, disclinations, dislocations, etc. [12]) which reduce the spacing between some atoms in the lattice and increase it for others. This will change the magnitude of the exchange interactions between electrons on adjacent atoms, which will manifest itself in our model as the coupling constant $J$ assuming a range of values.

This alteration — replacing a constant $J$ with a set of random $J_i$ which differ for each lattice site — complicates the theoretical treatment of our models considerably. Both of the theoretical methods discussed in the previous section are weakened considerably by random couplings. The Suzuki-Trotter mapping now produces a two dimensional system (figure 2.4.1) with anisotropic and highly correlated couplings which are hard to treat with the methods of classical statistical mechanics. If we instead express the system as a continuum
fermionic theory, the randomness in the couplings means we can no longer pass to the continuum limit by writing down dimensionless creation and annihilation operators as we did in section 2.3.2. For example, obtaining the low-energy excitation spectrum requires the numerical diagonalization of large random matrices [10].

We describe methods designed to treat random chains in section 3.4, but we can also appreciate the effects of randomness in a qualitative way. Even if we assume the couplings are uncorrelated random variables, we should expect coincidences where all the couplings in a region are stronger or weaker than average. These anomalous clusters are responsible for much of the phenomena random systems produce. Due to the statistical origin of these clusters, much of the calculation done with disordered systems takes on a flavor of percolation theory — although the percolation is usually of such a specific type that one can’t make explicit use of it.

2.4.2 The Harris criterion

The first question to ask when considering disorder is whether we need to consider disorder at all — that is, given a fixed point of a pure system and a specific type of randomness, we want to know whether the randomness is a relevant operator. If randomness is irrelevant (in the sense of section 2.1.2), then if we perturb the system by adding a small amount of randomness the RG flow will simply bring it back to the pure system’s fixed point. If the randomness is relevant, the system will flow away to points unknown and the macroscopic system will be described by a different fixed point entirely. We can decide which of these
scenarios takes place through a simple scaling argument known as the Harris criterion [42].

It follows from the central limit theorem that the variance of the sum of $n$ random couplings will be of order $\sqrt{n}$, independent of the coupling distribution as $n \to \infty$. This means that in $d$ dimensions lattice regions of size $L$ will display an average local coupling $C_L$ that deviates from the global average $\bar{C}$ by a factor of $L^{d/2}$. If, for a fixed deviation $|\bar{C} - C_L|$, these regions are larger than the correlation length $\xi$, they will still be relevant when the renormalization group reaches the length scale set by $\xi$; otherwise they’ve been averaged out and do not change the macroscopic fixed point behavior. We define the correlation length through the critical exponent $\xi(C) \sim |\bar{C} - C|^{-\nu}$, so this requirement translates to

$$L \ll \xi \Rightarrow |\bar{C} - C|^{-2/d} \ll |\bar{C} - C|^{-\nu} \Rightarrow \nu \geq \frac{2}{d}$$

which is the Harris criterion. In the case of the Heisenberg antiferromagnet, we have $d = 1$ and $\nu = 1$ [21], so randomness will be a relevant perturbation. We discuss the details of its effects in section 3.4.
Chapter 3

More specific background

3.1 Entanglement

We now shift our attention from many-body quantum mechanics to two-body quantum mechanics and discuss the phenomenon of entanglement. Entanglement is a phenomenon which is the hallmark of essentially quantum-mechanical behavior in a system. While other characteristic features of the quantum state (such as noncommuting observables) have been well understood for decades, all but the simplest aspects of entanglement remain open questions [11].

3.1.1 Entanglement defined

The concept of entanglement is easy to illustrate. Consider the spin-1 state $|\phi\rangle = |1\rangle$ and the singlet state $|\psi\rangle = (|1\rangle - |1\rangle)/\sqrt{2}$ of two spin-1/2 objects $A$ and $B$. We can write down the density matrix for the complete system $\rho_{AB} = |\psi\rangle\langle\psi|$ and obtain the density matrix describing one part of it by tracing out the degrees of freedom associated with the other part; our notation is $\rho_A = \text{Tr}_B[\rho_{AB}]$. We refer to $\rho_A$ and $\rho_B$ as the reduced density matrices obtained from $\rho_{AB}$.

Taking the partial trace of the spin-1 state tells us that, taken in isolation, both $A$ and $B$ are in the pure state $|1\rangle$, and we can reconstruct the whole density matrix since $\rho_A \otimes \rho_B = \rho_{AB}$. Neither of these properties holds for the singlet: taken in isolation, both spins are in a completely unpolarized mixed state, and $\rho_A \otimes \rho_B \neq \rho_{AB}$. This is an
unexpected result — we know that \( \rho_A \) literally contains all the information about system \( A \), since we obtain the expectation value of any operator \( O \) on \( A \) via \( \text{Tr}[O \rho_A] \). One can just as easily say the same thing about \( \rho_B \), so when we add up all the pieces of the system we should have a complete description of the system.

The fact that this doesn’t happen in the singlet is an example of an obvious result of linear algebra having profound physical consequences: at least part of the information describing the system must be, in some sense, nonlocal. We call this property \textit{entanglement}, and we can define it more generally in the following way: If any quantum state composed into parts \( A,B,C \cdots \) has a density matrix \( \rho \) that cannot be written as a tensor product \( \rho_A \otimes \rho_B \otimes \cdots \) of any states \( \rho_A, \rho_B \cdots \) of its components\(^1\), then that state is entangled. More specifically, we can speak of there being entanglement between parts \( A, B, \) etc.

3.1.2 The Schmidt decomposition

In performing entanglement calculations we consider partitioned systems, which raises questions not commonly considered in elementary quantum mechanics. It should come as no surprise that we need additional mathematical tools to answer these questions. Chief among them is the Schmidt decomposition\(^2\) of a bipartite quantum system [40, 20].

\[
|\psi\rangle = \sum_i c_i |u_i\rangle_A |v_i\rangle_B
\]

with \( \langle u_i | u_j \rangle = \delta_{ij} \) and \( \langle v_i | v_j \rangle = \delta_{ij} \). This manipulation is non-trivial: we know we could write the arbitrary state as a double sum \( \sum_{ij} c_{ij} |u_i\rangle |v_j\rangle \) for any basis, but here we’re able to reduce this to a single sum over both subspaces simultaneously. The utility of the Schmidt decomposition becomes clear when we go to take the partial trace of a density matrix. We then have

\[
\rho_{AB} = \langle \psi | \langle \psi | = \sum_{ij} c_i^* c_j |u_i\rangle \langle u_j| \otimes |v_i\rangle \langle v_j|
\]

which means that

\[
\rho_A = \sum_i |c_i|^2 |u_i\rangle \langle u_j|; \rho_B = \sum_i |c_i|^2 |v_i\rangle \langle v_j|.
\]

In other words, the Schmidt basis is the one that simultaneously diagonalizes both reduced density matrices. In numerical work one can make use of the singular value decomposition

\(^1\)Note that this means \( \rho_A, \) etc., can be any state, not just \( \text{Tr}_{BC \cdots} \rho \).

\(^2\)Some authors also use the term ‘polar decomposition’ [35].
Frequently, one instead proceeds in the reverse direction: the vectors of the Schmidt basis can be found by diagonalizing the reduced density matrices.

### 3.1.3 Von Neumann entropy

We now come to the question of quantifying entanglement. We know that if a state isn’t a tensor product state it must be entangled, but in what way can we claim a state is “more entangled” than another? Our earlier definition of entanglement made reference to concepts such as “the information in part $A$”. While that discussion was on a qualitative level, we can make the idea of “information” qualitative following ideas first introduced by Claude Shannon. According to the results of classical information theory, the unique measure of information a random variable is capable of providing about the rest of the world is simply the entropy of its probability distribution: $H(X) = \sum_x \Pr(x) \log \Pr(x)$. The derivation is straightforward (see [35]) but we omit it here for brevity’s sake.

At this point all we’ve done is assigned a name to a function. One of Shannon’s major accomplishments was showing that entropy measures information in the sense that if we have distributions $A, B$ with entropies $H_A$ and $H_B$, we can use $B$ to store everything we need to know to reconstruct $A$ perfectly if and only if $H_B \geq H_A$. This is known as the noiseless coding theorem: we’re using $B$ to encode information about $A$, and we assume that the encoding/decoding process happens without any mistakes$^3$.

The fundamental objects of quantum mechanics are density matrices and state vectors, not probability distributions. The generalization of the noiseless coding theorem to quantum states was proved in [43] by Schumacher, who showed that if one starts with an entangled bipartite pure state $AC$, one can “transpose” the entanglement between $A$ and $C$ onto entanglement between some $B$ and $C$ with perfect fidelity if and only if $S(\rho_A) \leq S(\rho_B)$, where $S$ is the von Neumann entropy:

$$E(\rho_{AB}) = - \text{Tr} [\rho_A \log \rho_A] = - \text{Tr} [\rho_B \log \rho_B]$$  \hspace{1cm} (3.1)

Von Neumann originally derived this quantity as the thermodynamic entropy of a statistical ensemble of quantum states.

$^3$Shannon originally developed these ideas in the context of electrical engineering.
3.2 Beyond the Von Neumann entanglement

Despite the fact that quantum information theory makes use of no physics beyond quantum mechanics, equation 3.1 is essentially the only certain result in the theory of entanglement as of this writing. Schumacher’s argument fails for mixed bipartite states since one can no longer define the fidelity of reproduction in an appropriate way for ensembles of states. Furthermore, information theory as a whole is defined in terms of binary relations, so it’s even less clear how one could extend his argument to cover simultaneous mutual entanglement between more than two parts. This latter case subsumes the former, since we may use the Schmidt decomposition to write the density matrix of any bipartite mixed system as the partial trace of a tripartite pure state (see [40]). We briefly summarize the current state of these questions; see [11] for a recent review.

3.2.1 The bipartite mixed state

The prevalent argument on this question goes as follows: consider a source that continuously produces systems in the specified state. One then performs a specified class of operations on these systems in order to transform them into a reference state (of maximal entanglement). One can then define a so-called ‘entanglement of distillation’, which is the number of states (actually, the asymptotic ratio of states) it takes to reproduce the reference state. Of course, it would be equally valid to consider the ‘entanglement of formation’, the number of specified mixed states that can be produced from one reference state.

This is a reasonable way to approach the problem, perhaps made more appealing by the obvious parallels with thermodynamics\textsuperscript{4} and heat engines — one could imagine speaking of “entanglement reservoirs”, etc. There are a number of serious problems with the above approach, though: except for the case of a $2 \times 2$ state system, it’s not known how to express these measures as a function of the density matrix; instead, they are defined as suprema over classes of states, which makes them rather difficult to compute in practice. More serious, though, is the fact that they don’t agree: it can be shown that for any state, the entanglement of formation is always greater than or equal to the entanglement of distillation, with equality only for pure states (in which case both measures reduce to equation 3.1.)

---

\textsuperscript{4}Recent work [34] has called this paradigm into question.
In fact, it’s an open question to determine whether a general mixed state is entangled at all. The most reliable test appears to be the positive partial transpose criterion: one transposes the vectors corresponding to one part of the system only. If the resulting density matrix is no longer a positive operator (i.e., if some of its eigenvalues are negative), the state is entangled. This criterion has an intriguing physical interpretation when the system are spins: then partial transposition corresponds to reversing the direction of time for one part of the system only. It’s intuitively clear that if the density matrix of the system remains physically valid after this operation, there can be no correlation between the parts of the system.

Unfortunately, this is not a complete criterion for entanglement, since examples of entangled systems have been found with a positive partial transpose! These are referred to as “bound” entangled states which are regarded as having weaker entanglement than “normal” states; for example, the entanglement of distillation of all bound entangled states is zero.

### 3.2.2 Multipartite mixed states

Even less is known for the problem of multipartite entanglement. One interesting result is that a single scalar measure of entanglement is insufficient, since there are fundamentally different ways for a multipartite state to be entangled [47, 41]. By “different”, we mean that states in different classes can’t be mapped on to each other by a restricted class of basis transformations — we can map any state to any other using a general unitary transformation on $\rho_{ABC}$, but generically this transformation won’t respect the integrity of the partitions of the system. Instead, we restrict the class of allowable transformations to local operations (i.e. the group $U_A \otimes U_B \otimes U_C$ of individual unitary transformations on the parts) and classical communication (i.e. creating non-quantum correlations such as ferromagnetic order).

In [47], it’s proved that even if we only require that these transformations map one state to another with nonzero probability, there are still two inequivalent classes of intrinsic

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5The time reversal operator reverses all momenta, including angular momenta, so we have $|m_z\rangle \rightarrow |-m_z\rangle$.
6To satisfy the reader’s curiosity, an example is · · ·
7The precise definition of the set of allowable transformations is still a matter of some controversy; however, all authors agree that the following operations should be permissible.
three-party entanglement, neither of which can be expressed in terms of bipartite relations. Examples of states from the two classes are

\[ |GHZ\rangle = \frac{1}{\sqrt{2}} (|111\rangle + |111\rangle) \]

and

\[ |W\rangle = \frac{1}{\sqrt{3}} (|111\rangle + |111\rangle + |111\rangle) \]

In a nutshell, the inequivalence is proved by the fact that \(GHZ\) states only have two terms in their Schmidt decomposition while \(W\) states have three, and the number of terms is invariant under the class of operations considered. As one might guess, the number of inequivalent states increases combinatorially with the number of partitions involved [41] and also with the size of the Hilbert space of the parts.

### 3.3 Entanglement in quantum critical phenomena

In the modern theory of phase transitions, all the critical behavior of a system is determined by the divergence of relevant correlation lengths — by analogy with field theory, one can think of the correlations as driving all other observed behavior. Entanglement is the uniquely quantum mechanical analogue of the classical correlation function; isn’t it logical, then, that it should play the main role in quantum phase transitions?

This appealing point of view has yet to receive much theoretical or experimental elaboration, primarily due to the still-unclear nature of entanglement. One very relevant detail that complicates the analogy is the fact that entanglement is a limited resource [46, 41]: in an ordered phase, a classical Ising spin may be correlated with arbitrarily many other spins, but if (for example) a quantum spin is in a singlet state with another spin it cannot be entangled with any other spin. The presence of incommensurate multiparticle entangled states also complicates any quantitative discussion of entanglement in many-body systems.

Nevertheless, even at this stage interesting observations have been made. Nearly all of the results obtained so far pertain to exactly soluble, isotropic quantum spin systems: the Heisenberg chain, the XX and XY models (anisotropic limits of the Heisenberg chain that fall into different universality classes) and the transverse field Ising model. The substantial literature on these systems and their quantum phase transitions, combined with the fact
that their degrees of freedom have Hilbert spaces of low dimensionality, make these models a logical first step in addressing the broader issues alluded to above.

The most straightforward measure of entanglement one can measure during a quantum phase transition is just the bipartite entanglement between two neighboring spins. These will not be in a pure state, so one must employ the numerical method mentioned in section 3.2.1 to calculate the entanglement of formation. This is the approach taken in [36] and later [38]. In [36], it was found that the antiferromagnetic ground state maximized their entanglement measure when considered in terms of all translationally invariant states with total spin 0 (although it wasn’t a maximum relative to all possible states).

Strangely enough, [38] found that the nearest-neighbor concurrence was not maximized at the critical point, although the next-nearest neighbor concurrence apparently was. In addition, for certain parameter values these entanglement measures were greater at (low) finite temperature than at zero temperature. In interpreting their results, Osbourne and Nielsen noted that the entanglement measure they considered was not rescaleable and hence could not be a universal property of the system. They also drew attention to the problem entanglement sharing posed for answering this question.

Indeed, it had been noted earlier [48] that the interactions in the XY chain could produce multiparticle entangled states (such as the GHZ state mentioned earlier), so it seems likely that only looking at the bipartite entanglement between two spins will miss much of the entanglement structure present in the system as a whole (if, in fact, there is any). The results of [1] support this view; they considered the entanglement between two spins as a function of the distance between them and found that the entanglement of formation was undetectable beyond the second nearest neighbor.

Latorre et. al. [24, 32] have taken the different approach of examining the entanglement between a block of \( L \) spins and the rest of the chain:

![Diagram of entanglement between a block of L spins and the rest of the chain.](image)

where one traces out the spins in the shaded region. This is a better way to pose the problem for several reasons: the block of spins is more amenable to scaling concepts. More importantly, the spin chain as a whole is in a pure state, so the correct measure of entanglement for this scenario is the von Neumann entropy (equation 3.1) which is known to be
the unique measure for the case of a bipartite pure state. They performed this calculation numerically for $L \lesssim 200$ for four exactly soluble models. In each case they found that the block entanglement of critical chains diverged as $\log L$, while away from the critical point the entanglement was nonextensive.

In chapter 4 we will take these findings as the starting point for our own investigations. Before we do, we need to introduce the renormalization group framework we’ll be using to study the disordered chains.

### 3.4 The Strong Disorder Renormalization Group

Within the framework of the renormalization group, we can see that adding randomness to the coupling constants of an isotropic system can have one of three possible effects on its macroscopic behavior [30]:

1. The disorder may be an irrelevant operator, in the sense that as an RG is run the distribution of couplings gets narrower and narrower until we recover the isotropic system at the fixed point. Indeed, since an RG is effectively a microscopic averaging process, we might expect this to be the default behavior for disordered systems.

2. The system may flow to a fixed point with some changed distribution of couplings that still has a finite second moment; we might call this a ‘finite disorder fixed point’. Spin glasses are thought to fall into this category [23]; see also [19].

3. Finally, we could imagine that the randomness is self-reinforcing, so that the distribution becomes increasingly broad as the RG runs and the second moment diverges at an ‘infinite disorder fixed point’.

The final case will describe the systems we study in detail in this thesis. The infinite disorder condition has the potential to drastically simplify calculations: at the fixed point, we may safely assume that given two bonds, one will be much stronger than the other, which may be treated perturbatively\(^8\). This condition makes the strong disorder renormalization group (SDRG) possible.

\(^8\)This is somewhat reminiscent of dilute bond models, where one simply removes a random set of links from the lattice the isotropic system is defined on, but has the significant difference that the bond strengths are all relative.
The essential idea of the strong disorder renormalization group is that at each step one selects the strongest remaining coupling and puts the subsystem conjugate to that coupling in its ground state. The couplings between this subsystem and everything else are, by the strong disorder assumption, much weaker, so they can be treated by second-order perturbation theory and effective couplings across the subsystem are generated. These new couplings are added to the coupling probability distribution as the strongest couplings are removed. One writes down an RG flow equation describing the evolution of the probability distribution under this process and solves it for fixed point distributions.

We note that these ideas are conceptually related to the more general density matrix renormalization group (see [49]) which is usually employed in numerical studies of non-random chains, although historically the strong disorder RG was proposed first (in [16]). Dasgupta and Ma employed it to study the random Heisenberg chain [16]; their results were significantly extended by Fisher [21] who was able to treat the case of general isotropy as well as other models [22]; see [23] for a review.

3.5 Application of the SDRG to antiferromagnetic spin chains

3.5.1 Random spin-1/2 Heisenberg chain

Following [16], we consider the isotropic spin-1/2 heisenberg antiferromagnet with random couplings:

\[ H = \sum_i J_i \left( \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z \right) \]

and denote the strongest coupling by \( J_k \). The operator conjugate to this is \( \vec{\sigma}_k \cdot \vec{\sigma}_{k+1} \), so switching to the total spin basis we know this term has a singlet ground state with energy \( E_S^0 = -3J_k/4 \) and a triplet excited state with energy \( E_t^0 = J_k/4 \).

The part of the hamiltonian that couples to these spins is \( H' = J_{k-1} \sigma_{k-1} \cdot \vec{\sigma}_k + J_{k+1} \sigma_{k+1} \cdot \vec{\sigma}_k \). If we meet the strong randomness condition, we may assume that \( J_k \gg J_{k-1}, J_{k+1} \), and so the low energy behavior is well described by putting spins \( k \) and \( k+1 \) into their ground state and treating their interaction with the rest of the system as a perturbation. In the total spin basis of spins \( k-1 \) and \( k+2 \), we obtain

\[ E_s^0 + \langle s | H_0 | s \rangle + \sum_t \left| \langle s | H'_t | t \rangle \right|^2 = E_s^0 - \frac{3(J_{k-1}^2 + J_{k+1}^2)}{16J_k} + \frac{J_{k-1}J_{k+1}}{2J_k} \sigma_{k-1} \cdot \sigma_{k+2} \]
in other words, we obtain an effective coupling consisting of a constant term (which we ignore) and a new Heisenberg interaction between spins \( k - 1 \) and \( k + 2 \) with effective strength \( J' = \frac{J_{k-1}J_{k+1}}{2J_k} \ll J_{k-1}, J_{k+1} \) in the strong disorder approximation. This multiplicative relation suggests that it would be most appropriate to measure bond strengths on a logarithmic scale, so following [21] we abbreviate \( \Gamma = -\log \Omega \) and set \( \zeta_i = \log \Omega/J_i \) where \( \Omega \) is the strength of the strongest remaining coupling. The recursion simply becomes \( \zeta' = \zeta_1 + \zeta_3 - \log 2 \), since the strongest bond has by definition \( \zeta = 0 \). Weak couplings have large \( \zeta \), and as the RG is run the probability distribution \( \rho(\zeta|\Gamma) \) of their strengths grows increasingly broad, so we expect \( \max(\zeta_1, \zeta_3) \gg \log 2 \) and we drop this constant term from the recursion relation. We write our RG flow equation as

\[
\frac{\partial \rho(\zeta, \Gamma)}{\partial \Gamma} = \left[ \frac{\partial \rho}{\partial \zeta} + \rho(0, \Gamma) \int_0^\infty d\zeta_1 \int_0^\infty d\zeta_2 \rho(\zeta_1, \Gamma) \rho(\zeta_2, \Gamma) \delta(\zeta - \zeta_1 - \zeta_2) \right] (3.2)
\]

The first step in finding a fixed point of this is to rewrite it in terms of scale-invariant (aka dimensionless) quantities [21]. From the definition of \( \zeta \), we know it will scale as the first power of \( \Gamma \), so we redefine \( \eta = \zeta/\Gamma \) and \( \rho(\zeta, \Gamma) = Q(\eta, \Gamma)/\Gamma \) to obtain

\[
\Gamma \frac{\partial Q}{\partial \Gamma} = \left[ Q + (1 + \eta) \frac{\partial Q}{\partial \eta} \right] + Q^0 Q \otimes Q
\]

(3.3)

where in the last term we’ve abbreviated \( Q(0, \Gamma) \equiv Q^0 \) and expressed the double integral as a convolution (since, after all, that’s what it is). Note that \( \Gamma \) only enters into equation 3.3 as a logarithmic derivative; in other words we can rewrite its left hand side as \( \partial Q/\partial t \) with an “RG time”

\[
t = \log \Gamma
\]

(3.4)

As the RG is run, successive generations of effective couplings are generated with ever-broader distributions (which, after all, is why we obtain a strong disorder fixed point) so we must integrate over longer and longer intervals in \( \Gamma \) to decimate the same number of bonds. If we choose to parameterize the energy scale in terms of \( t \), though, the decimation happens at a constant rate, which will simplify later analysis.
In [21], Fisher found that the only non-singular fixed point distribution satisfying the above equation has the remarkably simple form

\[ Q^*(\eta) = \theta(\eta)e^{-\eta} \implies \Pr(J | \Omega) = -\frac{1}{\Omega \log J} \left( \frac{\Omega}{J} \right)^{1-1/\Gamma} \theta(\Omega - J) \] (3.5)

where \( \theta(x) \) is simply the Heaviside step function.

### 3.5.2 The random singlet ground state

Qualitatively, we can describe the above procedure as forming a singlet across the strongest remaining bond as the energy scale of the RG is lowered. After the RG runs for a while, we can expect the generic bond to be formed over a previously generated effective coupling, so expressed in terms of the original spins our ground state will look something like figure 3.5.2: in other words, a collection of singlet bonds of various lengths, some of which will be arbitrarily long. This is called a random singlet phase, first predicted in [7] from numerical calculations. Whenever we take a step in the Fisher RG and eliminate all bonds with strengths between 0 and \( d \Gamma \), we eliminate a fraction \( 2Q^0 d\Gamma / \Gamma \) of the remaining spins\(^9\), which means the fraction \( n \) of spins still left follows

\[ \frac{dn}{d\Gamma} = \frac{-2Q^0}{\Gamma^n} \]

and at the fixed point we have \( n \sim \Gamma^{-2} \) since \( Q^0 = 1 \). Equivalently, we can say that the bonds formed at an energy scale \( \Gamma \) have a length on the order of \( L = n^{-1} = \Gamma^2 \).

The random singlet state generalizes readily to higher spin: in the valence bond picture, each site only forms valence bonds with one other site, which can be arbitrarily far away. See figure 3.5.2. We denote the fixed point that generates a random singlet state out of spin-\( J \) degrees of freedom by \( RS_J \). We don’t need to make any changes to the Fisher RG to describe these higher spin fixed points; in general we obtain them when the amplitude

\(^9\)At every decimation, we remove three couplings and two spins and create one new effective coupling, so the number of spins remains the same as the number of couplings.
of the randomness is much stronger than the screening from other valence bonds, causing all the valence bonds in a singlet to be formed successively. This point will be more clearly explained by a general treatment of the higher spin random Heisenberg model, which is our next topic.

3.5.3 Higher spin

We recall our qualitative description of the higher-spin Heisenberg ground state from section 2.2.3. In that discussion we were able to sweep through phases that were topologically equivalent to the original valence bond phases by adjusting the amount of explicit dimerization in our couplings. Now we add randomness (whose amplitude we parameterize by $R$) to the couplings:

$$J_i = J(1 + \delta(-1)^i) \exp(R\eta_i)$$

where the $\eta_i$ have mean zero and variance one. We ask ourselves what the phase diagram looks like in the $R - \delta$ plane under the valence bond ansatz.

All the valence bond solid phases have a finite energy gap, so they will be stable when we add weak amounts of randomness — the randomness just represents a perturbation away from the corresponding valence bond hamiltonian. As we saw from our discussion above, the spin-1/2 Heisenberg chain we obtain at the $R = 0$ critical points is unstable with respect to any weak randomness, so for any $R \neq 0$ we obtain the spin-1/2 random singlet ground state.

We can also guess what happens for very large randomness and $\delta = 0$: we obtain the spin-$J$ random singlet state. If we move off to $\delta \neq 0$, we cause the spin-$J$ singlets to preferentially terminate on one of the sublattices, and we obtain a phase that’s topologically equivalent to one of the completely dimerized valence bond states (depending on the sign of $\delta$).

We now try to fill in what happens between these two extremes: on the one hand, we
have $2J + 1$ distinct domains and $2J$ critical lines representing $RS_{1/2}$ states. On the other, we have just two phases separated by an $RS_J$ critical line. To make these match up, we must have a series of multicritical points (which we denote by $P_N$) where $N \geq 3$ distinct phases become energetically equivalent; in other words the behavior of the system is left invariant under any permutation of this set of domains. For $J = 1, 3/2$ this (along with the reflection symmetry along the $\delta$ axis) fixes the form of the phase diagram completely: For

Figure 3.3: Phase diagrams for the spin-1 and spin-3/2 antiferromagnetic chains as a function of randomness and dimerization.

$S > 3/2$ there are a variety of ways to draw the diagram, which are controlled by additional couplings in the interaction which we haven’t considered so far. Because of the symmetry in $\delta$, we know that in the generic case we only have $P_3$ and $P_4$ fixed points for any $S$; obtaining $P_5$ and higher requires fine tuning of these additional couplings\(^\text{10}\). Having now described

Figure 3.4: The three possible phase diagrams for the spin-2 antiferromagnetic chain. We can switch between them by tuning some additional parameter in the system, such as the next-nearest neighbor coupling [15]. Generically we expect to see either the first or last diagram for any physical system; the second requires fine tuning of the parameters.

this second family of fixed points, we now present the strong disorder renormalization group used to study them.

\(^{10}\)Phrased another way, each successive $P_N$ is described by a critical surface of dimension one less that that of $P_{N-1}$. 
### 3.5.4 The renormalization group treatment

Remarkably, Damle and Huse found that Fisher’s RG treatment described in section 3.5.1 could be extended to arbitrarily high spin in a relatively straightforward way. We follow the presentation of [15]; previous related ideas are expressed in [14, 25]. For the spin-$J$ chain we have $N = 2J + 1$ domains to work with (which we refer to using greek letters $0 \leq \alpha, \beta, \gamma \cdots \leq N - 1$), and the magnitude of a free spin on the boundary between domains of type $\alpha$ and $\beta$ is simply $|\alpha - \beta|/2$.

![Figure 3.5: Diagram of how the Damle-Huse RG is set up. We show a cartoon depiction of a spin-2 chain near a permutation-symmetric multicritical point — note that for clarity we haven’t shown the effects of randomness on the domains. The arrowheads represent the unpaired spins that arise at domain boundaries; in reality the spin degrees of freedom will be spread out over many lattice sites. Effective couplings are generated between the unpaired spins as shown.](image)

The focus now shifts to these domain wall spins: we seek to form an effective spin $j_{13}$ from the low-energy states of two adjacent domain wall spins $j_{12}$ and $j_{23}$, just as in the original Fisher RG. We have a subtlety that even though we’re dealing with an antiferromagnet, domain wall spins can add ferromagnetically if the domain labels form a monotonic sequence. In principle this means that we now have positive and negative couplings, but since this only changes the sign (and not the magnitude) of couplings to the new spin we need only keep track of their absolute magnitude.

In an nutshell, there’s no major conceptual change in the RG equations in going from $N = 2$ to $N > 2$; we just need to do extra bookkeeping to keep track of the domain labels. For our convenience we define $\rho_\alpha$ to be the probability that a specific domain is of type $\alpha$ and $W_{\alpha\beta}$ to be the probability of occurrence of the domain sequence $\alpha\beta$ (i.e., a domain of type $\alpha$ followed by one of type $\beta$). We then define

$$V_{\alpha\beta} = \Pr(\left\{\begin{smallmatrix} \alpha & \gamma & \beta \\ \downarrow & \\ \downarrow \end{smallmatrix}\right\}) = \sum_\gamma W_{\alpha\gamma} P_{\beta}^\gamma W_{\gamma\beta}$$

(3.6)
as the probability for a new junction $\alpha \gamma \beta \rightarrow \alpha \beta$ to be formed from the decimation of any bond. The Damle-Huse RG equation for the coupling distribution $P_\alpha$ for each domain $\alpha$ is then

$$
\frac{\text{Change}}{\text{in } P_\alpha} = \text{(rescaling)} + \text{(renormalization)} + \text{Pr} \left( \frac{\alpha \sqrt{\alpha}}{\text{expected strength of new bonds}} \right) - \text{Pr} \left( \text{bonds over duplicate domain} \right)
$$

which translates to

$$
\frac{\partial P_\alpha}{\partial \Gamma} = \frac{\partial P}{\partial \zeta} + P^0 P(\zeta) + V_{\alpha \alpha} [P_\alpha \otimes P_\alpha - P_\alpha]
$$

This equation for $P$ can be reduced to a rescaled version of 3.2, so we recover Fisher’s solution $P_\alpha(\zeta|\Gamma) = (N-1)e^{-(N-1)\zeta/\Gamma}/\Gamma$. The quantities $W_{\alpha \beta}, \rho_\alpha$ governing the distribution of the domains follow their own renormalization group equations, but their fixed point values become obvious given the domain permutation symmetry. In effect, this symmetry means that we’re only allowed to test whether two domains are the same or different; individual domain labels become meaningless. Therefore, we have $\rho_\alpha = 1/N$ for any $\alpha$, and similarly $W_{\alpha \beta} = 1/(N-1)$ for any $\alpha \neq \beta$. Since we aren’t interested in the scaling behavior of these quantities, we omit their RG equations.

We are interested in the distribution of bond lengths, however, since we want to compare that result with what we found in section 3.5.2. The RG equation for the fraction of remaining spins $n$ is simple; at each step in $\Gamma$ we remove the fraction that were decimated by the RG. If the decimation results in two domains of the same type being next to each other, we need to remove one of them as well. This tells us

$$
\frac{dn}{d\Gamma} = -n \left[ \sum_\alpha \rho_\alpha P^{\alpha \beta}_\alpha + \sum_\alpha \rho_\alpha V_{\alpha \alpha} \right]
$$

At the fixed point the former sum evaluates to $(N-1)/\Gamma$ while the latter is $1/\Gamma$; therefore we have $n \sim \Gamma^{-N}$ and we expect the bonds formed at energy scales of $\Gamma$ to have a length on the order of $L^N$, in agreement with the $N = 2$ result.

This concludes our exposition of the families of fixed points $RS_J$ and $P_N$ and the strong disorder renormalization group frameworks used to study them. These techniques will form the starting point for the original work done for this thesis, which we now describe.
Chapter 4

Original Results

4.0.5 Introduction and motivation

The work done for this thesis was motivated by a number of interesting conjectures about the block entanglement of quantum systems made in [32, 24]:

1. They conjecture that the block entanglement always decreases along RG flows from high-energy to low-energy fixed points. This might seem obvious, since we expect the low-energy fixed point to have fewer degrees of freedom to entangle, but we recall that a generic RG involves both a decimation of degrees of freedom and a rescaling. It’s quite conceivable that the rescaling operations could cause the density of entanglement to progressively increase, so we have no reason to believe that the entanglement would decrease monotonically along the flows.

2. They also notice that the asymptotic block entanglement they obtain is identical to a different quantity, the geometric entropy [13] of the field theory one obtains for the spin systems via the Jordan-Wigner transformation. This leads them to claim that the entanglement properties they find are consequences of the underlying conformal invariance of the models they chose.

If one assumes the conformal invariance property (2), the monotonicity property (1) follows automatically for one-dimensional systems, due to Zamolodchikov’s c-theorem [4]. This result establishes that the central charge of a conformal field theory never increases along
renormalization group flows; since the geometric entropy of a conformal theory is proportion-
tional to this quantity, the first conjecture follows automatically.

Examining fixed points with strong randomness will shed some light on these issues, since none of the fixed points discussed in section 3.4 are conformally invariant. One can obtain a qualitative feel for why this is so from the Suzuki-Trotter mapping (figure 2.4.1): under strong disorder, the pattern of couplings one obtains is extremely anisotropic and any conformal map on the potential implied by this distribution will result in a drastically different distribution. There are model systems with weak randomness where one can use various techniques [6] to perform an explicit average over the randomness and obtain an isotropic theory from a random one; however, the conformal field theories produced in this way have a central charge of zero, which implies an unentangled ground state by the result of [13]. In addition, there’s no guarantee that the averaged theory one obtains is conformally invariant in the first place, and arguments have been given [28] that strong randomness breaks conformal invariance irrevocably.

Moreover, while Latorre et. al. performed their calculations for four quantum critical points, we’re considering two infinite families of critical points (the $RS_J$ and $PN$ fixed points). Since all the points in a family are described by trivially similar RG equations, we can in principle calculate the block entanglement for all of them. This point is relevant because in section 4.4.3 we discuss how the set of RG flows between these fixed points constitutes a nontrivial test of the monotonicity conjecture.

Another reason to look at the scaling of block entanglement in random systems is that it’s a calculation which may be done comparatively easily and accurately within the context of the strong disorder renormalization group. From the point of view of entanglement, randomness has the effect of breaking the existing degeneracy in energy space. An obvious consequence of the result of entanglement sharing is that the entanglement present in the random singlet ground state is only bipartite in nature; we can make a similar argument for the permutation-symmetric fixed point. Due to the confusion that exists over how to measure multiparticle entanglement, we can be more confident in our ability to account for all the entanglement in a system.
Whereas [24, 32] have to employ a rather involved chain of manipulations\(^1\) to obtain the entanglement, for our systems we can estimate the same quantities through comparatively simple statistical arguments and the strong disorder renormalization group. Ultimately we will be forced to switch over to numerical methods, but the part of the problem that we can solve analytically will yield some insight into the nature of the problem.

Therefore, the task we set for ourselves is to evaluate the block entanglement at the fixed points described in the previous chapter and compare the results against the views of Latorre et. al. We now turn to these calculations.

### 4.1 Entanglement calculations for spin-1/2

We now make use of the strong disorder renormalization group to calculate the entanglement between a block of \(L\) spins and the rest of the system for the random antiferromagnets introduced above. In this section we restrict ourselves to the easier spin-1/2 case. We set up the calculation as follows:

\[
E_{RS_{\frac{1}{2}}}(L) \sim \left(\text{RG time to decimate a block of } L \text{ spins}\right) \times 2 \left(\text{Rate at which singlets form across boundary}\right) \times \left(\text{Bits of entanglement per singlet}\right)
\]

where we introduce the notation \(E_{RS_J}\) to denote the block entanglement associated with the spin-\(J\) random singlet state. Strictly speaking, we should write the right hand side as an integral over the RG time, but we’re only interested in the \(L \to \infty\) behavior of \(E\); this means that the integral will be dominated by the value of the integrand at the strong disorder fixed point, which is where all the quantities are to be evaluated.

We obtain the factor of 2 simply because in 1D the boundary of the block consists of two separate pieces — since we’re really only interested in how the entanglement scales as \(L \to \infty\), we calculate the rate singlets form across a single partition between two semi-infinite chains and multiply this by two to get the entanglement at both ends of the block.

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Obviously, we get one bit of entanglement per singlet formed. From the previous discussion, we know that the RG time \(t\) and the average length \(L\) of new bonds are related to the RG energy scale \(\Gamma\) by \(t = \log \Gamma\) and \(L \sim \Gamma^2\); together these mean that the first factor is equal to \(1/2 \log L\). All that remains for us to do is calculate the probability that a singlet forms across the partition during a given RG time step.

\(^1\)For an idea of what’s involved, see figure 5 of [32].
4.1.1 Entanglement bit rate for the spin-1/2 chain

To answer this question, we need to keep track of more information as we do the RG since we’re focusing our attention on the bond crossing the partition (hereafter referred to as “the partition bond”). To do this, we simply give it its own distribution \( W(\eta, \Gamma) \); all other bonds remain statistically indistinguishable and continue to have strengths chosen from \( Q(\eta, \Gamma) \). \( W \) obeys its own RG equation, which is not too different from the equation for \( Q \) but includes some extra terms:

\[
\frac{\partial W}{\partial t} = W + (1 + \eta) \frac{\partial W}{\partial \eta} + W^0 Q \otimes Q + 2Q^0 (W \otimes Q - W) \tag{4.1}
\]

The first two terms arise from the same change of variables and rescaling we encountered in the equation for \( Q \). The third term describes the partition bond being decimated and replaced with a new bond formed from its neighbors. The final term accounts for those circumstances in which one of the bond’s two neighbors hit the top of the distribution, and the partition bond is incorporated into the resulting new bond.

Our task is to find the fixed point distribution \( \dot{W} = 0 \). We fortunately already have the analogous solution for \( Q \), so we might as well put it to good use: we define a function \( f(\eta, t) \) so that \( W = fQ \). We substitute this and the fixed point solution for \( Q \) (equation 3.5) into equation 4.1 to obtain

\[
\dot{W} = f(\eta)e^{-\eta} + (1 + \eta) \left( \frac{\partial f}{\partial \eta} e^{-\eta} - f(\eta)e^{-\eta} \right) + f(0) \eta e^{-\eta} + 2e^{-\eta} \int_0^\eta d\eta' f(\eta') - 2f(\eta)e^{-\eta}
\]

where the step function has been suppressed — i.e, the domain of this equation is \( \eta \geq 0 \). We can factor out \( e^{-\eta} \), but we’re still faced with integrals over and derivatives of \( f \) appearing in the same equation. We get around this by simply defining

\[
F(\eta, t) = \int_0^\eta d\eta' f(\eta')
\]

and note that \( \partial F/\partial \eta |_{\eta=0} = f(\eta_0) \) by the fundamental theorem of calculus. We finally obtain a second order differential equation in \( F \),

\[
-\eta f(0) = -(2 + \eta) \frac{\partial F}{\partial \eta} + (1 + \eta) \frac{\partial^2 F}{\partial \eta^2} + 2F
\]

which has the analytical solution\(^2\)

\[
F(\eta) = \frac{1}{2} f(0)(\eta^2 + 4\eta + 3) + C_1 (1 + \eta) - \frac{C_2}{2e} \left( e^{1+\eta}(\eta + 2) - (1 + \eta)^2 Ei(1 + \eta) \right)
\]

\(^2\)Here we treated \( f(0) \) as an ordinary constant independent of \( F \); the solution we obtain is self-consistent so this is justified.
where $\text{Ei}(z) = -\int_{-z}^{\infty} dt e^{-t}/t$ is the exponential integral. We now set boundary conditions to fix the constants of integration $C_1$ and $C_2$. An obvious requirement is the normalization $\int d\eta\ W = \int d\eta\ f e^{-\eta} = 1$. We have $\text{Ei}(1+\eta) \sim e^{1+\eta}/\eta$ as $\eta \to \infty$, so we see that

$$\lim_{\eta \to \infty} \frac{C_2}{2e} \left( e^{1+\eta}(\eta+2) - (1+\eta)^2\text{Ei}(1+\eta) \right) = \frac{C_2}{2} e^\eta \left( \eta + 2 - \frac{(1+\eta)^2}{\eta} \right) = -\frac{C_2}{2\eta} e^{-\eta}$$

When we multiply this term by $e^{-\eta}$ and integrate over the range $[0, \infty)$, it diverges to $-\infty$; therefore we need $C_2 = 0$. Normalizing the remaining terms results in the constraint $4C_1 - 3f(0) = 1$, while evaluating our solution at $C_2 = 0, \eta = 0$ gives us $f(0) = 2/3C_1$. Together these imply that $C_1 = 1/2$ and $f(0) = 1/3$, so we finally obtain

$$E_{RS_1}(L) \sim \left( \frac{1}{2} \log L \right) \times \frac{2}{3} \text{ bits}$$

or, generalizing to singlets of spin $J$,

$$E_{RS_J}(L) \sim \frac{1}{3} \log L \log_2(2J+1) \text{ bits} \quad (4.2)$$

### 4.2 Entanglement calculations for arbitrary spin

We now consider spin chains with $N > 2$ domains and switch to the language (and RG formalism) of [15] which we discussed in section 3.5.4. A first step is to rewrite equation 3.7 using the notation of the previous section; we apply a rescaling $(N-1)\xi/\Gamma \to \eta, P \to (N-1)Q/\Gamma$ to obtain

$$\Gamma \frac{\partial Q}{\partial \Gamma} = Q + (\eta + N-1)\frac{\partial Q}{\partial \eta} + (N-2)Q^0Q + Q^0(Q \otimes Q) \quad (4.3)$$

Note that this means that at the fixed point we have $Q^*(\eta) = e^{-\eta}$, as before (as can be verified by substitution), and our RG timescale is still defined by equation 3.4. Since we now have $L \sim \Gamma^N$, though, it now takes $\log L/N$ units of RG time to completely decimate a block of $L$ bonds — the block takes longer to decimate because if the types of neighboring domains don’t match, we only decimate one bond instead of two.

We want to repeat the chain of reasoning in the previous section as much as possible, but this is complicated by the fact that under the rules of the Damle-Huse RG the partition

\footnote{Recall that in the $N = 2$ RG, one decimation step involved removing the current strongest bond and its two neighbors and replacing them with a new effective bond, for a net loss of two bonds.}
bond can change into a spin sitting on top of the partition. This happens whenever we decimate the domain lying across the partition and its neighbors are of different types: instead of merging to forming a new domain across the partition, the neighbors remain distinct with a spin on their boundary. Since the spin lies exactly on the partition, it’s ambiguous whether this should count as an entanglement-generating event.

Furthermore, the bonds on either side of the spin may be decimated, resulting in spins being added to it (as depicted above). This may happen arbitrarily often; when the new neighboring domains are of the same type the merge to become a new partition bond. We call the object formed by this process a “spin tree”; ignoring the domains for a moment it simply refers to the sequential addition of a collection of spins on either side of the partition to form an object with total spin zero.

We assert that these spin trees produce a quantifiable amount of entanglement across the partition; we show how in section 4.3.2. The form our entanglement calculation takes is now

\[
E_{\Pi_N}(L) \sim \left( \frac{1}{N} \log L \right) \times 2 \left[ \frac{\text{Rate at which singlets form across boundary}}{\text{Bits of entanglement per singlet}} \right] \times \left( \frac{\text{Rate at which spin trees are completed}}{\text{Bits of entanglement per tree}} \right)
\]

(4.4)

The evaluation of these quantities, in particular the last one, is significantly less straightforward than the calculation of the previous section. We leave the discussion of spin trees for the next section and concentrate on the first three quantities here.

4.2.1 Singlet formation rate

The analysis of section 4.1.1 is still valid (or straightforwardly generalizable) whenever trees aren’t involved. We redefine \(W(\eta)\) to be the probability that the partition bond isn’t in a tree and has strength \(\eta\) and introduce a new variable \(T\) to denote the probability that a spin lies on the partition and we’re in a tree. Our normalization condition for \(W\) therefore changes to \(\int d\eta \, W = 1 - T\).

A tree is born when the partition bond is decimated and the domains on either side are of different type. Trees are terminated by the formation of a singlet at their root, which requires the two domains on either side of the root to be of the same type. Based on these considerations we can write down the RG equation for \(T\) at the permutation-symmetric
fixed point as

$$\frac{\partial T}{\partial t} = 0 = (N - 2)W^0 - 2TQ^0$$

(4.5)

We expect to recover our results from section 4.1.1 by examining the $N = 2$ case. Here setting $N = 2$ requires that $T = 0$; no trees can be formed with only two domains. For general $N$ we’ll also need to know $W^0$, which we turn to now.

We wrote down the generalized RG equation for the distribution $W$ by enumerating all the ways in which the partition bond can change over the course of the RG. Of course, we have the same shift and rescaling terms as in equation 4.3: these cover all situations where the partition bond is hit and removed, so we don’t need to include an additional loss term for when a tree is begun. When we aren’t in a tree we find ourselves in the situation described by equation 4.1, with the only changes coming from the decimation of the partition bond or one of its neighbors. We finally need to add a source term to describe the situations when a tree terminates and a new partition bond is formed from the domains that were on either side of the partition. For this to happen we need three conditions: we need to be in a tree, one of the two domains on either side of the partition needs to be decimated, and the new neighboring bonds need to be of the same type. In other words, this event happens with a probability $T \times 2V_{aa}$ (see equation 3.6) and the new partition bond’s strength will be drawn from the distribution $Q \otimes Q$. The complete RG equation at the permutation symmetric fixed point is then

$$\frac{\partial W}{\partial t} = W + (\eta + N - 1)\frac{\partial W}{\partial \eta} + W^0Q \otimes Q + 2Q^0(W \otimes Q - W) + 2TQ^0Q \otimes Q$$

(4.6)

This reproduces equation 4.1 for $N = 2$ — in fact, they’re sufficiently similar that we can solve this in the same way. Again defining $F(\eta) = \int_0^\eta d\eta'W(\eta')/e^{-\eta'}$ we obtain

$$-(N - 1)W^0\eta = 2F - (\eta + N)\frac{\partial F}{\partial \eta} + (\eta + N - 1)\frac{\partial^2 F}{\partial \eta^2}$$

with the boundary condition $F(0) = 0$. The other constant of integration we obtain is again set equal to zero by requiring $W$ to be normalizable; once again the general solution involves a term of the form $C_2\eta e^{-\eta}Ei(\eta + N - 1)$ which requires $C_2 = 0$ as demonstrated before. This yields

$$W(\eta) = W^0e^{-\eta}\frac{N\eta + N - 1}{N - 1}$$

---

The factor of $V_{aa}$ we just mentioned reduces to $Q^0$ when we make the change of variables $P \rightarrow Q$ and divide out common factors of $\Gamma$ and $(N - 1)$ as we did in obtaining equation 4.3 from equation 3.7.
We obtain $W^0$ by imposing normalization:

$$\int_0^\infty d\eta \ W = 1 \Rightarrow W^0 \frac{2N - 1}{N - 1} = 1 - \frac{1}{2} (N - 2)W^0 = 1 - T$$

Combining this result with equation 4.5, we find that

$$W^0 = \frac{N - 1}{N(N + 1)} \quad (4.7)$$

and

$$T = \frac{(N - 2)(N - 1)}{N(N + 1)} \quad (4.8)$$

These are key pieces of information we need in order to determine the entanglement — we form singlets at a rate $W^0$ and finish trees at a rate $2Q^0T$. We now calculate the expected entanglement we obtain from each of these events, starting with singlet formation.

### 4.2.2 Expected entanglement from singlets

In the Damle-Huse RG, we can still generate singlet bonds across decimated domains, but now the singlets can be formed out of objects of different spin — for example, if a domain of type 4 is decimated and both its neighbors are of type 1, we generate a spin-3/2 singlet bond. If we have $N$ domains, we can generate singlets with spin as high as $(N - 1)/2$ in this way. We know that a spin-$J$ singlet provides $\log_2 (2J + 1)$ bits of entanglement, so we now calculate the expected entanglement contribution from the singlets as

$$\langle \text{Bits of entanglement per singlet} \rangle = \frac{1}{2} (N-1) \sum_{J = \frac{1}{2}}^{\frac{1}{2} (N-1)} \Pr(J) \log_2 (2J + 1). \quad (4.9)$$

At the permutation-symmetric critical point, the distribution of spins appearing in the RG is straightforward to obtain since the spins are determined by differences between adjacent domains. Any specific sequence of $k$ domains will occur with probability $\left[ N(N - 1)^{k-1} \right]^{-1}$, and the spin at the boundary between two domains $\alpha \beta$ will have magnitude $J = |\beta - \alpha|/2$. 

We need to make an important distinction about the class of $P_N$ fixed points here, since as we saw in section 3.5.3 we can obtain $P_N$ fixed points in any spin-$J$ model that has $J \geq (N - 1)/2$. Therefore, for the purposes of entanglement we should really be referring to $P_N\{D_1, D_2 \cdots D_N\}$ fixed points, where the $D_i$ identify the subset of the $2J + 1$ domains that participate in the permutation symmetry at this fixed point. This additional distinction is
of course irrelevant for the strong disorder RG treatment, since that was only concerned with bond strengths — the exact identity of the fixed point only matters when we go to ask questions about the spin distributions.

In this section and the remainder of this paper we will restrict ourselves to the symmetric $P_N\{1, 2, \cdots N\}$ case\(^5\) for the sake of brevity. Our analysis is unchanged in the general case (i.e, the methods we describe below apply to any $P_N$ fixed point) but without this specialization we simply have too many options to consider.

We get singlets from domain sequences like $\alpha \beta \alpha$, so we can write the probability that a given singlet will be a spin-$J$ singlet as

$$\Pr(J) = 2 \sum_{\beta=1}^{N-2J} \frac{1}{N(N-1)^2} = 2 \frac{N-2J}{N(N-1)}$$

where the factor of two arises from considering the two cases $\alpha < \beta$ and $\alpha > \beta$ in the domain sequence $\alpha \beta \alpha$. Unfortunately, trying to take the expected value of $\log_2(2J + 1)$ using this distribution involves evaluating sums of the form $\sum j \log j$, which cannot be put in closed form. However, we can evaluate equation 4.9 for any fixed $N$ (see figure 4.2.2).

\[\text{Figure 4.1: Plot of expected number of singlet bits vs. number of domains } N. \text{ Squares indicate the exact summation (equation 4.9). The dotted and continuous lines show the asymptotic expansion (equation 4.11) up to the second and third terms respectively.}\]

and obtain the asymptotic behavior by approximating the sum by an integral, which tells us that

$$\lim_{N \to \infty} \left\langle \text{Bits of entanglement per singlet} \right\rangle \sim \log_2 N - \frac{3}{2 \log 2} + \frac{3 \log_2 N}{N}$$

\(^5\)An example for $P_5$ is shown in the center panel of figure 3.5.3.
The next highest order correction is negative, so this estimate is an upper bound on the large $N$ behavior. As figure 4.2.2 shows, it's in fact an upper bound for $N \geq 5$ and a very close estimate.

### 4.3 Calculating entanglement from spin trees

In the last section we were able to evaluate three of the four unknown quantities in equation 4.4. We now turn our attention to the spin trees and their contribution to the entanglement. In this section we describe in more detail what we mean by a “spin tree” and present a method for calculating the entanglement across the partition generated by an arbitrary tree. In the following section we return to the broader question of the block entanglement associated with the $N$ domain permutation symmetric multicritical point.

#### 4.3.1 Terminology

Our discussion of spin trees will be facilitated if we introduce several specific terms. All spin trees have the generic form depicted above: they begin when the bond over the partition is eliminated by the RG and end with the formation of a singlet. In between, a certain number of spins are added; we try to calculate the entanglement between all the spins on the left and right sides. The height $H$ of the tree is the total number of spins involved. In order to specify a tree, we first draw the unlabeled pattern of lines, which we call specifying the topology of the tree. We can label the branches with spins, and to be more specific we can assign fixed domain labels to the regions between the branches (with the constraint that

![Figure 4.2: Spin tree diagram](image)
the magnitudes of the spins are determined by the differences between adjacent domains). Note that different domain labellings can give rise to the same spin tree.

4.3.2 Entanglement calculation

In the singlets we’ve been studying earlier, two spin-$J$ objects on either side of the partition combine to form an object with total spin zero; this fact indicates that the two spins are entangled. The spin tree is simply a generalization of this situation involving the combination of arbitrary numbers of spins. Because spins on either side of the partition are involved, we know that any tree makes a well-defined contribution to the block entropy. For a given tree, the computation of this entanglement is straightforward if tedious: the tree as a whole is in a pure state, so the von Neumann entropy (equation 3.1) is the proper measure of entanglement to use. We can construct the state vector for the tree by adding the individual spins one at a time using the familiar Clebsch-Gordan coefficients; the reduced density matrix can be obtained from forming the outer product and tracing out all spins on one side of the partition.

We can delegate this work to a computer (see appendix A.1), but the size of the reduced density matrix increases exponentially with the number of spins in the tree so this method rapidly becomes impractical. We can make the calculation simpler both computationally and conceptually by performing operations on the spin tree itself before its entanglement is evaluated. We can do this by making use of more advanced results from the theory of angular momentum; specifically, the Wigner $6j$ coefficients let us rewrite the topology of a given tree as follows:

\[
\begin{align*}
\begin{array}{c}
\begin{array}{c}
\hline
j_1 \quad j_2 \quad j_3 \\
\hline
j
\end{array}
\end{array}

\end{align*}
\]

\[
\begin{align*}
\begin{array}{c}
\begin{array}{c}
\hline
j_1 \quad j_2 \quad j_3 \\
\hline
j
\end{array}
\end{array}
\end{align*}
\]

\[
\begin{align*}
\sum_i \sqrt{(2j + 1)(2i + 1)(-1)^{j_1+j_2+j_3+j_T}} \left( \begin{array}{ccc} j_1 & j_2 & j \\ j_3 & j_T & i \end{array} \right) \begin{array}{c}
\begin{array}{c}
\hline
j_1 \quad j_2 \quad j_3 \\
\hline
j
\end{array}
\end{array}
\end{align*}
\]  \hspace{1cm} (4.12)

\[
\begin{align*}
\sum_j \sqrt{(2i + 1)(2j + 1)(-1)^{j_1+j_2+j_3+j_T}} \left( \begin{array}{ccc} j_1 & j_2 & i \\ j_T & j_3 & j \end{array} \right) \begin{array}{c}
\begin{array}{c}
\hline
j_1 \quad j_2 \quad j_3 \\
\hline
j
\end{array}
\end{array}
\end{align*}
\]  \hspace{1cm} (4.13)

with the tableaux of spin magnitudes in the above equations being the standard notation for the $6j$ symbol. The above equations simply express the familiar operation of expanding a quantum mechanical state (the left hand side) in terms of a specified basis (the right hand side) — we emphasize that all this follows from the elementary relations of angular
momentum theory; the $6j$ symbols don’t express any new physical content but are merely a convenient algebraic device that lets us add spins in a basis-independent manner (i.e., without having to worry about the $m_z$ quantum numbers). For this reason the $6j$ symbols are sometimes called recoupling coefficients.

For ease of presentation we absorb the numerical prefactors into the definition of a new symbol — note that this is nonstandard notation:

$$(-1)^{j_1+j_2+j_3+j_T} \sqrt{(2i+1)(2j+1)} \begin{pmatrix} j_1 & j_2 & i \\ j_T & j_3 & j \end{pmatrix} \equiv \begin{bmatrix} j_1 & j_2 & i \\ j_T & j_3 & j \end{bmatrix}$$

The limits on the sum over the new spin $i$ are set by the requirement that all the spin additions depicted in the diagram on the right hand side be physically realizable: for example in the right-hand side of equation 4.12 we must be able to obtain a spin of magnitude $i$ by adding $j_2$ and $j_3$ as well as by adding $j_1$ and $j_T$. In the language of $6j$ coefficients, this is realized by having the coefficient vanish unless its entries satisfy four triangle inequalities. If we consider the arguments to the $6j$ symbol to be labeled as they are in equation 4.12, triangle inequalities must be satisfied by $(j_1, j_2, j)$, $(j_1, j_T, i)$, $(j_3, j_2, i)$ and $(j_3, j_T, j)$; equivalently, this means the range of summation for $i$ in equation 4.12 is

$$\max (|j_T - j_1|, |j_3 - j_2|) \leq i \leq \min (j_T + j_1, j_3 + j_2)$$

with an analogous relation holding for equation 4.13.

Note that in equations 4.12 or 4.13 the “inputs” $j_1, j_2$ etc. might have arisen from previous addition of spins. This lets us apply these relations repeatedly to a given tree in order to transform it into a more convenient form: namely, we can write any spin tree as a superposition of spin-$J$ singlets in a canonical way by “defoliating” the “trunk” of the spin tree. Consider this tree as an example — the oval denotes the position of the next spin to be expanded according\(^6\) to equation 4.12 or 4.13:

\(^6\)Since there are only two inequivalent configurations locally, there’s never any ambiguity as to which equation to use.
The value of this set of manipulations should be clear from the above exercise: in the last line we only have a single singlet bond across the partition, so the entanglement of any tree in the final sum will simply be $\log_2(2i_3 + 1) = \log_2(2i_4 + 1)$. The $6j$ symbols let us rewrite any spin tree as a sum of singlets in this fashion.

In other words, whereas previously we wrote the density matrix in terms of combinations of the $|l_1, m_{l_1}\rangle, |l_2, m_{l_2}\rangle, \cdots |r_1, m_{r_1}\rangle, |r_2, m_{r_2}\rangle, \cdots$ basis states, we can now write it in the $|i_1 i_2 i_3 \cdots \rangle$ basis: we only need to work with the magnitudes of the spins.

This new basis is orthonormal; we have $\langle i_1 \cdots i_n | j_1 \cdots j_n \rangle = \prod_k \delta_{i_k j_k}$. We can rewrite the basis states as $|i_1 \cdots i_n\rangle = \{|i^L\rangle \otimes |i^R\rangle\}$, where $\{|i^L\rangle \}$ ($\{|i^R\rangle\}$) refers to the set of new spins on the left (right) side of the partition. This unfortunately means that the basis is not bi-orthogonal: when we take the partial trace of $|\{i^L\}\rangle \otimes |\{i^R\}\rangle$, the reduced states

$$\text{Tr}_R \left[ \sum_{\{i^L\}, \{i^R\}} C (\{i^L\}, \{i^R\}) |\{i^L\}\rangle \otimes |\{i^R\}\rangle \right] = \sum_{\{i^L\}} |\{i^L\}\rangle \otimes |\{i^R\}\rangle$$

Each of the reduced $|\{i^L\}\rangle$ states is degenerate with a multiplicity equal to the number of allowable values for the $\{i^R\}$ given the magnitude of the singlet $i^L_n = i^R_n$. To find the correct weights for the singlet basis states, we need to perform a Schmidt decomposition on

---

7The reason that we can get away with this kind of compression is that the class of spin tree states one can construct from a given collection of spins is a subset of measure 0 of the set of all possible states those spins can be in. The old basis spans this larger Hilbert space while the new basis spans the space of spin trees.
each of the subspaces given by the projection of $|\{i^L\}\rangle$ onto the possible singlet magnitudes $i_n^L$.

In other words, the defoliation algorithm puts the density matrix of the spin tree in a block diagonal form, with each block labeled by a different value of the singlet magnitude $i_n^L = i_n^R$. Qualitatively, the reason we don’t completely diagonalize the matrix is that the only thing the reduced state $|\{i^L\}\rangle$ “knows” about the other quantum numbers of the other side is the singlet magnitude $i_n^R$. By diagonalizing the reduced density matrices, the Schmidt basis mixes the information on either side and lifts the degeneracy.

In practical terms, this means we haven’t escaped the need to calculate matrix eigenvalues in order to obtain the entanglement. It might seem that this algorithm accomplishes no real simplification, but we’ve transformed the problem from finding the eigenvalues of one large matrix to finding the eigenvalues of several smaller matrices. Since finding the eigenvalues of an $N \times N$ matrix takes of order $N^3$ arithmetic operations and the sum of the sizes of the new matrices is less than the size of the old density matrix, we always wind up doing fewer operations (although the number of operations still scales as $N^{3/2}$; we only obtain a smaller proportionality constant). Similar considerations apply to the storage space required. One would like to obtain a greater improvement, but we have been unable to come up with a decomposition algorithm that does a better job of diagonalizing the density matrix while still yielding a decomposition in terms of state whose entanglement is already known.

### 4.3.3 Tree height

We see from equation 4.8 that as $N$ increases we expect to be spending all of our time in spin trees. It’s important to know if this takes the form of a succession of many small trees or a few large trees, since the entanglement of large trees is difficult to calculate explicitly. Fortunately, the permutation symmetry of the fixed point means we can easily write down the distribution of tree heights $\Pr(H)$. To start a new tree, we need a sequence of three

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*See previous footnote.

*Strictly speaking, we should also include the number of operations needed to evaluate a 6$j$ symbol, which is a nontrivial effort: it involves a sum over factorials (see appendix A.1) so in principle it could be the dominant computation for large trees. However, one may use lookup tables to evaluate 6$j$ symbols with small arguments very efficiently [45]; in our calculations (presented in section 4.4) the matrix manipulations took the most computer time.
different domains (the middle of which gets decimated); there are \( N(N - 1)(N - 2) \) ways this can happen. We add spins to the tree by decimating one of the domains on either side of it; if the new neighboring domain is of the same type as the other neighbor the tree terminates but in the other \((N - 2)\) cases the tree continues. These considerations yield the probability that a given tree has height \( H \) — it’s the probability of \((H - 3)\) continuations and 1 termination:

\[
Pr(H) = \frac{1}{N - 1} \left( \frac{N - 2}{N - 1} \right)^{H - 3} \quad (4.14)
\]

In particular, we note that \( \langle H \rangle = N + 1 \), so although we can generate arbitrarily large trees at any \( N \), most trees are quite short. On the other hand, there are \( N(N - 1) [2(N - 2)]^{H - 3} \) different types of trees with a given \( N, H \). By “different types of trees”, we mean different domain colorings — one can obtain the same pattern of spins from different domain colorings, but enumerating these is a more difficult problem in combinatorics. We note that because of the finite number of domains, not all possible orders of adding a given set of spins result in a physical spin tree.

### 4.4 Statistical properties of spin trees

Summarizing the results we’ve obtained so far, namely equations 4.4, 4.7, 4.7 and 4.10, we have

\[
E_{P_N} = \left( \frac{2}{N} \log L \right) \times \left[ \frac{2(N - 1)}{N(N + 1)} \langle \log_2(2J + 1) \rangle_N + 2 \frac{(N - 2)(N - 1)}{N(N + 1)} \langle E_{trees} \rangle_N \right] \quad (4.15)
\]

We now find ourselves in the position of being able to investigate almost any property of the entanglement of spin trees numerically but not analytically. In particular, we must abandon our original goal of evaluating equation 4.10 and obtaining the entanglement for general \( N \): the most we can do is to examine trees on a case-by-case basis. For low \( N \) we can obtain a good estimate for the expected entanglement from a tree by systematically generating all trees up to some size \( H \), evaluating their entanglement and weighting the results according to equation 4.14. See appendix A.1 for the details of how this is done.

Due to time constraints, we’ve only been able to evaluate the expected entanglement from trees to acceptable accuracy for \( N = 3 \); by examining all trees with \( H \leq 12 \) we estimated the average entanglement from trees to be 1.458 bits; the expected entanglement
from singlets is 1.195 bits which implies that $E_{P_3} \approx 0.590 \times \log L$ bits. Of course, for these types of numbers to be meaningful, we need some way of estimating the contributions from all the trees with sizes above the cutoff that we neglect.

### 4.4.1 Estimating error

In order for our numerical estimates of the entanglement from trees to be useful, we need some way to estimate the error we accumulate by only doing calculations for trees up to a finite height. For a given $N, H$ we know the number of different trees and the probability with which they occur (equation 4.14); we just need a bound on the amount of entanglement we get. Our earlier considerations show that the bipartite entanglement is limited by the size of the hilbert space of the smaller subsystem, so to obtain the maximum entanglement we consider an evenly balanced tree. The von Neumann entropy is maximized if the density matrix eigenvalues are uniformly distributed, so our upper bound is

$$\langle E\text{\scriptsize\text{\textsc{tree}}} \rangle_{N,H} \leq \frac{H}{2} \langle \log_2 (2J + 1) \rangle$$

This is only an upper bound on the average entanglement of all trees at fixed $N, H$; if we label the domains appropriately we can always construct a tree\textsuperscript{10} whose component spins add up to more than $H\langle J \rangle$. We’ve already discussed the evaluation of $\langle \log_2 (2J + 1) \rangle$ in section 4.2.2, so putting all these pieces together we have

$$\text{Error} < \sum_{h=H+1}^{\infty} \frac{4}{N} (2(N-1))^{1-h} \times \frac{h}{2} \times \left( \log_2 N - \frac{3}{2\log 2} + \frac{3\log_2 N}{N} \right)$$

where the first factor is the probability of obtaining any tree with fixed $N, h$ and the third factor is the upper bound on $\langle \log_2 (2J + 1) \rangle$ given by equation 4.11. Evaluating the sum in $h$, we obtain our bound on the remaining expected entanglement:

$$\text{Error} < \frac{(2(N+3)\log N - 3N)(N + H - 1)}{4N\log 2} \left( \frac{N - 2}{N - 1} \right)^H$$

### 4.4.2 Some plots

To get a feel for the behavior of spin tree entropy, there’s no substitute for working out concrete examples. To that end, we employed the Mathematica code listed in appendix A.1\textsuperscript{10}For example, in $N = 3$ if we draw a tree with many spins being successively added from the same side of the partition, we can assign domains so that all those spins are spin-1 even though in the system as a whole $\text{Pr}(J = 1) = 1/3$. \textsuperscript{10}
to automatically generate a large number of spin trees and evaluate their entanglement. We restricted our efforts to \( N \leq 10 \) and \( H \leq 12 \) in the interests of computational time. Although the numerical results we present in this section are by no means extensive enough to form airtight conclusions about the behavior of trees in the general case, we can make a number of interesting observations.

The most immediately self-evident question that arises is to examine entanglement as a function of the number of spins in the tree. This will let us examine the degree to which the upper bound we derived in the previous section overestimates the average entropy. The data for \( N = 3 \) and \( N = 10 \) are plotted in figure 4.4.2; the behavior for intermediate values of \( N \) is qualitatively similar. The entanglement from individual trees is represented as a small dot; in order to keep the dots from piling up on top of each other at the integer values of \( H \) we perturb the x coordinate of the point by a random amount. This allows one to get a feel for the distribution of entanglement values at fixed \( N, H \). We notice that this distribution is not completely uniform: at low \( N \) and \( H \) it appears to be made up of a series of irregularly spaced bands. We return to this observation, but for now we turn to the question of the accuracy of our upper bound (equation 4.16) which we plot as a solid line. The average entanglements of trees at fixed \( N, H \) are plotted as squares with 1\( \sigma \) error bars reflecting the width of the distribution. As we can see, the upper bound overestimates the actual average by roughly a factor of two. To be more exact in this statement, we plot histograms of the entanglements at fixed \( N, H \) divided by the value specified in equation 4.16 in figure 4.4.2. We don’t have enough data to make any definitive claims here, but we can see that the ratios seem to cluster around roughly 0.6 independent of \( N \). The irregular nature of the distributions is probably a sign that we need to sample higher \( H \). Next, we return to the question of the entanglement distributions themselves. We expect the the distribution to consist of a finite set of discrete values for \( H = 3 \), since for these trees the singlet decomposition can only include one term. Since the entanglement of larger trees can be expressed as a weighted sum over singlets, it’s perhaps not too surprising that this discrete structure should persist for low \( H \), where the amount of possible mixing between the weights is still small. For the most part, the discrete structure fades out rather quickly and already at (for example) \( N = 10, H = 8 \) we can see the distribution is smooth and presumably indicative of behavior in the large \( H \) case.
We can gain a more quantitative description of the entanglement distributions by constructing histograms at fixed $N, H$. We plot entanglement distributions for $N = 6$ in figure 4.4.2 and for $N = 10$ in figure 4.4.2. The data at $N = 6$ (and all other values of $N$) was collected by systematic construction of all possible trees below a threshold height while the $N = 10$ data was acquired through random sampling\textsuperscript{11}. We can clearly make the initial discrete distribution of singlet entanglements $\log_2 2J + 1$ and see that these peaks become less prominent with greater $H$; what’s unexpected is the apparent emergence of new discrete values for entanglement (for example, at roughly 3.55 bits and $N = 10$, $H = 7$ or 8). Presumably this means that certain specific singlet decompositions are common to many different trees; it seems doubtful that one could achieve a combinatoric understanding of why this happens.

We now reconsider the question of why our upper bound was so inaccurate. We relied on three assumptions: that the average tree is evenly balanced, the magnitudes of its component spins are consistent with the distribution of spin magnitudes for the system as a whole, and that the entropy of the eigenvalues of the reduced density matrix is maximized. We know the first two are correct as $H \to \infty$, so the third becomes suspect in light of the observation we made above. To investigate this, we can directly plot the entanglement as a function of the size of the smaller reduced hilbert space. In figure 4.4.2 we do this for a set of representative $N$ and $H$. The reason why we segment the data in this way is because only considering trees below a cutoff $H$ will bias this plot: for any value of the size of the smaller reduced hilbert space, we can make chains whose other reduced hilbert space is arbitrarily large. The line in these plots represents the absolute upper bound we get by maximizing the von Neumann entropy; surprisingly many trees get very close to this limit.

We can make this more precise by plotting histograms of the entanglement normalized by the smaller reduced hilbert space size; this is done in figures 4.4.2 and 4.4.2. Although we need more data for a definitive conclusion, we see that for low $H$ the distributions are peaked at the maximum possible value. For increasing $H$, it appears that the peak moves over. We can understand this behavior in terms of the mixing of the distributions of singlet weights.

\textsuperscript{11}Thanks to the permutation symmetry at the $P_N$ fixed point, we know all trees with a given $N$ and $H$ are equally probable.
4.4.3 The large N limit

The most immediate application of our Mathematica routines is to obtain an estimate of the expected entanglement contribution from an average tree at a given $N$-domain permutation-symmetric fixed point, and in the previous section we did this for small $N$. We have an infinite number of fixed points to investigate, however, and as $N$ increases the number of trees we need to examine to obtain a good estimate increases exponentially.

In fact, the large $N$ limit of this problem is of interest for several reasons. As the number of domains goes to infinity, the role they play in determining the spin trees becomes progressively less important. When only a few domains are available, the set of possible spin trees is restricted. For example, with $N = 3$ it’s impossible to generate a tree in which a spin-1 is added immediately after another spin-1 is added on the opposite side: although this is reasonable from the viewpoint of spin addition, there’s no way to assign domains to make this happen. As we increase the number of domains, restrictions such as this become less severe, which might simplify the problem.

The primary motivation for considering the $N \to \infty$ limit comes from Latorre et. al.’s monotonicity conjecture. If entanglement never decreased along renormalization group flows in the systems we’re considering, this would mean that the entanglement at a $P_N$ fixed point will always be greater than the entanglement at the corresponding $RS_{(N-1)/2}$ singlet fixed point, since in the spin-$(N-1)/2$ system exhibiting the $P_N\{1,2,\cdots,N\}$ fixed point we always have this arrangement of critical lines. We’ve found the entanglement of the $RS_J$ fixed point for all $J$ already (equation 4.2), and although we haven’t found a closed form expression for the entanglement of the $P_N$ fixed points we can write down its large $N$ behavior based on the considerations that arose in section 4.4.1; namely we expect that

$$E_{P_N} \sim \left(\frac{2}{N}\log L\right) \left(\frac{2(N-2)(N-1)}{N(N+1)}\right) \times C_E \times \left\langle \frac{H}{2} \log_2(2J+1) \right\rangle$$

which is simply relation 4.4 after neglecting the contribution to the entanglement from singlet formation, since we’ve seen that the singlet formation rate ($W^0$) goes to zero as $N \to \infty$. The final factor was dealt with in section 4.4.1; we also have the result from section 4.3.3 that $\langle H/2 \rangle = (N+1)/2$ and the fact that $\langle \log_2(2J+1) \rangle \sim \log_2 N$ from equation 4.11. We’ve inserted a new “fudge factor” $C_E < 1$ that accounts for the fact that the reduced density matrix eigenvalues are not uniformly distributed; the data plotted in
figure 4.4.2 suggest that for low \( N, H \) we have \( C_E \approx 0.6 \) but we’ve been unable to come up with a good argument for what its behavior should be at large \( N \).

Together these considerations mean that in the large \( N \) limit, we have \( E_P \sim 2C_E \log L \log_2 N \), which is to be compared with the result of \( E_{RS(N - 1)/2} = 1/3 \log L \log_2 N \). If we have \( C_E < 1/6 \), the monotonicity conjecture is disproven at some finite \( N \); however, this seems unlikely — one would expect the eigenvalue distribution in large trees to be more uniform if we think of each step of the defoliation algorithm as a mixing operation. Therefore we appear to have an infinite number of examples unholding this conjecture.
Figure 4.3: We plot entanglement versus the size of the tree for $N = 3$ and 10. The squares denote the average entanglement of all trees at fixed $N$ and $H$, while the straight line is given by the upper bound from equation 4.16. The positions of the points representing the entanglements of individual trees have been perturbed by random amounts in the $x$ direction in order to display their distribution.
Figure 4.4: Histograms of the entanglements divided by our upper bound (equation 4.16.)
Figure 4.5: Histograms of the entanglement values for $N = 6$ and various $H$. The units of the x axis are bits.
Figure 4.6: Histograms of the entanglement values for $N = 10$ and various $H$. The units of the x axis are bits.
Figure 4.7: Entanglement versus the size of the smaller of the reduced hilbert spaces, for representative values of $N$ and $H$. 
Figure 4.8: Histograms of the entanglement divided by the absolute upper bound imposed by the size of the smaller reduced hilbert space, for various $N$ and $H$. 
Figure 4.9: Continuation of the previous figure. Histograms of the entanglement divided by the absolute upper bound imposed by the size of the smaller reduced hilbert space, for various $N$ and $H$. 
Chapter 5

Conclusion

5.1 Discussion and conclusion

5.1.1 Entanglement measures

We begin our discussion with the observation that the spin tree diagrams we made use of are special cases of a general diagrammatic method of representing group theory calculations (see [9]), and one can generalize the $6j$ symbols to recouple different types of diagrams. The algorithm we presented in section 4.3.2 lets us rewrite a class of multiparticle states (the spin trees) in terms of a weighted sum of reference states (the spin-$J$ singlets) which are inequivalent from the point of view of entanglement.

One might imagine that if we could appropriately generalize our diagrammatic scheme to represent arbitrary states of several spins, one could perform a series of similar decomposition operations in order to write it in terms of a weighted sum of reference states representing the inequivalent multiparticle entanglement classes discussed in section 3.2.2. Although in general one would not be able to assign a definite number of bits to the entanglement contributed by the reference states with multiparticle entanglement, this would constitute a formal solution to the problem of quantifying pure state entanglement.

5.1.2 The entanglement calculations in context

Much is still uncertain about the nature of entanglement, how it should be quantified, and the role it plays in quantum phase transitions, yet the latter area contains many interesting
questions one would like to be able to answer. We would like to reemphasize the point that the analysis performed in this thesis represents one of the most straightforward answers to this issue given the current understanding of the former two in several senses.

We know that singlets are the simplest possible case of entanglement, and the spin trees constitute a nontrivial generalization of the singlet which is still amenable to direct analysis. Furthermore, randomness guarantees that the random singlet ground states generate no intrinsically multipartite entanglement, and the defoliation algorithm demonstrates that this does not occur for spin trees either.

The randomness also ensures that the ground state in either case can be written as the tensor product of clearly demarcated entangled structures; each singlet and spin tree when considered individually is a pure state. Therefore, we can be sure that the von Neumann entropy (equation 3.1) captures all the entanglement present and is the correct measure to use.

5.1.3 The monotonicity conjecture

Based on our arguments, we have good reason to believe that the infinite family of fixed points considered in this work and the infinite set of renormalization group flows between them all obey the monotonicity conjecture. While one cannot conclude anything from this result alone, it provides strong support for the view that entanglement is completely unrelated to conformal symmetry; if a system is described by a conformal field theory this only means that its entanglement is easy to calculate with the results of [13]. Except for the case of conformally invariant fixed points, the physical principles enforcing monotonicity remain unclear.
Appendix A

Appendices

A.1 Mathematica code listing

In this appendix we present a complete listing of all the mathematica code that was written for the thesis. The routines were written to perform three tasks: to construct and evaluate the von Neumann entropy of a reduced density matrix of a spin tree, to perform the singlet decomposition described in section 4.3.2, and to generate sets of spin trees according to certain parameters.

A.1.1 Explicit density matrix calculations

The most straightforward way to approach the spin tree entanglement calculation is simply to construct an explicit state vector in the $\sigma_z$ basis by summing the spins in the given order using Clebsch-Gordan coefficients, tracing out the undesired degrees of freedom in the resulting density matrix and solving for the eigenvalues. We describe an algorithm in the text which is an improvement on this process, but doing the calculation the straightforward way is a useful sanity check.

The algorithm itself is implemented in Mathematica except for the function evaluating the $6j$ symbol itself. Because Mathematica is an interpreted programming language, instructions run more slowly than in a compiled language such as C. We therefore obtain a significant performance improvement by replacing our use of the built-in Mathematica function SixJSymbol with a call (via the MathLink library) to an external C function which
evaluates the $6j$ symbol.

The C routine is based on that provided by Thomson [45], with minor corrections for programming style, so we do not provide a listing here. The $6j$ symbol is evaluated via Racah’s summation formula: if we first define for convenience

$$\Delta(i,j,k) = \sqrt{\frac{(a + b - c)! (a + c - b)! (b + c - a)!}{(a + b + c + 1)!}}$$

the $6j$ symbol is given by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{pmatrix} = (-1)^{j_1+j_2+j_4+j_5} \Delta(j_1,j_2,j_3) \Delta(j_1,j_5,j_6) \Delta(j_2,j_4,j_6) \Delta(j_5,j_4,j_3)$$

$$\times \sum_k (-1)^k (j_1 + j_2 + j_3 + j_4 + 1 - k)!$$

$$\times [k!(j_3 + j_6 - j_1 - j_4 + k)!(j_3 + j_6 - j_2 - j_5 + k)]^{-1}$$

$$\times [(j_1 + j_2 - j_3 - k)!(j_5 + j_4 - j_3 - k)!(j_1 + j_5 - j_6 - k)!(j_2 + j_4 - j_6 - k)]^{-1}$$

(A.1)

The limits on the sum are set by the requirement that we sum over all values of $k$ except those that would require us to take the factorial of a negative number. Inspection of the relation shows that this means that the sum is always finite, which is fortunate for computational work. Use of the `Timing` command reveals that with this external function call, evaluation of the $6j$ symbols accounts for only a minority of the total running time.

These commands load subroutine libraries called by the other functions:

`<< LinearAlgebra('MatrixManipulation')`  
`<< LinearAlgebra('Orthogonalization')`

These next functions allow us to specify the magnitudes of the spins in the tree and the order of their summation in a relatively straightforward way. The notation is that $a[j]$ creates a bare spin of magnitude $j$, and $p[j_T,j_1,j_2]$ adds the two expressions (bare or composite spins) in $j_1$ and $j_2$ to make an object with total spin $j_T$. Note that this notation can describe spin addition schemes of arbitrary topology (despite being rather hard to read in practice).

$$A\text{Spin}[j_] := \text{IdentityMatrix}[2*j + 1];$$
SpinPair[j_, s1_, s2_] := 
Module[{j1, j2},
  j1 = (Length[s1] - 1)/2;
  j2 = (Length[s2] - 1)/2;
  Return[Table[If[m > Max[j1 - j2, j2 - j1],
    Sum[ClebschGordan[{j1, m1}, {j2, m - m1}, {j, m}]*Flatten[Outer[Times, s1[[1 + j1 - m1]], s2[[1 + j2 - m + m1]]]], {m1, m - j2, j1}],
    If[m < Min[j1 - j2, j2 - j1],
    Sum[ClebschGordan[{j1, m1}, {j2, m - m1}, {j, m}]*Flatten[Outer[Times, s1[[1 + j1 - m1]], s2[[1 + j2 - m + m1]]]], {m1, -j1, m + j2}],
    If[j2 > j1,
    Sum[ClebschGordan[{j1, m1}, {j2, m - m1}, {j, m}]*Flatten[Outer[Times, s1[[1 + j1 - m1]], s2[[1 + j2 - m + m1]]]], {m1, -j1, j1}],
    Sum[ClebschGordan[{j1, m - m2}, {j2, m2}, {j, m}]*Flatten[Outer[Times, s1[[1 + j1 - m + m2]], s2[[1 + j2 - m2]]]], {m2, -j2, j2}]]], {m, j, -j, -1}];
];
a[j_] := ASpin[j];
p[j_, s1_, s2_] := SpinPair[j, s1, s2];

The following functions perform the actual calculation. Once a state vector has been
specified using the commands above, ReducedDM performs the partial trace over the specified
spins (one spin at a time) and VNEntangle returns the Von Neumann entropy of the density
matrix. VNEntEvals lists the eigenvalues of the matrix explicitly, and VNEntEsys also gives
the eigenvectors. All other functions are subroutines.

TraceOverOne[RhoSpinList_, n_] := 
Module[{vec, i},
  vec = Flatten[ReplacePart[Table[All, {2*Length[RhoSpinList[[2]] ]}], i, {{2*n - 1}, {2*n}}];
  {Sum[Apply[Part[RhoSpinList, 1, ##] & , vec], {i, 1, RhoSpinList[[2, n]]}], Drop[RhoSpinList[[2]], {n}]}];
ReducedDM[StateVector_, SpinList_, TraceOver_] :=
Module[{vec, rho, vec2},
  vec = {#, #} & /@ Reverse[Rest[SpinList]];
  ...
rho = Fold[Partition, Outer[Times, Flatten[StateVector], Flatten[StateVector]], vec];  
Fold[TraceOverOne, {rho, SpinList}, Reverse[Sort[TraceOver]]];

EntFun[x_] := If[x == 0, 0, x*Log[x]];
TensorFlatten[rho_] := Module[{rhoCopy},
rhoCopy = rho;
Do[rhoCopy = Map[BlockMatrix, rhoCopy, {i}], {i, Length[Dimensions[rho]] - 4, 0, -2}];
Return[rhoCopy];

VNEntangle[rho_] := -Tr[Map[EntFun, Eigenvalues[TensorFlatten[rho]]]]
VNEntEvals[rho_] := Module[{evals},
evals = Eigenvalues[TensorFlatten[rho]];
Print[evals];
Return[-Tr[Map[EntFun, evals]]];
]

VNEntESys[rho_] := Eigensystem[TensorFlatten[rho]]

A.1.2 Defoliation algorithm for entanglement calculation

The details of the algorithm are given in the main text; implementation is essentially straightforward. First, we define the coupling coefficient between different tree types and the Von Neumann entropy:

Off[General::spell1];
SixJay[v1_, v2_] := (-1)^(v1[[1]] + v2[[1]] + v1[[2]] + v2[[2]])*Sqrt[(2*v1[[3]] + 1)*(2*v2[[3]] + 1)]*SixJSymbol[v1, v2];
EntFun[x_] := If[x == 0, 0, x*Log[2, x]];

The following subroutines perform one step in the decomposition — i.e. they add a factor of one $6j$ symbol to the sum.

Unzip[data_] := Switch[data[[1, 4, 2]], l, UnzipRL[data], r, UnzipLR[data], c, Print[Error]];
UnzipLR[data_] := Module[{iter, min, max, s, newsml, newc}
iter = Unique[unzip];
s = Flatten[Take[data[[1]], 5, 1]];
min = Max[Abs[s[[2]] - s[[4]]], Abs[s[[1]] - s[[5]]]];
max = Min[s[[2]] + s[[4]], s[[1]] + s[[5]]];
newsml = Append[data[[2]], {iter, min, max}];
newc = data[[3]]*SixJay[Hold[Evaluate[{s[[1]], s[[2]], s[[3]]}, {s[[4]], s[[5]], iter}]]];
newsl = Insert[Drop[data[[1]], {2, 4}], {iter, r}, 2];
Return[{newsl, newsm, newc, Append[data[[4]], r]}];

UnzipRL[data_] := Module[{iter, min, max, s, newsm, newc, newsl},
iter = Unique[unzip];
s = Flatten[Take[data[[1]], 5, 1]];
min = Max[Abs[s[[1]] - s[[4]]], Abs[s[[2]] - s[[5]]]];
max = Min[s[[2]] + s[[5]], s[[1]] + s[[4]]];
newsm = Append[data[[2]], {iter, min, max}];
newc = data[[3]]*SixJay[Hold[Evaluate[{s[[1]], s[[2]], s[[3]]}, {s[[5]], s[[4]], iter}]]];
newsl = Prepend[Drop[Drop[data[[1]], 1], {2, 3}], {iter, l}];
Return[{newsl, newsm, newc, Append[data[[4]], l]}];

This subroutine constructs and finds the eigenvalues of the reduced density matrix for a given singlet magnitude— note that this density matrix only describes a subspace of the complete Hilbert space. Note that in the last line we’ve specified numerical (rather than analytic) evaluation of the eigenvalues: this is because only polynomials of low degree can be solved analytically.

SameFunc[x_, y_] := Take[x, 2] === Take[y, 2];
RDMEigenvals[x_] := Module[{Lindex, Rindex, vect, rdm, sing},
vect = Transpose[x];
sing = vect[[1, 1]];
Lindex = Union[vect[[2]]];
Rindex = Union[vect[[3]]];
If[Length[Lindex] == 1 || Length[Rindex] == 1,
(*Trivial case ... *)
Return[{sing, {Tr[Map[#^2 &, vect[[4]]]]}}];
(*Else form RDM and return eigenvals*)
vect[[2]] = Flatten[vect[[2]]] /. (#1 -> Position[Lindex, #1]) & /@ Lindex;
vect[[3]] = Flatten[vect[[3]]] /. (#1 -> Position[Rindex, #1]) & /@ Rindex;
vect = Transpose[Take[vect, -3]];
stuff = Complement[
Flatten[Table[{i, j, 0}, {i, 1, Length[Lindex]}, {j, 1, Length[Rindex]}], 1],
vect, SameTest -> SameFunc];
vect = Sort[Join[vect, stuff]][[All, 3]];
rdm = Tr[Partition[Outer[
Finally, we have the main function, \texttt{Unzipper}, which performs the decomposition, calculates the eigenvalues contributed by each singlet and computes the entanglement.

\begin{verbatim}
TestFn[x_] := Length[x[[1]]] > 3;
CollectFn[v_] := {v[[1, 1]], Plus @@ Transpose[v][[2]]};
DuplicateEVs[v_] := Module[{sing},
    sing = 2*v[[1]] + 1;
    Return[Flatten[Map[Table[#/sing, {sing}] &, v[[2]]]]];
]
Unzipper[spinlist_] := Module[{data, weights, evals, qnl, qnr},
data = {spinlist, {}, 1, {}};
data = NestWhile[Unzip, data, TestFn, 1];
qnl = data[[2, Flatten[Position[data[[4]], l]], 1]];
qnr = data[[2, Flatten[Position[data[[4]], r]], 1]];
weights = {};
(Do[weights = Append[weights, {Last[qnl], qnl, qnr, ReleaseHold[data[[3]]]], #1] &)
weights = Split[Sort[weights, OrderedQ[{#1[[1]], #2[[1]]}] &], #1[[1]] == #2[[1]] &];
weights = RDMEigenvals /@ weights;
evals = Flatten[Map[DuplicateEVs, weights]];
Return[-Tr[EntFun /@ evals]];]
\end{verbatim}

\subsection{A.1.3 Systematic tree generation}

In order to obtain a good estimate for the entanglement, we need to evaluate many trees. Ultimately it proves most economical to have the computer generate the trees automatically, which also reduces the likelihood of mistakes for large trees.

This function returns a list of all possible tree topologies of a given height.

\begin{verbatim}
TreeSkel[h_] := Module[{iterVars, iterRange, iterates},
    Switch[h, 3, Return[{{1, r, 1}}]],
\end{verbatim}
iterVars = Table[Unique[treeskel], {h - 3}];
iterRange = Map[{#, 1, 2} &, iterVars];
iterates = Map[Hold[{l, r}[[#]]] &, iterVars];
Return[
    Partition[Flatten[
        Apply[
            Table[ReleaseHold[Join[{l, r, l}, iterates]], ##] &,
                   iterRange]
    ], h]
];

The following functions are subroutines used for manipulating the tree's adjacency matrix.

AppendColumns1[mat1_, mat2_] :=
    If[Length[mat1] == 0, mat2,
        If[Length[mat2] == 0, mat1,
            AppendColumns[mat1, mat2]]];
AppendRows1[mat1_, mat2_] :=
    If[Length[mat1] == 0, mat2,
        If[Length[mat2] == 0, mat1,
            AppendRows[mat1, mat2]]];
AddRows[mat_, target_, source_] := Module[{m},
    m = mat;
    m[[target]] = m[[target]] + m[[source]]; Return[m];
];
DeleteColumn[mat_, n_] := Module[{l},
    l = Dimensions[mat][[2]];
    Return[AppendRows1[TakeColumns[mat, n - 1], TakeColumns[mat, -(l - n)]]];
];
DeleteRow[mat_, n_] := Module[{l},
    l = Dimensions[mat][[1]];
    Return[AppendColumns1[TakeRows[mat, n - 1], TakeRows[mat, -(l - n)]]];
];
OneMove[mat_, n_] := DeleteRow[DeleteColumn[AddRows[mat, n - 2, n], n], n];

These are subroutines used in assigning domain labels ("colorings") to the bare tree. Given a partially labeled tree, these routines return all possible labelings of the next domain that don't conflict with the labels already assigned.
ColorSub[adj_, cols_, colorings_] := Partition[Flatten[
Map[ColorSubSub[adj, cols, #] & , colorings]], Length[adj]];

ColorSubSub[adjacency_, colors_, pat_] := Module[{n, n2, options},
n = Position[pat, 0][[1, 1]];  
n2 = Flatten[Position[adjacency[[n]], 1]];  
options = Complement[colors, Map[pat[[#]] & , n2]];  
Return[Table[ReplacePart[pat, options[[i]], n], {i, 1, Length[options]}]]];

PadColoring[pat_, v_] :=
Fold[ReplacePart[#1, #1[[#2 - 2]], #2] &,
Fold[Insert[#1, 0, #2 + 1] &, pat, Reverse[v]],
v + Range[Length[v]]];

This subroutine converts the domain labels into spin magnitudes and formats the resulting spin tree into the notation expected by the Unzipper function.

SpinFn[v_, i_, j_] := Abs[v[[i]] - v[[j]]]/2;

ColorsToSpins[v_] := Module[{len, center, landr, ans},
len = Length[v];
Switch[len,
  3, Return[{{SpinFn[v, 2, 1], l}, {SpinFn[v, 3, 1], r}, {SpinFn[v, 3, 2], c}, {SpinFn[v, 3, 2], l}, {0, c}}];,
  4, Return[{{SpinFn[v, 2, 1], l}, {SpinFn[v, 3, 1], r}, {SpinFn[v, 3, 2], c}, {SpinFn[v, 4, 2], l}, {SpinFn[v, 4, 3], c}, {SpinFn[v, 4, 3], r}, {0, c}}];,
  _,
  center = Table[SpinFn[v, i, i - 1], {i, 4, len - 1}];
  landr = Table[SpinFn[v, i, i - 2], {i, 4, len - 1}];
  ans =
  Join[{{{SpinFn[v, 2, 1], l}, {SpinFn[v, 3, 1], r}, {SpinFn[v, 3, 2], c}}},
  Table[{{landr[[i]], If[EvenQ[i], r, 1]}, {center[[i]], c}}, {i, 1, Length[center]}],
  If[EvenQ[len],
  {{{SpinFn[v, len, len - 2], l}, {SpinFn[v, len, len - 1], c}, {SpinFn[v, len, len - 1], r}}},
  {{{SpinFn[v, len, len - 2], l}, {SpinFn[v, len, len - 2], r}}}] ];
  Return[Append[Partition[
  Flatten[Select[ans, ! MemberQ[#, {0, 2, 2}] &]], 2], {0, c}]]];
This is the main body of the routine: given a tree topology, we return a list of spin trees resulting from all allowed domain labelings. We know that the spins assigned to a tree won’t change under a relabeling $0 \rightarrow N - 1, 1 \rightarrow N - 2, \cdots$, so we fix this symmetry by requiring that the first domain assigned is less than $N/2$ (with appropriate care taken in the care that $N$ is odd).

```
AllTreeColorings[t_, n_] := Module[{colors, domains, runs, num, adjacency, colorings},
  colors = Range[n];
  domains = Append[Drop[Prepend[t, 0], -2], 0];
  runs1 = Flatten@Position[
    Apply[SameQ, Partition[domains, 2, 1], {1}], True];
  runs2 = Reverse[runs1 + Range[Length[runs1]]];
  num = Length[domains] + Length[runs2];
  adjacency = Table[
    If[j == i + 1 || j == i + 2, 1, 0],
    {i, 1, num}, {j, 1, num}];
  adjacency = Transpose[Fold[OneMove, adjacency, runs2]]; (*colorings = {Table[0, {Length[domains]}]};
  colorings = Nest[ColorSub[adjacency, colors, #] &, colorings, Length[domains]];*)
  colorings = {Table[0, {Length[domains]}]};
  colorings = Nest[ColorSub[adjacency, colors, Range[Floor[n/2]], colorings]; (*domain label inversion symmetry*)
  If[EvenQ[n],
    colorings = Nest[
      ColorSub[adjacency, colors, #] &, colorings, Length[domains] - 1]; (*else*)
    colorings = ColorSub[adjacency, colors, colorings];
    colorings = Join[colorings, ColorSub[adjacency, Range[Ceiling[n/2]],
      {Prepend[Table[0, {Length[domains] - 1}], Ceiling[n/2]]}] ];
    colorings = Nest[ColorSub[adjacency, colors, #] &, colorings, Length[domains] - 2];
  ];
  Return[Map[ColorsToSpins, Map[PadColoring[#, runs1] &, colorings]]];
];
```
A.1.4 Random sampling of trees

We rapidly find ourselves in situations where creating all trees at a given $N,H$ exhausts available computing power. When this happens (for $N = 10$ in the text) we switch to random sampling of trees, which is carried out by these routines. The first generates a set of trees of random topology.

```
RandomInt[n_] := Random[Integer, {1, n}];
RTreeSkel[h_, n_] := Map[Join[{l, r, l}, #] &, Table[Random[Integer], {i, 1, n}, {j, 1, h - 3}] /. {0 -> l, 1 -> r} ];
```

The other routine, when given a tree of a specified topology, returns just one random assignment of domain labels to it. It operates recursively and is essentially copied from the systematic tree coloring routine.

```
RColorSub[adjacency_, colors_, pat_] := Module[{n, n2, options},
n = Position[pat, 0][[1, 1]];
n2 = Flatten[Position[adjacency[[n]], 1]];
options = Complement[colors, Map[pat[[#]] &, n2]];
options = options[[ RandomInt[Length[options]] ]] ];
Return[ReplacePart[pat, options, n]];
];
```

```
OneRandomColoring[t_, d_] := Module[{colors, domains, runs, num, adjacency, coloring},
colors = Range[d];
domains = Append[Drop[Prepend[t, 0], -2], 0];
runs1 = Flatten@Position[
    Apply[SameQ, Partition[domains, 2, 1], {1}], True];
runs2 = Reverse[runs1 + Range[Length[runs1]]];
num = Length[domains] + Length[runs2];
adjacency = Table[
    If[j == i + 1 || j == i + 2, 1, 0],
    {i, 1, num}, {j, 1, num}];
adjacency = Transpose[Fold[OneMove, adjacency, runs2]];
coloring = Table[0, {Length[domains]}];
coloring = RColorSub[adjacency, Range[Ceiling[d/2]], coloring];
(*domain label inversion symmetry*)
If[EvenQ[d],
]
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coloring = Nest[RColorSub[adjacency, colors, #] &, coloring, Length[domains] - 1];,
(*else*)
If[coloring[[1]] == Ceiling[d/2],
coloring = RColorSub[adjacency, Range[Ceiling[d/2]], coloring];,
coloring = RColorSub[adjacency, colors, coloring];
];
coloring = Nest[
RColorSub[adjacency, colors, #] &, coloring, Length[domains] - 2];
]
Return[ColorsToSpins[PadColoring[coloring, runs1]]];
];

A.1.5 Example of use

Commands of this type were used to generate the data discussed in section 4.4.2. This produces a table (broken up into several text files) of information about randomly sampled trees with $N = 10$ and $3 \leq H \leq 8$.

LHSSize[t_] := N[1.0*
   Tr[Map[2# + 1 &, Transpose[Cases[t, {_, l}][[1]]]]], Times];
RHSSize[t_] := N[1.0*
   Tr[Map[2# + 1 &, Transpose[Cases[t, {_, r}][[1]]]]], Times];
TrLength[t_] := (Length[t] + 1)/2;
Do[
   tr = Flatten[
      Table[Map[OneRandomColoring[#, 10] &, RTreeSkel[i, 25]], {i, 3, 8}], 1];
   Export[StringJoin["~/randtrees10n10x", ToString[qqq], ".txt"], Table[{TrLength[tr[[i]]], LHSSize[tr[[i]]], RHSSize[tr[[i]]], Unzipper[tr[[i]]]},{i, 1, Length[tr]}], 
   "Table"];
   Print[qqq];, {qqq, 1, 20}];
References


