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Mathematics and Statistics
Centre for Doctoral Training

Quantum spin systems, probabilistic representations and phase transitions

by

Benjamin Thomas Lees

Thesis

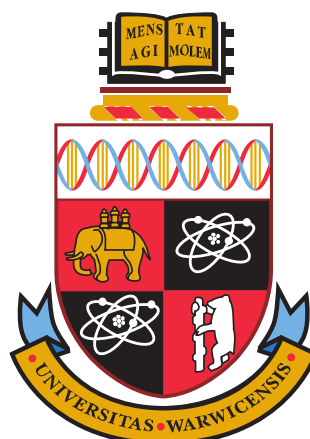
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Declarations

The work of this thesis has been carried out under the support of my supervisors, Daniel Ueltschi and Roman Kotecký. Parts of this thesis have already appeared in papers as follows:

- Chapter 4 is formed from Benassi, Lees and Ueltschi (2015) [10].
- Chapter 5 is formed from Lees (2014) [69].
- Section 6.2 contains work formed from Lees (2015) [70].
- Section 7.4 is formed from Kotecký and Lees (2016) [63].

Except for the areas noted above I declare that, to the best of my knowledge, the material in this thesis is original and my own work except where otherwise indicated or commonly known.

The material in this thesis is submitted to the University of Warwick for the degree of Doctor of Philosophy and has not been submitted to any other university or for any other degree.

Abstract

This thesis investigates properties of classical and quantum spin systems on lattices. These models have been widely studied due to their relevance to condensed matter physics.

We identify the ground states of an antiferromagnetic \mathbf{RP}^2 model, these ground states are very different from the ferromagnetic model and there was some disagreement over their structure, we settle this disagreement.

Correlation inequalities are proved for the spin- $\frac{1}{2}$ XY model and the ground state of the spin-1 XY model. This provides fresh results in a topic that had been stagnant and allows the proof of some new results, for example existence of some correlation functions in the thermodynamic limit.

The occurrence of nematic order at low temperature in a quantum nematic model is proved using the method of reflection positivity and infrared bounds. Previous results on this nematic order were achieved indirectly via a probabilistic representation. This result is maintained in the presence of a small antiferromagnetic interaction, this case was not previously covered.

Probabilistic representations for quantum spin systems are introduced and some consequences are presented. In particular, Néel order is proved in a bilinear-biquadratic spin-1 system at low temperature. This result extends the famous result of Dyson, Lieb and Simon [35].

Dilute spin systems are introduced and the occurrence of a phase transition at low temperature characterised by preferential occupation of the even or odd sublattice of a cubic box is proved. This result is the first of its type for such a mixed classical and quantum system. A probabilistic representation of the spin-1 Bose-Hubbard model is also presented and some consequences are proved.

Chapter 1

Introduction and outline

1.1 Introduction

It became clear in the last century that the classical view of elementary particles using classical mechanics is insufficient for a complete description of atomic phenomena. This is especially clear when considering the Hydrogen atom, according to classical mechanics the orbiting electron would continuously lose energy due to its radial acceleration causing it to spiral into the nucleus. However it is clear that this cannot be the case, the Hydrogen atom is stable over very long periods of time. A new theory applicable to fundamental particles is required. This theory is, of course, quantum mechanics. One aspect of quantum mechanics is that particles, even elementary particles, possess an “intrinsic” angular momentum known as *spin*. We will consider properties of systems of particles with interactions coming from their spins.

Statistical mechanics (both classical and quantum) is concerned with systems consisting of a large number of subsystems (e.g. particles) whose interaction produces macroscopic effects. This is known as thermodynamic behaviour and is obtained by some process of averaging over individual systems. This thermodynamic behaviour is described by equilibrium states (states of an isolated system after large amounts of time) consisting of macroscopic homogeneous regions (phases) which can be described by a finite number of parameters of the system. Making such a description of the thermodynamics of a system rigorous is difficult and has been a topic of intense study during the last century, we refer to [95]. This thesis will mainly concern itself with the infinite volume equilibrium states of systems and the phases which are present.

Quantum spin systems and phase transitions

Proving rigorous statements about quantum spin systems is a difficult task. We will often be informed by the expected phase diagram of the systems we consider. In certain situations one may be able to consider a quantum system as being a (small) perturbation of a classical model. This idea has led to positive results. It was shown in [20] that under certain conditions the low temperature phase diagram for a classical system accompanied by a small quantum perturbation is only a small perturbation of the zero temperature phase diagram of the classical system. Similar results were also obtained independently around the same time [29]. These results required finitely many ground states of the classical model. This requirement was lifted via a unitary conjugation of the system where the quantum perturbation lifts the ground-state degeneracy [30]. These results all rely on (extensions of) Pirogov-Sinai theory [91, 104] that systematically extends contour techniques, which find their origin in the work of Peierls [89] on the Ising model, to a wide class of models.

Proving the occurrence of phase transitions remains a major area of research in statistical mechanics. One sees from nature that physical changes such as condensation of a gas below the boiling point or magnetisation of a ferromagnetic material below the Curie temperature occur quite abruptly as (for example) the temperature of the system is lowered. Capturing this phenomenon mathematically is notoriously difficult. It can be characterised by non-analyticity of the *free energy*, f_Λ , of the system but for finite systems (with finitely many degrees of freedom) on space Λ (lattice, box,...) f_Λ is usually real analytic in each of its variables. There is, however, a solution. When studying phase transitions we are interested in very large systems. We work with the infinite volume limit $f = \lim_{|\Lambda| \rightarrow \infty} f_\Lambda$ and this limit may not be analytic in one or more variables. This raises another major issue; can we take this limit? The answer for many systems is yes. We take $|\Lambda| \rightarrow \infty$ as follows; let $\{\Lambda_n\}_{n \geq 1}$ be a collection of sublattices of some infinite reference lattice A (for example $A = \mathbb{Z}^d$), we say $\Lambda_n \rightarrow A$ as $n \rightarrow \infty$ if for every finite $\Lambda \subset A$ there is an $N \geq 1$ such that $\Lambda \subset \Lambda_n$ if $n \geq N$. We could take limits in a more general way if we wished (Van Hove) [95].

Often it will be very difficult to deduce that the free energy is not analytic directly. The free energy is defined as the logarithm of the *partition function*, divided by the volume. The functional derivatives of this free energy give, formally, correlations in the system with total mass given by the partition function. This suggests it may be more sensible to look at the *Gibbs measure/Gibbs state* that the partition function is the normalisation constant of (we will see its definition in Chapter 2). How we take the infinite volume limit of this Gibbs measure/state is open to some choice. We can take weak cluster points as $\Lambda \rightarrow \mathbb{Z}^d$ (and, if we want, take the limit in a more general way than above) with various

boundary conditions (see Section 2.1.1). Alternatively we could decide on some important property of these measures/states in finite dimensions and define an infinite dimensional analogue (in classical systems this is the DLR condition and in quantum systems it is the KMS condition). The existence of more than one infinite volume DLR/KMS state means that there is a phase transition of the system. In this thesis we will use both approaches but when taking the first approach we will always take periodic boundary conditions for convenience, see Section 2.2.5 for discussion on these points.

Once we know that such a limit exists we can attempt to prove that a phase transition occurs. Unsurprisingly this is notoriously difficult even when heuristic or numerical evidence suggests it should happen. For classical systems things are somewhat easier (despite still being difficult). For quantum systems there are extra difficulties coming from observables being operators, causing commutativity issues. One can use results from classical systems and transfer this to quantum spin systems for high spin [16], for example by using coherent states, but one must still have a way to deal with the quantum system to some extent.

It is well known that the set of infinite volume KMS states form a simplex and that in the extremal states truncated correlations decay. This means that showing the non-decay of some truncated correlation proves that there is not a unique KMS state, hence there is a phase transition. See, for example, [56, 103] for a discussion of such results. Many of the results on phase transitions in this thesis are achieved by proving long-range order, that is, the non-decay of a (spin-spin) correlation as the distance between the spin-carrying particles diverges, see (for example) chapters 5, 6 and 7. This non-decay of a correlations indicates some type of order (as opposed to disorder) of the spins in a system at a macroscopic scale.

Phase transitions are often accompanied by the breaking of an internal symmetry of the system, for example magnetisation may correspond to a discontinuity in one of the derivatives of the free energy [39], the symmetry is broken by the alignment of spins in the direction of an external field whose strength is reduced to zero. This alignment of spins over long distances is referred to as *ferromagnetic order*, in the classical case it means that the spins (unit vectors) point in the same direction, in the quantum case it means that the state of the system is strongly correlated to a state that is symmetric under switching of individual particles (for example a product state where each particle is in the same state). The rotational symmetry has been broken as one particular direction is preferred. In this thesis phase transitions will often correspond to a breaking of a rotational (more precisely $SU(2)$) symmetry, this is an example of a continuous symmetry. We will also see an example of a phase transition corresponding to the breaking of a discrete (translational) symmetry in Section 7.4. Two types of order will be of particular interest. The first is *antiferromagnetic order*, also referred to as *Néel order* after Louis Néel who first noted the occurrence, [83]. It is characterised in

the classical case by neighbouring spins pointing in opposite directions. The quantum case is characterised by strong correlation to a state of the system where neighbouring spins are opposite, for example in spin-1 the Néel state has spins alternating between the +1 and -1 eigenstate (see sections 2.2.2 and 2.2.5). The second type of order is *nematic order*, also called ferro-quadrupolar order. In the classical case this is characterised by spins aligning along the same axis but not necessarily pointing in the same direction or alternating direction, this is clearly a weaker order than Néel order. In the quantum case nematic order is more mysterious, in spin-1 it corresponds to being strongly correlated to the product state of the 0 eigenstate [113]. In this case the precise relationship between Néel and nematic order remains unknown. Nematic order has been a topic of interest due to its occurrence in Ni-based compounds such as $NiGa_2S_4$ [82, 114] and other compounds such as $PrCu_2$, $CeAg$ [79, 99]. There is also a related *staggered-nematic order*, also called antiferro-quadrupolar order, proposed for other compounds such as CeB_6 and $PrPb_3$ [80, 85], we will not discuss this order further as very little can be rigorously achieved. See Section 2.2.5 for more precise statements and definitions.

Some available methods for proving the occurrence of phase transitions

There are few methods available to prove a system undergoes a phase transition. The first was Peierls' method, which finds its origin in the the work of Peierls [89] and was developed for classical spin systems by Dobrushin [33] and Griffiths [51]. Extensions of Peierls' method were used to treat anisotropic quantum Heisenberg models by Ginibre [47] and Robinson [94]. This method shows spontaneous symmetry breaking, which implies a phase transition. However it can only deal with breaking of discrete symmetries.

It is known for translation invariant models on \mathbb{Z}^d that if continuous symmetry breaking occurs there is a gapless excitation spectrum. There is much literature on spectral gaps [5, 6, 7, 25] and recent interest has been piqued due to the possibility that systems with gapped ground states may support topological order.

For continuous symmetries it is known that in one or two dimensional lattice models there can be no breaking of the symmetry at positive temperatures. This result is usually attributed to Mermin and Wagner [78] who proved this was the case for the quantum Heisenberg model. Fisher and Jasnow [37] proved decay of two point correlations in the anisotropic case. The classical $O(n)$ model was covered in two dimensions by McBryan and Spencer [77] where power-law decay of two point correlations was proved, this was generalised to two dimensional classical systems with symmetry groups that are compact connected Lie groups [90].

Despite the theorem of Mermin and Wagner and its extensions there is a method (in fact it is essentially the only method currently available) for proving the occurrence of phase transitions in systems with continuous symmetries in dimensions three or more (and in the ground state of dimension two); the method of *reflection positivity*. See sections 2.1.3 and 2.2.6 for a discussion of reflection positivity. This method dates back to the remarkable work of Fröhlich, Simon and Spencer [43] who proved that a phase transition occurs in $(\phi \cdot \phi)_3^2$ quantum field theories and the classical isotropic Heisenberg model on a cubic lattice in dimension $d \geq 3$. The result was extended to quantum models in the now famous paper of Dyson, Lieb and Simon [35]. It was proved, in particular, that the isotropic spin- $\frac{1}{2}$ XY model and the Heisenberg antiferromagnet with spin $S \geq 1$ undergo a phase transition in dimension $d \geq 3$. This was extended to the XY model with spin $S \geq 1$ for the ground state in dimension $d \geq 2$ by Kennedy, Lieb and Shastry [58]. A proof for the quantum Heisenberg ferromagnet is absent, this model does not enjoy the very useful property of reflection positivity. This remains a big open problem.

A major drawback of reflection positivity is that it usually imposes very strictly requirements on the underlying structure (the lattice). It requires that the underlying lattice has significant reflection symmetry, such as a cubic lattice in \mathbb{Z}^d or the hexagonal lattice. Triangular lattices can not be dealt with in quantum models due to reflections through sites causing commutativity issues between each side of the reflection. There has been some work that does not require this spatial reflection symmetry by using the notion of *spin-reflection positivity*. This technique was used by Lieb to prove uniqueness of the ground state of the Hubbard model at half filling [73], both the attractive and repulsive case were considered. It was later shown that in the repulsive case there is *ferrimagnetic* order in the ground state on bipartite lattices (see [100] for a definition of ferrimagnetic order). The idea of spin-reflection positivity has been developed by Tasaki and Tian [107, 108].

Since these initial works the theory surrounding reflection positivity has seen much interest [39, 41, 42]. A consequence of reflection positivity is *Gaussian domination* which allows to obtain an *infrared bound*, a bound on the higher Fourier modes of (spin or particle) correlations. We will see this method used in Section 5.2, 6.2.6, 6.2.7, 6.2.8, 6.2.9 and 7.3.1. This was used in previously mentioned works [35, 43]. The result of Dyson, Lieb and Simon [35] was used by Neves and Perez to prove that there is Néel order in the ground state of the antiferromagnet for $d = 2$ and spin $S \geq 3/2$ [84]. Kennedy, Lieb and Shastry extended the result to the spin- $\frac{1}{2}$ antiferromagnet in $d = 3$ [58], the same authors also proved that there is a phase transition for the XY models for all spins $S \in \frac{1}{2}\mathbb{N}$ and dimensions $d \geq 2$ [59]. Other models such as the spin-1 bilinear-biquadratic exchange Hamiltonian have also benefited from the technique. It was shown in [106] that *Néel order* occurs in the ground

state of the antiferromagnetic case in dimensions $d = 2, 3$ if the biquadratic interaction is small enough. *Nematic order* was also shown in the ferromagnetic case if the biquadratic interaction is slightly stronger than the ferromagnetic interaction. This nematic order has also been proved to occur in spin-1 for a purely biquadratic interaction [69]. This is the content of Chapter 5. The result also holds in the presence of a small antiferromagnetic interaction however it is expected that the stronger Néel order is present here. Infrared bounds have also been used with probabilistic representations of quantum spin systems, this will be discussed in the sequel.

A further consequence of reflection positivity are *chessboard estimates*. See Section 2.2.7 for a discussion of chessboard estimates, we will use them in Section 7.4. These estimates can be used to show phase transitions in cases where infrared bounds cannot be used. Chessboard estimates find their origins in the work of Fröhlich and Lieb [39] and were developed subsequently [41, 42]. This method has been used on the q state Potts model with $q \gg 1$ [60]. It was used to prove the occurrence of a phase transition in the classical 120° model. The method has also been used to prove that if use of chessboard estimates provides proof of a phase transition in a classical spin system then there will also be a phase transition in the corresponding quantum spin model provided the magnitude of the quantum spin is large enough [16]. It has more recently been used to prove long range order in quantum dimer models [49]. The method can also be applied to diluted spin systems [23, 24] this is the content of Section 7.4. Chessboard estimates allow to prove breaking of discrete symmetries. For example in [24] it was shown that for certain annealed classical models on bipartite lattices there is a phase characterised by the preferential occupation of either the even or odd sublattice.

Correlation inequalities

Correlation functions are often of interest. If we knew everything about correlations of a system we would usually know everything about the system as they often characterise the distribution. In this thesis we will often be concerned with two-point correlations and their behaviour in the infinite volume limit. It is not trivial to prove that these correlations exist in infinite volume. Despite this there are results using correlation inequalities. These inequalities date back to the work of Griffiths [51] for the Ising model. They have been very useful for classical models for establishing infinite volume limits of correlation functions, proving the monotonicity of spontaneous magnetisation and to establish inequalities on critical exponents. Quantum systems have proved more difficult to study. Ginibre proposed a general setting under which correlation inequalities hold [48]. This included many classi-

cal systems and some quantum systems. Proving that a given quantum system satisfies the requirement of this framework is difficult. It has been shown that the quantum XY model fits this setting for spin- $\frac{1}{2}$ and the ground state in spin-1 [10], this is the content of Chapter 4. Correlation inequalities had previously been shown for the quantum XY model with pair interactions [45]. Inequalities for (untruncated) correlations in more general models were proposed in [40].

Probabilistic representations of quantum spin systems

Useful connections between many-body quantum systems and probabilistic models have seen growing recent interest. These representations date back to Feynman but since then there has been much work. It is expected that there are deep connections between the Bose gas and models of spatial random permutations [110] however this has not been rigorously proved. For quantum spin systems this work dates back to the work of Tóth [107] who used an interacting self-avoiding random walk representation of the Heisenberg ferromagnet to bound the pressure. A similar model for the antiferromagnet was introduced by Aizenman and Nachtergaele [2]. These models were combined and extended by Ueltschi [111]. We explain this model in Section 6.1. A connection between the probabilistic representation and various quantum spin systems was proved. For example for the nematic region of a general spin-1 bilinear-biquadratic interaction where it was proved that nematic order occurs for $d \geq 5$. It was also shown that in the presence of a purely biquadratic interaction on a bipartite lattice there is Néel order. The work of Crawford, Ng and Starr [28] on emptiness formation makes use of the model, as does the work of Björnberg and Ueltschi [19] on decay of correlations in the presence of a transverse magnetic field. We also consider the same spin-1 model [70] using and developing another loop model introduced in [81]. In this work it was shown that there is Néel order for a large range of parameters of an antiferromagnet interaction accompanied by a nematic interaction in dimension $d \geq 3$. This work also obtained some inequalities for different correlation functions that seemed very hard to obtain otherwise. We will see this work in Section 6.2.

These models have also seen significant interest from a purely probabilistic perspective. For probabilistic models such as those presented in [2, 69, 81, 111] it has been shown that macroscopic loops occur in the infinite volume limit, this is equivalent to symmetry breaking in the corresponding quantum models. It remains an open problem to rigorously describe the structure of these macroscopic loops (indeed there are expected to be multiple macroscopic loops). It is conjectured [111, 113] that these loops have a Poisson Dirichlet structure with parameter depending on the interactions. For example the loop model corre-

sponding to the ferromagnet is expected to have a PD(2) structure whereas for the nematic region PD($\frac{3}{2}$) is expected. Proof of such a result would provide much information on spin-spin correlations. For example, as mentioned in the prequel, proof of phase transitions can be achieved through proof of the non-decay of some relevant spin correlation by showing that the Cesàro average of the correlations is bounded away from zero. This result does not give information on the correlation between specific sites (other than that some unknown sites have a spin correlation that is bounded away from zero). Using the conjectured structure of macroscopic loops an explicit expression for spin correlations between sites can be obtained that becomes exact in the large volume, large distance limit. Recent work by Kotecký, Miłoś and Ueltschi [65] showed occurrence of macroscopic cycles for the random interchange process on the hypercube. Work by Schramm [98] and Berestycki [11] proved that the random interchange model on the complete graph undergoes a phase transition characterised by the emergence of infinite cycles whose sizes satisfy a Poisson Dirichlet law. It has recently been proved by Björnberg that large cycles also appear when permutations receive a weighting of $\theta^{\#cycles}$ where $\theta > 1$. Probabilistic representations have also been used to explore other properties of quantum spin systems. They were used to bound the emptiness formation probability (the probability that a region has all spins in the same eigenspace) for the Heisenberg antiferromagnet [28], to investigate gapped ground states of systems with continuous symmetries [5] and to classify pure Gibbs states of certain spin systems [111, 113].

Dilute spin systems and systems of itinerant particles

Systems where spin-carrying particles are itinerant have also received much attention in the literature. One such example is the Hubbard model. As mentioned before this model was studied using the method of spin-reflection positivity with great success. The model is very relevant as a system of many electrons for the study of ferromagnetism. In particular, if the spin interaction is neglected, is the Coulomb interaction a possible cause of ferromagnetic ordering [107]? Experiments on Bosons in optical lattices have also renewed interest in the Bose-Hubbard model. The Bose-Hubbard model has some significant differences with the Hubbard model, which models fermions, due to the system allowing many particles to occupy the same site. One can also include a spin interaction with this model and study the effect of this interaction. We will do this in Section 7.5. Bosons with spin are relevant to the theory of ^3He super-fluidity [68]. They have also been discussed due to connections with multicomponent Bose-Einstein condensation, [97, 105]. It was shown that in the absence of explicit spin interactions the system has a groundstate that is fully polarised. The case of explicit spin interactions has also been dealt with [57], it was shown that the structure of

the ground state only depends on the sign of the spin-dependent term. Various authors have looked at systems involving explicit spin-1 interactions using perturbative methods [54, 61] or using a mean-field approach [88, 92].

One can also consider systems where particles may not possess a spin that interacts with its neighbours (e.g. systems with impurities). These dilute spin systems have only limited results in the quantum case, although the classical case has seen some positive progress. The case of the Potts model with a large number of states was studied under annealed dilution, it was shown that the model has a phase where staggered order occurs; order characterised by preferential occupation of the even or odd sublattice for a system on a bipartite lattice [23]. This was later extended to classical systems with continuous spin [24]. Extending such results to a quantum system will be the content of Section 7.4.

1.2 Key results

In chapters 5 and 6 we consider a spin-1 quantum spin system with a bilinear-biquadratic interaction. We prove that Néel order occurs when the sign of the bilinear interaction is negative (the antiferromagnetic case) and the sign of the biquadratic interaction is positive (the nematic case) and not too large compared to the bilinear interaction (Theorem 6.2.6, found in [70]). This result extends the famous result of Dyson, Lieb and Simon [35] by handling the terms coming from the biquadratic interaction and therefore allowing an explicit region where Néel order occurs to be identified. We also prove that for the bilinear interaction accompanied by a small antiferromagnetic interaction nematic order is present (Theorem 5.1.1, found in [69]). This result applies to the region of the phase diagram that is expected to be antiferromagnetic. This raises the interesting question of the connection between nematic and Néel order for this quantum model.

In Section 7.4 we present a dilute quantum spin system. We consider dilution coming from site annealing. It is proved that for some region of the systems parameters and low enough temperature there is a phase transition categorised by preferential occupation of the odd or even sublattice (Theorem 7.4.1, found in [63]). Such results had previously been obtained for classical systems but this result is (to our knowledge) the first result for quantum spin systems.

In Chapter 4 we prove correlation inequalities for the quantum XY model. Proving correlation inequalities for quantum systems has been difficult, with limited results. We are able to treat the spin- $\frac{1}{2}$ case at all temperatures and the spin-1 case in the ground state. This is based on [10].

1.3 Outline of thesis

In Chapter 2 some theory for the general setting of classical and quantum spin systems on a lattice is presented. For classical systems we outline the set up for a classical spin system on a lattice as well as examples of some well known classical spin systems. We then discuss the issues of defining infinite volume systems such as DLR states. The property of reflection positivity for classical spin systems is also introduced. For quantum systems we outline the set up for a quantum spin system on a lattice including the definition and properties of quantum spin operators. Examples of some well known quantum spin systems including ones that will be considered in later chapters are given. There is then a discussion on the issues of defining infinite volume systems such as the evolution operator and KMS states, as well as some theorems on infinite volume limits of thermodynamic functions and a precise definition of Néel and nematic order. The property of reflection positivity for quantum spin systems is introduced and some of its consequences are discussed. We conclude this chapter with a small result concerning double commutators of matrices that may be of use when using the Falk-Bruch inequality [36], as is done several times in this thesis.

In Chapter 3 we present a brief result on the ground states of a particular classical spin system. This model will be referred to as the staggered nematic model but is also referred to as the antiferromagnetic \mathbf{RP}^2 model. We prove that the ground states of this model have a certain chessboard structure characterised by a high degeneracy despite being frustration free.

In Chapter 4 we show the positivity or negativity of truncated correlation functions in the quantum XY model with spin- $\frac{1}{2}$ (at any temperature) and spin-1 (in the ground state). These Griffiths-Ginibre inequalities of the second kind generalise an earlier result of Gallavotti. This is achieved by proving that the system under consideration fits the general framework presented by Ginibre [48]. In order to treat the spin-1 case we use the ideas of Nachtergaele [81] by representing a spin-1 system as a projection of two spin- $\frac{1}{2}$ systems onto the spin triplet.

Chapter 5 is based on the paper [69]. We introduce a spin-1 quantum nematic model (also known as a biquadratic model) and prove that this model undergoes a phase transition at low temperature in high dimension of the lattice. This result extends the work [3] to the quantum case. It also complements the work of Biskup, Chayes and Starr [16] whose methods proved the occurrence of a phase transition for this model in high ($\gg 1$) spin. It is then proved that this result is maintained if a small antiferromagnetic interaction is added.

In Chapter 6 we introduce several probabilistic representations for quantum spin systems

that have seen interest in recent years. To begin we introduce the Aizenman-Nachtergaele-Tóth-Ueltschi representation and prove the connection with quantum spin systems. Section 6.2 begins with the content of [70]. The loop model introduced by Nachtergaele [81] is presented and several results concerning the connection between spin and loop correlations are proved. It is proved that for a general spin-1 interaction that is $SU(2)$ invariant there is a phase transition (Néel order, or equivalently occurrence of macroscopic loops) for a large region of the model parameters at low temperature and for lattice dimension three or above. An alternate proof from [70] is provided that uses the loop model directly, reflection positivity is an essential tool. A result related to nematic order (which was relevant in Chapter 5) is then proved, a discussion on what is needed to improve this to a proof of nematic order is included. These two results are then reproved using the method of space-time reflection positivity introduced in [17]. This result offers a slight improvement over the previous result concerning Néel order.

In Chapter 7 we consider several quantum lattice systems where sites are allowed to have particle occupation numbers other than 1. In Section 7.1 the setting for a lattice system with quenched dilution is presented and an example of both a classical and quantum quenched system is given. In Section 7.2 the setting for a lattice system with annealed dilution is presented. In Section 7.3 it is proved that there is a phase transition for an annealed Heisenberg model whenever there is also a phase transition for the non-diluted system as long as the particle density is sufficiently close to 1. This section serves to show the (simple) adaptation of a well known result to the annealed case and also as a warm up to the next section. Section 7.4 is based on the paper [63]. It is proved for a quantum annealed system that for some values of the systems parameters and low temperatures there is a phase transition characterised by distinct states that prefer occupation of either the even or odd sublattice of the (bipartite) lattice. Finally Section 7.5 introduces a model of itinerant Bosons on a lattice (the Bose-Hubbard model) where particles interact according to a general spin-1 interaction. A probabilistic representation for this model is derived which is of a similar flavour to those seen in Chapter 6. This representation is used to derive expressions for off diagonal correlations and spin correlations between particles in terms of probabilities of events in the loop model.

Chapter 2

Setting for classical and quantum spin systems on a lattice

2.1 Classical spin systems on a lattice

2.1.1 Setting and examples

Consider a finite lattice, Λ , with a set of edges, \mathcal{E} . In examples we will take $\Lambda \subset \mathbb{Z}^d$ to be a box with nearest neighbour edges, \mathcal{E} , or the discrete torus in dimension d . Each $x \in \Lambda$ will have an associated classical spin, $\mathbf{S}_x \in \Omega$, where $\Omega \subset \mathbb{R}^N$ is a closed set (discrete or continuous). Denote by $\mathbf{S}_\Lambda = \{\mathbf{S}_x\}_{x \in \Lambda} \in \Omega^\Lambda$ a spin configuration consisting of a spin for each $x \in \Lambda$. We call a configuration, \mathbf{S}_{Λ^c} , of spins outside Λ a boundary condition. Particles at sites connected by an edge will interact according to their spins. For $A \subset \mathbb{Z}^d$ we denote by ϕ_A a function depending only on $\{\mathbf{S}_x\}_{x \in A}$. In order to describe the energy of a spin system we specify its *Hamiltonian*. The Hamiltonian will involve interactions ϕ_A for $A \cap \Lambda \neq \emptyset$. For the Hamiltonian to be well defined we require translation invariant interactions and a decay condition for the norm of the interactions:

1. $\phi_A(\{\mathbf{S}_x\}_{x \in A}) = \phi_{A+\mathbf{a}}(\tau_{\mathbf{a}}\{\mathbf{S}_x\}_{x \in A})$, $\mathbf{a} \in \mathbb{Z}^d$ where $\tau_{\mathbf{a}}$ is the translation operator by \mathbf{a} .
 2. $\sum_{A \ni 0} \|\phi_A\| < \infty$ where $\|\cdot\|$ is some appropriately chosen norm.
- (2.1.1)

For $\mathbf{S} = (\mathbf{S}_\Lambda, \mathbf{S}_{\Lambda^c})$ the most general Hamiltonian can then be written as

$$H_\Lambda(\mathbf{S}) = \sum_{\substack{A \subset \mathbb{Z}^d \text{ finite} \\ A \cap \Lambda \neq \emptyset}} \phi_A(\{\mathbf{S}_x\}_{x \in A}), \quad (2.1.2)$$

the conditions (2.1.1) ensure the sum is well defined. There are many excellent references on this topic, for example [13, 95] and references therein.

The law of spin configurations, \mathbf{S}_Λ , is then given by a *Gibbs distribution* at *inverse temperature* β of the form $e^{-\beta H_\Lambda(\mathbf{S})} \mu(d\mathbf{S}_\Lambda)$ where μ is some *a priori* Borel product measure on Ω^Λ . $\beta \geq 0$ is given by $\beta = \frac{1}{K_B T}$ where T is the temperature in Kelvins and $K_B = 1.38 \times 10^{-23} \text{m}^2 \text{Kg s}^{-2} \text{K}^{-1}$ is Boltzmann's constant. We refer the reader to the literature [46, 56, 96, 103] for treatment of Gibbs measure theory. Note that we only define this measure for finite Λ . We now present some examples of classical spin systems.

1. *The Ising model.* This is undoubtedly the most famous model of lattice spins. We denote the spin at $x \in \Lambda$ by σ_x . The set of possible spins is $\Omega = \{-1, +1\}$ with the *a priori* measure, μ , the uniform measure. The Hamiltonian is given by

$$H_\Lambda(\sigma_\Lambda) = - \sum_{\substack{x,y \in \Lambda \\ |x-y|=1}} \sigma_x \sigma_y - \mu \sum_{i \in \Lambda} \sigma_i. \quad (2.1.3)$$

For $\mu = 0$ we can see that having neighbouring spins aligned leads to more energetically favourable configurations. Note that the configurations with lowest energy (the ground state configurations) correspond to all spins being either $+1$ or -1 , this configuration has energy $-|\mathcal{E}|$. The minus sign in the Hamiltonian means that it is a *ferromagnetic* model, removing it results in an *antiferromagnetic* model. The model was invented by Lenz [71] and studied by his student, Ising in the 1920's. Ising solved the system in dimension one, showing that there is no phase transition [55]. It was assumed that there was also no phase transition in dimension two, however it was shown by Peierls [89] that in fact there is a phase transition. The proof used the beautiful and now famous *Peierls' argument*, we shall see it in section 7.4. In the absence of an external field the two dimensional case was solved analytically by Onsager [86]. The subsequent literature on the Ising model is extremely large.

2. *The Potts model.* This model generalises the Ising model to more than two possible spin states. It was introduced by Renfrey Potts in his 1951 thesis. An excellent review of the Potts model can be found in Wu's article [115]. We have spins $\sigma_x \in \{1, \dots, q\}$, $q \in \mathbb{N}$, again with uniform *a priori* measure. The Hamiltonian is

$$H_\Lambda(\sigma_\Lambda) = - \sum_{\substack{x,y \in \Lambda \\ |x-y|=1}} \delta_{\sigma_x, \sigma_y}. \quad (2.1.4)$$

It is energetically favourable to have all spins aligned. In two dimensions there is a first order phase transition if $q > 4$ and a continuous transition when $q \leq 4$.

3. *The Heisenberg model.* This model is used to model both ferromagnetism and anti-ferromagnetism. It can be seen as a generalisation of the Potts model to continuous spins, \mathbf{S} , taking values in $\Omega = \mathbb{S}^2$ with *a priori* measure the Haar measure on the surface of \mathbb{S}^2 with total mass 1. The Hamiltonian is

$$H_\Lambda(\mathbf{S}_\Lambda) = -J \sum_{\substack{x,y \in \Lambda \\ |x-y|=1}} \mathbf{S}_x \cdot \mathbf{S}_y. \quad (2.1.5)$$

Taking $J > 0$ gives the *Heisenberg ferromagnet* and taking $J < 0$ gives the *Heisenberg antiferromagnet*. Note that on a bipartite lattice the sign of J does not matter as we can flip all the spins on the even sublattice to effectively switch the sign of J . This model has an obvious $O(3)$ symmetry. It was famously shown that in $d \geq 3$ the ferromagnet exhibits a phase transition [43]. The proof used the method of reflection positivity and infrared bounds that will feature often in this thesis. It was known due to the Mermin-Wagner theorem [78] and its extensions that no such phase transition could occur for $d \leq 2$. Note that we could also take a more general model where $\Omega = \mathbb{S}^N$ for other values of $N \in \mathbb{N}$, this is called the $O(N)$ model. The $O(N)$ model has (unsurprisingly) an $O(N)$ symmetry. Formally the Ising model is the $O(1)$ model.

4. *The nematic model.* This is a model of liquid crystals. We refer the reader to [31] for theory on the physics of liquid crystals. The spins, \mathbf{S}_x , take values in $\Omega = \mathbb{S}^2$ as in the Heisenberg model. The Hamiltonian is

$$H_\Lambda(\mathbf{S}_\Lambda) = -J \sum_{\substack{x,y \in \Lambda \\ |x-y|=1}} (\mathbf{S}_x \cdot \mathbf{S}_y)^2. \quad (2.1.6)$$

This model is invariant under reversal of any spins due to the square in the interaction. The case $J > 0$ and $J < 0$ are not equivalent in this model and in fact behave quite differently. For $J > 0$ ground state configurations will involve nearest neighbour spins being aligned in the same direction. It has been proved that the system undergoes a phase transition in dimension $d \geq 3$ [3]. The quantum version of this model will be the topic of Chapter 5. For $J < 0$ the ground state configurations are more complicated [8, 9, 60], this will be the context of chapter 3.

2.1.2 Infinite volume Gibbs measures

For the models presented in Section 2.1.1 we considered only finite Λ . To consider the infinite volume limit of these models we must make sense of both the Hamiltonian and the

Gibbs measures. The problem is that neither are well defined for infinite volumes. We will deal with $\Lambda \subset \mathbb{Z}^d$ and for convenience consider only Λ that are boxes centered at the origin. We can take more general sets as in [95] (e.g. the limit in the sense of Van Hove) but for us boxes will be sufficient. If we wish to consider spins on the entirety of \mathbb{Z}^d we must take into account spins outside of Λ . For a system with Hamiltonian $H_\Lambda(\mathbf{S}_\Lambda)$ and boundary condition \mathbf{S}_{Λ^c} at inverse temperature β we define the systems *partition function* by

$$Z_\Lambda(\mathbf{S}_{\Lambda^c}, \beta) = \int_{\Omega^\Lambda} \mu(d\mathbf{S}_\Lambda) e^{-\beta H_\Lambda(\mathbf{S})}. \quad (2.1.7)$$

Expectations in this system will be given by the *Gibbs states*

$$\langle f \rangle_{\mathbf{S}_{\Lambda^c}, \beta} = \frac{1}{Z_\Lambda(\mathbf{S}_{\Lambda^c}, \beta)} \int_{\Omega^\Lambda} \mu(d\mathbf{S}_\Lambda) f(\mathbf{S}) e^{-\beta H_\Lambda(\mathbf{S})}, \quad (2.1.8)$$

denote the associated measure by $\mu_\Lambda(\cdot | \mathbf{S}_{\Lambda^c}, \beta)$. The two standard ways of defining infinite volume Gibbs states are either to consider weak cluster points of $\langle \cdot \rangle_{\mathbf{S}_{\Lambda^c}, \beta}$ as $\Lambda \rightarrow \mathbb{Z}^d$ with various boundary conditions or to use the *DLR* condition [13, 32] (named after Dobrushin, Lanford and Ruelle).

Definition 2.1.1. *For Hamiltonian, H , on \mathbb{Z}^d and inverse temperature, β , a measure, μ , on $\Omega^{\mathbb{Z}^d}$ is called an infinite volume Gibbs measure if for every finite $\Lambda \subset \mathbb{Z}^d$ and μ -a.e. boundary condition we have that μ satisfies the DLR condition*

$$\mu(\cdot | \mathbf{S}_{\Lambda^c}) = \mu_\Lambda(\cdot | \mathbf{S}_{\Lambda^c}, \beta). \quad (2.1.9)$$

The set of all infinite volume Gibbs states, \mathcal{G}_β , for a given β is of interest. \mathcal{G}_β is a weakly closed convex set. When $|\mathcal{G}_\beta| > 1$ we say that the system undergoes a phase transition. We can show that the Ising model undergoes a phase transition by taking Λ to be a box in \mathbb{Z}^d centred at the origin with boundary conditions all set to +1 or all set to -1. This is the famous result of Peierls whose beautiful contour method will be seen in Section 7.4.

2.1.3 Reflection positivity for classical models

Reflection positivity (RP) is one of the main tools of this thesis. Although it will mainly be applied to quantum systems it is useful to first consider the classical version of this property. The technique was developed in the now famous works of Dyson, Fröhlich, Isreal, Lieb, Simon and Spencer [35, 41, 42, 43]. Reflection positivity requires a great deal of symmetry of the lattice, namely reflection symmetry in any plane bisecting edges. For this reason we will work with the d -dimensional torus, \mathbb{T}_L , of side length, $L \in 2\mathbb{N}$. Note that the torus also

has symmetry under reflections through planes of sites and for classical systems we can also use RP for such reflections. Let R be a reflection in a plane splitting \mathbb{T}_L into two halves, $\mathbb{T}_1, \mathbb{T}_2$. We have $R\mathbb{T}_1 = \mathbb{T}_2$. Denote by \mathcal{A}_1 the set of all functions $\Omega^{\mathbb{T}_L} \rightarrow \mathbb{R}$ that only depend on spins in \mathbb{T}_1 . R acts on such functions by reflecting sites, for example $R(\mathbf{S}_x) = \mathbf{S}_{Rx}$.

Definition 2.1.2. *We say a state $\langle \cdot \rangle$ is reflection positive with respect to a reflection, R , if for any $f, g \in \mathcal{A}_1$*

$$\langle fRg \rangle = \langle gRf \rangle, \quad (2.1.10)$$

$$\langle fRf \rangle \geq 0. \quad (2.1.11)$$

The content of this definition is mainly in the second condition, the first condition usually follows from the structure of the lattice. Trivially the product measure, $\mu(d\mathbf{S}_\Lambda)$, is RP. One can think of RP as an inner product condition, the function $f, g \rightarrow \langle fRg \rangle$ is a positive-semidefinite, symmetric bilinear form. From this we have the Cauchy-Schwarz inequality

$$(\langle fRg \rangle)^2 \leq \langle fRf \rangle \langle gRg \rangle. \quad (2.1.12)$$

This is the main tool for using reflection positivity. Using this it can be proved [13, 41] that for a reflection, R , in a plane bisecting edges the Gibbs measure for β will be reflection positive if its associated Hamiltonian can be written in the form

$$H_\Lambda = -A - RA - \sum_{\alpha} B_{\alpha}RB_{\alpha}, \quad (2.1.13)$$

for $A, B_{\alpha} \in \mathcal{A}_1$. We will see how to apply this property to prove the occurrence of a phase transition in later chapters. Note that all of the examples in Section 2.1.1 can be brought to RP form. For example for the Hamiltonian 2.1.6 we reason as follows: for spin \mathbf{S} define a 3×3 matrix Q by

$$Q_{\alpha\beta} := \mathbf{S}^{\alpha}\mathbf{S}^{\beta} - \frac{1}{3}\delta_{\alpha\beta}. \quad (2.1.14)$$

Note that Q is a traceless matrix and for two spins $\mathbf{S}_x, \mathbf{S}_y$ we have

$$Tr(Q_x Q_y) = \sum_{\alpha, \beta=1}^3 (Q_x)_{\alpha\beta} (Q_y)_{\alpha\beta} = (\mathbf{S}_x \cdot \mathbf{S}_y)^2 - \frac{1}{3}. \quad (2.1.15)$$

This form was used in [3] to prove the occurrence of a phase transition for $J > 0$.

2.2 Quantum spin systems on a lattice

2.2.1 Setting

In this section we will present a general setting for a quantum spin system on a lattice and discuss topics such as infinite volume Gibbs states and reflection positivity. We will then have the tools required to move into the later chapters. Some of the setting for quantum spin systems on a lattice bears a resemblance to the classical setting. However the two settings depart in some major ways. Let Λ be a finite lattice with a set of edges, \mathcal{E} . We will usually take $\Lambda \subset \mathbb{Z}^d$ to be a box with a set of nearest neighbour edges, \mathcal{E} . We denote by \mathcal{H} a finite dimensional local Hilbert space. For each $x \in \Lambda$ denote by \mathcal{H}_x a copy of \mathcal{H} . Let \mathcal{A} be the algebra of operators on \mathcal{H} and let \mathcal{A}_x be its copy for $x \in \Lambda$. For a subset $A \subset \Lambda$ we define a Hilbert space, \mathcal{H}_A , and algebra of operators, \mathcal{A}_A , by

$$\mathcal{H}_A = \otimes_{x \in A} \mathcal{H}_x, \quad (2.2.1)$$

$$\mathcal{A}_A = \otimes_{x \in A} \mathcal{A}_x. \quad (2.2.2)$$

We can define a partial order on these algebras. For $A \subset B$, and $a \in \mathcal{A}_A$ we identify the operator $a \otimes \mathbb{1}_{B \setminus A}$ in \mathcal{A}_B . We use this to say $\mathcal{A}_{\Lambda'} \subset \mathcal{A}_\Lambda$ if $\Lambda' \subset \Lambda$. An interaction $\phi = \{\phi_A\}$ for $A \cap \Lambda \neq \emptyset$ is then a family of operators satisfying:

1. $\phi_A \in \mathcal{A}_A$. (2.2.3)

2. $\phi_{A+a} = \tau_a \phi_A$ where τ_a is the translation operator $\mathcal{A}_A \rightarrow \mathcal{A}_{A+a}$. (2.2.4)

3. $\phi_A^* = \phi_A$. (2.2.5)

For $r > 0$ we introduce a norm on interactions given by

$$\|\phi\|_r = \sum_{A \ni 0} \|\phi_A\| e^{r|A|}. \quad (2.2.6)$$

With this norm the space of interactions is a Banach space. For a given interaction and finite Λ we can define a Hamiltonian by

$$H_\Lambda = \sum_{\substack{A \subset \mathbb{Z}^d \text{ finite} \\ A \cap \Lambda \neq \emptyset}} \phi_A, \quad (2.2.7)$$

and finite volume Gibbs states at inverse temperature $\beta \geq 0$ by

$$\langle \cdot \rangle_{\Lambda, \beta} = \frac{1}{Z_{\Lambda, \beta}} \text{Tr} \cdot e^{-\beta H_{\Lambda}}, \quad (2.2.8)$$

with the partition function $Z_{\Lambda, \beta} = \text{Tr} e^{-\beta H_{\Lambda}}$. We will define more general states in Section 2.2.4 when the infinite volume limit will be studied.

2.2.2 Spin operators

Many quantum spin systems, including all those considered in this thesis, are defined via interactions involving *spin operators*. It is known that quantum models behave in some way similarly to their classical counterparts at finite temperature (but there are some significant differences!). It is the case that as the spin parameter $S \rightarrow \infty$ we recover the classical spin system however a rigorous treatment of this is still missing. There have been precise statements for the free energy of certain systems as $S \rightarrow \infty$ [12, 44, 72, 101]. We now present an introduction to these operators and their properties¹. For $S \in \frac{1}{2}\mathbb{N}$ consider the matrices (S^1, S^2, S^3) on \mathbb{C}^{2S+1} generating a $(2S+1)$ -dimensional irreducible representation of $\mathfrak{su}(2)$. They satisfy the commutation relations

$$[S^{\alpha}, S^{\beta}] = i \sum_{\gamma} \mathcal{E}_{\alpha\beta\gamma} S^{\gamma}, \quad (2.2.9)$$

for $\alpha, \beta, \gamma \in \{1, 2, 3\}$ and $\mathcal{E}_{\alpha\beta\gamma}$ the Levi-Civita symbol ($= 1(-1)$ if (α, β, γ) is an even (odd) permutation of $(1, 2, 3)$ and 0 else). Denote $\mathbf{S} = (S^1, S^2, S^3)$, we take the normalisation

$$\mathbf{S} \cdot \mathbf{S} = S(S+1)\mathbb{1}. \quad (2.2.10)$$

These properties uniquely define the S^i up to unitary transformations (see [102] Section VIII.4). The case $S = \frac{1}{2}$ gives $\frac{1}{2}$ the Pauli spin matrices:

$$S^1 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^2 = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.2.11)$$

For $S = 1$ we have the following matrices:

$$S^1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (2.2.12)$$

¹Several results concerning spin matrices were communicated to me by Daniel Ueltschi.

For general $S \in \mathbb{N}$ we prove the existence of these matrices by construction. For $a \in \{-S, \dots, S\}$ let $\{|a\rangle\}$ be an orthonormal basis of \mathbb{C}^{2S+1} . Denote the spin raising/lowering operators by S^\pm . We define S^3, S^\pm by

$$\begin{aligned} S^3|a\rangle &= a|a\rangle, \\ S^+|a\rangle &= \sqrt{S(S+1) - a(a+1)}|a+1\rangle, \\ S^-|a\rangle &= \sqrt{S(S+1) - a(a-1)}|a-1\rangle, \end{aligned} \tag{2.2.13}$$

with $S^+|S\rangle = S^-|-S\rangle = 0$. Then taking $S^1 = \frac{1}{2}(S^+ + S^-)$ and $S^2 = \frac{1}{2i}(S^+ - S^-)$ gives matrices S^1, S^2, S^3 satisfying (2.2.9) and (2.2.10). Note that $S^\pm = S^1 \pm iS^2$.

Lemma 2.2.1. *For Hermitian matrices S^1, S^2, S^3 satisfying (2.2.9) and (2.2.10) each S^i has eigenvalues $\{-S, -S+1, \dots, S\}$.*

Proof. We prove the claim for S^3 . We have

$$\begin{aligned} S^+S^- &= S(S+1) - (S^3)^2 + S^3, \\ S^-S^+ &= S(S+1) - (S^3)^2 - S^3. \end{aligned} \tag{2.2.14}$$

Then if $|a\rangle$ is an eigenvector of S^3 with eigenvalue a we have

$$\begin{aligned} \|S^+|a\rangle\|^2 &= \langle a|S^-S^+|a\rangle = S(S+1) - a^2 - a, \\ \|S^-|a\rangle\|^2 &= \langle a|S^+S^-|a\rangle = S(S+1) - a^2 + a. \end{aligned} \tag{2.2.15}$$

Hence we must have $|a| \leq S$ and $S^+|a\rangle = 0 \iff a = S$. Now as $[S^3, S^+] = S^+$ we have that $S^3S^+|a\rangle = (a+1)S^+|a\rangle$. From this we see that if $a < S$ is an eigenvalue so is $a+1$. Similarly for S^- if $a > -S$ is an eigenvalue so is $a-1$. Hence the set of eigenvalues is $\{-S, \dots, S\}$. \square

Spin matrices are well behaved under rotations. For $\mathbf{u} \in \mathbb{R}^3$ define $S^{\mathbf{u}} = \mathbf{u} \cdot \mathbf{S}$, we have

$$[S^{\mathbf{u}}, S^{\mathbf{v}}] = iS^{\mathbf{u} \times \mathbf{v}}. \tag{2.2.16}$$

Lemma 2.2.2. *If $R_{\mathbf{u}}\mathbf{v}$ is the result of rotating vector \mathbf{v} by angle $\|\mathbf{u}\|$ around \mathbf{u} then*

$$e^{-iS^{\mathbf{u}}} S^{\mathbf{v}} e^{iS^{\mathbf{u}}} = S^{R_{\mathbf{u}}\mathbf{v}}. \tag{2.2.17}$$

To prove this identity let $\mathbf{u} \rightarrow s\mathbf{u}$ and differentiate both sides with respect to s , one finds they satisfy the same ODE.

If we look at two spins with operators $S_1^i = S^i \otimes \mathbb{1}$ and $S_2^i = \mathbb{1} \otimes S^i$ on $\mathbb{C}^{2S+1} \otimes \mathbb{C}^{2S+1}$ the following lemma is well known.

Lemma 2.2.3. *The matrix $(\mathbf{S}_1 + \mathbf{S}_2)^2$ has eigenvalues $J(J+1)$ where $J \in \{0, 1, \dots, 2S\}$. The subspace corresponding to J has degeneracy $2J+1$. Further $[S_1^i + S_2^i, (\mathbf{S}_1 + \mathbf{S}_2)^2] = 0$ for $i = 1, 2, 3$ and the eigenvalues of $S_1^i + S_2^i$ in sector J are $-J, \dots, J$.*

More generally for particles on a lattice Λ with spins we take the operator S_x^i for $i = 1, 2, 3$ to be shorthand for the operator $S_x^i \otimes Id_{\Lambda \setminus \{x\}}$. We use the notation $|a, b\rangle = |a\rangle \otimes |b\rangle$ etc.

2.2.3 Examples

1. *The quantum Ising model.* Consider a graph (Λ, \mathcal{E}) with sites $x \in \Lambda$ having a spin- $\frac{1}{2}$ degree of freedom and \mathcal{E} a set of edges. The Hamiltonian is

$$H_\Lambda = -\lambda \sum_{\{x,y\} \in \mathcal{E}} S_x^3 S_y^3 - \delta \sum_{x \in \Lambda} S_x^1. \quad (2.2.18)$$

H_Λ acts on the Hilbert space $\otimes_{x \in \Lambda} \mathbb{C}^2$. S^i are the spin- $\frac{1}{2}$ matrices. The parameters $\lambda, \delta > 0$ are the spin-coupling and transverse field intensities, respectively. This model was introduced in [75] where its ground state and free energy were found exactly. It has since been widely studied, for example in [52] where ground state entanglement in dimension $d = 1$ was studied and in [18] where it was shown that the system undergoes a unique sharp phase transition.

2. *The anisotropic Heisenberg model.* The Hamiltonian is given by

$$H_\Lambda = - \sum_{\{x,y\} \in \mathcal{E}} (J_1 S_x^1 S_y^1 + J_2 S_x^2 S_y^2 + J_3 S_x^3 S_y^3) \quad (2.2.19)$$

where $-1 \leq J_1, J_2, J_3 \leq 1$ and S^i are the spin- S operators. Taking all $J_i = J$ gives the Heisenberg ferromagnet for $J > 0$ and the Heisenberg antiferromagnet for $J < 0$. Taking $J_1 = J_3 \neq 0$ and $J_2 = 0$ gives the XY model. Note that for the XY model on a bipartite lattice the sign of J_1 does not matter as the spins can be reversed on half the sites by the operators $e^{i\pi S_x^2}$. It is known that on a bipartite lattice the antiferromagnet has a unique ground state [74], however the exact structure is unknown. It is also known that the antiferromagnet undergoes a phase transition [35]. By contrast for the ferromagnet there is an entire $O(3)$ symmetry of the ground states that can be identified (see for example [113]) but it remains a huge open problem to prove the occurrence of a phase transition.

3. *The bilinear-biquadratic exchange Hamiltonian.* The Hamiltonian is given by

$$H_\Lambda = - \sum_{\{x,y\} \in \mathcal{E}} \left(J_1 (\mathbf{S}_x \cdot \mathbf{S}_y) + J_2 (\mathbf{S}_x \cdot \mathbf{S}_y)^2 \right). \quad (2.2.20)$$

The case $J_1 = 0 < J_2$ is the content of chapter 5, it is proved that there is nematic order. The first result on phase transitions for this model is the famous result of Dyson, Lieb and Simon [35] for $J_1 < 0 = J_2$ and $S \geq 1, d \geq 3$ or $S \geq 1/2, d \geq 4$. Kennedy, Lieb and Shastry extended this result to the case $(S, d) = (1/2, 3)$ [58]. For $S = 1$ and $d \geq 3$ it was shown [70] that Néel order is actually present in a large portion of the quadrant $J_1 < 0 < J_2$. For example in $d = 3$ Néel order is proved for $0 \leq J_2 < -2.161J_1$, this is the content of Section 6.2.6. Section 6.2.8 improves this to $0 \leq J_2 < -4.431J_1$ in $d = 3$. These regions increase in size as d increases. In the limit $d \rightarrow \infty$ we have Néel order for the entire quadrant. In the region $J_2 < 0$ very little is known. One result is for the AKLT model [1] for $S = 1$ where the presence of a “massive” phase was presented, in agreement with Haldane’s conjecture. It was shown in [111] that for $0 < J_2 \leq J_1/2$ there is nematic order on a cubic lattice in \mathbb{Z}^d for $d \geq 5$ at low temperature. For $J_1 = 0 < J_2$ it was shown that there is the stronger Néel order. Similar results were found independently in [106] for the ground state in dimensions three for $0 < J_1 \leq J_2/2 < 1.332J_1$, it was also shown that there is Néel order in dimensions two and three for $0 \leq J_2 < -0.188J_1$ and $0 \leq J_2 < -1.954J_1$ respectively. For the Heisenberg ferromagnet with $(S, d) = (1/2, 3)$ there are several results bounding the pressure, [26, 107]. Sharp bounds were recently found [27].

4. *The orbital compass model.* The Hamiltonian on \mathbb{Z}^2 is

$$H_\Lambda = \sum_{\{x,y\} \in \mathcal{E}} \begin{cases} S_x^1 S_y^1 & \text{if } y = x \pm e_1, \\ -S_x^3 S_y^3 & \text{if } y = x \pm e_3. \end{cases} \quad (2.2.21)$$

This model has been studied in several works [21, 34, 38, 53, 87] using numerical techniques, evidence points towards a phase transition in dimension 2 for spin- $\frac{1}{2}$.

5. *The plaquette orbital model.* The Hamiltonian on \mathbb{Z}^2 is

$$H_\Lambda = - \sum_{\{x,y\} \in \mathcal{E}} \begin{cases} J_1 S_x^1 S_y^1 & \text{if } x \text{ even/odd and } y = x \pm e_1 \text{ or } y = x \pm e_2, \\ J_2 S_x^3 S_y^3 & \text{if } x \text{ odd/even and } y = x \pm e_1 \text{ or } y = x \pm e_2. \end{cases} \quad (2.2.22)$$

It was shown in [15] this model exhibits orientational long-range order at low temperatures in one of the two lattice directions for S large enough. The case of lower spins, in particular spin- $\frac{1}{2}$, remains open.

2.2.4 Infinite volume states and the KMS condition

We can construct *infinite volume Gibbs states* from cluster points of $\langle \cdot \rangle_{\Lambda, \beta}$ for $\Lambda \rightarrow \mathbb{Z}^d$. We observe that by taking the spiral order on \mathbb{Z}^d it is an ordered set. With this order $\langle \cdot \rangle_{\Lambda, \beta}$ is then a net (a sequence indexed by \mathbb{Z}^d rather than \mathbb{N}) and by compactness of the set of observables there exist converging subnets. We will take Λ to be a box centred at the origin, this will be sufficient for our needs. The equivalent of the DLR condition for quantum systems is the KMS condition (named after Kubo, Martin and Schwinger [66, 76]). In order to state this condition we must introduce the *time evolution operator*.

Definition 2.2.4. For a Hamiltonian H_Λ of the form in (2.2.7), $a \in \mathcal{A}_\Lambda$, and $t \in \mathbb{C}$ we define the time evolution, $\alpha_t^{(\Lambda)}(a)$, of a by t as

$$\alpha_t^{(\Lambda)}(a) = e^{itH_\Lambda} a e^{-itH_\Lambda}. \quad (2.2.23)$$

In finite volume we have the following identity by cyclicity of the trace for $a, b \in \mathcal{A}_\Lambda$:

$$\begin{aligned} \langle a \alpha_t^{(\Lambda)}(b) \rangle_{\Lambda, \beta} &= \frac{1}{Z_{\Lambda, \beta}} \text{Tr} a e^{itH_\Lambda} b e^{-itH_\Lambda} e^{-\beta H_\Lambda} \\ &= \frac{1}{Z_{\Lambda, \beta}} \text{Tr} e^{itH_\Lambda + \beta H_\Lambda} b e^{-itH_\Lambda - \beta H_\Lambda} a e^{-\beta H_\Lambda} = \langle \alpha_{t-i\beta}^{(\Lambda)}(b) a \rangle_{\Lambda, \beta}. \end{aligned} \quad (2.2.24)$$

This identity in infinite volume is the KMS condition. Before we state the KMS condition precisely we need a time evolution operator for infinite volume. For infinite volume systems we cannot use the Hilbert space $\otimes_{x \in \mathbb{Z}^d} \mathcal{H}_x$ as it is non-separable. Instead we define the *algebra of quasi-local observables* by

$$\mathcal{A} = \overline{\mathcal{A}_0}, \quad \text{where} \quad \mathcal{A}_0 = \bigcup_{\Lambda \text{ finite}} \mathcal{A}_\Lambda, \quad (2.2.25)$$

where the overbar means the norm closure. A *state* is a positive normalised linear functional ρ on \mathcal{A} i.e. it has the properties

$$1. \quad \rho(\mathbb{1}) = 1 \quad (2.2.26)$$

$$2. \quad \rho(A^*A) \geq 0. \quad (2.2.27)$$

The following lemma is well known, see [93] for a proof.

Lemma 2.2.5. For $t \in \mathbb{R}$ and interaction $\{\phi_A\}$ with $\|\phi\|_r < \infty$ for some $r > 0$ there exists a

unique bounded operator $\alpha_t : \mathcal{A} \rightarrow \mathcal{A}$ such that

$$\lim_{\Lambda \nearrow \mathbb{Z}^d} \|\alpha_t^{(\Lambda)}(a) - \alpha_t(a)\| = 0 \quad \forall a \in \mathcal{A}_0, \quad (2.2.28)$$

$$\alpha_{s+t}(a) = \alpha_s(\alpha_t(a)) \quad \forall s, t \in \mathbb{C}, \quad (2.2.29)$$

for $\Lambda \rightarrow \mathbb{Z}^d$ along a sequence Λ_n of sets such that any finite set is contained in all Λ_n 's once n is large enough. $\alpha_t(A)$ has an analytic continuation to $t \in \mathbb{C}$ for every $A \in \mathcal{A}_0$.

Definition 2.2.6. A state ρ on \mathcal{A} satisfies the KMS condition for a Hamiltonian H if for every $a, b \in \mathcal{A}$

$$\rho(a\alpha_t(b)) = \rho(\alpha_{t-i\beta}(b)a). \quad (2.2.30)$$

It is known ([56] Theorem III.3.8) that every equilibrium state for an interaction, ϕ , is a KMS state for ϕ . The existence of more than one KMS state ensures a phase transition. A major tool for proving the occurrence of a phase transition is reflection positivity.

2.2.5 Phase transitions for quantum systems

In this section we will briefly outline some known results involving phase transitions including the existence of the infinite volume limit of some physical quantities and the relation relevance of correlations. We will also define quantities such as the Néel and nematic correlation functions that are relevant for Néel and nematic order discussed in Chapter 1. For notions of thermodynamic limits we follow the treatment in [95].

To begin we introduce a slightly different norm on interactions. For an interaction, ϕ , satisfying (2.2.3), (2.2.4) and (2.2.5), we define the norm

$$\|\phi\|_0 = \sum_{X \ni 0} \frac{\|\phi_X\|}{|X|}. \quad (2.2.31)$$

Recall the norm $\|\phi\|_r$, $r > 0$ (2.2.6), we have trivially that $\|\phi\|_0 \leq \|\phi\|_r$ (with the interpretation that the right side could be infinite). Denote $\mathcal{B} = \{\phi : \|\phi\|_0 < \infty\}$ and let $\mathcal{B}_0 \subset \mathcal{B}$ be those interaction in \mathcal{B} with finite range (i.e. there is an $N > 0$ such that $\phi_X = 0$ for $|X| > N$).

For Hamiltonian, $H_\Lambda(\phi) = \sum_{\substack{A \subset \mathbb{Z}^d \text{ finite} \\ A \cap \Lambda \neq \emptyset}} \phi_A$, with associated partition function $Z_\Lambda(\phi) = \text{Tr} e^{-H_\Lambda(\phi)}$ (we have absorbed the β into the interaction for notational convenience) we define the *free energy* of the system as

$$f_\Lambda(\phi) = -\frac{1}{|\Lambda|} \log Z_\Lambda(\phi). \quad (2.2.32)$$

The following proposition can be found in [95].

Proposition 2.2.7. *If $\phi, \psi \in \mathcal{B}$ then*

$$|f_\Lambda(\phi) - f_\Lambda(\psi)| \leq \|\phi - \psi\|_0, \quad (2.2.33)$$

further, f_Λ is convex on \mathcal{B} .

We now want to introduce the thermodynamic limit. In future chapters we will take the limit $\Lambda \rightarrow \mathbb{Z}^d$ along a sequence of boxes but here we introduce a slightly more general notion. For $a = (a_1, \dots, a_d) \in \mathbb{Z}^d$ with $a_i > 0$ for each i , define $\Lambda(a) = \{x \in \mathbb{Z}^d : 0 \leq x_i < a_i \text{ for } i = 1, \dots, d\}$. For $n \in \mathbb{Z}^d$ we define $\Lambda_n = \Lambda(a) + na$ as the translate of $\Lambda(a)$ by na . For $\Lambda \subset \mathbb{Z}^d$ denote by $N_a^+(\Lambda)$ the number of sets, Λ_n , such that $\Lambda_n \cap \Lambda \neq \emptyset$ and by $N_a^-(\Lambda)$ the number of sets, Λ_n , such that $\Lambda_n \subset \Lambda$.

Definition 2.2.8. *We say that sets Λ tend to infinity in the sense of Van Hove if*

$$N_a^-(\Lambda) \rightarrow \infty, \quad N_a^-(\Lambda)/N_a^+(\Lambda) \rightarrow 1. \quad (2.2.34)$$

We will denote this by $\lim_{|\Lambda| \rightarrow \infty}$ or $\lim_{\Lambda \nearrow \mathbb{Z}^d}$.

The following theorem can be found in [93].

Theorem 2.2.9. *If $\phi \in \mathcal{B}$ then the following limit exists and is finite*

$$f(\phi) = \lim_{\Lambda \rightarrow \infty} f_\Lambda(\phi), \quad (2.2.35)$$

where the limit is in the sense of Van Hove. Further, f is convex on \mathcal{B} and for $\phi, \psi \in \mathcal{B}$

$$|f(\phi) - f(\psi)| \leq \|\phi - \psi\|_0. \quad (2.2.36)$$

As was mentioned in Chapter 1, in finite volume the important quantities of the system such as its free energy will be real analytic in each of their variables. This may not be the case in infinite volume. The first problem, taking an infinite volume limit, can be overcome as we saw in Theorem 2.2.9. We take the view that phase transitions correspond to points of non-analyticity of a thermodynamic function. It is known ([95, Section 5.7]) that the functional derivative of the free energy with respect to a k -body potential ($\phi_X \in \phi$ with $|X| = k$) is, formally, the k -body correlation function. This means that passing between different analytic portions of f through a singularity corresponds to a point of discontinuity of the correlation functions. From this we see that the existence of multiple KMS states (which characterise the equilibrium states) ensures a phase transition. Note that this argument is far from rigorous, however, we adopt the view that this is the correct approach to phase

transitions.

Although this thesis is interested in phase transitions at low temperatures there are several results concerning the absence of phase transitions, for example the following theorem can be found in [40].

Theorem 2.2.10. *Assume that*

$$\beta\|\phi\|_{N+1} < (2N)^{-1}, \quad (2.2.37)$$

then there exists a unique KMS state at inverse temperature β .

The set of KMS states forms a simplex (in fact a Choquet simplex) [56, Theorem IV.3.12]. It is known [56, Section IV] that in the extremal states truncated correlations (those of the form $\langle AB \rangle - \langle A \rangle \langle B \rangle$) decay. This property will be extremely useful as we will often prove that a phase transition occurs by proving that a given (truncated) correlation does not decay. We will generally consider periodic boundary conditions for convenience. If one wished to identify different KMS states it is often helpful to consider infinite volume limits with different boundary conditions. There are two correlations of particular interest to us.

Definition 2.2.11. *Let H_Λ be a Hamiltonian which is a function of the spin- S operators given in Section 2.2.2 with Gibbs states at inverse temperature β given by $\langle \cdot \rangle_{\Lambda, \beta}$. We define the Néel correlation function as $(-1)^{\|x-y\|} \langle S_x^3 S_y^3 \rangle_{\Lambda, \beta}$ with $x, y \in \Lambda$ and $\|x-y\|$ the lattice distance between x and y . We similarly define the nematic correlation function as $\langle (S_x^3)^2 (S_y^3)^2 \rangle_{\Lambda, \beta} - \langle (S_x^3)^2 \rangle_{\Lambda, \beta} \langle (S_y^3)^2 \rangle_{\Lambda, \beta}$.*

Analogously to the classical case we say a system exhibits Néel order (resp. nematic order) if the Néel (resp. nematic) correlation function does not decay in the infinite volume limit.

It is worth noting that Néel order is also referred to as antiferromagnetic order or antiferro-dipolar order and that nematic order is also referred to as ferro-quadrupolar order. The method of *reflection positivity* will allow us to show such order by showing that the *Cesàro mean* does not decay.

2.2.6 Reflection positivity for quantum models

We now present some general theory of reflection positivity (RP) for quantum models, again we refer to previous literature [13, 16, 35, 39, 41, 42, 43]. We work with the d -dimensional torus, \mathbb{T}_L , of side length, $L \in 2\mathbb{N}$. It is possible to work on other lattices that have a lot of reflection symmetry, for example the hexagonal/honeycomb lattice. Unlike the classical case, in the quantum case we cannot use reflections through planes of sites due to operators on each side of the reflection plane no longer commuting. Let R be a reflection in a plane bisecting edges splitting \mathbb{T}_L into two halves, $\mathbb{T}_1, \mathbb{T}_2$. We have $R\mathbb{T}_1 = \mathbb{T}_2$. Denote by \mathcal{A}_1 the

algebra of operators on $\otimes_{x \in \mathbb{T}_1} \mathcal{H}_x$. We identify $A \in \mathcal{A}_1$ with the operator $A \otimes \mathbb{1}_{\mathbb{T}_2} \in \mathcal{A}$. R acts on such operators by reflecting sites, for example the spin operators: $R(\mathbf{S}_x) = \mathbf{S}_{R_x}$. The reflection acts as an involution $R : \mathcal{A}_1 \rightarrow \mathcal{A}_2$ as $R(A_1 \otimes \mathbb{1}_{\mathbb{T}_2}) = \mathbb{1}_{\mathbb{T}_1} \otimes RA_1$ for $A_1 \in \mathcal{A}_1$. The following definition is analogous to definition 2.1.2.

Definition 2.2.12. A state, $\langle \cdot \rangle$, on $\mathcal{A}_{\mathbb{T}_L}$ is reflection positive with respect to reflection R if for every $A, B \in \mathcal{A}_1$

$$\langle \overline{AR(B)} \rangle = \overline{\langle BR(A) \rangle}, \quad (2.2.38)$$

$$\langle \overline{AR(A)} \rangle \geq 0. \quad (2.2.39)$$

As in the classical case it follows that if $\langle \cdot \rangle$ is RP with respect to R then for every $A, B \in \mathcal{A}_1$

$$(\langle \overline{AR(B)} \rangle)^2 \leq \langle \overline{AR(A)} \rangle \langle \overline{BR(B)} \rangle. \quad (2.2.40)$$

A sufficient condition for RP, analogous to (2.1.13) for the classical case, is proved in [35]: For a reflection, R , through edges the Gibbs states associated to Hamiltonian H_L acting on $\mathcal{A}_{\mathbb{T}_L}$ are reflection positive if

$$H_L = A + \overline{R(A)} - \int \rho(d\alpha) B_\alpha \overline{R(B_\alpha)}, \quad (2.2.41)$$

where $A, B_\alpha \in \mathcal{A}_1$ and ρ is a finite measure. We refer to [35] for a proof. Note that each of the examples in Section 2.2.3 can be written in this form. This is more clear for some systems than for others. For example for the bilinear-biquadratic exchange Hamiltonian with $J_1 = 0 < J_2$ it is not immediately clear how to write H_Λ in this form however it will be shown in Chapter 5 how this can be achieved.

Two consequences of RP are Gaussian domination, which we will see in sections 5.2, 6.2.6, 6.2.7, 6.2.8, 6.2.9 and 7.3.1 and chessboard estimates, which we will see in Section 7.4. The reader is encouraged to consult some of the many references on Gaussian domination [13, 35, 41, 42, 43] and chessboard estimates [13, 16, 39, 41, 42, 60]. Chessboard estimates are used to control the energy of contours in contour expansions, see [20, 29, 30, 64] for work on contour expansions. As Gaussian domination and its important consequence, infrared bounds, will be seen in several places in this thesis we leave this property for now and instead explain chessboard estimates.

2.2.7 Chessboard estimates

This section will introduce the general setting of chessboard estimates. Let $\langle \cdot \rangle$ be a state satisfying the properties of reflection positivity in definition 2.2.12 on $\mathbb{T}_L = \mathbb{Z}^d / L\mathbb{Z}^d$ (the torus with L^d sites that can be identified with $(-L, L]^d \cap \mathbb{Z}^d$) and define

$$\mathbb{T}_B = \{0, 1, \dots, B-1\}^d \quad (2.2.42)$$

for $B \in \mathbb{Z}$ dividing L . Further denote by $\mathbb{T}_B + B\mathbf{t}$ the translation of \mathbb{T}_B by $B\mathbf{t} \in \mathbb{Z}^d$. We see

$$\mathbb{T}_L = \bigcup_{\mathbf{t} \in \mathbb{T}_{L/B}} (\mathbb{T}_B + B\mathbf{t}). \quad (2.2.43)$$

We know an operator $A \in \mathcal{A}_{\mathbb{T}_B}$ can be identified with $A \otimes \mathbb{1} \in \mathcal{A}_{\mathbb{T}_L}$. For $\mathbf{t} \in \mathbb{T}_{L/B}$ with $|\mathbf{t}| = 1$ let $R_{\mathbf{t}}$ be the reflection between edges on the side of \mathbb{T}_B corresponding to \mathbf{t} . Define

$$\hat{\mathcal{R}}_{\mathbf{t}}(A) = \overline{R_{\mathbf{t}}(A)}. \quad (2.2.44)$$

For other \mathbf{t} 's we define $\hat{\mathcal{R}}_{\mathbf{t}}$ by a sequence of reflections (this doesn't depend on the choice of sequence). Now we state the chessboard estimate, the proof can be found in [16].

Theorem 2.2.13. *Suppose $\langle \cdot \rangle$ is reflection positive for any reflection between sites. Then if $A_1, \dots, A_m \in \mathcal{A}_{\mathbb{T}_B}$ and $\mathbf{t}_1, \dots, \mathbf{t}_m \in \mathbb{T}_{L/B}$ are distinct,*

$$\left\langle \prod_{j=1}^m \hat{\mathcal{R}}_{\mathbf{t}_j}(A_j) \right\rangle \leq \prod_{j=1}^m \left\langle \prod_{\mathbf{t} \in \mathbb{T}_{L/B}} \hat{\mathcal{R}}_{\mathbf{t}}(A_j) \right\rangle^{(B/L)^d}. \quad (2.2.45)$$

The proof involves repeatedly applying (2.2.40) to tile the A_j 's throughout the lattice.

2.2.8 Double commutators of spin operators

In this section we present a result concerning double commutators of symmetric matrices. Our motivation is the Falk-Bruch inequality which was proposed independently in two papers [35, 36]. For a system with Hamiltonian H , partition function Z_{β} , and Gibbs states $\langle \cdot \rangle_{\beta}$,

$$\frac{1}{2} \langle A^* A + A A^* \rangle_{\beta} \leq \frac{1}{2} \sqrt{(A, A)_{Duh}} \sqrt{\langle [A^*, [H, A]] \rangle_{\beta}} + \frac{1}{\beta} (A, A)_{Duh} \quad (2.2.46)$$

where $(\cdot, \cdot)_{Duh}$ is the *Duhamel inner product*

$$(A, B)_{Duh} = \frac{1}{Z_{\beta}} \int_0^{\beta} ds \text{Tr} A^* e^{-sH} B e^{-(\beta-s)H}. \quad (2.2.47)$$

This inequality will be essential in future chapters and has been essential in past major works. The importance of this inequality means that the double commutator on the right side is also important for computation. When we use this inequality in the sequel we will be dealing with symmetric matrices.

Proposition 2.2.14. *Suppose A, B are real symmetric $n \times n$ matrices, then*

$$[B, A] \neq 0 \Rightarrow [A, [B, A]] \neq 0. \quad (2.2.48)$$

Proof. Let $\{f_i\}_{i=1}^n$ be an eigenbasis of B with corresponding eigenvalues $\{\lambda_i\}_{i=1}^n$ ($Bf_i = \lambda_i f_i$). If $[B, A] \neq 0$ there is an f_m that is not an eigenvector of A , hence there is an f_m such that

$$\begin{aligned} [B, A]f_m &= (B - \lambda_m)Af_m, \\ [B, A]f_m &\neq 0. \end{aligned} \quad (2.2.49)$$

Indeed if not then $[B, A]f_i = 0$ for any shared eigenvector of A and B and also for other eigenvectors of B but we know $[B, A] \neq 0$. Denote by f_k an eigenvector satisfying (2.2.49) with the least eigenvalue. We thus have (as $[B, A]$ is skew symmetric) for some $i \neq k$

$$\begin{aligned} 0 \neq f_i^T [B, A]f_k &= f_i^T B A f_k - f_i^T A \lambda_k f_k = \sum_j \left((f_i^T B f_j) (f_j^T A f_k) - (f_i^T A f_j) (f_j^T \lambda_k f_k) \right) \\ &= \lambda_i f_i^T A f_k - \lambda_k f_i^T A f_k = \underbrace{(\lambda_i - \lambda_k)}_{\geq 0} \underbrace{f_i^T A f_k}_{=f_k^T A f_i}. \end{aligned} \quad (2.2.50)$$

Where the inequality $\lambda_i - \lambda_k \geq 0$ follows as $[B, A]$ is skew-symmetric. Now suppose that $[A, [B, A]] = 0$, we consider two cases:

Case 1 $A[B, A] = 0$: Then $0 = \sum_j (f_k^T A f_j) (f_j^T [B, A]f_k) = \sum_j (\lambda_j - \lambda_k) (f_k^T A f_j)^2 > 0$ where the equality is due to A being symmetric. This is a contradiction.

Case 2 $A[B, A] \neq 0$: As A, B are symmetric $A[B, A]$ is skew symmetric, hence $f_j^T (A[B, A])f_j = 0 \forall j$. We calculate as follows:

$$0 = f_k^T (A[B, A])f_k = \sum_j (f_k^T A f_j) (f_j^T [B, A]f_k) = \sum_j (\lambda_j - \lambda_k) (f_j^T A f_k)^2. \quad (2.2.51)$$

This means that for every j either $f_j^T A f_k = 0$ or $\lambda_j = \lambda_k$. However as $(\lambda_i - \lambda_k) f_i^T A f_k \neq 0$ and $\lambda_i - \lambda_k \geq 0$ from above we have $(\lambda_i - \lambda_k) (f_i^T A f_k)^2 > 0$ and $(\lambda_j - \lambda_k) (f_j^T A f_k)^2 \geq 0 \forall j$. Hence $[A, [B, A]] \neq 0$. This completes the proof. \square

Chapter 3

Classical staggered nematic ground states

Spin models with nearest neighbour ferromagnetic interactions have simple and easily described ground states using the symmetries of the Hamiltonian. For antiferromagnetic interactions on bipartite lattices the equivalence with the ferromagnetic interactions provides an equally simple description of the ground states. On non-bipartite lattices the situation is quite different, antiferromagnetic models experience frustration and have highly degenerate ground states. For example the antiferromagnetic Ising model on a triangular lattice is maximally frustrated. We consider a model of nematic liquid crystals involving spins placed on a cubic lattice with nearest neighbour interactions of the form $J(\sigma_x \cdot \sigma_y)^2$ with each $\sigma \in \mathbb{S}^2$. For $J < 0$ the system exhibits a phase transition at low temperatures [3]. The ground states of this system correspond to all spins being aligned. The case of the lattice-gas with longer range interactions was also studied in lower dimensions with success [4]. It was also shown that with the addition of a small ferromagnetic interaction the system has an intermediate phase with non-zero nematic order parameter but zero magnetisation [22]. For $J > 0$ the system behaves very differently, this case will be the focus of the current article. Monte Carlo studies suggest the occurrence of a phase transition in this model for low temperatures [8, 9, 62]. The ground states for $J > 0$ are more complicated, they are characterised by chessboard configurations with the spins on the even (odd) sublattice taking the same fixed value and spins on the odd (even) sublattice having free choice on a copy of \mathbb{S}^1 perpendicular to spins on the even (odd) sublattice. These ground states are highly degenerate. Kohring and Shrock [62] noted that these configurations had a nonzero disordering entropy but believed that the true ground states were more complicated, we prove that this is not the case.

3.1 The model and main result

We will work on a finite bipartite lattice, $\Lambda_L \subset \mathbb{Z}^d$,

$$\Lambda_L = \left\{ -\frac{L}{2} + 1, \dots, \frac{L}{2} \right\}^d, \quad (3.1.1)$$

with nearest neighbour edges with periodic boundary conditions, \mathcal{E}_L . Let Λ_A (Λ_B) denote the even (odd) sublattice. At each $x \in \Lambda_L$ we assign a classical spin $\sigma_x \in \mathbb{S}^2$, hence we have state space $\Omega_{\Lambda_L} = (\mathbb{S}^2)^{\Lambda_L}$. The Hamiltonian of the system is

$$H_{\mathbf{h}}(\sigma) = 2 \sum_{\{x,y\} \in \mathcal{E}_L} (\sigma_x \cdot \sigma_y)^2 - \sum_{x \in \Lambda_L} h_x \left((\sigma_x^3)^2 - \frac{1}{3} \right). \quad (3.1.2)$$

Here σ_x^i denotes the i^{th} component of the spin at $x \in \Lambda_L$. Notice the model does not see any difference between σ_x and $-\sigma_x$. The partition function is

$$Z(\beta, \Lambda_L, \mathbf{h}) = \int_{\Omega_{\Lambda_L}} d\sigma e^{-\beta H_{\mathbf{h}}(\sigma)}, \quad (3.1.3)$$

with inverse temperature $\beta \geq 0$ and $d\sigma$ the Haar measure on Ω_{Λ_L} with $\int_{\Omega_{\Lambda_L}} d\sigma = 1$. We will take $\mathbf{h} = \mathbf{0}$ and write $H_{\mathbf{0}}(\sigma) = H(\sigma)$ and $Z(\beta, \Lambda_L, \mathbf{0}) = Z(\beta, \Lambda_L)$. Expectations are given by

$$\langle \cdot \rangle_{\beta} = \frac{1}{Z(\beta, \Lambda_L)} \int_{\Omega_{\Lambda_L}} d\sigma \cdot e^{-\beta H(\sigma)}. \quad (3.1.4)$$

We want to understand the ground states of this system. Intuitively the possible configurations will have nearest neighbours with perpendicular spins. We will call uniform measures on such configurations ground-states and we will see this is justified. The states adopted by the system at low temperature are the chessboard states, where spins on one sublattice are equal (up to sign) and spins of the second sublattice lie on a circle perpendicular to the spins on the first, see Fig. 3.1. Before we state our main result we must introduce the chessboard measure, this will be the limiting measure of our system as we shall see.

Definition 3.1.1. *We define the chessboard measure, ρ as follows: Let $D \subset \Omega_{\Lambda_L}$ then*

$$\rho(D) = \frac{1}{2} \left(\int_D d\alpha \prod_{x \in \Lambda_A} (\delta(\sigma_x - \alpha) + \delta(\sigma_x + \alpha)) \prod_{x \in \Lambda_B} dv_{\alpha}(\sigma_x) + \int_D d\alpha \prod_{x \in \Lambda_B} (\delta(\sigma_x - \alpha) + \delta(\sigma_x + \alpha)) \prod_{x \in \Lambda_A} dv_{\alpha}(\sigma_x) \right) \quad (3.1.5)$$

where $d\alpha$ is the Haar measure on \mathbb{S}^2 with $\int_{\Omega_{\Lambda_A}} d\alpha = 1$ and v_{α} is the Haar measure on the set of $u \in \mathbb{S}^2$ such that $u \cdot \alpha = 0$, again with total weight 1.

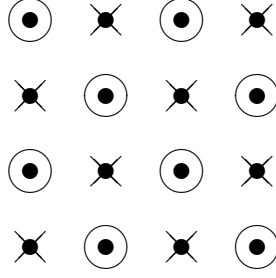


Figure 3.1: Illustration of a possible chessboard configuration. Here the crosses denote that spins on one sublattice are pointing into (or out of) the page, the spins on the other sublattice can take any value on the circle parallel to the plane of the page.

Theorem 3.1.2. For L even and any continuous bounded function f on Ω_{Λ_L}

$$\lim_{\beta \rightarrow \infty} \frac{1}{Z(\beta, \Lambda_L)} \int_{\Omega_{\Lambda_L}} d\sigma f(\sigma) e^{-\beta H(\sigma)} = \int_{\Omega_{\Lambda_L}} f(\sigma) d\rho(\sigma). \quad (3.1.6)$$

3.2 Proof of theorem 3.1.2

The proof of Theorem 3.1.2 will be split into several parts. First we will prove that our expectations concentrate onto the ground-states described above. For $\varepsilon > 0$ let

$$D_\varepsilon = \{\sigma \in \Omega_{\Lambda_L} : \exists \{x, y\} \in \mathcal{E}_L \text{ s.t. } |\sigma_x \cdot \sigma_y| \geq \varepsilon\}, \quad (3.2.1)$$

$$G_\varepsilon = D_\varepsilon^c = \{\sigma \in \Omega_{\Lambda_L} : |\sigma_x \cdot \sigma_y| < \varepsilon \forall \{x, y\} \in \mathcal{E}\}. \quad (3.2.2)$$

Then D_ε consists of those states that are ‘far away’ from ground-states. We first show that $\langle \cdot \rangle_\beta$ converges to the uniform measure on $G = \bigcap_{\varepsilon > 0} G_\varepsilon$, denoted by μ .

Lemma 3.2.1. For any $\varepsilon > 0$ we have that $\langle \mathbb{1}_{D_\varepsilon} \rangle_\beta \rightarrow 0$ as $\beta \rightarrow \infty$.

Proof.

$$\langle \mathbb{1}_{D_\varepsilon} \rangle_\beta = \frac{\int_{D_\varepsilon} d\sigma e^{-\beta H(\sigma)}}{\int_{D_\varepsilon} d\sigma e^{-\beta H(\sigma)} + \int_{D_\varepsilon^c} d\sigma e^{-\beta H(\sigma)}} \leq \frac{\int_{D_\varepsilon} d\sigma e^{-2\beta \varepsilon^2}}{\int_{D_\varepsilon^c} d\sigma e^{-\beta H(\sigma)}} \leq \frac{e^{-2\beta \varepsilon^2}}{\int_{D_\varepsilon^c} d\sigma e^{-\beta H(\sigma)}}. \quad (3.2.3)$$

To estimate the denominator we let β be large enough that $1/\sqrt{\beta} < \varepsilon$, then

$$\int_{D_\varepsilon^c} d\sigma e^{-\beta H(\sigma)} \geq \int_{D_{1/\sqrt{\beta}}^c} d\sigma e^{-\beta H(\sigma)} \geq \int_{D_{1/\sqrt{\beta}}^c} d\sigma e^{-2d|\Lambda_L|} \geq e^{-2d|\Lambda_L|} A_\sigma(D_{1/\sqrt{\beta}}^c). \quad (3.2.4)$$

Where $A_\sigma(D_{1/\sqrt{\beta}}^c)$ is the area of $D_{1/\sqrt{\beta}}^c$ under the Haar measure. We have

$$A_\sigma(D_{1/\sqrt{\beta}}^c) \leq A_\sigma\left(\left\{|\sigma_0 \cdot \sigma_{e_1}| < \frac{1}{\sqrt{\beta}}\right\}\right)^{d|\Lambda_L|} = A_\sigma\left(\left\{|\sigma_{e_1}^1| < \frac{1}{\beta}\right\}\right)^{d|\Lambda_L|} = \left(\sqrt{1 - \frac{1}{\beta}}\right)^{d|\Lambda_L|}. \quad (3.2.5)$$

Hence $\langle \mathbb{1}_{D_\varepsilon} \rangle \leq e^{-2\beta\varepsilon^2} e^{2d|\Lambda_L|} A_\sigma(D_{1/\sqrt{\beta}}^c)^{-1} \rightarrow 0$ as $\beta \rightarrow \infty$ for any $\varepsilon > 0$. \square

Lemma 3.2.2. *We have that $\langle \cdot \rangle_\beta \rightarrow \mu$ as $\beta \rightarrow \infty$.*

Proof. We prove the equivalent statement that $\limsup_{\beta \rightarrow \infty} \langle \mathbb{1}_C \rangle_\beta \leq \mu(C)$ for any closed $C \subset \Omega_{\Lambda_L}$. Firstly if $C \subset D_\varepsilon$ for some ε then by Lemma 3.2.1 $\limsup_{\beta \rightarrow \infty} \langle \mathbb{1}_C \rangle_\beta = 0 = \mu(C)$. If $A_\sigma(C)$ is the area under the Haar measure on Ω_{Λ_L} of C then if $A_\sigma(C) = 0$ we have $\limsup_{\beta \rightarrow \infty} \langle \mathbb{1}_C \rangle_\beta = 0 \leq \mu(C)$. Suppose $A_\sigma(C) \neq 0$ and $C \cap G_\varepsilon \neq \emptyset \forall \varepsilon > 0$ then

$$\limsup_{\beta \rightarrow \infty} \langle \mathbb{1}_C \rangle_\beta = \limsup_{\beta \rightarrow \infty} \frac{1}{Z_{\beta, \Lambda_L}} \int d\sigma \mathbb{1}_{C \cap G_\varepsilon} e^{-\beta H(\sigma)} \leq \limsup_{\beta \rightarrow \infty} \frac{1}{Z_{\beta, \Lambda_L}} A_\sigma(C \cap G_\varepsilon) \quad \forall \varepsilon > 0. \quad (3.2.6)$$

Hence we need a lower bound on the partition function, this is easy to obtain,

$$Z(\beta, \Lambda_L) \geq \int d\sigma \mathbb{1}_{G_\varepsilon} e^{-\beta H(\sigma)} \geq A_\sigma(G_\varepsilon) e^{-2\beta\varepsilon^2 d|\Lambda_L|} \quad \forall \varepsilon > 0. \quad (3.2.7)$$

If we take $\varepsilon = 1/\beta$ we finally have

$$\limsup_{\beta \rightarrow \infty} \langle \mathbb{1}_C \rangle_\beta \leq \limsup_{\beta \rightarrow \infty} \frac{A_\sigma(C \cap G_{1/\beta})}{A_\sigma(G_{1/\beta}) e^{-2d|\Lambda_L|/\beta}} = \mu(C). \quad (3.2.8)$$

\square

What we want now is that of all possible ground-states we will μ -a.s. be in the set of chessboard states. Hence the limiting measure will be a uniform measure on chessboard configurations, i.e. the chessboard measure. This gives us Theorem 3.1.2 for indicator functions, for general functions we use the standard machinery of measure theory.

Now we must define the set of ‘approximate chessboard states’, $C_{\varepsilon, \delta}$. We initially define

$$\widetilde{C}_{\varepsilon, \delta} = \{\sigma \in G_\varepsilon : |\sigma_x - \sigma_y| \in [\delta, 2 - \delta]^c \forall x, y \in \Lambda_A \text{ or } |\sigma_w - \sigma_z| \in [\delta, 2 - \delta]^c \forall w, z \in \Lambda_B\}. \quad (3.2.9)$$

So now we have relaxed the configurations so that spins may occupy small regions around the spin of the groundstate configuration that $\sigma \in G_\varepsilon$ approximates. However we could have an approximate ground state where spins on the ‘fixed’ (to within distance δ) sublattice are slowly rotated as we move in some direction across Λ , if Λ is large enough and the rotation

gradual enough we could end up with a state with a small energy (comparable to a state in $\widetilde{C}_{\varepsilon,\delta}$) where we could appear to be in different states in $\widetilde{C}_{\varepsilon,\delta}$ depending on where we were looking. To avoid this scenario we could take ε to be small enough but then ε must depend on Λ_L . Instead we make our proper definition as follows

$$C_{\varepsilon,\delta} = \{\sigma \in G_\varepsilon : |\sigma_x - \sigma_y| \in [\delta, 2 - \delta]^c \ \forall \text{ next nearest neighbours } x, y \in \Lambda_A \text{ or} \\ \forall \text{ next nearest neighbours } x, y \in \Lambda_B\}. \quad (3.2.10)$$

Then

$$\widetilde{C}_{\varepsilon,2\delta/dL} \subset C_{\varepsilon,2\delta/dL} \subseteq \widetilde{C}_{\varepsilon,\delta} \subset C_{\varepsilon,\delta}. \quad (3.2.11)$$

We will see that we require $\delta < \varepsilon$. We therefore take $\delta = \varepsilon/2$. If we can show that

$$|G_\varepsilon \setminus C_{\varepsilon,\varepsilon/dL}|/|C_{\varepsilon,\varepsilon/dL}| \rightarrow 0 \text{ as } \varepsilon \rightarrow 0 \quad (3.2.12)$$

then we will be done. Intuitively approximate chessboard states will be preferred because they give the most possible choice. $|\Lambda_L|/2$ of the sites have a choice from an entire strip around a copy of $\mathbb{S}^1 \subset \mathbb{S}^2$ and other states will not have such choice.

Now we can estimate the sizes of G_ε and $C_{\varepsilon,\varepsilon/2}$. The area of $\widetilde{C}_{\varepsilon,\varepsilon/2}$ gives a lower bound on the area of $C_{\varepsilon,\varepsilon/2}$. Suppose that $|\sigma_x - \sigma_y| \in [\varepsilon/2, 2 - \varepsilon/2]^c \ \forall x, y \in \Lambda_A$. All spins on sites in Λ_A lie on one of two spherical caps defined by a cone with vertex $(0, 0, 0)$ and circular base of diameter $\varepsilon/2$ lying on \mathbb{S}^2 . These caps have combined surface area (Haar measure)

$$\left(1 - \sqrt{1 - \frac{\varepsilon^2}{16}}\right) = \frac{\varepsilon^2}{32} + \frac{\varepsilon^4}{128} + O(\varepsilon^6). \quad (3.2.13)$$

Because we also require $|\sigma_x \cdot \sigma_y| < \varepsilon \ \forall \{x, y\} \in \mathcal{E}$ the spins on Λ_B must lie on a strip around \mathbb{S}^2 consisting of vectors approximately perpendicular to all vectors in the spherical cap. This explains our requirement that $\delta < \varepsilon$ as the strip only exists in this case. With a little thought and a suitably drawn diagram we can see that, for $\delta = \varepsilon/2$, this strip is defined by an arc of a circle with angle

$$2 \cos^{-1} \left(\frac{\varepsilon^2}{4} + \sqrt{\frac{\varepsilon^4}{16} - \frac{17\varepsilon^2}{16} + 1} \right) \leq \theta \leq 2 \cos^{-1} \left(\frac{\varepsilon^2}{4} - \sqrt{\frac{\varepsilon^4}{16} - \frac{17\varepsilon^2}{16} + 1} \right). \quad (3.2.14)$$

This strip has surface area given by $\sin(\theta)$ and (recall we have $\int_{\Omega_\Lambda} d\sigma = 1$) we have

$$\frac{3\varepsilon}{4} + \frac{3\varepsilon^2}{32} + \frac{63\varepsilon^5}{2048} + O(\varepsilon^7) \leq \sin(\theta) \leq \frac{5\varepsilon}{4} - \frac{5\varepsilon^2}{32} - \frac{65\varepsilon^5}{2048} + O(\varepsilon^7). \quad (3.2.15)$$

Hence, because in an approximate chessboard configuration the sites on one sublattice can take spins on spherical caps and sites on the other sublattice can take spins on a strip around \mathbb{S}^2 we have (noting the symmetry under swapping of the sublattices) the bound

$$\begin{aligned} |C_{\varepsilon, \varepsilon/dL}| &\geq 2 \left[\left(\frac{\varepsilon^2}{32} + \frac{\varepsilon^4}{128} \right) \times \left(\frac{3\varepsilon}{4} + \frac{3\varepsilon^2}{32} + \frac{63\varepsilon^5}{2048} \right) \right]^{|\Lambda_L|/2} + O(\varepsilon^{13|\Lambda_L|/2}) \\ &= 2 \left(\frac{3}{128} \right)^{|\Lambda_L|/2} \varepsilon^{3|\Lambda_L|/2} + O(\varepsilon^{2|\Lambda_L|}) \end{aligned} \quad (3.2.16)$$

The following lemma completes the proof of Theorem 3.1.2.

Lemma 3.2.3. *For some $k \geq 1$*

$$|G_\varepsilon \setminus C_{\varepsilon, \varepsilon/dL}| \leq O(\varepsilon^{3|\Lambda_L|/2+k}). \quad (3.2.17)$$

Proof. For concreteness we will work in $d = 2$, the proof can easily be generalised to higher dimensions. Let $\sigma \in G_\varepsilon$. Consider a site $x = (x_1, x_2) \in \Lambda_L$, when looking at the set of possible spins for site x there are two cases:

1. $|\sigma_{(x_1-1, x_2)} - \sigma_{(x_1, x_2-1)}| \in \left[\frac{\varepsilon}{2}, 2 - \frac{\varepsilon}{2} \right]^c$, then σ_x can lie in a strip of area $O(\varepsilon)$.
2. $|\sigma_{(x_1-1, x_2)} - \sigma_{(x_1, x_2-1)}| \in \left[\frac{\varepsilon}{2}, 2 - \frac{\varepsilon}{2} \right]$, then because we need $|\sigma_{(x_1-1, x_2)} \cdot \sigma_x| < \varepsilon$ and $|\sigma_{(x_1, x_2-1)} \cdot \sigma_x| < \varepsilon$, σ_x must lie in intersection of two strips (defined by $\sigma_{(x_1-1, x_2)}$ and $\sigma_{(x_1, x_2-1)}$) tilted at an angle of $\phi > 2 \arcsin \frac{\varepsilon}{4}$ to each other. This means the spin lies in a section of the sphere defined by a rhombus of side ε and hence area $O(\varepsilon^2)$.

If $\sigma \notin C_{\varepsilon, \varepsilon/dL}$ at least one pair of sites must be in case 2, hence locally approximate chessboard configurations are preferable. Let \mathcal{B} be the set of states in G_ε with sites $x, y \in \Lambda_L$ such that there is a region $U_x \ni x$ that has an approximate chessboard configuration and no neighbourhood of y is compatible with the same approximate chessboard configuration. Note $\mathcal{B} = G_\varepsilon \setminus C_{\varepsilon, \varepsilon/dL}$. Hence there must be a contour $\gamma \subset \Lambda_L$ surrounding the approximate chessboard state at x . From above we know this contour can only have spins on an area of order at least $\varepsilon^{|\gamma|}$ higher than an approximate chessboard state would. Let $c > 1$ be a constant such that the number of contours of length n on Λ_L is bounded by c^n then

$$\frac{A_\sigma(\mathcal{B})}{A_\sigma(C_{\varepsilon, \varepsilon/dL})} \leq \binom{|\Lambda_L|}{2} \sum_\gamma \varepsilon^{|\gamma|} \leq \binom{|\Lambda_L|}{2} \sum_{n \geq 1} c^n \varepsilon^n = \binom{|\Lambda_L|}{2} \frac{c\varepsilon}{1 - c\varepsilon} \rightarrow 0 \text{ as } \varepsilon \rightarrow 0. \quad (3.2.18)$$

This shows that $A_\sigma(\mathcal{B}) \leq O(\varepsilon)A_\sigma(G_\varepsilon)$, completing the proof. \square

Chapter 4

Correlation inequalities for the quantum XY model

4.1 Introduction & results

In his extension of Griffiths' inequalities, Ginibre proposed a setting that also applies to quantum spin systems [48]. The goal of this chapter is to show that the quantum XY model fits the setting, at least with $S = \frac{1}{2}$ and $S = 1$. It follows that many truncated correlation functions take a fixed sign.

Let Λ denote the (finite) set of sites that host the spins. The Hilbert space of the model is $\mathcal{H}_\Lambda = \otimes_{x \in \Lambda} \mathbb{C}^{2S+1}$ with $S \in \frac{1}{2}\mathbb{N}$. Let $S^i, i = 1, 2, 3$ denote usual spin operators on \mathbb{C}^{2S+1} ; that is, they satisfy the commutation relations $[S^1, S^2] = iS^3$, and other relations obtained by cyclic permutation of the indices 1, 2, 3. They also satisfy the identity $(S^1)^2 + (S^2)^2 + (S^3)^2 = S(S+1)$. Finally, let $S_x^i = S^i \otimes \mathbb{1}_{\Lambda \setminus \{x\}}$ denote the spin operator at site x . We consider the Hamiltonian

$$H_\Lambda = - \sum_{A \subset \Lambda} \left(J_A^1 \prod_{x \in A} S_x^1 + J_A^2 \prod_{x \in A} S_x^2 \right). \quad (4.1.1)$$

Here, J_A^i is a nonnegative coupling constant for each subset of $A \subset \Lambda$ and each spin direction $i \in \{1, 2\}$. The expected value of an observable a (that is, an operator on \mathcal{H}_Λ) in the Gibbs state with Hamiltonian H_Λ and at inverse temperature $\beta > 0$ is

$$\langle a \rangle = \frac{1}{Z(\Lambda)} \text{Tr } a e^{-\beta H_\Lambda}, \quad (4.1.2)$$

where the normalisation $Z(\Lambda)$ is the partition function

$$Z(\Lambda) = \text{Tr } e^{-\beta H_\Lambda} . \quad (4.1.3)$$

Traces are taken in \mathcal{H}_Λ . We also consider Schwinger functions that are defined for $s \in [0, 1]$ by

$$\langle a; b \rangle_s = \frac{1}{Z(\Lambda)} \text{Tr } a e^{-s\beta H_\Lambda} b e^{-(1-s)\beta H_\Lambda} . \quad (4.1.4)$$

Our first result holds for $S = \frac{1}{2}$ and all temperatures.

Theorem 4.1.1. *Assume that $J_A^i \geq 0$ for all $A \subset \Lambda$ and all $i \in \{1, 2\}$. Assume also that $S = \frac{1}{2}$. Then for all $A, B \subset \Lambda$, and all $s \in [0, 1]$, we have*

$$\begin{aligned} \left\langle \prod_{x \in A} S_x^1, \prod_{x \in B} S_x^1 \right\rangle_s - \left\langle \prod_{x \in A} S_x^1 \right\rangle \left\langle \prod_{x \in B} S_x^1 \right\rangle &\geq 0; \\ \left\langle \prod_{x \in A} S_x^1, \prod_{x \in B} S_x^2 \right\rangle_s - \left\langle \prod_{x \in A} S_x^1 \right\rangle \left\langle \prod_{x \in B} S_x^2 \right\rangle &\leq 0. \end{aligned}$$

Clearly, other inequalities can be generated using spin symmetries. The corresponding inequalities for the classical XY model have been proposed in [67].

The proof of Theorem 4.1.1 can be found in Section 4.3. It is based on Ginibre's structure [48]. It is simpler than Gallavotti's, who used an ingenious approach based on the Trotter product formula, on a careful analysis of transition operators, and on Griffiths' inequalities for the classical Ising model [45]. Our proof allows us to go beyond pair interactions.

A consequence of Theorem 4.1.1 is the monotonicity of certain spin correlations with respect to the coupling constants:

Corollary 4.1.2. *Under the same assumptions as in the above theorem, we have for all $A, B \subset \Lambda$ that*

$$\begin{aligned} \frac{\partial}{\partial J_A^1} \left\langle \prod_{x \in B} S_x^1 \right\rangle &\geq 0; \\ \frac{\partial}{\partial J_A^1} \left\langle \prod_{x \in B} S_x^2 \right\rangle &\leq 0. \end{aligned}$$

The first inequality states that correlations increase when the coupling constants increase (in the same spin direction). The second inequality is perhaps best understood classically; if the first component of the spins increases, the other components must decrease because

the total spin is conserved. Corollary 4.1.2 follows immediately from Theorem 4.1.1 since

$$\frac{1}{\beta} \frac{\partial}{\partial J_A^i} \left\langle \prod_{x \in B} S_x^j \right\rangle = \int_0^1 \left[\left\langle \prod_{x \in B} S_x^j; \prod_{x \in A} S_x^i \right\rangle_s - \left\langle \prod_{x \in B} S_x^j \right\rangle \left\langle \prod_{x \in A} S_x^i \right\rangle \right] ds. \quad (4.1.5)$$

We use this corollary in Section 4.2 to give a partial construction of infinite-volume Gibbs states.

The case of higher spins, $S > \frac{1}{2}$, is much more challenging, but we have obtained an inequality that is valid in the ground state of the $S = 1$ model. Recall that the states $\langle \cdot \rangle$ and $\langle \cdot \rangle_s$, defined in Eqs (4.1.2) and (4.1.4), depend on the inverse temperature β .

Theorem 4.1.3. *Assume that $J_A^i \geq 0$ for all $A \subset \Lambda$ and all $i \in \{1, 2\}$. Assume also that $S = 1$. Then for all $A, B \subset \Lambda$, and all $s \in [0, 1]$, we have*

$$\begin{aligned} \lim_{\beta \rightarrow \infty} \left[\left\langle \prod_{x \in A} S_x^1; \prod_{x \in B} S_x^1 \right\rangle_s - \left\langle \prod_{x \in A} S_x^1 \right\rangle \left\langle \prod_{x \in B} S_x^1 \right\rangle \right] &\geq 0; \\ \lim_{\beta \rightarrow \infty} \left[\left\langle \prod_{x \in A} S_x^1; \prod_{x \in B} S_x^2 \right\rangle_s - \left\langle \prod_{x \in A} S_x^1 \right\rangle \left\langle \prod_{x \in B} S_x^2 \right\rangle \right] &\leq 0. \end{aligned}$$

The proof of this theorem can be found in Section 4.4. It uses Theorem 4.1.1.

4.2 Infinite volume limit of correlation functions

Infinite volume limits of Gibbs states are notoriously delicate issues; we show in this section that Theorem 4.1.1 (and Corollary 4.1.2) give partial but useful information: For Gibbs states “with + boundary conditions”, the infinite volume limits of many correlation functions exist.

Let us recall the notion of infinite volume limit. Let $(t_\Lambda)_{\Lambda \subset \subset \mathbb{Z}^d}$ be a sequence of real or complex numbers, indexed by finite subsets of \mathbb{Z}^d . We say that $t_\Lambda \rightarrow t$ as $\Lambda \nearrow \mathbb{Z}^d$ if

$$\lim_{n \rightarrow \infty} t_{\Lambda_n} = t \quad (4.2.1)$$

along every sequence (Λ_n) of increasing finite subsets that tends to \mathbb{Z}^d . That is, the sequence satisfies $\Lambda_{n+1} \supset \Lambda_n$, and, for any finite $A \subset \subset \mathbb{Z}^d$, there exists n_A such that $\Lambda_n \supset A$ for all $n \geq n_A$.

We assume the interaction is finite-range: There exists R such that $J_A^i = 0$ whenever

$\text{diam } A > R$. Let Λ_R denote the enlarged domain

$$\Lambda_R = \{x \in \mathbb{Z}^d : \text{dist}(x, \Lambda) \leq R\}. \quad (4.2.2)$$

Let $\partial_R \Lambda = \Lambda_R \setminus \Lambda$ be the exterior boundary of Λ . We consider the Hamiltonian $H_{\Lambda_R}^\eta$ with field on the exterior boundary:

$$H_{\Lambda_R}^\eta = - \sum_{A \subset \Lambda_R} \left(J_A^1 \prod_{x \in A} S_x^1 + J_A^2 \prod_{x \in A} S_x^2 \right) - \eta \sum_{x \in \partial_R \Lambda} S_x^1. \quad (4.2.3)$$

Temperature does not play a rôle in this section so we set $\beta = 1$. The relevant (finite volume) Gibbs state is the linear functional that, to any operator a on \mathcal{H}_Λ , assigns the value

$$\langle a \rangle_\Lambda^{(+)} = \lim_{\eta \rightarrow \infty} \frac{\text{Tr } a e^{-H_{\Lambda_R}^\eta}}{\text{Tr } e^{-H_{\Lambda_R}^\eta}}. \quad (4.2.4)$$

Traces are taken in \mathcal{H}_{Λ_R} (and a on \mathcal{H}_Λ is identified with $a \otimes \mathbb{1}_{\partial_R \Lambda}$ on \mathcal{H}_{Λ_R}). We comment below on the relevance of this definition for Gibbs states. But first, we observe that the limit $\eta \rightarrow \infty$ exists.

Proposition 4.2.1. *For all operators a on \mathcal{H}_Λ , the limit in (4.2.4) exists and is equal to*

$$\langle a \rangle_\Lambda^{(+)} = \frac{\text{Tr } a e^{-H_\Lambda^{(+)}}}{\text{Tr } e^{-H_\Lambda^{(+)}}},$$

where traces are taken in \mathcal{H}_Λ and

$$H_\Lambda^{(+)} = - \sum_{A \subset \Lambda} \left(J_A^1 \prod_{x \in A} S_x^1 + J_A^2 \prod_{x \in A} S_x^2 \right) - \sum_{\substack{A \subset \Lambda_R \\ A \cap \partial_R \Lambda \neq \emptyset}} 2^{-|A \cap \partial_R \Lambda|} J_A^1 \prod_{x \in A \cap \Lambda} S_x^1.$$

Proof. We can add a convenient constant to the Hamiltonian without changing the corresponding Gibbs state, so we consider

$$\text{Tr } a \exp \left\{ \sum_{A \subset \Lambda_R} \left(J_A^1 \prod_{x \in A} S_x^1 + J_A^2 \prod_{x \in A} S_x^2 \right) + \eta \sum_{x \in \partial_R \Lambda} \left(S_x^1 - \frac{1}{2} \right) \right\}. \quad (4.2.5)$$

We have

$$\lim_{\eta \rightarrow \infty} e^{\eta(S_x^1 - \frac{1}{2})} = P_x^+, \quad (4.2.6)$$

where P_x^+ is the projector onto the eigenstates of S_x^1 with eigenvalue $\frac{1}{2}$. Writing $P_A^+ =$

$\prod_{x \in A} P_x^+$, we have

$$\begin{aligned} P_{\partial_R \Lambda}^+ \left(\prod_{x \in A} S_x^1 \right) P_{\partial_R \Lambda}^+ &= 2^{-|A \cap \partial_R \Lambda|} \left(\prod_{x \in A \cap \Lambda} S_x^1 \right) P_{\partial_R \Lambda}^+, \\ P_{\partial_R \Lambda}^+ \left(\prod_{x \in A} S_x^2 \right) P_{\partial_R \Lambda}^+ &= 0 \quad \text{if } A \cap \partial_R \Lambda \neq \emptyset. \end{aligned} \quad (4.2.7)$$

Then, since the Trotter expansion converges uniformly in η , we have

$$\begin{aligned} &\lim_{\eta \rightarrow \infty} \text{Tr} a \exp \left\{ \sum_{A \subset \Lambda_R} \left(J_A^1 \prod_{x \in A} S_x^1 + J_A^2 \prod_{x \in A} S_x^2 \right) + \eta \sum_{x \in \partial_R \Lambda} \left(S_x^1 - \frac{1}{2} \right) \right\} \\ &= \lim_{n \rightarrow \infty} \lim_{\eta \rightarrow \infty} \text{Tr} a \left[\left(1 + \frac{1}{n} \sum_{A \subset \Lambda_R} \left(J_A^1 \prod_{x \in A} S_x^1 + J_A^2 \prod_{x \in A} S_x^2 \right) \right) e^{\frac{1}{n} \eta \sum_{x \in \partial_R \Lambda} \left(S_x^1 - \frac{1}{2} \right)} \right]^n \\ &= \lim_{n \rightarrow \infty} \text{Tr} a \left[1 - \frac{1}{n} H_{\Lambda}^{(+)} \right]^n \\ &= \text{Tr} a e^{-H_{\Lambda}^{(+)}}. \end{aligned} \quad (4.2.8)$$

□

The challenge is to prove that $\langle a \rangle_{\Lambda}^{(+)}$ converges as $\Lambda \nearrow \mathbb{Z}^d$, for any operator a on $\mathcal{H}_{\Lambda'}$ with $\Lambda' \subset \subset \mathbb{Z}^d$ (again, a on $\mathcal{H}_{\Lambda'}$ is identified with $a \otimes \mathbb{1}_{\Lambda \setminus \Lambda'}$ on \mathcal{H}_{Λ} with $\Lambda \supset \Lambda'$). We can use the correlation inequalities to establish the existence of the infinite volume limit for certain operators a .

Theorem 4.2.2. *For every finite $A \subset \subset \mathbb{Z}^d$ and every $i \in \{1, 2\}$, $\langle \prod_{x \in A} S_x^i \rangle_{\Lambda}^{(+)}$ converges as $\Lambda \nearrow \mathbb{Z}^d$.*

Proof. If $\Lambda \subset \Lambda'$, let us define the Hamiltonian

$$H_{\Lambda, \Lambda'_R}^{\eta} = - \sum_{A \subset \Lambda'_R} \left(J_A^1 \prod_{x \in A} S_x^1 + J_A^2 \prod_{x \in A} S_x^2 \right) - \eta \sum_{x \in \Lambda'_R \setminus \Lambda} S_x^1. \quad (4.2.9)$$

Adapting the proof of Proposition 4.2.1, we can check that we have, for all operators on \mathcal{H}_{Λ} ,

$$\langle a \rangle_{\Lambda}^{(+)} = \lim_{\eta \rightarrow \infty} \frac{\text{Tr} a e^{-H_{\Lambda, \Lambda'_R}^{\eta}}}{\text{Tr} e^{-H_{\Lambda, \Lambda'_R}^{\eta}}}, \quad (4.2.10)$$

where traces are taken in $\mathcal{H}_{\Lambda'_R}$. Corollary 4.1.2 implies that

$$\frac{\text{Tr} \left(\prod_{x \in A} S_x^1 \right) e^{-H_{\Lambda, \Lambda'_R}^{\eta}}}{\text{Tr} e^{-H_{\Lambda, \Lambda'_R}^{\eta}}} \geq \frac{\text{Tr} \left(\prod_{x \in A} S_x^1 \right) e^{-H_{\Lambda'_R}^{\eta}}}{\text{Tr} e^{-H_{\Lambda'_R}^{\eta}}}; \quad (4.2.11)$$

the opposite inequality holds when $\prod S_x^1$ is replaced by $\prod S_x^2$. Thus $\langle \prod_{x \in A} S_x^i \rangle_{\Lambda}^{(+)}$ is mono-

tone decreasing for $i = 1$, and monotone increasing for $i = 2$. It is also bounded, so it converges. \square

Finally, let us comment on the relevance of this Gibbs state with + boundary conditions. Consider the case of the isotropic XY model, where $J_A^1 = J_A^2$ for all $A \subset \subset \mathbb{Z}^d$. At low temperatures, the infinite volume state $\langle \cdot \rangle^{(+)} = \lim_{\Lambda \nearrow \mathbb{Z}^d} \langle \cdot \rangle_{\Lambda}^{(+)}$ is expected to be extremal and to describe a system with spontaneous magnetisation in the direction 1 of the spins. One can apply rotations in the 1-2 plane to get all other (translation-invariant) extremal Gibbs states. Much work remains to be done to make this rigorous, but Theorem 4.2.2 seems to be a useful step.

4.3 The case $S = \frac{1}{2}$

We can define the spin operators as $S^i = \frac{1}{2}\sigma^i$, where the σ^i s are the Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.3.1)$$

It is convenient to work with the Hamiltonian with interactions in the 1-3 spin directions, namely

$$H_{\Lambda} = - \sum_{A \subset \Lambda} \left(J_A^1 \prod_{x \in A} S_x^1 + J_A^3 \prod_{x \in A} S_x^3 \right). \quad (4.3.2)$$

Following Ginibre [48], we introduce the product space $\mathcal{H}_{\Lambda} \otimes \mathcal{H}_{\Lambda}$. Given an operator a on \mathcal{H}_{Λ} , we consider the operators a_+ and a_- on the product space, defined by

$$a_{\pm} = a \otimes \mathbb{1} \pm \mathbb{1} \otimes a. \quad (4.3.3)$$

The Gibbs state in the product space is

$$\langle\langle \cdot \rangle\rangle = \frac{1}{Z(\Lambda)^2} \text{Tr} \cdot e^{-H_{\Lambda,+}}, \quad (4.3.4)$$

where $H_{\Lambda,+} = H_{\Lambda} \otimes \mathbb{1} + \mathbb{1} \otimes H_{\Lambda}$. Without loss of generality, we set $\beta = 1$ in this section. We also need the Schwinger functions in the product space, namely

$$\langle\langle \cdot; \cdot \rangle\rangle_s = \frac{1}{Z(\Lambda)^2} \text{Tr} \cdot e^{-sH_{\Lambda,+}} \cdot e^{-(1-s)H_{\Lambda,+}}. \quad (4.3.5)$$

Lemma 4.3.1. For all observables a, b on \mathcal{H}_Λ , we have

$$\begin{aligned}\langle ab \rangle - \langle a \rangle \langle b \rangle &= \frac{1}{2} \langle\langle a_- b_- \rangle\rangle, \\ \langle a; b \rangle_s - \langle a \rangle \langle b \rangle &= \frac{1}{2} \langle\langle a_-; b_- \rangle\rangle_s.\end{aligned}$$

Proof. It is enough to prove the second line. The right side is equal to

$$\begin{aligned}\langle\langle a_-; b_- \rangle\rangle_s &= \frac{1}{Z(\Lambda)^2} \left[\text{Tr}(a \otimes \mathbb{1}) e^{-sH_{\Lambda,+}} (b \otimes \mathbb{1}) e^{-(1-s)H_{\Lambda,+}} \right. \\ &\quad + \text{Tr}(\mathbb{1} \otimes a) e^{-sH_{\Lambda,+}} (\mathbb{1} \otimes b) e^{-(1-s)H_{\Lambda,+}} \\ &\quad - \text{Tr}(\mathbb{1} \otimes a) e^{-sH_{\Lambda,+}} (b \otimes \mathbb{1}) e^{-(1-s)H_{\Lambda,+}} \\ &\quad \left. - \text{Tr}(a \otimes \mathbb{1}) e^{-sH_{\Lambda,+}} (\mathbb{1} \otimes b) e^{-(1-s)H_{\Lambda,+}} \right].\end{aligned}\tag{4.3.6}$$

The first two lines of the right side give $2\langle a; b \rangle_s$ and the last two lines give $2\langle a \rangle \langle b \rangle$. \square

Next, a simple lemma with a useful formula.

Lemma 4.3.2. For all operators a, b on \mathcal{H}_Λ , we have

$$(ab)_\pm = \frac{1}{2} a_+ b_\pm + \frac{1}{2} a_- b_\mp.$$

The proof is straightforward algebra. Notice that both terms of the right side have *positive* factors. Now comes the key observation that leads to positive (and negative) correlations.

Lemma 4.3.3. There exists an orthonormal basis on $\mathbb{C}^2 \otimes \mathbb{C}^2$ such that $S_+^1, S_-^1, S_+^3, -S_-^3$ have nonnegative matrix elements.

As a consequence, there exists an orthonormal basis of $\mathcal{H}_\Lambda \otimes \mathcal{H}_\Lambda$ such that $S_{x,+}^1, S_{x,-}^1, S_{x,+}^3$, and $-S_{x,-}^3$ have nonnegative matrix elements.

Proof of Lemma 4.3.3. For $\varepsilon_1, \varepsilon_2 = \pm$, let $|\varepsilon_1, \varepsilon_2\rangle$ denote the eigenvectors of $S^3 \otimes \mathbb{1}$ and $\mathbb{1} \otimes S^3$ with respective eigenvalues $\frac{1}{2}\varepsilon_1$ and $\frac{1}{2}\varepsilon_2$. It is well-known that $S^1 \otimes \mathbb{1} |\varepsilon_1, \varepsilon_2\rangle = \frac{1}{2} |-\varepsilon_1, \varepsilon_2\rangle$ and similarly for $\mathbb{1} \otimes S^1$. The convenient basis in $\mathbb{C}^2 \otimes \mathbb{C}^2$ consists of the following four elements:

$$\begin{aligned}p_+ &= \frac{1}{\sqrt{2}}(|++\rangle + |--\rangle), & q_+ &= \frac{1}{\sqrt{2}}(|-+\rangle + |+-\rangle), \\ p_- &= \frac{1}{\sqrt{2}}(|++\rangle - |--\rangle), & q_- &= \frac{1}{\sqrt{2}}(|-+\rangle - |+-\rangle).\end{aligned}\tag{4.3.7}$$

Direct calculations show that

$$\begin{aligned}
(p_+, S_+^1 q_+) &= (q_+, S_+^1 p_+) = 1, \\
(p_-, S_-^1 q_-) &= (q_-, S_-^1 p_-) = 1, \\
(p_+, S_+^3 p_-) &= (p_-, S_+^3 p_+) = 1, \\
(q_+, S_-^3 q_-) &= (q_-, S_-^3 q_+) = -1.
\end{aligned} \tag{4.3.8}$$

All other matrix elements are zero. \square

Proof of Theorem 4.1.1 for $S = \frac{1}{2}$. We use Lemma 4.3.1 in order to get

$$\left\langle \prod_{x \in A} S_x^1; \prod_{x \in B} S_x^1 \right\rangle_s - \left\langle \prod_{x \in A} S_x^1 \right\rangle \left\langle \prod_{x \in B} S_x^1 \right\rangle = \frac{1}{2} \left\langle \left(\prod_{x \in A} S_x^1 \right)_-; \left(\prod_{x \in B} S_x^1 \right)_- \right\rangle_s. \tag{4.3.9}$$

In order to make visible the sign of the right side, we expand the exponentials in Taylor series, so as to get a positive linear combination of terms of the form

$$\text{Tr}_{\mathcal{H}_\Lambda \otimes \mathcal{H}_\Lambda} \left(\prod_{x \in A} S_x^1 \right)_- (-H_{\Lambda,+})^k \left(\prod_{x \in B} S_x^1 \right)_- (-H_{\Lambda,+})^\ell \tag{4.3.10}$$

with $k, \ell \in \mathbb{N}$. Expanding $(-H_{\Lambda,+})^k$ and $(-H_{\Lambda,+})^\ell$, we get a positive linear combination of

$$\text{Tr}_{\mathcal{H}_\Lambda \otimes \mathcal{H}_\Lambda} \left(\prod_{x \in A} S_x^1 \right)_- \prod_{i=1}^k \left(\prod_{x \in A_i} S_x^{\varepsilon_i} \right)_+ \left(\prod_{x \in B} S_x^1 \right)_- \prod_{j=1}^\ell \left(\prod_{x \in A'_j} S_x^{\varepsilon'_j} \right)_+ \tag{4.3.11}$$

with $\varepsilon_i, \varepsilon'_j \in \{1, 3\}$. Further, all products $(\prod S_x^i)_\pm$ can be expanded using Lemma 4.3.2 in polynomials of $S_{x,\pm}^i$, still with positive coefficients. Finally, observe that the total number of operators $S_{x,-}^3$, $x \in \Lambda$, is always even; then each $S_{x,-}^3$ can be replaced by $-S_{x,-}^3$. We now have the trace of a polynomial, with positive coefficients, of matrices with nonnegative elements (by Lemma 4.3.3). This is positive.

The second inequality (with S^3 instead of S^2) is similar. The only difference is that $(\prod S_x^3)_-$ gives a polynomial where the number of $S_{x,-}^3$ is odd. Hence the negative sign. \square

4.4 The case $S = 1$

This section is much more involved, and our result is sadly restricted to the ground state. Our strategy is inspired by the work of Nachtergaele on graphical representations of the Heisenberg model with large spins [81]. We consider a system where each site hosts a

pair of spin $\frac{1}{2}$ particles. The inequalities of Theorem 4.1.1 apply. By projecting onto the triplet subspaces, one gets a correspondence with the original spin 1 system. We prove that all ground states of the new model lie in the triplet subspace, so the inequality can be transferred. These steps are detailed in the rest of the section.

It is perhaps worth noticing that the tensor products in this section play a different rôle than those in Section 4.3.

4.4.1 The new model

We introduce the new lattice $\tilde{\Lambda} = \Lambda \times \{1, 2\}$. The new Hilbert space is

$$\tilde{\mathcal{H}}_{\Lambda} = \otimes_{x \in \Lambda} (\mathbb{C}^2 \otimes \mathbb{C}^2) \simeq \otimes_{x \in \tilde{\Lambda}} \mathbb{C}^2. \quad (4.4.1)$$

Let R^i be the following operator on $\mathbb{C}^2 \otimes \mathbb{C}^2$:

$$R^i = \frac{1}{2}(\sigma^i \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^i). \quad (4.4.2)$$

Here, σ^i are the Pauli matrices in \mathbb{C}^2 as before. We denote $R_x^i = R^i \otimes \mathbb{1}_{\Lambda \setminus \{x\}}$ the corresponding operator at site $x \in \Lambda$. As before, we choose the interactions to be in the 1-3 spin directions; the Hamiltonian on $\tilde{\mathcal{H}}_{\Lambda}$ is

$$\tilde{H}_{\Lambda} = - \sum_{A \subset \Lambda} \left(J_A^1 \prod_{x \in A} R_x^1 + J_A^3 \prod_{x \in A} R_x^3 \right). \quad (4.4.3)$$

The coupling constants J_A^i are the same as those of the original model on \mathcal{H}_{Λ} . The expected value of an observable a in the Gibbs state with Hamiltonian \tilde{H}_{Λ} is

$$\langle a \rangle^{\sim} = \frac{1}{\tilde{Z}(\Lambda)} \text{Tr } a e^{-\beta \tilde{H}_{\Lambda}}, \quad (4.4.4)$$

where the normalisation $\tilde{Z}(\Lambda)$ is the partition function

$$\tilde{Z}(\Lambda) = \text{Tr } e^{-\beta \tilde{H}_{\Lambda}}. \quad (4.4.5)$$

We similarly define Schwinger functions $\langle \cdot; \cdot \rangle_s^{\sim}$ for $s \in [0, 1]$.

It is useful to rewrite \tilde{H}_{Λ} as the Hamiltonian of spin $\frac{1}{2}$ particles on the extended lattice $\tilde{\Lambda}$. Given a subset $X \subset \tilde{\Lambda}$, we denote $\text{supp}X$ its natural projection onto Λ , i.e.

$$\text{supp}X = \{x \in \Lambda : (x, 1) \in X \text{ or } (x, 2) \in X\}. \quad (4.4.6)$$

We also denote $D(\tilde{\Lambda})$ the family of subsets of $\tilde{\Lambda}$ where each site of Λ appears at most once. Notice that $|D(\tilde{\Lambda})| = 3^{|\Lambda|}$. Finally, let us introduce the coupling constants

$$\tilde{J}_X^i = \begin{cases} 2^{-|X|} J_{\text{supp}X}^i & \text{if } X \in D(\tilde{\Lambda}), \\ 0 & \text{otherwise.} \end{cases} \quad (4.4.7)$$

From these definitions, we can write \tilde{H}_Λ using Pauli operators as

$$\tilde{H}_\Lambda = - \sum_{X \subset \tilde{\Lambda}} \left(\tilde{J}_X^1 \prod_{x \in X} \sigma_x^1 + \tilde{J}_X^3 \prod_{x \in X} \sigma_x^3 \right). \quad (4.4.8)$$

4.4.2 Correspondence with the spin 1 model

The Hilbert space at a given site, $\mathbb{C}^2 \otimes \mathbb{C}^2$, is the orthogonal sum of the triplet subspace (that is, the symmetric subspace, which is of dimension 3) and of the singlet subspace (of dimension 1). Let P^{triplet} denote the projector onto the triplet subspace, and let $P_\Lambda^{\text{triplet}} = \otimes_{x \in \Lambda} P^{\text{triplet}}$. We define a new Gibbs state, namely

$$\langle a \rangle' = \frac{1}{Z'(\Lambda)} \text{Tr } a P_\Lambda^{\text{triplet}} e^{-\beta \tilde{H}_\Lambda}, \quad (4.4.9)$$

with partition function $Z'(\Lambda) = \text{Tr } P_\Lambda^{\text{triplet}} e^{-\beta \tilde{H}_\Lambda}$. In order to state the correspondence between the models with different spins, let $V : \mathbb{C}^3 \rightarrow \mathbb{C}^2 \otimes \mathbb{C}^2$ denote an isometry such that

$$\begin{aligned} V^* V &= \mathbb{1}_{\mathbb{C}^3}, \\ V V^* &= P^{\text{triplet}}, \end{aligned} \quad (4.4.10)$$

One can check that $S^i = V^* R^i V$, $i = 1, 2, 3$, give spin operators in \mathbb{C}^3 . Let $V_\Lambda = \otimes_{x \in \Lambda} V$. For all observables on $a \in \mathcal{H}_\Lambda$, we have the identity

$$\langle a \rangle = \langle V_\Lambda a V_\Lambda^* \rangle'. \quad (4.4.11)$$

4.4.3 All ground states lie in the triplet subspace

Let $Q_{\Lambda,A}$ be the projector onto triplets on A , and singlet on $\Lambda \setminus A$:

$$Q_{\Lambda,A} = \left(\otimes_{x \in A} P^{\text{triplet}} \right) \otimes \left(\otimes_{x \in \Lambda \setminus A} (1 - P^{\text{triplet}}) \right). \quad (4.4.12)$$

One can check that $[R_x^i, Q_{\Lambda, A}] = 0$ for all $i = 1, 2, 3$, all $x \in \Lambda$, and all $A \subset \Lambda$. Further, since the operators R^i give zero when applied on singlets, we have

$$Q_{\Lambda, A} \tilde{H}_\Lambda = -Q_{\Lambda, A} \sum_{B \subset A} \left(J_B^1 \prod_{x \in B} R_x^1 + J_B^3 \prod_{x \in B} R_x^3 \right). \quad (4.4.13)$$

Lemma 4.4.1. *The ground state energy of \tilde{H}_Λ is a strictly decreasing function of $J_{A'}^i$, for all $i = 1, 3$ and all $A \subset \Lambda$.*

It follows from this lemma and Eq. (4.4.13) that all ground states lie in the subspace of $Q_{\Lambda, \Lambda} = P_\Lambda^{\text{triplet}}$. To see this, note that $Q_{\Lambda, A}$ has the effect of setting $J_B^i = 0$ for $B \not\subset A$. Then if $A' \supset A$, $Q_{\Lambda, A'} \tilde{H}_\Lambda$ has larger coupling constants for those B such that $B \not\subset A$ but $B \subset A'$ (other coupling constants are unaffected). Hence having more sites in the triplet subspace leads to strictly lower energy.

Proof of Lemma 4.4.1. We actually prove the result for the hamiltonian (4.4.8) and the couplings \tilde{J}_X^i , which implies the lemma. With $E_0(a)$ denoting the ground state energy of the operator a , we show that

$$E_0\left(\tilde{H}_\Lambda - \varepsilon \prod_{x \in Y} \sigma_x^1\right) < E_0(\tilde{H}_\Lambda), \quad (4.4.14)$$

for any $\varepsilon > 0$, and any $Y \subset \tilde{\Lambda}$. Let ψ_0 denote the ground state of \tilde{H}_Λ . It is also eigenstate of $e^{-\tilde{H}_\Lambda}$ with the largest eigenvalue. Using the Trotter product formula, we have

$$e^{-\tilde{H}_\Lambda} = \lim_{n \rightarrow \infty} \left[\left(1 + \frac{1}{n} \sum_{X \subset \tilde{\Lambda}} \tilde{J}_X^1 \prod_{x \in X} \sigma_x^1 \right) e^{\frac{1}{n} \sum_{X \subset \tilde{\Lambda}} \tilde{J}_X^3 \prod_{x \in X} \sigma_x^3} \right]^n, \quad (4.4.15)$$

which, in the basis where the Pauli matrices are given by (4.3.1), is a product of matrices with nonnegative elements. By a Perron-Frobenius argument, ψ_0 can be chosen as a linear combination of the basis vectors with nonnegative coefficients. Then

$$E_0\left(\tilde{H}_\Lambda - \varepsilon \prod_{x \in Y} \sigma_x^1\right) \leq \left(\psi_0, \left(\tilde{H}_\Lambda - \varepsilon \prod_{x \in Y} \sigma_x^1 \right) \psi_0 \right) = E_0(\tilde{H}_\Lambda) - \varepsilon \left(\psi_0, \left(\prod_{x \in Y} \sigma_x^1 \right) \psi_0 \right). \quad (4.4.16)$$

If $(\psi_0, (\prod_{x \in Y} \sigma_x^1) \psi_0) \neq 0$, then it is positive and the conclusion follows. Otherwise, let $\hat{H}_\Lambda = \tilde{H}_\Lambda - c \mathbb{1}$ with c large enough so that all eigenvalues of \hat{H}_Λ are negative. If $(\psi_0, (\prod_{x \in Y} \sigma_x^1) \psi_0) = 0$, using $(\prod_{x \in Y} \sigma_x^1)^2 = 4^{-|Y|} \mathbb{1}$, we have

$$\left(\psi_0, \left(\hat{H}_\Lambda - \varepsilon \prod_{x \in Y} \sigma_x^1 \right)^2 \psi_0 \right) = E_0(\hat{H}_\Lambda)^2 + (4^{-|Y|} \varepsilon)^2. \quad (4.4.17)$$

This implies that $E_0(\hat{H}_\Lambda - \varepsilon \prod_{x \in Y} \sigma_x^1) < E_0(\hat{H}_\Lambda)$, hence the strict inequality (4.4.14).

One can replace σ_x^1 with σ_x^3 and prove Inequality (4.4.14) in the same fashion; indeed, one can choose a basis where σ^3 is like σ^1 in (4.3.1), and σ^1 is like $-\sigma^3$. \square

4.4.4 Proof of Theorem 4.1.3

We can assume that for any $x \in \Lambda$, there exist $i \in \{1, 3\}$ and $A \ni x$ such that $J_A^i > 0$ — the extension to the general case is straightforward. Since all ground states lie in the triplet subspace, we have for all subsets $A, B \subset \Lambda$ and for all $s \in [0, 1]$,

$$\begin{aligned}
\lim_{\beta \rightarrow \infty} \left\langle \prod_{x \in A} S_x^1; \prod_{x \in B} S_x^1 \right\rangle_s &= 2^{-|A|-|B|} \sum_{\substack{X \in D(\tilde{\Lambda}) \\ \text{supp} X = A}} \sum_{\substack{Y \in D(\tilde{\Lambda}) \\ \text{supp} Y = B}} \lim_{\beta \rightarrow \infty} \left\langle \prod_{x \in X} \sigma_x^1; \prod_{x \in Y} \sigma_x^1 \right\rangle_s^{\sim} \\
&\geq 2^{-|A|-|B|} \sum_{\substack{X \in D(\tilde{\Lambda}) \\ \text{supp} X = A}} \sum_{\substack{Y \in D(\tilde{\Lambda}) \\ \text{supp} Y = B}} \lim_{\beta \rightarrow \infty} \left\langle \prod_{x \in X} \sigma_x^1 \right\rangle^{\sim} \left\langle \prod_{x \in Y} \sigma_x^1 \right\rangle^{\sim} \quad (4.4.18) \\
&= \lim_{\beta \rightarrow \infty} \left\langle \prod_{x \in A} S_x^1 \right\rangle \left\langle \prod_{x \in B} S_x^1 \right\rangle.
\end{aligned}$$

We used Theorem 4.1.1. We have obtained the first inequality of Theorem 4.1.3. The second inequality follows in the same way.

Chapter 5

Long-range order for the spin-1 Heisenberg model with a small antiferromagnetic interaction

This chapter is based on the paper [69]. We look at the general $SU(2)$ invariant spin-1 Heisenberg model and prove nematic order occurs for some values of the model parameters. As we have seen, this family includes the well known Heisenberg ferromagnet and antiferromagnet as well as the interesting nematic (biquadratic) and the largely mysterious staggered-nematic interaction. We use of a type of matrix representation of the interaction making clear several identities that would not otherwise be noticed. This representation can be seen as an adaptation of (2.1.14) to the quantum case. Inspiration is taken from the proof for the classical case [3]. We use the method of reflection positivity in order to obtain an infrared bound, that is, a bound on the Fourier transform of the correlation in question. One can then easily show that the correlation function does not decay if the infrared bound is sufficiently strong. The infrared bound proven in [35] allows to show a phase transition for the antiferromagnet. It is straightforward to extend this result to a model with an antiferromagnetic interaction accompanied by a small nematic (biquadratic) interaction. However when the nematic interaction is too large the result will no longer apply. This chapter follows the approach of [35], starting with the nematic model, obtaining a lower bound that involves some other correlation functions. This bound can be shown to be positive for low temperatures by relating these correlations to probabilities in the random loop model introduced in [2] and presented in Chapter 6. It is then easy to show (due to reflection positivity of the antiferromagnetic interaction) that adding an antiferromagnetic interaction will maintain the positivity of the lower bound, providing the interaction is small enough.

5.1 The spin-1 SU(2)-invariant model

Denote by S^1, S^2 and S^3 the spin-1 matrices. Denote $\mathbf{S} = (S^1, S^2, S^3)$. Consider a pair (Λ_L, \mathcal{E}) of a lattice $\Lambda_L \subset \mathbb{Z}^d$ and a set of edges \mathcal{E} between points in Λ_L . Here we will take

$$\Lambda_L = \left\{ -\frac{L}{2} + 1, \dots, \frac{L}{2} \right\}^d, \quad (5.1.1)$$

for integer L . For the set of edges \mathcal{E} we take nearest-neighbour with periodic boundary conditions. Recall the operators S_x^i for $i = 1, 2, 3$ with $S_x^i \otimes Id_{\Lambda_L \setminus \{x\}}$. The Hamiltonian of interest is the general Spin-1 SU(2)-invariant Hamiltonian with a two-body interaction, it is known that this can be written as

$$H_{\Lambda_L}^{J_1, J_2} = -2 \sum_{\{x, y\} \in \mathcal{E}} \left(J_1 (\mathbf{S}_x \cdot \mathbf{S}_y) + J_2 (\mathbf{S}_x \cdot \mathbf{S}_y)^2 \right). \quad (5.1.2)$$

The phase diagram for this model is only partially understood. If $J_2 = 0$ and $J_1 < 0$ we have the Heisenberg antiferromagnet that is known to undergo a phase transition at low temperatures [35]. As the interaction when $J_2 > 0$ is reflection positive it is also possible to extend this result to $J_2 > 0$ when the ratio J_1/J_2 is sufficiently small. The line $J_1 = 0$ has been shown to exhibit Néel order for low temperatures when $J_2 > 0$ [111], for $J_2 < 0$ there are few rigorous results, it would be a challenging task to obtain results. The line $J_2 = J_1/3 < 0$ is the AKLT model [1].

The main result of this chapter is to show that there is a phase transition in this model for $J_2 > 0$ and $J_1 < 0$ with $|J_1|$ sufficiently small compared to $|J_2|$, the statement will be made precise below.

First we define the partition function and Gibbs states of our model as

$$Z_{\beta, \Lambda_L}^{J_1, J_2} = \text{Tr} e^{-\beta H_{\Lambda_L}^{J_1, J_2}}, \quad (5.1.3)$$

$$\langle \cdot \rangle_{\beta, \Lambda_L}^{J_1, J_2} = \frac{1}{Z_{\beta, \Lambda_L}^{J_1, J_2}} \text{Tr} \cdot e^{-\beta H_{\Lambda_L}^{J_1, J_2}}, \quad (5.1.4)$$

where $\beta > 0$ is the inverse temperature. The quantity of interest is then the correlation

$$\rho(x) = \left\langle \left((S_0^3)^2 - \frac{2}{3} \right) \left((S_x^3)^2 - \frac{2}{3} \right) \right\rangle_{\beta, \Lambda_L}^{J_1, J_2}. \quad (5.1.5)$$

This correlation is specifically of interest for spin-1, in general spin- S $\frac{2}{3}$ will be replaced with $\frac{1}{3}S(S+1)$. The result is then given by the following theorem.

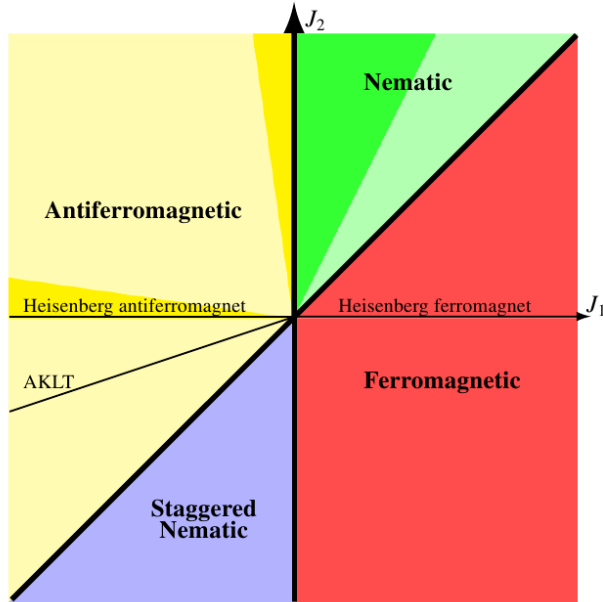


Figure 5.1: The phase diagram for the general SU(2) invariant spin-1 model. Some regions have rigorous proofs that the expected order is indeed correct. The line $J_1 < 0, J_2 = 0$ is the Heisenberg antiferromagnet where antiferromagnetic order has been proven [35], this region extends slightly into the dark yellow region. Increasing the size of this dark yellow region will be the focus of Section 6.2.6 The dark green region has nematic order at low temperatures [111], with Néel order on the line $J_2 > 0, J_1 = 0$, the adjacent dark yellow region also has long range order, however only the nematic correlation function has been shown not to decay, antiferromagnetic order is expected here but is not yet proved.

Theorem 5.1.1. *Let $S = 1, J_2 > 0, L$ be even and $d \geq 5$. Then there exists $J_1^0 < 0, \beta_0$ and $C = C(\beta, J_1) > 0$ such that if $J_1^0 < J_1 \leq 0$ and $\beta > \beta_0$ then*

$$\frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \rho(x) \geq C.$$

for all L large enough.

The proof of the result will be in two steps, first the result will be proved for $J_1 = 0$, this will be the content of the next section. Second it will be shown how the result for $J_1 = 0$ extends to sufficiently small $J_1 < 0$, this should come as no surprise as the interaction is reflection positive for $J_1 < 0$ hence adding a small interaction in this direction should not alter the result too much.

5.2 The model $J_2 > 0, J_1 = 0$

We will now consider the so-called quantum nematic model $J_2 > 0, J_1 = 0$, the aim is to prove long-range order for this model using a similar approach to the proofs in [35, 41, 42, 43]. To do this we will use a representation that is an analogue of the matrix representation used in [3]. Care must be taken as now we are working with matrices rather than vectors and so commutativity becomes an issue. We introduce an external field, \mathbf{h} , to the Hamiltonian

$$H_{\Lambda_L, \mathbf{h}}^{0,1} = -2 \sum_{\{x,y\} \in \mathcal{E}} (\mathbf{S}_x \cdot \mathbf{S}_y)^2 - \sum_{x \in \Lambda_L} h_x \left((S_x^3)^2 - \frac{1}{3} S(S+1) \mathbb{1} \right). \quad (5.2.1)$$

Here $\mathbb{1}$ is the identity matrix. Equilibrium states are given by

$$\langle A \rangle_{\beta, \Lambda_L, \mathbf{h}}^{0,1} = \frac{1}{Z_{\beta, \Lambda_L, \mathbf{h}}^{0,1}} \text{Tr} A e^{-\beta H_{\Lambda_L, \mathbf{h}}^{0,1}}. \quad (5.2.2)$$

Note that the J_2 has been absorbed into the parameter β . Using the direct analogue of [3] will not work here, the reason is that reflection positivity will fail as $\overline{S^2} = -S^2$. We will instead use a matrix representation of a Hamiltonian that is unitarily equivalent to (5.2.1). From now on we will work with the following Hamiltonian

$$H_{\Lambda_L, \mathbf{h}}^U = -2 \sum_{\{x,y\} \in \mathcal{E}} (S_x^1 S_y^1 - S_x^2 S_y^2 + S_x^3 S_y^3)^2 - \sum_{x \in \Lambda_L} h_x \left((S_x^3)^2 - \frac{1}{3} S(S+1) \mathbb{1} \right), \quad (5.2.3)$$

and partition function

$$Z_{\Lambda_L, \beta, \mathbf{h}}^U = \text{Tr} e^{-\beta H_{\Lambda_L, \mathbf{h}}^U}. \quad (5.2.4)$$

Similarly to before, equilibrium states are given by

$$\langle A \rangle_{\Lambda_L, \beta, \mathbf{h}}^U = \frac{1}{Z_{\Lambda_L, \beta, \mathbf{h}}^U} \text{Tr} A e^{-\beta H_{\Lambda_L, \mathbf{h}}^U}. \quad (5.2.5)$$

As Λ_L has a bipartite structure, $\Lambda_L = \Lambda_e \cup \Lambda_o$ where Λ_e, Λ_o are the even and odd sublattices, respectively. We define $U = \prod_{x \in \Lambda_e} e^{i\pi S_x^2}$ we have

$$U^{-1} H_{\Lambda_L, \mathbf{h}}^U U = H_{\Lambda_L, \mathbf{h}}^{0,1}. \quad (5.2.6)$$

Note that this leaves $\rho(x)$ unchanged. Before the theorem we introduce integrals,

$$I_d = \frac{1}{(2\pi)^d} \int_{[-\pi, \pi]^d} \sqrt{\frac{\varepsilon(k + \pi)}{\varepsilon(k)}} \left(\frac{1}{d} \sum_{i=1}^d \cos k_i \right)_+ dk, \quad (5.2.7)$$

$$J_d = \frac{1}{(2\pi)^d} \int_{[-\pi, \pi]^d} \frac{1}{\varepsilon(k)} dk \quad (5.2.8)$$

where

$$\varepsilon(k) = 2 \sum_{i=1}^d (1 - \cos k_i). \quad (5.2.9)$$

We have $I_d < \infty$ for $d \geq 3$ and it can be shown that $I_d \rightarrow 0$ as $d \rightarrow \infty$ [58]. We have the following result:

Theorem 5.2.1. *Let $S = 1$. Assume $\mathbf{h} = 0$ and L is even with $d \geq 3$. Then we have the bound*

$$\liminf_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \rho(x) \geq \liminf_{L \rightarrow \infty} \left(\rho(e_1) - I_d \sqrt{\langle S_0^1 S_0^3 S_{e_1}^1 S_{e_1}^3 \rangle_{\Lambda_L, \beta, \mathbf{0}}^U} - \frac{1}{2\beta} J_d \right). \quad (5.2.10)$$

If this lower bound is strictly positive it implies a phase transition, note that the lower bound is valid in any dimension $d \geq 3$, in $d \leq 2$ J_d is not finite, hence no phase transition. This is consistent with the well known Mermin-Wagner theorem [78]. Using the loop model introduced in [2] and extended in [111] we can relate the expectations in the lower bound to the probability of the event E_{0, e_1} , that two nearest neighbours are in the same loop as

$$\rho(e_1) = \frac{2}{9} \mathbb{P}[E_{0, e_1}], \quad \langle S_0^1 S_0^3 S_{e_1}^1 S_{e_1}^3 \rangle_{\Lambda_L, \beta, \mathbf{h}}^U = \frac{1}{3} \mathbb{P}[E_{0, e_1}]. \quad (5.2.11)$$

So we can write the lower bound as $\sqrt{\mathbb{P}[E_{0, e_1}]} \left(\frac{2}{9} \sqrt{\mathbb{P}[E_{0, e_1}]} - \frac{I_d}{\sqrt{3}} \right) - \frac{1}{2\beta} J_d$. This means a sufficiently large lower bound on $\mathbb{P}[E_{0, e_1}]$ will allow to show the lower bound is positive in high enough dimension for β large. Note that the dependence on β is hidden in \mathbb{P} , we shall see the dependence in Chapter 6.

Proposition 5.2.2. *For $d \geq 1$, $S = 1$ and L even. In the limit $\beta \rightarrow \infty$ we have the lower bound*

$$\mathbb{P}[E_{0, e_1}] \geq \frac{2}{5}. \quad (5.2.12)$$

Putting this bound into the theorem and computing I_d for various d shows that there is a positive lower bound (and hence phase transition) for $d \geq 5$ if β is large enough ((5.2.12) will be weaker for $\beta < \infty$ but we will have a lower bound $\frac{2}{5} - o(\beta)$).

Proof. For any state $\psi \in \otimes_{x \in \Lambda_L} \mathbb{C}^3$ we have that in the ground state

$$\lim_{\beta \rightarrow \infty} \langle H_{\Lambda_L}^{0,1} \rangle_{\Lambda_L, \beta} \leq \langle \psi, H_{\Lambda_L, \mathbf{0}}^{0,1} \psi \rangle. \quad (5.2.13)$$

We pick the Néel state, $\psi_{Néel}$, as a trial state

$$\psi_{Néel} = \otimes_{x \in \Lambda_L} |(-1)^x\rangle. \quad (5.2.14)$$

We have used Dirac notation here where $S^3|a\rangle = a|a\rangle$. For the left of (5.2.13) we recall that for x and y nearest neighbours $(\mathbf{S}_x \cdot \mathbf{S}_y)^2$ has three terms of the form $(S_x^i)^2(S_y^i)^2$, having expectation $\frac{2}{9}\mathbb{P}[E_{0,e_1}] + \frac{4}{9}$ independent of i , three terms of the form $S_x^i S_x^j S_y^i S_y^j$ having expectation $\frac{1}{3}\mathbb{P}[E_{0,e_1}]$ independent of i and j (this is due to the equivalent roles of i and j coupled with $(S_x^i S_x^j)^T = \pm S_x^j S_x^i$ where the sign depends on the value of i or j) and finally three terms of the form $S_x^i S_x^j S_y^j S_y^i$ having zero expectation. This gives

$$\lim_{\beta \rightarrow \infty} \langle H_{\Lambda_L}^{0,1} \rangle_{\Lambda_L, \beta} = -2 \sum_{\{x,y\} \in \Lambda_L} \left[\frac{2}{3}\mathbb{P}[E_{0,e_1}] + \frac{4}{3} + \mathbb{P}[E_{0,e_1}] \right] = -2d|\Lambda_L| \frac{5\mathbb{P}[E_{0,e_1}] + 4}{3}. \quad (5.2.15)$$

For the right side of (5.2.13) it can be checked that, for $S = 1$, $(\mathbf{S}_x \cdot \mathbf{S}_y)^2 = P_{xy} + 1$ where $\frac{1}{3}P_{xy}$ is the projector onto the spin singlet. Hence

$$\langle 1, -1 | (\mathbf{S}_x \cdot \mathbf{S}_y)^2 | 1, -1 \rangle = \langle 1, -1 | P_{xy} + 1 | 1, -1 \rangle = 2, \quad (5.2.16)$$

from this we see that the right side of (5.2.13) is $-4d|\Lambda_L|$. Inserting each of these values into (5.2.13) and rearranging gives the claim of the proposition. \square

Note that if one could find a state with lower energy than the Néel state this lower bound could be improved and hence potentially the theorem strengthened to show phase transitions in lower dimensions. However the problem of finding lower energy states does not appear an easy one.

The rest of the section will be dedicated to the proof of Theorem 5.2.1. We will proceed with calculations for general spin until it becomes necessary to restrict to the case $S = 1$. Fortunately for this Hamiltonian we can find a matrix representation. Define Q_x as

$$Q_x = \begin{pmatrix} (S_x^1)^2 - \frac{1}{3}S(S+1) & S_x^1 i S_x^2 & S_x^1 S_x^3 \\ S_x^1 i S_x^2 & (S_x^2)^2 - \frac{1}{3}S(S+1) & i S_x^2 S_x^3 \\ S_x^1 S_x^3 & i S_x^2 S_x^3 & (S_x^3)^2 - \frac{1}{3}S(S+1) \end{pmatrix}. \quad (5.2.17)$$

We introduce the operation \mathcal{TR} , which is the sum of diagonal entries of matrices of the

form of Q_x , however this ‘trace’ will return an operator, not a number, so we distinguish it from the normal trace. As an example we see that $\mathcal{TR}(Q_x) = 0$, the zero matrix. We have the relation (note that below we do *not* mean ‘normal’ matrix multiplication, we only write $Q_x Q_y$ for convenience as explained in the remark).

$$\mathcal{TR}(Q_x Q_y) = (S_x^1 S_y^1 - S_x^2 S_y^2 + S_x^3 S_y^3)^2 - \frac{1}{3} S^2 (S + 1)^2 \mathbb{1}. \quad (5.2.18)$$

Remark 5.2.3. *We must be careful here, as we are working with a matrix of matrices, as to what we mean by multiplication. The representation (5.2.17) is not at all essential to the proof, the advantage of using it is that once (5.2.18) has been verified other relations can be stated much more concisely and clearly and easily checked, these relations are not at all obvious or easy to come up with without using (5.2.18).*

By the product $Q_x Q_y$ we follow the ‘normal’ matrix multiplication with the added stipulation that for the i^{th} diagonal entry of $Q_x Q_y$ the operator S^i will appear first. For example in entry $\{1, 1\}$ of $Q_x Q_y$ there is the term $S_x^1 i S_x^2 S_y^1 i S_y^2$, in the entry $\{2, 2\}$ this term will become $i S_x^2 S_x^1 i S_y^2 S_y^1$, this ensures that we have each of the cross terms in the right-hand side of (5.2.18). For off-diagonal entries we are not concerned as we are always taking a ‘trace’.

In the case $x \neq y$ less care is needed as components of \mathbf{S}_x and \mathbf{S}_y commute (in fact $\mathcal{TR} Q_x Q_y = \mathcal{TR} Q_y Q_x$, hence we must only take care that the product order of components of spin at the same site is maintained).

We also have that $\mathcal{TR} Q_x^2 = C_x^S - \frac{1}{3} S^2 (S + 1)^2$ acting on \mathcal{H}_x . In $S = 1$

$$C_x^1 = \begin{pmatrix} 2 & 0 & 2 \\ 0 & 0 & 0 \\ 2 & 0 & 2 \end{pmatrix}_x. \quad (5.2.19)$$

Using this we can represent our interaction as

$$(S_x^1 S_y^1 - S_x^2 S_y^2 + S_x^3 S_y^3)^2 = \frac{1}{2} (C_x^S + C_y^S - \mathcal{TR} [(Q_x - Q_y)^2]). \quad (5.2.20)$$

We introduce the field v on Λ_L with value $v_x \in \mathbb{R}$ at the site $x \in \Lambda_L$. We denote by \mathbf{v} the field of 3×3 matrices on Λ_L such that each \mathbf{v}_x has one non-zero entry, the entry $\{3, 3\}$ being $v_x \in \mathbb{R}$. We define

$$H(v) = \sum_{\{x,y\} \in \mathcal{E}} (\mathcal{TR} [(Q_x - Q_y)^2] - C_x^S - C_y^S) - \sum_{x \in \Lambda_L} (\Delta v)_x \left((S_x^3)^2 - \frac{1}{3} S(S + 1) \right), \quad (5.2.21)$$

$$Z(v) = \text{Tr} e^{-\beta H(v)}. \quad (5.2.22)$$

Note that from (5.2.20) $H(v) = H_{\Lambda_L, \Delta v}^U$. Here we have used the lattice Laplacian and below we use the inner product $(f, g) = \sum_{x \in \Lambda_L} f_x g_x$ with the identity $(f, -\Delta g) = \sum_{\{x, y\} \in \mathcal{E}} (f_x - f_y)(g_x - g_y)$. Then we can calculate as follows:

$$\begin{aligned} H(v) &= \sum_{\{x, y\} \in \mathcal{E}} \left\{ \mathcal{TR} \left[\left(Q_x + \frac{\mathbf{v}_x}{2} - Q_y - \frac{\mathbf{v}_y}{2} \right)^2 \right] - \mathcal{TR} \left[(Q_x - Q_y)(\mathbf{v}_x - \mathbf{v}_y) \right] \right. \\ &\quad \left. - C_x^S - C_y^S + (v_x - v_y) \left((S_x^3)^2 - (S_y^3)^2 \right) - \frac{1}{4} (v_x - v_y)^2 \right\} \quad (5.2.23) \\ &= \sum_{\{x, y\} \in \mathcal{E}} \left\{ \mathcal{TR} \left[\left(Q_x + \frac{\mathbf{v}_x}{2} - Q_y - \frac{\mathbf{v}_y}{2} \right)^2 \right] - C_x^S - C_y^S \right\} - \frac{1}{4} (v, -\Delta v). \end{aligned}$$

We must check carefully when dealing with the cross terms $(Q_x - Q_y)(\mathbf{v}_x - \mathbf{v}_y)$ and $(\mathbf{v}_x - \mathbf{v}_y)(Q_x - Q_y)$, they are not equal but $\mathcal{TR}(Q_x - Q_y)(\mathbf{v}_x - \mathbf{v}_y) = \mathcal{TR}(\mathbf{v}_x - \mathbf{v}_y)(Q_x - Q_y)$, so the calculation is correct. From this it makes sense to define the following Hamiltonian and partition function:

$$H'(v) = H(v) + \frac{1}{4} (v, -\Delta v), \quad (5.2.24)$$

$$Z'(v) = \text{Tr} e^{-\beta H'(v)}. \quad (5.2.25)$$

Now the property of Gaussian Domination is

$$Z(v) \leq Z(0) e^{\frac{\beta}{4} (v, -\Delta v)} \iff Z'(v) \leq Z'(0), \quad (5.2.26)$$

as in the classical case it follows from reflection positivity. The proof of the following reflection positivity lemma follows from Trotter's formula. As in the classical case, reflection positivity is a very powerful tool, for more information see [13, 14, 16, 35, 39, 41, 42, 43, 109, 111, 112].

Lemma 5.2.4. *Let $\mathcal{H} = h \otimes h$, $\dim h < \infty$, fix a basis. Let A, B, C_i, D_i for $i = 1, \dots, k$ be matrices in h , then*

$$\begin{aligned} &\left| \text{Tr}_{\mathcal{H}} \exp \left\{ A \otimes \mathbb{1} + \mathbb{1} \otimes B - \sum_{i=1}^k (C_i \otimes \mathbb{1} - \mathbb{1} \otimes D_i)^2 \right\} \right|^2 \\ &\leq \text{Tr}_{\mathcal{H}} \exp \left\{ A \otimes \mathbb{1} + \mathbb{1} \otimes \bar{A} - \sum_{i=1}^k (C_i \otimes \mathbb{1} - \mathbb{1} \otimes \bar{C}_i)^2 \right\} \quad (5.2.27) \\ &\quad \times \text{Tr}_{\mathcal{H}} \exp \left\{ \bar{B} \otimes \mathbb{1} + \mathbb{1} \otimes B - \sum_{i=1}^k (\bar{D}_i \otimes \mathbb{1} - \mathbb{1} \otimes D_i)^2 \right\} \end{aligned}$$

where \bar{A} is the complex conjugate of A .

Before we prove reflection positivity for our partition function we should calculate the trace in $Z'(v)$, recall how we have defined our multiplication.

$$\begin{aligned} \mathcal{TR} \left[\left(Q_x + \frac{\mathbf{v}_x}{2} - Q_y - \frac{\mathbf{v}_y}{2} \right)^2 \right] &= \left((S_x^1)^2 - (S_y^1)^2 \right)^2 + \left((S_x^2)^2 - (S_y^2)^2 \right)^2 \\ &\quad + \left((S_x^3)^2 + \frac{\mathbf{v}_x}{2} - (S_y^3)^2 - \frac{\mathbf{v}_y}{2} \right)^2 + \left(S_x^1 i S_x^2 - S_y^1 i S_y^2 \right)^2 \\ &\quad + \left(S_x^1 S_x^3 - S_y^1 S_y^3 \right)^2 + \left(i S_x^2 S_x^3 - i S_y^2 S_y^3 \right)^2 \\ &\quad + \left(i S_x^2 S_x^1 - i S_y^2 S_y^1 \right)^2 + \left(S_x^3 S_x^1 - S_y^3 S_y^1 \right)^2 + \left(S_x^3 i S_x^2 - S_y^3 i S_y^2 \right)^2. \end{aligned} \tag{5.2.28}$$

Now we have enough information to use the Lemma, let $R : \Lambda_L \rightarrow \Lambda_L$ be a reflection that swaps Λ_1 and Λ_2 where $\Lambda = \Lambda_1 \cup \Lambda_2$, each such reflection defines two sub-lattices of Λ_L in this way, we split the field $v = (v_1, v_2)$ on the sub-lattices Λ_1 and Λ_2 .

Lemma 5.2.5. For $S \in \frac{1}{2}\mathbb{N}$ and any reflection, R , across edges and $v = (v_1, v_2)$

$$Z((v_1, v_2))^2 \leq Z((v_1, Rv_1))Z((Rv_2, v_2)).$$

Proof. We cast $Z'(v)$ in RP form. Let

$$A = -\beta \sum_{\{x,y\} \in \mathcal{E}_1} \mathcal{TR} \left[\left(Q_x + \frac{\mathbf{v}_x}{2} - Q_y - \frac{\mathbf{v}_y}{2} \right)^2 \right] - \beta d \sum_{x \in \Lambda_1} C_x^S, \tag{5.2.29}$$

B = same in Λ_2 ,

where \mathcal{E}_1 is the set of edges in Λ_1 and we note that the term C_x^S occurs d times in the sum over \mathcal{E} for each $x \in \Lambda_L$. Further define

$$\begin{aligned} C_i^1 &= \sqrt{\beta} (S_{x_i}^1)^2, & D_i^1 &= \sqrt{\beta} (S_{y_i}^1)^2. \\ C_i^2 &= \sqrt{\beta} (S_{x_i}^2)^2, & D_i^2 &= \sqrt{\beta} (S_{y_i}^2)^2. \\ C_i^3 &= \sqrt{\beta} \left((S_{x_i}^3)^2 + \frac{\mathbf{v}_{x_i}}{2} \right), & D_i^3 &= \sqrt{\beta} \left((S_{y_i}^3)^2 + \frac{\mathbf{v}_{y_i}}{2} \right). \\ C_i^4 &= \sqrt{\beta} S_{x_i}^1 i S_{x_i}^2, & D_i^4 &= \sqrt{\beta} S_{y_i}^1 i S_{y_i}^2. \\ C_i^5 &= \sqrt{\beta} S_{x_i}^1 S_{x_i}^3, & D_i^5 &= \sqrt{\beta} S_{y_i}^1 S_{y_i}^3. \\ C_i^6 &= \sqrt{\beta} i S_{x_i}^2 S_{x_i}^3, & D_i^6 &= \sqrt{\beta} i S_{y_i}^2 S_{y_i}^3. \\ C_i^7 &= \sqrt{\beta} i S_{x_i}^2 S_{x_i}^1, & D_i^7 &= \sqrt{\beta} i S_{y_i}^2 S_{y_i}^1. \\ C_i^8 &= \sqrt{\beta} S_{x_i}^3 S_{x_i}^1, & D_i^8 &= \sqrt{\beta} S_{y_i}^3 S_{y_i}^1. \\ C_i^9 &= \sqrt{\beta} S_{x_i}^3 i S_{x_i}^2, & D_i^9 &= \sqrt{\beta} S_{y_i}^3 i S_{y_i}^2. \end{aligned} \tag{5.2.30}$$

Here $\{x_i, y_i\}$ are edges crossing the reflection plane with $x_i \in \Lambda_1$ and $y_i \in \Lambda_2$. Because $\overline{S_x^1} = S_x^1$, $\overline{S_x^3} = S_x^3$, $\overline{iS_x^2} = iS_x^2$ we see from the previous lemma that $Z'((v_1, v_2))^2 \leq Z'((v_1, Rv_1))Z'((Rv_2, v_2))$, from which the result follows. \square

The Gaussian domination inequality (5.2.26) follows from this just as in the classical case, a proof can be found in [35]. The next step in the classical case was to obtain an infrared bound for the correlation function $\rho(x)$, we cannot do this directly but we can obtain an infrared bound for the *Duhamel correlation function*.

Definition 5.2.6. For matrices A, B we define the Duhamel correlation function $(A, B)_{Duh}$ as

$$(A, B)_{Duh} = \frac{1}{Z(0)} \frac{1}{\beta} \int_0^\beta ds \text{Tr} A^* e^{-sH(0)} B e^{-(\beta-s)H(0)}.$$

Note that this is an inner product.

Now to use this correlation function we must first fix our definition of the Fourier transform

$$\begin{aligned} \mathcal{F}(f)(k) &= \hat{f}(k) = \sum_{x \in \Lambda_L} e^{-ikx} f(x) & k \in \Lambda_L^*, \\ f(x) &= \frac{1}{|\Lambda|} \sum_{k \in \Lambda_L^*} e^{ikx} \hat{f}(k) & x \in \Lambda_L. \end{aligned} \quad (5.2.31)$$

where

$$\Lambda_L^* = \frac{2\pi}{L} \left\{ -\frac{L}{2} + 1, \dots, \frac{L}{2} \right\}^d, \quad (5.2.32)$$

Lemma 5.2.7. For $S \in \frac{1}{2}\mathbb{N}$ and L even we have the following infrared bound

$$\mathcal{F} \left((S_0^3)^2 - \frac{1}{3}S(S+1), (S_x^3)^2 - \frac{1}{3}S(S+1) \right)_{Duh}(k) \leq \frac{1}{2\beta\varepsilon(k)}. \quad (5.2.33)$$

Proof. We begin as usual by choosing $v_x = \eta \cos(kx)$ for $k \in \Lambda_L^*$, then from Taylor's theorem and using $h = \Delta v = -\varepsilon(k)v$ we see

$$Z(v) = Z(0) + \frac{1}{2} \left(h, \frac{\partial^2 Z(v)}{\partial h_x \partial h_y} \Big|_{h=0} h \right) + O(\eta^4). \quad (5.2.34)$$

Using the Duhamel formula

$$e^{\beta(A+B)} = e^{\beta A} + \int_0^\beta ds e^{sA} B e^{(\beta-s)(A+B)} \quad (5.2.35)$$

with $A = H(0)$ and $B = -\sum_{x \in \Lambda_L} (\Delta v)_x \left((S_x^3)^2 - \frac{1}{3}S(S+1) \right)$ gives

$$\frac{1}{Z(0)} \frac{\partial^2 Z(v)}{\partial h_x \partial h_y} \Big|_{h=0} = \beta^2 \left((S_x^3)^2 - \frac{1}{3}S(S+1), (S_y^3)^2 - \frac{1}{3}S(S+1) \right)_{Duh}. \quad (5.2.36)$$

Putting this together we have

$$\begin{aligned}
Z(\mathbf{v}) - O(\eta^4) &= \\
&= Z(0) + \frac{1}{2}Z(0)(\eta\varepsilon(k)\beta)^2 \sum_{x,y \in \Lambda_L} \cos(kx) \cos(ky) \left((S_x^3)^2 - \frac{1}{3}S(S+1), (S_y^3)^2 - \frac{1}{3}S(S+1) \right)_{Duh} \\
&= Z(0) + \frac{1}{2}Z(0)\beta^2\eta^2\varepsilon(k)^2 \mathcal{F} \left((S_0^3)^2 - \frac{1}{3}S(S+1), (S_y^3)^2 - \frac{1}{3}S(S+1) \right)_{Duh} \sum_{x \in \Lambda_L} \cos^2(kx).
\end{aligned} \tag{5.2.37}$$

Also

$$e^{-\frac{1}{4}\beta(\mathbf{v}, \Delta \mathbf{v})} = e^{\frac{1}{4}\beta\varepsilon(k)\eta^2 \sum \cos^2(kx)}, \tag{5.2.38}$$

comparing the order η^2 terms gives the result. \square

To transfer the infrared bound to the normal correlation function we would like to use the Falk-Bruch inequality [36]:

$$\frac{1}{2}\langle A^*A + AA^* \rangle \leq (A, A)_{Duh} + \frac{1}{2} \sqrt{(A, A)_{Duh} \langle [A^*, [H_{\Lambda_L, \mathbf{h}}^U, A]] \rangle}. \tag{5.2.39}$$

If we attempt to use this inequality with $A = \mathcal{F} \left((S_x^3)^2 - \frac{1}{3}S(S+1) \right) (k)$ and $H = \beta H_{\Lambda_L, \mathbf{0}}^U$, we must calculate the double commutator to find $\langle [A^*, [H_{\Lambda_L, \mathbf{h}}^U, A]] \rangle$. In general spins this is a huge calculation, instead we specialise to the case $S = 1$. In this case we can calculate as below, it uses several special properties of the Spin-1 matrices. To make use of this inequality we note that

$$\begin{aligned}
&\mathcal{F} \left\langle \left\langle \left((S_0^3)^2 - \frac{1}{3}S(S+1) \right) \left((S_x^3)^2 - \frac{1}{3}S(S+1) \right) \right\rangle_{\Lambda_L, \mathbf{0}}^U \right\rangle (k) \\
&= \sum_{x \in \Lambda_L} e^{-ikx} \left\langle \left\langle \left((S_0^3)^2 - \frac{1}{3}S(S+1) \right) \left((S_x^3)^2 - \frac{1}{3}S(S+1) \right) \right\rangle_{\Lambda_L, \mathbf{0}}^U \right\rangle \\
&= \frac{1}{|\Lambda_L|} \sum_{x,y \in \Lambda} e^{-ik(x-y)} \left\langle \left\langle \left((S_x^3)^2 - \frac{1}{3}S(S+1) \right) \left((S_y^3)^2 - \frac{1}{3}S(S+1) \right) \right\rangle_{\Lambda_L, \mathbf{0}}^U \right\rangle \\
&= \frac{1}{|\Lambda_L|} \left\langle \mathcal{F} \left((S_x^3)^2 - \frac{1}{3}S(S+1) \right) (-k) \mathcal{F} \left((S_y^3)^2 - \frac{1}{3}S(S+1) \right) (k) \right\rangle_{\Lambda_L, \mathbf{0}}^U.
\end{aligned} \tag{5.2.40}$$

This relation holds for other correlation functions, including the Duhamel correlation func-

tion, but for Duhamel

$$\begin{aligned} & \mathcal{F}\left((S_0^3)^2 - \frac{1}{3}S(S+1), (S_x^3)^2 - \frac{1}{3}S(S+1)\right)_{Duh}(k) \\ &= \frac{1}{|\Lambda_L|} \left(\mathcal{F}\left((S_x^3)^2 - \frac{1}{3}S(S+1)\right)(k), \mathcal{F}\left((S_y^3)^2 - \frac{1}{3}S(S+1)\right)(k) \right)_{Duh}, \end{aligned} \quad (5.2.41)$$

there is no $-k$ because of the definition of the Duhamel correlation function and the equality $(\mathcal{F}[(S_x^3)^2])(k)^* = \mathcal{F}[(S_x^3)^2](-k)$.

First we prove a preliminary lemma regarding the double commutator

Lemma 5.2.8. For $S = 1$, $A = \mathcal{F}\left((S_x^3)^2 - \frac{2}{3}\right)(k)$ and $H = \beta H_{\Lambda_L, 0}$ we have

$$\langle [A^*, [H, A]] \rangle_{\Lambda_L, \mathbf{0}}^U = 8\beta |\Lambda_L| \varepsilon(k + \pi) \langle S_0^1 S_0^3 S_{e_1}^1 S_{e_1}^3 \rangle_{\Lambda_L, \mathbf{0}}^U$$

where e_1 is the first basis vector in \mathbb{Z}^d .

Proof. The proof is just a calculation, although it is somewhat complicated, we begin by noting that in the case $S = 1$ the matrices $(S^i)^2$ and $(S^j)^2$ commute and $(S^i)^3 = S^i$ for $i, j = 1, 2, 3$.

$$\begin{aligned} [H, A] &= -2\beta \sum_{x, y: \{x, y\} \in \mathcal{E}} e^{-ikx} \left[(S_x^1 S_y^1 - S_x^2 S_y^2 + S_x^3 S_y^3)^2, (S_x^3)^2 \right] \\ &= -2\beta \sum_{x, y: \{x, y\} \in \mathcal{E}} e^{-ikx} \left[(S_x^1 S_x^3 S_y^1 S_y^3 - S_x^1 S_x^2 S_y^1 S_y^2 - S_x^2 S_x^1 S_y^2 S_y^1 \right. \\ &\quad \left. - S_x^2 S_x^3 S_y^2 S_y^3 + S_x^3 S_x^1 S_y^3 S_y^1 - S_x^3 S_x^2 S_y^3 S_y^2), (S_x^3)^2 \right]. \end{aligned} \quad (5.2.42)$$

The square terms have dropped out as they commute with $(S_x^3)^2$, as does the constant term $S(S+1)/3$. Now we calculate the commutator for each term in the sum, here we make use of the fact that $S^i S^j S^i = 0$ for $i \neq j$, $i, j = 1, 2, 3$ for $S = 1$.

$$\begin{aligned} [H, A] &= -2\beta \sum_{x, y: \{x, y\} \in \mathcal{E}} e^{-ikx} \left(S_x^1 S_x^3 S_y^1 S_y^3 + \overbrace{[(S_x^3)^2, S_x^1 S_x^2]}^{=0} S_y^1 S_y^2 + \overbrace{[(S_x^3)^2, S_x^2 S_x^1]}^{=0} S_y^2 S_y^1 \right. \\ &\quad \left. - S_x^2 S_x^3 S_y^2 S_y^3 - S_x^3 S_x^1 S_y^3 S_y^1 + S_x^3 S_x^2 S_y^3 S_y^2 \right) \\ &= +2\beta \sum_{x, y: \{x, y\} \in \mathcal{E}} e^{-ikx} \left([S_x^2 S_y^2, S_x^3 S_y^3] + [S_x^3 S_y^3, S_x^1 S_y^1] \right). \end{aligned} \quad (5.2.43)$$

Now calculating the commutator of these products and using the spin commutation relations

we obtain

$$[H, A] = 2\beta i \sum_{x,y:\{x,y\} \in \mathcal{E}} e^{-ikx} \underbrace{\left(S_x^2 S_x^3 S_y^1 + S_x^3 S_x^1 S_y^2 + S_x^1 S_y^3 S_y^2 + S_x^2 S_y^1 S_y^3 \right)}_{f(\mathbf{S}_x, \mathbf{S}_y)}. \quad (5.2.44)$$

Now we can use this to calculate the double commutator, firstly we split the commutator into the sum of two similar terms

$$\begin{aligned} [A^*, [H, A]] &= 2\beta i \sum_{x,y:\{x,y\} \in \mathcal{E}} e^{-ikx} \left[e^{ikx} (S_x^3)^2 + e^{iky} (S_y^3)^2, f(\mathbf{S}_x, \mathbf{S}_y) \right] \\ &= 2\beta i \sum_{x,y:\{x,y\} \in \mathcal{E}} \left[(S_x^3)^2, f(\mathbf{S}_x, \mathbf{S}_y) \right] + \cos(k(x-y)) \left[(S_y^3)^2, f(\mathbf{S}_x, \mathbf{S}_y) \right]. \end{aligned} \quad (5.2.45)$$

We can calculate each of these commutators separately, the first double commutator can be calculated as follows

$$\begin{aligned} \left[(S_x^3)^2, f(\mathbf{S}_x, \mathbf{S}_y) \right] &= \left[(S_x^3)^2, S_x^2 S_x^3 S_y^1 + S_x^3 S_x^1 S_y^2 + S_x^1 S_y^3 S_y^2 + S_x^2 S_y^1 S_y^3 \right] \\ &= -S_x^2 S_x^3 S_y^1 + iS_x^3 S_x^2 S_y^3 S_y^2 + iS_x^2 S_x^3 S_y^3 S_y^2 \\ &\quad + S_x^3 S_x^1 S_y^2 - iS_x^3 S_x^1 S_y^3 S_y^1 - iS_x^1 S_x^3 S_y^1 S_y^3. \end{aligned} \quad (5.2.46)$$

We recognise the commutator relations above to finally give

$$\left[(S_x^3)^2, f(\mathbf{S}_x, \mathbf{S}_y) \right] = iS_x^2 S_x^3 S_y^2 S_y^3 + iS_x^3 S_x^2 S_y^3 S_y^2 - iS_x^3 S_x^1 S_y^3 S_y^1 - iS_x^1 S_x^3 S_y^1 S_y^3. \quad (5.2.47)$$

For the other commutator we follow the previous calculation almost exactly and in fact we find the two commutators are equal

$$\left[(S_y^3)^2, f(\mathbf{S}_x, \mathbf{S}_y) \right] = \left[(S_x^3)^2, f(\mathbf{S}_x, \mathbf{S}_y) \right]. \quad (5.2.48)$$

To finish the calculation we take expectations

$$\begin{aligned} \langle [A^*, [H, A]] \rangle_{\Lambda_L, \mathbf{0}}^U &= \\ &= -4\beta |\Lambda_L| \sum_{i=1}^d (1 + \cos(k_i)) \left\langle S_0^2 S_0^3 S_{e_i}^2 S_{e_i}^3 + S_0^3 S_0^2 S_{e_i}^3 S_{e_i}^2 - S_0^3 S_0^1 S_{e_i}^3 S_{e_i}^1 - S_0^1 S_0^3 S_{e_i}^1 S_{e_i}^3 \right\rangle_{\Lambda_L, \mathbf{0}}^U \end{aligned} \quad (5.2.49)$$

now use the identities $(S^3 S^2)^T = -S^2 S^3$ and $(S^3 S^1)^T = S^1 S^3$ and get

$$\begin{aligned}
\langle [A^*, [H, A]] \rangle_{\Lambda_L, \mathbf{0}}^U &= -8\beta |\Lambda_L| \sum_{i=1}^d (1 + \cos(k_i)) \langle S_0^2 S_0^3 S_{e_i}^2 S_{e_i}^3 - S_0^3 S_0^1 S_{e_i}^3 S_{e_i}^1 \rangle_{\Lambda_L, \mathbf{0}}^U \\
&= 8\beta |\Lambda_L| \sum_{i=1}^d (1 + \cos(k_i)) \langle 2S_0^2 S_0^3 S_{e_i}^2 S_{e_i}^3 \rangle_{\beta, \Lambda_L, \mathbf{0}}^{0, J_2} \\
&= 8\beta |\Lambda_L| \varepsilon(k + \pi) \langle S_0^1 S_0^3 S_{e_1}^1 S_{e_1}^3 \rangle_{\beta, \Lambda_L, \mathbf{0}}^{0, J_2}.
\end{aligned} \tag{5.2.50}$$

On the second line we have used that $US_{e_1}^2 S_{e_1}^3 = -S_{e_1}^2 S_{e_1}^3 U$ to move from states $\langle \cdot \rangle_{\Lambda_L, \mathbf{0}}^U$ to states $\langle \cdot \rangle_{\beta, \Lambda_L, \mathbf{0}}^{0, J_2}$ and on the third line we have used that each cross term $\langle S_x^i S_x^j S_y^i S_y^j \rangle_{\beta, \Lambda_L, \mathbf{0}}^{0, J_2}$ has the same expectation value. Now simply note that the above correlation is the same in $\langle \cdot \rangle_{\Lambda_L, \mathbf{0}}^U$ and in $\langle \cdot \rangle_{\beta, \Lambda_L, \mathbf{0}}^{0, J_2}$. \square

Using this in Falk-Bruch we have the bound

$$\hat{\rho}(k) \leq \sqrt{\langle S_0^1 S_0^3 S_{e_1}^1 S_{e_1}^3 \rangle_{\beta, \Lambda_L, \mathbf{0}}^{0, J_2}} \sqrt{\frac{\varepsilon(k + \pi)}{\varepsilon(k)}} + \frac{1}{2\beta \varepsilon(k)}. \tag{5.2.51}$$

The possibility of obtaining a result is not ruled out for other values of S , I expect it to be the case for other values of S , but computing the double commutator in Falk-Bruch becomes extremely complicated.

Now using the Fourier transform in the following way:

$$\left\langle \left((S_0^3)^2 - \frac{2}{3} \right) \left((S_y^3)^2 - \frac{2}{3} \right) \right\rangle_{\Lambda_L, \mathbf{0}}^{0, J_2} = \frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \rho(x) + \frac{1}{|\Lambda|} \sum_{k \in \Lambda_L^* \setminus \{0\}} e^{ik \cdot y} \hat{\rho}(x)(k) \tag{5.2.52}$$

with $y = e_1$ we get the lower bound

$$\frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \rho(x) \geq \rho(e_1) - \frac{\sqrt{\langle S_0^1 S_0^3 S_{e_1}^1 S_{e_1}^3 \rangle_{\beta, \Lambda_L, \mathbf{0}}^{0, J_2}}}{|\Lambda_L|} \sum_{k \in \Lambda_L^* \setminus \{0\}} \sqrt{\frac{\varepsilon(k + \pi)}{\varepsilon(k)}} \left(\frac{1}{d} \sum_{i=1}^d \cos k_i \right)_+ - \frac{1}{2\beta \varepsilon(k)}. \tag{5.2.53}$$

This proves Theorem 5.2.1. \square

5.3 Extending to $J_1 < 0$

The aim of this section is to extend the proof of Theorem 5.2.1 to a proof of Theorem 5.1.1. The proof of long-range order for $J_1 < 0$ is a straightforward extension of the previous results. Like before we will work with a Hamiltonian that is Unitarily equivalent to $H_{\Lambda_L, \mathbf{0}}^{J_1, J_2}$, we also introduce an external field \mathbf{h} as before. Recall the unitary operator $U = \prod_{x \in \Lambda_e} e^{i\pi S_x^2}$, let

$$\tilde{H}_{\Lambda_L, \mathbf{h}}^U = U H_{\Lambda_L, \mathbf{0}}^{J_1, J_2} U^{-1} - \sum_{x \in \Lambda_L} h_x \left((S_x^3)^2 - \frac{1}{3} S_x(S_x + 1) \right). \quad (5.3.1)$$

The effect of the unitary operator here is to replace S_x^1 and S_x^3 in $H_{\Lambda_L, \mathbf{0}}^{J_1, J_2}$ with $-S_x^1$ and $-S_x^3$ respectively. By using the representation (5.2.17) we can write $\tilde{H}_{\Lambda_L, \mathbf{0}}^U$ as

$$\begin{aligned} \tilde{H}_{\Lambda_L, \mathbf{0}}^U = & - \sum_{\{x, y\} \in \mathcal{E}} \left[J_1 \left((S_x^1 - S_y^1)^2 - (S_x^2 - S_y^2)^2 + (S_x^3 - S_y^3)^2 \right) \right. \\ & \left. - J_2 \left(\mathcal{T}\mathcal{R}[(Q_x - Q_y)^2] \right) + C_{\Lambda_L}(J_1, J_2) \right]. \end{aligned} \quad (5.3.2)$$

Then as to before we introduce the field v and associated 3×3 field of matrices \mathbf{v} . Define

$$\begin{aligned} \tilde{H}(v) = & - \sum_{\{x, y\} \in \mathcal{E}} \left[J_1 \left((S_x^1 - S_y^1)^2 - (S_x^2 - S_y^2)^2 + (S_x^3 - S_y^3)^2 \right) \right. \\ & \left. - J_2 \left(\mathcal{T}\mathcal{R} \left[\left(Q_x + \frac{\mathbf{v}_x}{2} - Q_y - \frac{\mathbf{v}_y}{2} \right)^2 \right] \right) + C_{\Lambda_L}(J_1, J_2) \right] - \frac{1}{4}(v, -\Delta v), \end{aligned} \quad (5.3.3)$$

$$\tilde{Z}(v) = \text{Tr} e^{-\beta \tilde{H}(v)}, \quad (5.3.4)$$

and

$$\tilde{H}'(v) = \tilde{H}(v) + \frac{1}{4}(v, -\Delta v), \quad (5.3.5)$$

$$\tilde{Z}'(v) = \text{Tr} e^{-\beta \tilde{H}'(v)}. \quad (5.3.6)$$

From this reflection positivity follows just as in Lemma 5.2.5, with the obvious changes to A and B and the extra terms

$$\begin{aligned} C_i^{10} &= \sqrt{-J_1} S_{x_i}^1, & D_i^{10} &= \sqrt{-J_1} S_{y_i}^1, \\ C_i^{11} &= \sqrt{-J_1} i S_{x_i}^2, & D_i^{11} &= \sqrt{-J_1} i S_{y_i}^2, \\ C_i^{12} &= \sqrt{-J_1} S_{x_i}^3, & D_i^{12} &= \sqrt{-J_1} S_{y_i}^3, \end{aligned} \quad (5.3.7)$$

(recall that $J_1 < 0$). From this we obtain the Gaussian domination inequality

$$\widetilde{Z}(v) \leq \widetilde{Z}(0)e^{\frac{\beta}{4}(v, -\Delta v)} \iff \widetilde{Z}'(v) \leq \widetilde{Z}'(0), \quad (5.3.8)$$

just as before. We also obtain the same infrared bound as in Lemma 5.2.7, with an identical proof

$$\mathcal{F}\left((S_0^3)^2 - \frac{1}{3}S(S+1), (S_x^3)^2 - \frac{1}{3}S(S+1)\right)_{Duh}(k) \leq \frac{1}{2\beta\varepsilon(k)}. \quad (5.3.9)$$

Again the results up to here work for general $S \in \frac{1}{2}\mathbb{N}$, at this point we must specialise to $S = 1$ to be able to calculate the quantities in the double commutator of the Falk-Bruch inequality. From this we can see that by using Falk-Bruch inequality with $A = \mathcal{F}\left((S_x^3)^2 - \frac{2}{3}\right)(k)$ and $H = \beta\widetilde{H}_{\Lambda, \mathbf{0}}^U$ the linearity of the double commutator means that there will be an extra term in the analogous result to Lemma 5.2.8 equal to $\langle J_1[A^*, [-2 \sum_{\{x,y\} \in \mathcal{E}} (\mathbf{S}_x \cdot \mathbf{S}_y), A]] \rangle$. This will result in the IRB analogous to (5.2.51) potentially being larger, weakening the result. If $|J_1|$ is small enough this weakening will not be too severe so as to make the lower bound analogous to the bound in Theorem 5.2.1 negative in cases where we know the original lower bound was positive. This ensures that we have a positive lower bound $C = C(\beta, J_1)$ in Theorem 5.1.1 when β and $|J_1|$ are small enough. It is worth noting that for the same reason as just described, extending the result of Dyson, Lieb and Simon [35] to $J_2 > 0$ also requires that $|J_2|$ is small. This means the two results will not overlap, leaving part of the quadrant $J_1 \leq 0 \leq J_2$ still open to investigation in Chapter 6.

Chapter 6

Probabilistic representations of quantum spin systems

In this chapter we consider random loop representations of various quantum spin systems. We begin by introducing the Aizenman-Nachtergaele-Tóth-Ueltschi model and mention some results obtained using the model. We then introduce the ‘multi-line’ model of Nachtergaele and prove its relation to quantum spin systems. Using this relation it is shown that for dimensions 3 and above Néel order occurs for a large range of values of the relative strength of the bilinear ($-J_1$) and biquadratic ($-J_2$) interaction terms of a general two-body $SU(2)$ invariant spin-1 interaction. We also prove results related to nematic order. The proofs use the method of reflection positivity and infrared bounds. Links between spin correlations and loop correlations are also proved. We look at the general $SU(2)$ invariant spin-1 Heisenberg model with a two-body interaction

$$H_{\Lambda}^{J_1, J_2} = - \sum_{\{x, y\} \in \mathcal{E}} \left(J_1 (\mathbf{S}_x \cdot \mathbf{S}_y) + J_2 (\mathbf{S}_x \cdot \mathbf{S}_y)^2 \right). \quad (6.0.1)$$

Here we will have $x \in \Lambda \subset \mathbb{Z}^d$ and \mathcal{E} the set of nearest neighbour edges. The operators $\mathbf{S} = (S^1, S^2, S^3)$ are the spin-1 matrices, see Section 6.2.4 for details of the model. The work in [111] shows that in the region $0 \leq J_1 \leq \frac{1}{2}J_2$ the system exhibits *nematic order* in the thermodynamic limit if the temperature is low enough and the dimension is high enough. Nematic order was also shown independently using different methods in [106]. It is also shown that if Λ is bipartite there will be *Néel* order for $J_1 = 0 \leq J_2$ at low temperature. This corresponds to the occurrence of infinite loops in the related loop model. Alternatively in $d \leq 2$ infinite loops should not occur, it is proved in [40] that this is the case for $J_2 = 0$, the extension to $J_2 > 0$ should be straightforward.

6.1 The Aizenman-Nachtergaele, Tóth, Ueltschi representation

In this section we discuss Ueltschi's extension [113] of the probabilistic representation introduced in the work of Aizenman and Nachtergaele [2] and Tóth [107]. Both these works considered the spin- $\frac{1}{2}$ Heisenberg model. It was shown in [113] that the representations can be combined and extended to cover the spin- $\frac{1}{2}$ XY model and higher spin models. The equivalence of the loop and spin models will be proved and several results concerning long-range order will be stated. We begin by introducing the loop model.

6.1.1 The Loop Model

We work on a finite graph (Λ, \mathcal{E}) with Λ the set of vertices and \mathcal{E} the set of edges. For $\beta > 0$ we attach to each edge $\{x, y\} \in \mathcal{E}$ an interval $[0, \beta]$. We further define a Poisson point process on each edge $\{x, y\} \times [0, \beta]$ consisting of two types of events. The events are crosses, with intensity u and double bars, with intensity $1 - u$, for $u \in [0, 1]$. Let ρ denote the process of an independent Poisson process on each edge $\{x, y\} \times [0, \beta]$ with the above intensities. To a realisation ω of this process we can associate a set of loops, $\mathcal{L}(\omega)$ (\mathcal{L} maps from realisations of the process to positive integers). These loops are best understood pictorially, see Fig. 6.1. We define them mathematically as follows. A loop of length l is a closed trajectory $\gamma : [0, \beta l]_{per} \rightarrow \Lambda \times [0, \beta]_{per}$ following certain rules:

- γ is piecewise differentiable with derivative ± 1 at points of differentiability.
- γ is injective at its points of differentiability.
- If s is a point of non-differentiability then $\{\gamma(s-), \gamma(s+)\} \in \mathcal{E} \times \{x, y\}$.

Loops that are the same up to reparameterisation are identified. The events are incorporated into the loops as the points of non-differentiability. Starting at a point $(x, t) \in \Lambda \times [0, \beta]_{per}$ we move upwards until an event is reached. If the event is a cross we cross it to the other associated edge and continue moving upwards, if the event is a double bar we cross it to the associated edge and reverse direction. See, for example, [50, 65, 111] for further information on the state space, $\Omega_{\Lambda, \beta}$, for loop ensembles. The partition function, $Y_{\theta}^{(u)}(\Lambda, \beta)$ is given by

$$Y_{\theta}^{(u)}(\Lambda, \beta) = \int \rho(d\omega) \theta^{|\mathcal{L}(\omega)|}, \quad (6.1.1)$$

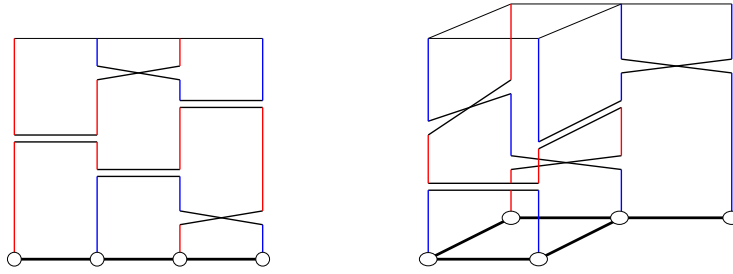


Figure 6.1: Example of realisations of ρ from [113] with loops coloured.

where the integral is over $\Omega_{\Lambda, \beta}$ (we will omit the region of integration from integrals unless it is *not* $\Omega_{\Lambda, \beta}$). The measure is given by

$$\mathbb{P}(d\omega) = \frac{1}{Y_{\theta}^{(u)}(\Lambda, \beta)} \rho(d\omega) \theta^{|\mathcal{L}(\omega)|}, \quad (6.1.2)$$

hence a realisation, ω , has weight $\theta^{|\mathcal{L}(\omega)|}$, this leads to very complicated dependencies on the events of ρ . There are three main events of interest. The first is that points $(x, 0)$ and (y, t) are in the same loop, denoted $E_{x,y,t}$. Other events are that $(x, 0)$ and (y, t) are in the same loop and have either the same or opposite vertical direction at these points, denoted by $E_{x,y,t}^+$ and $E_{x,y,t}^-$ respectively.

6.1.2 Connection with spin systems

We begin by defining space-time spin configurations, piecewise constant functions

$$\sigma : \Lambda \times [0, \beta]_{per} \rightarrow \{-S, -S + 1, \dots, S\}. \quad (6.1.3)$$

For a realisation, ω , of ρ we say σ is compatible with ω if it is constant on the vertical segments of each loop in $\mathcal{L}(\omega)$ and flips sign when crossing a double bar. Denote the set of all compatible configurations by $\Sigma(\omega)$. More precisely, a compatible configuration, σ is a function that is piecewise constant on each $x \in \Lambda$ which must satisfy certain restrictions. The value $\sigma_{x,t}$ must be constant in t for each $x \in \Lambda$ unless an event is encountered on an edge containing x . If a cross is encountered at $(\{x, y\}, t) \in \mathcal{E} \times [0, \beta]$ we must have that $\sigma_{x,t-} = \sigma_{y,t+}$ and $\sigma_{y,t-} = \sigma_{x,t+}$. If a bar is encountered at $(\{x, y\}, t) \in \mathcal{E} \times [0, \beta]$ we must have that $\sigma_{x,t-} = -\sigma_{y,t-}$ and $\sigma_{y,t+} = -\sigma_{x,t+}$. Note that each loop has $(2S + 1)$ possible assignments of spin for a compatible configuration, hence for $\theta = 2S + 1$

$$Y_{2S+1}^{(u)}(\Lambda, \beta) = \int \rho(d\omega) \sum_{\sigma \in \Sigma(\omega)} 1. \quad (6.1.4)$$

We now define two operators, T_{xy}, P_{xy} on local Hilbert spaces $\mathcal{H}_x \otimes \mathcal{H}_y$. We define these operators by

$$T_{xy}|a, b\rangle = |b, a\rangle, \quad (6.1.5)$$

$$P_{xy} = \sum_{a,b=-S}^S (-1)^{a-b} |a, -a\rangle \langle b, -b|, \quad (6.1.6)$$

and define a Hamiltonian

$$H_\Lambda^{(u)} = - \sum_{\{x,y\} \in \mathcal{E}} (uT_{xy} + (1-u)P_{xy} - 1). \quad (6.1.7)$$

This Hamiltonian is relevant for the spin-1 system. Another Hamiltonian is introduced in [113] that is relevant to the spin- $\frac{1}{2}$ model. We denote by $Z^{(u)}(\Lambda, \beta)$ and $\langle \cdot \rangle_{\Lambda, \beta}^{(u)}$ the usual partition function and Gibbs states. The following equality is proved in [113], we present it here

$$\int (2S+1)^{|\mathcal{L}(\omega)|} \rho(d\omega) = Z^{(u)}(\Lambda, \beta). \quad (6.1.8)$$

Proof. We use Trotter's formula

$$\text{Tr} e^{-\beta H_\Lambda^{(u)}} = \lim_{N \rightarrow \infty} \text{Tr} \left(\prod_{\{x,y\} \in \mathcal{E}} \left[1 - \frac{\beta}{N} + \frac{\beta}{N} (uT_{xy} + (1-u)P_{xy}) \right] \right)^N. \quad (6.1.9)$$

Now expanding the trace and inserting a resolution of the identity between each factor we have

$$\text{Tr} e^{-\beta H_\Lambda^{(u)}} = \lim_{N \rightarrow \infty} \sum_{\sigma^{(1)}, \dots, \sigma^{(N)}} \prod_{i=1}^N \left\langle \sigma^{(i)} \left| \prod_{\{x,y\} \in \mathcal{E}} \left[1 - \frac{\beta}{N} + \frac{\beta}{N} (uT_{xy} + (1-u)P_{xy}) \right] \right| \sigma^{(i+1)} \right\rangle. \quad (6.1.10)$$

The sum is over all configurations $\sigma^{(i)} \in \{-S, \dots, S\}^\Lambda$ with $\sigma^{(N+1)} \equiv \sigma^{(1)}$. Note that if we view $\sigma^{(i)}$ as the space-time spin configuration between events $i-1$ and i in realisation ω of ρ then T_{xy} corresponds to crosses and P_{xy} corresponds to bars. Note the identity

$$\exp \left\{ - \sum_{\{x,y\} \in \mathcal{E}} (uT_{xy} + (1-u)P_{xy} - 1) \right\} = \int \rho(d\omega) \prod_{(x_i, y_i, t) \in \omega}^* R_{x_i y_i}^{(i)} \quad (6.1.11)$$

where \prod^* is the time ordered product of events in the realisation, ω , of ρ and each $R_{x_i y_i}^{(i)}$ is an event $(T_{x_i y_i}, P_{x_i y_i})$ on the edge $\{x_i, y_i\}$ at time t . Using this and taking the limit $N \rightarrow \infty$ gives (6.1.8). \square

For this model it is also shown that

$$\langle S_x^i S_y^i \rangle_{\Lambda, \beta}^{(u)} = \frac{1}{3} S(S+1) (\mathbb{P}[E_{x,y,t}^+] - \mathbb{P}[E_{x,y,t}^-]), \quad (6.1.12)$$

$$\langle (S_x^i)^2 (S_y^i)^2 \rangle_{\Lambda, \beta}^{(u)} - \langle (S_x^i)^2 \rangle_{\Lambda, \beta}^{(u)} \langle (S_y^i)^2 \rangle_{\Lambda, \beta}^{(u)} = \frac{1}{45} S(S+1)(2S-1)(2S+3) \mathbb{P}[E_{x,y,t}]. \quad (6.1.13)$$

The proof involves a similar expansion as the proof of (6.1.8). Similar results will be presented for Nachtergaele's loop model in Proposition 6.2.3 hence the reader is directed there for the methods of the proof. It is also proved that for $d \geq 3$ and $u \in [0, \frac{1}{2}]$ if S is small enough then there is a $c > 0$ such that

$$\lim_{\beta \rightarrow \infty} \liminf_{|\Lambda| \rightarrow \infty} \frac{1}{|\Lambda|} \sum_{x \in \Lambda} \mathbb{P}[E_{0,x,0}] \geq c, \quad (6.1.14)$$

where the limit $|\Lambda| \rightarrow \infty$ is taken along cubic lattices of even side length. This result can be translated into results for corresponding spin models. For $S = 1$ we take Hamiltonian

$$H = - \sum_{\{x,y\} \in \mathcal{E}} J_1 \mathbf{S}_x \cdot \mathbf{S}_y + J_2 (\mathbf{S}_x \cdot \mathbf{S}_y)^2 \quad (6.1.15)$$

then for $0 < J_1 \leq \frac{1}{2} J_2$ it is shown that there is nematic order at low temperatures for $d \geq 5$. In fact for $0 = J_1 < J_2$ there is Néel order in $d \geq 5$ at low temperatures. This result fits nicely with the results concerning Néel order via the loop representation of Nachtergaele.

6.2 Existence of Néel order in the $S=1$ bilinear-biquadratic Heisenberg model via random loops

This section is mainly based on the paper [70]. We present the main result and then introduce the model. Several secondary theorems are also proved using similar methods.

6.2.1 Main result

We use the method of reflection positivity and infrared bounds on a the loop model introduced in [81]. Links between correlations in the spin model and probabilities of events in the loop model are also derived in Section 6.2.5. We focus on the quadrant $J_1 \leq 0 \leq J_2$ for (6.1.15), see Fig. 6.2. We prove results for Néel and nematic correlations using both 'normal' and space-time reflection positivity. The following result concerning Néel order follows from proposition 6.2.3 a), theorem 6.2.6 and the discussion that follows. For the

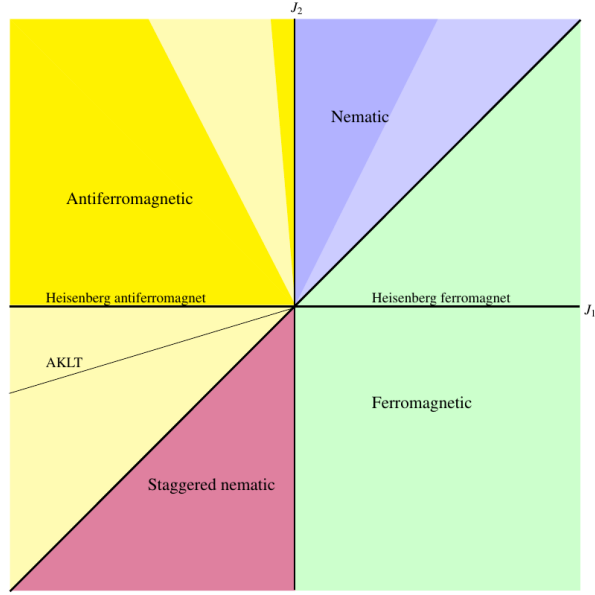


Figure 6.2: The phase diagram for the general SU(2) invariant spin-1 model. Regions that are shaded darker have rigorous proofs of the relevant phases. The line $J_1 < 0, J_2 = 0$ is the Heisenberg antiferromagnet where antiferromagnetic order has been proven [35], Néel order extends into the dark yellow region. The dark blue region $0 \leq J_1 \leq \frac{1}{2}J_2$ has nematic order at low temperatures [111], with Néel order on the line $J_2 > 0, J_1 = 0$. The adjacent dark yellow region has been proved to exhibit nematic order in high enough dimension [69]. Antiferromagnet order is expected here but is not yet proved.

precise statements see Section 6.2.6.

Theorem. For $\Lambda \subset \mathbb{Z}^d$ a box of even side length, L , and $d \geq 3$ there exists $\alpha = \alpha(d) > 0$ and $0 < \beta_0 < \infty$ such that for $J_1 \leq 0 \leq J_2$ if $-J_1/J_2 > \alpha$ and $\beta > \beta_0$ there exists $c = c(\alpha, d, \beta) > 0$ such that

$$\liminf_{L \rightarrow \infty} \frac{1}{L^d} \sum_{x \in \Lambda} (-1)^{\|x\|} \langle S_0^3 S_x^3 \rangle_{\Lambda, \beta} \geq c. \quad (6.2.1)$$

Furthermore $\alpha(d) \rightarrow 0$ as $d \rightarrow \infty$.

Analogous theorems are also proved for nematic correlations. It is shown in the discussion after Theorem 6.2.6 that this sum is positive for β large enough if

$$I_d K_d < (-4J_1)/(-J_1 + 4J_2). \quad (6.2.2)$$

I_d and K_d are integrals to be introduced in (6.2.64). Their values for various d are given in the table below.

d	I_d	K_d
3	0.349882	1.15672
4	0.253950	1.09441
5	0.206878	1.06754
6	0.177716	1.05274

It can be shown [35, 58] that $I_d \rightarrow 0$ and $K_d \rightarrow 1$ as $d \rightarrow \infty$ and that both are decreasing in d . This means we can prove that the region where Néel order occurs will increase to the entire quadrant $J_1 \leq 0 \leq J_2$ as $d \rightarrow \infty$ i.e. the ratio $\alpha(d)$ is decreasing. In $d = 3$ there is Néel order in the spin system for $-J_1/J_2 < 0.46$, this is a triangular region of angle 65° measured from the J_1 axis.

Reflection positivity for this quadrant is already known, for $J_1 < 0 = J_2$ it was shown in [35] and for $J_1 = 0 < J_2$ one can see Lemma 6.2.13 ([69] Lemma 3.4) for an explicit proof. It was proved in [35] that Néel order occurs for $J_1 < 0 = J_2$, it is clear the result extends to a neighbourhood of the axis for $J_1 < 0 < J_2$ with J_2/J_1 sufficiently small. However it is impossible to extend the result concerning Néel order any significant amount without some new results. This is where the loop model has been essential. Indeed in [35] an infrared bound is obtained of the form

$$\langle \widehat{S_0^3, S_x^3} \rangle_{Duh}(k) \leq \frac{1}{2(-J_1)\varepsilon(k)} \quad (6.2.3)$$

where $(A, B)_{Duh}$ is the Duhamel correlation function and $\varepsilon(k) = 2 \sum_{i=1}^d (1 - \cos k_i)$ for $k \in \Lambda^*$. Notice that this bound becomes weaker as $|J_1|$ decreases (equivalently on the unit circle as $|J_1|/|J_2|$ decreases). Transferring this bound to $\langle \widehat{S_0^3 S_x^3} \rangle_\beta(k)$ requires the Falk-Bruch inequality which would involve dealing with the term $\langle [\widehat{S_{-k}^3}, [J_2 (\mathbf{S}_x \cdot \mathbf{S}_y)^2, \widehat{S_k^3}]] \rangle_\beta$. After some calculation one obtains correlations in Proposition 6.2.3 such as $\langle S_x^1 S_y^1 S_x^3 S_y^3 \rangle_\beta$. Hence to work directly in the quantum system using the methods of [35] one must obtain good bounds on these correlations. Simple bounds such as taking the operator norm are not sufficient due to the weakening of (6.2.3) as $|J_1|/|J_2|$ decreases. Without using the loop model it is not clear how to obtain such bounds currently.

The random loop model is presented in sections 6.2.2 and 6.2.3. The spin-1 Heisenberg model is introduced in Section 6.2.4. In Section 6.2.5 the connection between the loop model and the quantum system is proved. In particular it is shown how to write various correlation functions in terms of probabilities of events in the loop model, some of these correlations are also presented in [113]. In Section 6.2.6 the main result concerning Néel order is presented and proved. Section 6.2.7 presents and proves an analogous result for nematic correlations, both sections 6.2.6 and 6.2.7 rely on reflection positivity of the loop

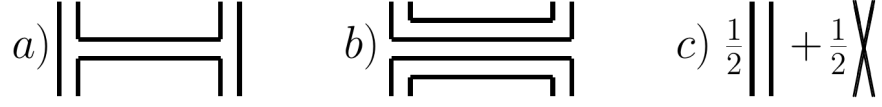


Figure 6.3: Events of the process ρ_{J_1, J_2} , a) represents single bars, b) represents double bars and c) represents the uniform measure on vertical segments being either parallel or crossing.

model. Sections 6.2.8 and 6.2.9 present results analogous to sections 6.2.6 and 6.2.7 respectively using space-time reflection positivity.

6.2.2 The random loop model

We now introduce the loop model presented in [81]. To begin we take a finite set of vertices, Λ , with a set of edges, $\mathcal{E} \subset \{\{x, y\} | x, y \in \Lambda, x \neq y\}$. We associate to this lattice a new lattice, $\tilde{\Lambda}$, and edge set, $\tilde{\mathcal{E}}$:

$$\tilde{\Lambda} = \Lambda \times \{0, 1\}, \quad (6.2.4)$$

$$\tilde{\mathcal{E}} = \{\{(x, i), (y, j)\} | i, j \in \{0, 1\}, \{x, y\} \in \mathcal{E}\}. \quad (6.2.5)$$

There are two lattice sites in $\tilde{\Lambda}$ for every site in Λ and four edges in $\tilde{\mathcal{E}}$ for each edge in \mathcal{E} . We will write x_0, x_1 in place of $(x, 0), (x, 1)$.

For $\beta > 0$ consider a process, ρ_{J_1, J_2} , consisting of a Poisson point process on $\mathcal{E} \times [0, \beta]$ and a uniform measure on segments of $\Lambda \times [0, \beta]$ between events of the Poisson point process. The Poisson point process has two events that we will refer to as ‘single bars’ and ‘double bars’. Note that this process is on the edge set \mathcal{E} , the events define corresponding events on the edge set $\tilde{\mathcal{E}}$. The single bars will occur at rate $-2J_1$ and double bars at rate J_2 for $J_1 \leq 0 \leq J_2$. The rate for the single bars is written in this way to be consistent with the connection to the quantum spin system that will be introduced in Section 6.2.4. The interval $[0, \beta]$ will be referred to as a time interval. The uniform measure is on two possibilities, “crossing” and “parallel”. How to build loops from these events is described in detail below, see Fig. 6.3 for pictorial representations of the events. The construction is much in analogue with Section 6.1.

We first define the single and double bars. Single bars occur at a point (x, y, t) for $\{x, y\} \in \mathcal{E}$. We define the corresponding geometric event on $\tilde{\mathcal{E}}$ as a bar joining x_1 and y_0 at time t . Double bars occur at a point (x, y, t) and the corresponding event on $\tilde{\mathcal{E}}$ is a bar joining x_1 and y_0 and a bar joining x_0 and y_1 , both at time t . A *loop* of length l is then a map $\gamma : [0, \beta l]_{per} \rightarrow \tilde{\Lambda} \times [0, \beta]_{per}$ such that $\gamma(s) \neq \gamma(t)$ if $s \neq t$, γ is piecewise differentiable with

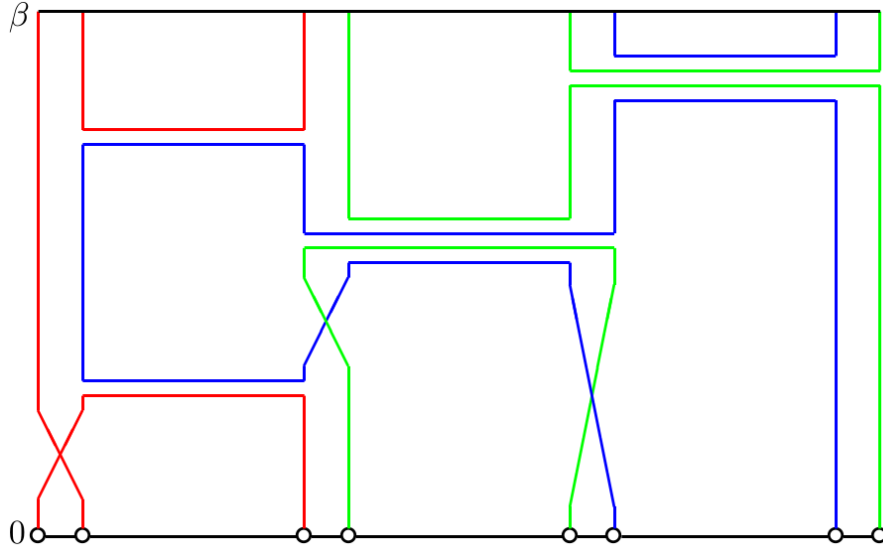


Figure 6.4: An example realisation with loops coloured in red, green and blue. Here there are four sites in the underlying Λ and for this realisation $|\mathcal{L}(\omega)| = 3$.

derivate ± 1 where it exists. If s is a point of non-differentiability then $\{\gamma(s-), \gamma(s+)\} \in \tilde{\mathcal{E}}$. Loops with the same support and different parameterisations are identified. For a realisation ω of ρ_{J_1, J_2} we associate a set of loops as follows: Starting at a point $(x_i, s) \in \tilde{\Lambda} \times [0, \beta]$ we move upwards (i.e. in direction of increasing s). If a bar is met at time t it is crossed and we then continue in the opposite direction from (y_j, t) , where y_j is the other site associated to the bar. Each maximal vertical segment between bars $(x_0, x_1) \times [s, t]$ (i.e. bars involving the site x occur at times s and t and no bar involving x occurs for u such that $s < u < t$) is either parallel (nothing happens) or crossing (the sites x_0 and x_1 are exchanged). If time β is reached the periodic time conditions mean we continue in the same direction starting from time 0. We denote by $\mathcal{L}(\omega)$ the set of all loops associated to a realisation ω . Loops are most easily understood pictorially, see Fig. 6.4. Note that the loops could be defined via a Poisson point process on $\tilde{\mathcal{E}} \times [0, \beta]$ where bars can occur between x_i and y_j with each (i, j) being equally likely. However one would still need to introduce the crossing or parallel events so that it is still possible to have x_0 and x_1 in the same loop even when there is no bar occurring on any edge containing x .

For this loop model we have partition function

$$Y_\theta^{J_1, J_2}(\beta, \Lambda) = \int \rho_{J_1, J_2}(d\omega) \theta^{|\mathcal{L}(\omega)|}. \quad (6.2.6)$$

Here $\theta > 0$ is a parameter and ρ_{J_1, J_2} is the probability measure corresponding to a Pois-

son point process of intensity $-2J_1$ for single bars and J_2 for double bars. The relevant probability measure is then

$$\mathbb{P}(d\omega) = \frac{1}{Y_\theta^{J_1, J_2}(\beta, \Lambda)} \rho_{J_1, J_2}(d\omega) \theta^{|\mathcal{L}(\omega)|}. \quad (6.2.7)$$

We are interested in sets of realisations, ω , where certain points of $\tilde{\Lambda} \times [0, \beta]$ are in the same loop. Probabilities of these events are connected to correlations in the spin-1 quantum system presented in Section 6.2.4, they will be required in the proof of Néel order in Section 6.2.6. Particular events of interest will be denoted pictorially, see Fig. 6.5. These events are defined and denoted as follows.

- a) The event that sites x_i and y_j are connected (in the same loop). Note that the probability of x_i and y_j being connected is independent of i and j . Denoted $E[x_i - y_j]$.
- b) The event that x_0 and x_1 are connected, y_0 and y_1 are connected but there is no connection from any x_i to any y_j . Denoted $E \left[\begin{array}{c} x_0 \quad y_0 \\ \text{---} \text{---} \\ x_1 \quad y_1 \end{array} \right]$.
- c) The event that x_0 and y_0 are connected, x_1 and y_1 are connected but x_0 and x_1 are not connected. Denoted $E \left[\begin{array}{c} x_0 \text{---} y_0 \\ \text{---} \text{---} \\ x_1 \text{---} y_1 \end{array} \right]$. We can also have x_0 and y_1 connected and x_1 and y_0 connected but x_0 and x_1 not connected and denote the event in the analogous way. These events both have the same probability.
- d) The event that all four sites x_0, x_1, y_0, y_1 are connected. Denoted $E \left[\begin{array}{c} x_0 \quad y_0 \\ \text{---} \text{---} \\ x_1 \quad y_1 \end{array} \right]$.

The definition of bars means that if a loop is followed starting from a point $x_i \in \tilde{\Lambda}$ (by moving in either the up or down direction) then the direction it is travelling upon arriving at a point $y_j \in \tilde{\Lambda}$ in the same loop is determined only by the number of bars the loop has encountered between the sites. For example on a bipartite lattice defined by sublattices Λ_A and Λ_B such that $\{x, y\} \in \mathcal{E} \iff x \in \Lambda_A, y \in \Lambda_B$ the direction that x_i is left and y_j is entered will be the same if x and y are in the same sublattice and different if they are in different sublattices.

Sometimes the order in which sites are encountered along the loop will be important. In this case arrows will indicate the order that sites will be encountered in on following the loop (up to parameterisation). The events $E \left[\begin{array}{c} x_0 \rightarrow y_0 \\ \uparrow \quad \downarrow \\ x_1 \leftarrow y_1 \end{array} \right]$, $E \left[\begin{array}{c} x_0 \quad y_0 \\ \downarrow \quad \uparrow \\ x_1 \leftarrow y_1 \end{array} \right]$ and $E \left[\begin{array}{c} x_0 \rightarrow y_0 \\ \downarrow \quad \uparrow \\ x_1 \leftarrow y_1 \end{array} \right]$ are the events that all four sites are connected and are encountered along the loop in the order indicated by the arrows. For example the first event, $E \left[\begin{array}{c} x_0 \rightarrow y_0 \\ \uparrow \quad \downarrow \\ x_1 \leftarrow y_1 \end{array} \right]$, means that upon leaving site x_0 if we encounter y_0 before encountering x_1 then we will encounter y_1 and then x_1 before closing the loop. As this notation is potentially confusing (but also seemingly unavoidable) the reader will be told explicitly when the order is important. When wanting the probability of

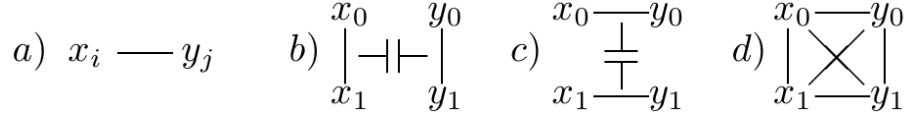


Figure 6.5: Pictures representing the set of realisations where the pictured connections are present.

these events we will drop the E from the notation, as below.

It is intuitively clear that $\mathbb{P}(x_0 \text{---} y_0)$ decays exponentially fast with respect to $\|x - y\|$ for β small. Hence $\mathbb{P}\left(\begin{smallmatrix} x_0 \text{---} y_0 \\ | \\ x_i \text{---} y_i \end{smallmatrix}\right)$ and $\mathbb{P}\left(\begin{smallmatrix} x_0 \text{---} y_0 \\ | \\ x_1 \text{---} y_1 \end{smallmatrix}\right)$ must also have exponential decay. $\mathbb{P}\left(\begin{smallmatrix} x_0 \text{---} y_0 \\ | \\ x_1 \text{---} y_1 \end{smallmatrix}\right)$ should depend weakly on $\|x - y\|$ for small enough β . For $\|x - y\|$ large enough the probability may approach $\mathbb{P}(x_0 \text{---} x_1)^2$, it is not clear how to prove or disprove such a relation at this time.

6.2.3 Space-time spin configurations

In order to make the connection with spin systems we need the notion of a *space-time spin configuration*. The spin system we shall connect to is the spin-1 Heisenberg model, we shall make this connection via an intertwining that merges two spin- $\frac{1}{2}$ models. For this reason we will take $\theta = 2$ from Section 6.2.2 ($2S + 1$ for $S = \frac{1}{2}$). This is also the reason the lattice $\tilde{\Lambda}$ has two sites for every site in Λ . It is also possible to represent the spin- S model for general S by merging $2S$ spin- $\frac{1}{2}$ models, this will mean $\tilde{\Lambda}$ will have $2S$ sites for every site in Λ . See [81] for more details. This generalisation together with some results analogous to the ones presented here should be straightforward once the spin-1 model is understood. It is not immediately clear which results will still hold however, investigation is required.

From now on we take the cubic lattice in \mathbb{Z}^d with side length L , denoted Λ_L , with periodic boundary conditions. The edge set, \mathcal{E}_L , will consist of pairs of nearest neighbour lattice points. Precisely

$$\Lambda_L = \left\{ -\frac{L}{2} + 1, \dots, \frac{L}{2} \right\}^d, \quad (6.2.8)$$

$$\mathcal{E}_L = \{\{x, y\} \subset \Lambda_L \mid \|x - y\| = 1 \text{ or } |x_i - y_i| = L - 1 \text{ for some } i = 1, \dots, d\}. \quad (6.2.9)$$

Where $\|x - y\|$ is the graph distance between x and y . A space-time spin configuration is a function

$$\sigma : \tilde{\Lambda} \times [0, \beta]_{per} \rightarrow \left\{ -\frac{1}{2}, \frac{1}{2} \right\}. \quad (6.2.10)$$

$\sigma_{x_i, t}$ is piecewise constant in t for any x_i . We further define Σ to be the set of all such functions with a finite number of discontinuities. For a realisation of the process ω we

consider σ that are constant on the vertical segments of each loop in $\mathcal{L}(\omega)$ and that change value on crossing a bar. This restriction on configurations will allow to make the link with spin systems. We call such configurations *compatible* with ω and denote by $\Sigma^{(1)}(\omega)$ the set of all compatible configurations, this is analogous to Section 6.1. The following relation holds as we work on a bipartite lattice, meaning fixing a configuration's value at some (x_i, t) determines the configuration on the entire loop containing (x_i, t) :

$$|\Sigma^{(1)}(\omega)| = 2^{|\mathcal{L}(\omega)|}, \quad (6.2.11)$$

from which we can obtain

$$Y_2^{J_1, J_2}(\beta, \Lambda) = \int \rho_{J_1, J_2}(d\omega) \sum_{\sigma \in \Sigma^{(1)}(\omega)} 1. \quad (6.2.12)$$

We further define the set $\Sigma_{x_i, y_j}^{(1)}(\omega) \supset \Sigma^{(1)}(\omega)$ to be compatible configurations along with configurations that flip spin at points $(x_i, 0)$ or $(y_j, 0)$ (or both) but are otherwise compatible.

When the occurrence of macroscopic loops is proved we will not require the condition that compatible configurations flip value on crossing a bar, in fact this condition would add an unnecessary extra complication. Hence we further define $\Sigma^{(2)}(\omega)$ to be configurations that are constant on loops (and hence do not flip value at bars). $\Sigma_{x_i, y_j}^{(2)}(\omega) \supset \Sigma^{(2)}(\omega)$ denotes the set of configurations in $\Sigma^{(2)}(\omega)$ along with configurations that flip spin at points $(x_i, 0)$ or $(y_j, 0)$ (or both) but are otherwise consistent with the definition of $\Sigma^{(2)}(\omega)$.

As in [111] we will later need a more general setting for the measure on space-time spin configurations. We consider a Poisson point process on $\tilde{\mathcal{E}} \times [0, \beta]$ with events being specifications of the local spin configuration. We will consider discontinuities involving two pairs of sites (x_0, x_1, y_0, y_1) . The objects of the process will be a set of allowed configurations at these sites immediately before and after t . We can denote these events as

$$\frac{\sigma_{x_0, t+} \sigma_{x_1, t+} \quad \sigma_{y_0, t+} \sigma_{y_1, t+}}{\sigma_{x_0, t-} \sigma_{x_1, t-} \quad \sigma_{y_0, t-} \sigma_{y_1, t-}} \quad (6.2.13)$$

Implicit here is an ordering on Λ with $x < y$. An event A is a subset of $\{-1/2, 1/2\}^8$ and occurs with intensity $\iota(A)$. More precisely we let $\iota : \mathcal{P}(\{-1/2, 1/2\}^8) \rightarrow \mathbb{R}$ denote the intensities of the Poisson point process, denoted ρ_ι . Given a realisation, ξ , of ρ_ι let $\Sigma(\xi)$ be the set of configurations compatible with ξ meaning that $\sigma \in \Sigma(\xi)$ if

$$\frac{\sigma_{x_0, t+} \sigma_{x_1, t+} \quad \sigma_{y_0, t+} \sigma_{y_1, t+}}{\sigma_{x_0, t-} \sigma_{x_1, t-} \quad \sigma_{y_0, t-} \sigma_{y_1, t-}} \in A \text{ whenever } \xi \text{ contains the event } A \text{ at point } (x_0, x_1, y_0, y_1, t),$$

and $\sigma_{x_i, t}$ is otherwise constant in t . The measure is then given by ρ_ι with the counting measure on compatible configurations. We note that different intensities can give the same measure as in [111], for ι and ι' intensities it is shown in [111] that

$$\int \rho_\iota(d\xi) \int \rho_{\iota'}(d\xi') \sum_{\sigma \in \Sigma(\xi \cup \xi')} F(\sigma) = \int \rho_{\iota+\iota'}(d\xi) \sum_{\sigma \in \Sigma(\xi)} F(\sigma). \quad (6.2.14)$$

We want to write the Poisson point process involving bars in terms of intensities of specifications of spins. We require that specifications corresponding to single and double sets of bars have intensity $-2J_1$ and J_2 respectively. If we naively define $\tilde{\iota}$ by

$$\tilde{\iota} \left(\left\{ \frac{a' a}{a' c} \quad \frac{a b}{c b} \right\} \right) = -2J_1, \quad \tilde{\iota} \left(\left\{ \frac{a' a}{c' c} \quad \frac{a a'}{c c'} \right\} \right) = J_2. \quad (6.2.15)$$

For any $a, a', b, c, c' \in \{1/2, -1/2\}$, where the first event corresponds to single bars and the second event to double bars. We see there is an overlap on the specification

$$\frac{b a}{b c} \quad \frac{a b}{c b}$$

so this assignment of intensities of specifications cannot be correct. Simply removing the overlapping case from one of the specifications will result in events not having the required intensities. This suggests we should instead define ι by

$$\iota \left(\left\{ \frac{a' a}{c' c} \quad \frac{a a'}{c c'} \right\}_{a' \neq b} \right) = -2J_1, \quad \iota \left(\left\{ \frac{a' a}{a' c} \quad \frac{a b}{c b} \right\}_{a' \neq c'} \right) = J_2, \quad (6.2.16)$$

$$\iota \left(\left\{ \frac{b a}{b c} \quad \frac{a b}{c b} \right\} \right) = J_2 - 2J_1.$$

For any $a, a', b, c, c' \in \{1/2, -1/2\}$. Now each specification is disjoint from the other two and single and double sets of bars have intensities $-2J_1$ and J_2 respectively, as required. We also have $\iota(A) = 0$ for any other specification. Then

$$Y_2^{J_1, J_2}(\beta, \Lambda) = \int \rho_\iota(d\xi) \sum_{\sigma \in \Sigma(\xi)} 1. \quad (6.2.17)$$

This representation will be needed when we show reflection positivity of the loop model.

6.2.4 The general spin-1 SU(2) invariant Heisenberg model

Let S^1, S^2 and S^3 denote the spin-1 matrices as introduced in 2.2.2. Denote $\mathbf{S} = (S^1, S^2, S^3)$. We will use the following matrices:

$$S^1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (6.2.18)$$

Consider a pair (Λ, \mathcal{E}) of a lattice, $\Lambda \subset \mathbb{Z}^d$, and a set of edges, \mathcal{E} , between points in Λ . We will take Λ to be a box in \mathbb{Z}^d , hence Λ is bipartite. We denote by Λ_A and Λ_B the two disjoint lattices such that $\Lambda_A \cup \Lambda_B = \Lambda$ and every $e \in \mathcal{E}$ contains precisely one site from Λ_A and one site from Λ_B .

Recall we take the operator S_x^i for $i = 1, 2, 3$ to be shorthand for the operator $S_x^i \otimes Id_{\Lambda \setminus \{x\}}$. Recall the definition of $\tilde{\Lambda}$ and $\tilde{\mathcal{E}}$ above, we shall use these below.

The most general SU(2) invariant Hamiltonian with two-body interactions for spin-1 is

$$H_{\Lambda}^{J_1, J_2} = - \sum_{\{x, y\} \in \mathcal{E}} \left(J_1 (\mathbf{S}_x \cdot \mathbf{S}_y) + J_2 (\mathbf{S}_x \cdot \mathbf{S}_y)^2 \right). \quad (6.2.19)$$

We will soon drop the parameters J_1, J_2 from $H_{\Lambda}^{J_1, J_2}$ for readability. In this chapter we will be concerned with the region where $J_1 \leq 0 \leq J_2$. Associated to this Hamiltonian we have the following partition function and Gibbs states for $\beta > 0$:

$$Z_{\Lambda, \beta}^{J_1, J_2} = \text{Tr} e^{-\beta H_{\Lambda}^{J_1, J_2}}, \quad (6.2.20)$$

$$\langle \cdot \rangle_{\Lambda, \beta}^{J_1, J_2} = \frac{1}{Z_{\Lambda, \beta}^{J_1, J_2}} \text{Tr} \cdot e^{-\beta H_{\Lambda}^{J_1, J_2}}. \quad (6.2.21)$$

Again we shall drop the parameters J_1, J_2 from the notation.

The following new definitions come from Nachtergaele [81]. We introduce an isometry $V : \mathbb{C}^3 \rightarrow \mathbb{C}^2 \otimes \mathbb{C}^2$ with the property $VD^1(g) = (D^{\frac{1}{2}}(g))^{\otimes 2}V$ for $g \in SU(2)$ and D^S the spin- S representation of SU(2). Here the representation D^1 is given by the matrices (2.2.12) and $D^{\frac{1}{2}}$ is given by the Pauli matrices. It is clear such an isometry exists as we can define it for spin matrices and then extend by linearity (recall that the spin matrices generate the representation). From this we obtain the key relation

$$VS^i = (\sigma^i \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^i)V, \quad (6.2.22)$$

where σ^i are the spin- $\frac{1}{2}$ matrices (hence $2\sigma^i$ are the Pauli matrices). Further we have

$$V^*V = \mathbb{1} \text{ and } VV^* = P, \quad (6.2.23)$$

where P is the projection onto the spin triplet. Hence VS^i acts on $\mathbb{C}^2 \otimes \mathbb{C}^2$ and so using the notation as before $V_x S_x^i$ acts on $\otimes_{y \in \Lambda} \mathbb{C}^2 \otimes \mathbb{C}^2$. We make the following definition

$$R^i := VS^i V^*. \quad (6.2.24)$$

One can check that $R^i = (\sigma^i \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^i)$. To make expressions more concise we will also denote $A_X := \otimes_{x \in X} A_x$ for $X \subset \Lambda$. For these new operators we have a new Hamiltonian (note we have now dropped the J_1 and J_2 parameters)

$$\tilde{H}_\Lambda^{(1)} = - \sum_{\{x,y\} \in \mathcal{E}} \left(J_1 (\mathbf{R}_x \cdot \mathbf{R}_y) + J_2 (\mathbf{R}_x \cdot \mathbf{R}_y)^2 \right), \quad (6.2.25)$$

and associated Gibbs states

$$Z_{\tilde{\Lambda}, \beta}^{(1)} = \text{Tr } P_\Lambda e^{-\beta \tilde{H}_\Lambda^{(1)}}, \quad (6.2.26)$$

$$\langle \cdot \rangle_{\tilde{\Lambda}, \beta}^{(1)} = \frac{1}{Z_{\tilde{\Lambda}, \beta}^{(1)}} \text{Tr} \cdot P_\Lambda e^{-\beta \tilde{H}_\Lambda^{(1)}}. \quad (6.2.27)$$

The connection with the previous Gibbs state can easily be made explicit,

$$\langle A \rangle_{\tilde{\Lambda}, \beta} = \langle V_\Lambda A V_\Lambda^* \rangle_{\tilde{\Lambda}, \beta}^{(1)}. \quad (6.2.28)$$

We use Dirac notation in the following way: $|a, b\rangle$ denotes an element of the one site Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$ and $|a, b\rangle \otimes |c, d\rangle$ for two sites etc.

There are two operators of particular interest, both act on two sites. Firstly we define $\mathcal{S}^{(1)'}$ by its matrix elements

$$\langle a', b' | \otimes \langle c', d' | \mathcal{S}^{(1)'} | a, b \rangle \otimes | c, d \rangle = (-1)^{b-b'} \delta_{a,a'} \delta_{d,d'} \delta_{b,-c} \delta_{b',-c'}. \quad (6.2.29)$$

Geometrically this requires spin b and c and the spins b' and c' to be the negative of each other and also requires $a = a'$ and $d = d'$. This corresponds to the the single bars in the loop picture. The second operator, $\mathcal{D}^{(1)'}$, is also defined via its matrix elements

$$\langle a', b' | \otimes \langle c', d' | \mathcal{D}^{(1)'} | a, b \rangle \otimes | c, d \rangle = (-1)^{a-a'} (-1)^{b-b'} \delta_{a,-d} \delta_{b,-c} \delta_{a',-d'} \delta_{b',-c'}. \quad (6.2.30)$$

The geometrical interpretation this time is that of the double bars. The actual operators

needed are $\mathcal{S}^{(1)} = P\mathcal{S}^{(1)'}P$ and $\mathcal{D}^{(1)} = P\mathcal{D}^{(1)'}P$ in order to account for bars occurring between any x_i and y_j with each i and j from $\{0, 1\}$ being equally likely. Note here that from this definition we see that we require the spin value to change sign on crossing a bar as was mentioned in Section 6.2.3. There are also extra factors in $\mathcal{S}^{(1)}$ and $\mathcal{D}^{(1)}$ of $e^{i\pi a}$ for the bottom half of a bar (denoted \sqcap) and $e^{-i\pi a}$ for the top half of a bar (denoted \sqcup) where $a = \pm\frac{1}{2}$ is the spin value on the site in Λ_A associated to the bar. By direct computation of the matrix elements we can prove the relations

$$\mathcal{S}_{x,y}^{(1)} = -\frac{1}{2}\mathbf{R}_x \cdot \mathbf{R}_y + \frac{1}{2}P_{x,y}, \quad (6.2.31)$$

$$\mathcal{D}_{x,y}^{(1)} = (\mathbf{R}_x \cdot \mathbf{R}_y)^2 - P_{x,y}. \quad (6.2.32)$$

Using these relations we can rewrite the Hamiltonian in the region $J_1 \leq 0 \leq J_2$ as

$$\tilde{H}_{\tilde{\Lambda}}^{(1)} = - \sum_{\{x,y\} \in \mathcal{E}} \left(-2J_1 \mathcal{S}_{x,y}^{(1)} + J_2 \mathcal{D}_{x,y}^{(1)} + (J_1 + J_2)P_{x,y} \right). \quad (6.2.33)$$

We further introduce $\mathcal{S}^{(2)'}$ and $\mathcal{D}^{(2)'}$ by

$$\langle a', b' | \otimes \langle c', d' | \mathcal{S}^{(2)'} | a, b \rangle \otimes | c, d \rangle = \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'}, \quad (6.2.34)$$

$$\langle a', b' | \otimes \langle c', d' | \mathcal{D}^{(2)'} | a, b \rangle \otimes | c, d \rangle = \delta_{a,d} \delta_{b,c} \delta_{a',d'} \delta_{b',c'}. \quad (6.2.35)$$

We again need the symmetrised version of these operators $\mathcal{S}^{(2)} = P\mathcal{S}^{(2)'}P$ and $\mathcal{D}^{(2)} = P\mathcal{D}^{(2)'}P$. The corresponding Hamiltonian is

$$\tilde{H}_{\tilde{\Lambda}}^{(2)} = - \sum_{\{x,y\} \in \mathcal{E}} \left(-2J_1 \mathcal{S}_{x,y}^{(2)} + J_2 \mathcal{D}_{x,y}^{(2)} + (J_1 + J_2)P_{x,y} \right). \quad (6.2.36)$$

This Hamiltonian will be used when showing the occurrence of long loops. This Hamiltonian's Gibbs states will be denoted $\langle \cdot \rangle_{\tilde{\Lambda}, \beta}^{(2)}$.

6.2.5 The random loop representation

We can neglect the term $(J_1 + J_2)P_{x,y}$ in the Hamiltonian (6.2.33) and (6.2.36) and instead add $(2J_1 - J_2)\mathbb{1}$, this does not change the Gibbs states. Doing this allows to use a useful lemma from [2]

$$\exp \left\{ - \sum_{\{x,y\} \in \mathcal{E}} (uA_{x,y} + vB_{x,y} - u - v) \right\} = \int \rho(d\omega) \prod_{(x,y) \in \omega}^* C_{x,y}. \quad (6.2.37)$$

Here ρ is the measure associated to a Poisson point process on $\mathcal{E} \times [0, 1]$ with two events occurring with intensities u and v respectively. The product is ordered according to the times at which the events occur. C is either A or B depending on which event occurs. This is actually a slight extension of the lemma presented in [2]. From this we can obtain

$$\exp \left\{ - \sum_{\{x,y\} \in \mathcal{E}} \left(-2J_1 \mathcal{S}_{x,y}^{(n)} + J_2 \mathcal{D}_{x,y}^{(n)} + 2J_1 - J_2 \right) \right\} = \int \rho(d\omega) \prod_{(x_i, y_j) \in \omega}^* A_{x_i, y_j}^{(n)} \quad (6.2.38)$$

here each $A^{(n)}$ is one of $\mathcal{S}^{(n)}$ or $\mathcal{D}^{(n)}$, this holds for both systems $\tilde{H}_{\Lambda}^{(1)}$ and $\tilde{H}_{\Lambda}^{(2)}$. Again the product is ordered by the time events occur.

We now prove the connection between the loop model and the quantum system. This will enable us to understand certain important correlation functions. After this we should have the tools we need to calculate any two point correlation (at least ones involving only spin operators). The first thing to understand is the extra factor, which we shall denote by $z_{x_i, y_j}(\sigma, \omega)$, the product of all factors $e^{\pm i\pi a}$ from operators $\mathcal{S}^{(1)}$ and $\mathcal{D}^{(2)}$ corresponding to the bars in loop(s) containing x_i and y_j in a realisation ω of ρ_{J_1, J_2} . Again $a \in \{1/2, -1/2\}$ is the value that σ assigns to the portions of these loop(s) in the Λ_A sublattice (or if all of a loop is on the sublattice Λ_B a is given by the negative of the value assigned to the loop). The value of $z_{x_i, y_j}(\sigma, \omega)$ is specified by the following lemma:

Lemma 6.2.1. *For Λ bipartite we have for all i, j*

$$z_{x_i, y_j}(\sigma, \omega) = \begin{cases} 1 & \text{if } \sigma \in \Sigma^{(1)}(\omega) \\ (-1)^{\|x-y\|} & \text{if } \sigma \in \Sigma_{x_i, y_j}^{(1)}(\omega) \setminus \Sigma^{(1)}(\omega) \text{ and } \omega \in E[x_i - y_j]. \end{cases} \quad (6.2.39)$$

Before the proof we should note that the lemma says that the only dependence on σ is at x_i and y_j at time zero. If the spin does not flip at both sites that we get total factor 1, else it depends on which sublattices the sites are in. If the spin only flips at one site then there are no compatible configurations hence the value of the total extra factor is unimportant.

Proof. To begin note that we can take $(i, j) = (0, 0)$. The result for $(i, j) \neq (0, 0)$ follows as the choice of i or j does not affect which sublattice the two sites are in. Suppose $\sigma \in \Sigma^{(1)}(\omega)$. Moving upwards from x_0 the first bar encountered is \sqcap , the bars encountered then alternate between \sqcup and \sqcap . Moving downwards from x_0 we first encounter a bar \sqcup then alternate between \sqcap and \sqcup . This means we can make a matching between bars of the form \sqcap and bars of the form \sqcup . Because there are no spin flips at time zero all the bars \sqcap have factors $e^{i\pi a}$ and all the bars \sqcup have factor $e^{-i\pi a}$ where a is the spin value σ gives to x_0 at time zero. Hence we have full cancellation and are left with factor 1. If there were a spin flip then bars

between x_0 at time $0-$ and y_0 at time $0\pm$ would have factors $e^{i\pi(-a)}$ and $e^{-i\pi(-a)}$ for \sqcap and \sqcup respectively.

If $\sigma \in \Sigma_{x_0, y_0}^{(1)}(\omega) \setminus \Sigma^{(1)}(\omega)$ and $(-1)^{\|x-y\|} = 1$ and $\omega \in E[x_0-y_0]$, then x_0 and y_0 are in the same sublattice. We can thus deduce that the section of loop that moves upwards/downwards from x_0 crosses an even number of bars before reaching y_0 . This means that the loop containing x_0 and y_0 contains an even number of bars of each type (\sqcap or \sqcup). Hence we can make a matching of a bar \sqcup in one ‘half’ of the loop with a bar \sqcup in the other ‘half’ and the same with bars \sqcap , with some bars left over. The factors from bars in the matching will thus be 1 as the spin flip at x_0 at time 0 means one bar in each pair has factor $e^{\pm i\pi a}$ and one bar has factor $e^{\pm i\pi(-a)}$. Here by ‘half’ of a loop we mean the section that connects x_0 at time $0+$ with y_0 at time $0-$ or x_0 at time $0-$ with y_0 at time $0+$. There are still possibly some bars left over as each half of the loop may have a different number of bars in it. A moments thought reveals that there must be an even number of bars left, half of type \sqcap and half of type \sqcup . As the bars \sqcap have factor $e^{-i\pi(\pm a)}$ and the bars \sqcup have factor $e^{i\pi(\pm a)}$ we have full cancellation again and have total factor 1.

For the remaining case $\sigma \in \Sigma_{x_0, y_0}^{(1)}(\omega) \setminus \Sigma^{(1)}(\omega)$ and $(-1)^{\|x-y\|} = -1$ and $\omega \in E[x_0-y_0]$, we have x_0 and y_0 in different sublattices. We can see as last time that the factors from the ‘extra bars’ (that arise from each half of the loop having a different number of bars) will cancel as again there are equal numbers of \sqcap and \sqcup . For the remaining bars there are an odd number in each half of the loop, this means we can make a matching for all but two of the bars. The factors from bars in the matching will cancel each other. For the remaining two bars one is a \sqcap with factor $e^{i\pi(\pm a)}$ and one is a \sqcup with factor $e^{-i\pi(\mp a)}$ (the sign of a is opposite due to the spin flip at x_0 at time 0). This means the overall factor is $(\pm i)^2 = -1$. This completes the proof. \square

In light of Proposition 6.2.1 the following proposition can be proved in the same way as Theorem 3.2 in [111].

Proposition 6.2.2. *The partition functions $Z_{\tilde{\Lambda}, \beta}^{(i)}$ $i = 1, 2$ are given by*

$$Z_{\tilde{\Lambda}, \beta}^{(i)} = \int \rho(d\omega) \sum_{\Sigma^{(i)}(\omega)} \prod_{\{x_i, y_j\} \in \mathcal{E}} z_{x_i, y_j}(\sigma, \omega) = \int \rho(d\omega) 2^{|\mathcal{L}(\omega)|} = Y_2^{J_1, J_2}(\beta, \Lambda). \quad (6.2.40)$$

We also have the following identity, note that for $\tilde{H}_{\tilde{\Lambda}_L}^{(2)}$ the factor $z_{x_i, y_j}(\sigma, \omega)$ does not appear as there are no spin flips at bars.

$$\text{Tr}(\sigma^3 \otimes \mathbb{1})_x (\sigma^3 \otimes \mathbb{1})_y e^{-\beta \tilde{H}_{\tilde{\Lambda}}^{(i)}} = \int \rho(d\omega) \sum_{\Sigma^{(i)}(\omega)} \left(\prod_{\{x_i, y_j\} \in \mathcal{E}} z_{x_i, y_j}(\sigma, \omega) \right) \sigma_{x_0} \sigma_{y_0}, \quad (6.2.41)$$

where σ_{z_i} is the value of a space time configuration, σ , at time 0 and site z_i .

With the important details understood we can calculate some correlations in terms of probabilities in the loop model. The most important correlations here are the Néel and nematic correlations (Proposition 6.2.3 a) and b) respectively).

Proposition 6.2.3. For $i, j = 1, 2, 3$, $x \neq y$, $i \neq j$ and Λ bipartite

- a) $\langle S_x^i S_y^i \rangle_{\Lambda, \beta} = (-1)^{\|x-y\|} \mathbb{P}(x_0=y_0)$,
- b) $\langle (S_x^i)^2 (S_y^i)^2 \rangle_{\Lambda, \beta} - \langle (S_x^i)^2 \rangle_{\Lambda, \beta} \langle (S_y^i)^2 \rangle_{\Lambda, \beta} = -\frac{1}{36} + \frac{1}{4} \mathbb{P} \left(\begin{array}{c} x_0 \\ | \leftarrow | \\ x_1 \end{array} \begin{array}{c} y_0 \\ | \\ y_1 \end{array} \right) + \frac{1}{2} \mathbb{P} \left(\begin{array}{c} x_0 \leftarrow y_0 \\ | \leftarrow | \\ x_1 \leftarrow y_1 \end{array} \right) + \frac{1}{4} \mathbb{P} \left(\begin{array}{c} x_0 \rightleftarrows y_0 \\ | \leftarrow | \\ x_1 \rightleftarrows y_1 \end{array} \right)$,
- c) $\langle S_x^i S_x^j S_y^i S_y^j \rangle_{\Lambda, \beta} = \frac{1}{4} \left[(-1)^{\|x-y\|} \mathbb{P}(x_0=y_0) + \mathbb{P} \left(\begin{array}{c} x_0 \leftarrow y_0 \\ | \leftarrow | \\ x_1 \leftarrow y_1 \end{array} \right) \right]$,
- d) $\langle S_x^i S_x^j S_y^j S_y^i \rangle_{\Lambda, \beta} = \frac{1}{4} \left[(-1)^{\|x-y\|} \mathbb{P}(x_0=y_0) + \mathbb{P} \left(\begin{array}{c} x_0 \leftarrow y_0 \\ | \leftarrow | \\ x_1 \leftarrow y_1 \end{array} \right) \right]$,
- e) $\langle (S_x^i)^2 (S_y^j)^2 \rangle_{\Lambda, \beta} = \frac{5}{12} + \frac{1}{4} \left[\mathbb{P} \left(\begin{array}{c} x_0 \\ | \leftarrow | \\ x_1 \end{array} \begin{array}{c} y_0 \\ | \\ y_1 \end{array} \right) + \mathbb{P} \left(\begin{array}{c} x_0 \rightarrow y_0 \\ | \leftarrow | \\ x_1 \leftarrow y_1 \end{array} \right) - \mathbb{P} \left(\begin{array}{c} x_0 \rightleftarrows y_0 \\ | \leftarrow | \\ x_1 \rightleftarrows y_1 \end{array} \right) \right]$.

Proof. We will calculate the correlations in order. First note that each S^i plays an equivalent rôle, hence cyclic permutations of the indices (1, 2, 3) does not alter the expectation. Using this together with $(S^i S^j)^T = \pm (S^j S^i)$ (the sign depending on the value of i and j) means we can take $i = 3$ and $j = 1$. For each we will expand using (6.2.24) and (6.2.28).

Proof of a). First

$$\langle S_x^3 S_y^3 \rangle_{\Lambda, \beta} = \langle (\sigma^3 \otimes \mathbb{1} \otimes \sigma^3 \otimes \mathbb{1} + \sigma^3 \otimes \mathbb{1} \otimes \mathbb{1} \otimes \sigma^3 + \mathbb{1} \otimes \sigma^3 \otimes \sigma^3 \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^3 \otimes \mathbb{1} \otimes \sigma^3)_{x,y} \rangle_{\Lambda, \beta}^{(1)}. \quad (6.2.42)$$

We see that due to sites z_0 and z_1 being interchangeable for $z \in \Lambda$ each of the four terms in the sum have the same expectation. We also know from Proposition 6.2.2

$$\text{Tr} (\sigma^3 \otimes \mathbb{1})_x (\sigma^3 \otimes \mathbb{1})_y e^{-\beta \tilde{H}_\Lambda} = \int \rho(d\omega) \sum_{\Sigma^{(1)}(\omega)} \sigma_{x_0} \sigma_{y_0}. \quad (6.2.43)$$

We note that the integral differs from zero only on the set where x_0 and y_0 are connected. If x and y are in different sublattices the product of spin configuration values is $-\frac{1}{4}$, if in the same sublattice the product is $\frac{1}{4}$. We can deduce that

$$\langle S_x^3 S_y^3 \rangle_{\Lambda, \beta} = (-1)^{\|x-y\|} \mathbb{P}(x_0=y_0). \quad (6.2.44)$$

Proof of b). For the second correlation

$$(R_x^3)^2 = (\sigma^3 \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^3)_x^2 = \left(\frac{1}{2} \mathbb{1} \otimes \mathbb{1} + 2\sigma^3 \otimes \sigma^3 \right)_x. \quad (6.2.45)$$

We see that expanding as before gives

$$\langle (S_x^3)^2 \rangle_{\Lambda, \beta} = \langle (R_x^3)^2 \rangle_{\tilde{\Lambda}, \beta}^{(1)} = \frac{1}{Z_{\tilde{\Lambda}, \beta}^{(1)}} \int \rho(d\omega) \sum_{\sigma \in \Sigma^{(1)}(\omega)} \left(\frac{1}{2} + 2\sigma_{x_0} \sigma_{x_1} \right) = \frac{1}{2} + \frac{1}{2} \mathbb{P}(x_0 - x_1). \quad (6.2.46)$$

From this and the fact that $\langle (S_x^3)^2 \rangle_{\Lambda, \beta} = \frac{1}{3} \langle \mathbf{S}_x \cdot \mathbf{S}_x \rangle_{\Lambda, \beta} = \frac{2}{3}$ we can deduce that

$$\mathbb{P}(x_0 - x_1) = \frac{1}{3}. \quad (6.2.47)$$

For the first term in the correlation we again note that $\langle (S_x^3)^2 (S_y^3)^2 \rangle_{\Lambda, \beta} = \langle (R_x^3)^2 (R_y^3)^2 \rangle_{\tilde{\Lambda}, \beta}^1$.

We then calculate as before:

$$\begin{aligned} (R_x^3)^2 (R_y^3)^2 &= (\sigma^3 \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^3)_x^2 (\sigma^3 \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^3)_y^2 \\ &= \left(\frac{1}{2} \mathbb{1} \otimes \mathbb{1} + 2\sigma^3 \otimes \sigma^3 \right)_x \left(\frac{1}{2} \mathbb{1} \otimes \mathbb{1} + 2\sigma^3 \otimes \sigma^3 \right)_y \\ &= \left(\frac{1}{4} \mathbb{1}^{\otimes 4} + \sigma^3 \otimes \sigma^3 \otimes \mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes \sigma^3 \otimes \sigma^3 + 4(\sigma^3)^{\otimes 4} \right)_{x,y}. \end{aligned} \quad (6.2.48)$$

Now following through the same expansion as before we have

$$\langle (S_x^3)^2 (S_y^3)^2 \rangle_{\Lambda, \beta} = \frac{1}{Z_{\tilde{\Lambda}, \beta}^{(1)}} \int \rho(d\omega) \sum_{\sigma \in \Sigma^{(1)}(\omega)} \left(\frac{1}{4} + \sigma_{x_0} \sigma_{x_1} + \sigma_{y_0} \sigma_{y_1} + 4\sigma_{x_0} \sigma_{x_1} \sigma_{y_0} \sigma_{y_1} \right). \quad (6.2.49)$$

Using (6.2.47) and noting that the last term in the sum requires either two loops containing two of the sites x_0, x_1, y_0, y_1 each or one loop containing all four sites to give a non-zero contribution to the sum overall (if one site is not connected to any other its spin value can be $\pm \frac{1}{2}$ independently of other sites, averaging the integral on this set to zero) we have

$$\langle (S_x^3)^2 (S_y^3)^2 \rangle_{\Lambda, \beta} - \langle (S_x^3)^2 \rangle_{\Lambda, \beta} \langle (S_y^3)^2 \rangle_{\Lambda, \beta} = -\frac{1}{36} + \frac{1}{4} \mathbb{P} \left(\begin{array}{c} x_0 \text{---} y_0 \\ | \text{---} | \\ x_1 \text{---} y_1 \end{array} \right) + \frac{1}{2} \mathbb{P} \left(\begin{array}{c} x_0 \text{---} y_0 \\ | \text{---} | \\ x_1 \text{---} y_1 \end{array} \right) + \frac{1}{4} \mathbb{P} \left(\begin{array}{c} x_0 \text{---} y_0 \\ | \text{---} | \\ x_1 \text{---} y_1 \end{array} \right). \quad (6.2.50)$$

The probability $\mathbb{P} \left(\begin{array}{c} x_0 \text{---} y_0 \\ | \text{---} | \\ x_1 \text{---} y_1 \end{array} \right)$ comes with twice the weight because there are two ways to connect both sites at x to different sites at y (but only one way both sites at x can be connected and both sites at y can be connected).

Proof of c). For the third correlation we use the same expansion

$$\langle S_0^1 S_0^3 S_x^1 S_x^3 \rangle_{\Lambda, \beta} = \frac{4}{Z_{\tilde{\Lambda}, \beta}^{(1)}} \text{Tr} (\sigma^1 \sigma^3 \otimes \mathbb{1} + \sigma^1 \otimes \sigma^3)_x (\sigma^1 \sigma^3 \otimes \mathbb{1} + \sigma^1 \otimes \sigma^3)_y P_{\Lambda} e^{-\beta \tilde{H}_{\tilde{\Lambda}}^{(1)}}. \quad (6.2.51)$$

The factor 4 has come from grouping together terms such as $\sigma^1 \otimes \sigma^3$ and $\sigma^3 \otimes \sigma^1$ that have

the same expectation. A useful observation at this stage is that $\sigma^1 \sigma^3 = \frac{-i}{2} \sigma^2$. Calculating further and noting that the two cross terms in the above product have the same expectation we see

$$\langle S_0^1 S_0^3 S_x^1 S_x^3 \rangle_{\Lambda, \beta} = 4 \left\langle -\frac{1}{4} \sigma^2 \otimes \mathbb{1} \otimes \sigma^2 \otimes \mathbb{1} - i \sigma^2 \otimes \mathbb{1} \otimes \sigma^1 \otimes \sigma^3 + \sigma^1 \otimes \sigma^3 \otimes \sigma^1 \otimes \sigma^3 \right\rangle_{\tilde{\Lambda}, \beta}^{(1)}. \quad (6.2.52)$$

From the symmetric roles of σ^i for $i = 1, 2, 3$ and part a) we know the first term is $-\frac{(-1)^{\|x-y\|}}{4} \mathbb{P}(x_0-y_0)$. For the second term we need $\langle \sigma^2 \otimes \mathbb{1} \otimes \sigma^1 \otimes \sigma^3 \rangle_{\tilde{\Lambda}, \beta}^{(1)}$. This is the expectation of a matrix with purely imaginary entries, due to the one appearance of σ^2 . Now we note three pieces of information that allow us to calculate this expectation. All the matrices $e^{-\beta \tilde{H}_{\tilde{\Lambda}}^{(1)}}$, $P_{\tilde{\Lambda}}$, σ^1 , σ^2 and σ^3 are Hermitian. The matrices σ^i are acting on different sites in $\tilde{\Lambda}$ and hence they commute. $e^{-\beta \tilde{H}_{\tilde{\Lambda}}^{(1)}}$ and $P_{\tilde{\Lambda}}$ commute and have real entries. This means taking the adjoint of the operator leaves the expectation unchanged. Because the operator is purely imaginary we should obtain the negative of what we started with on taking the adjoint. Hence the correlation must be zero.

For the last term we expand as in Proposition 6.2.2 and obtain

$$\langle \sigma^1 \otimes \sigma^3 \otimes \sigma^1 \otimes \sigma^3 \rangle_{\tilde{\Lambda}, \beta}^{(1)} = \frac{1}{Z_{\tilde{\Lambda}, \beta}^{(1)}} \int \rho(d\omega) \sum_{\sigma \in \Sigma_{x_0, y_0}^{(1)}(\omega)} z_{x_0, y_0}(\sigma, \omega) \langle \sigma_{\cdot, 0+} | \sigma^1 \otimes \sigma^3 \otimes \sigma^1 \otimes \sigma^3 | \sigma_{\cdot, 0-} \rangle \quad (6.2.53)$$

Here $\sigma_{\cdot, 0\pm}$ denotes the full spin configuration for some $\sigma \in \Sigma_{x_0, y_0}(\omega)$ at time $0\pm$ respectively. Also note that as σ^1 flips spins and σ^3 does not the set of space-time spin configurations $\Sigma_{x_0, y_0}^{(1)}(\omega)$ is the correct set. We could expand the set of configurations we sum over to include configurations that flip spin at sites x_1 and y_1 at time zero but these would not be compatible with σ^3 acting at time zero at those sites hence they would not contribute. Recall that a loop that contains a site that spin flips at time zero cannot contain only one such site, hence the set of configurations that contribute to the integral is $E[x_0-y_0]$. Again the set of configurations where one of the sites x_1 or y_1 is not connected to any of the other three does not contribute to the integral. Combining these two facts we see that the only sets of configurations that contribute to the integral are those where there are two loops each containing two sites (one with x_0 and y_0 and the other with x_1 and y_1), or one loop containing all four sites. For the case of two loops there is one factor of $z_{x_0, y_0}(\sigma, \omega) = (-1)^{\|x-y\|}$ from the loop containing x_0 and y_0 (where σ^1 acts). Another factor of $(-1)^{\|x-y\|}$ comes from the loop containing x_1 and y_1 and the condition that the spin flips on crossing a bar. Note that for the first loop there is no such factor coming from spin flips at bars because $\sigma^1 | \pm \frac{1}{2} \rangle = +\frac{1}{2} | \mp \frac{1}{2} \rangle$ hence there is a factor of $+\frac{1}{2}$ regardless of the spin value at the site. For the case of one loop containing all sites the order that sites occur in the loop is important, this is because both σ^1 and σ^3 are

acting at sites in the loop. If, when following the loop, the site y_1 appears directly before or after the site x_1 then the section of loop between these sites follows the normal rule of flipping spins at bars (or if we follow the loop the other way we pass through two spin flips at time zero as well, these cancel each other out as far as the product of spins at sites x_1 and y_1 is concerned). This means we have a factor of $(-1)^{\|x-y\|}$ as before. If one of the sites x_0 or y_0 appears between sites x_1 and y_1 on the loop the effect of the extra spin flip changes the sign of the factor coming from the product of spins, giving a factor of $-(-1)^{\|x-y\|}$. As before we also have the factor $z_{x_0, y_0}(\sigma, \omega) = (-1)^{\|x-y\|}$ in both cases. This means the correlation is

$$\langle \sigma^1 \otimes \sigma^3 \otimes \sigma^1 \otimes \sigma^3 \rangle_{\tilde{\Lambda}, \beta}^{(1)} = \frac{1}{16} \left[\mathbb{P} \left(\begin{array}{c} x_0 \text{---} y_0 \\ \text{---} x_1 \text{---} y_1 \end{array} \right) + \mathbb{P} \left(\begin{array}{c} x_0 \text{---} y_0 \\ \uparrow \text{---} \downarrow \\ x_1 \text{---} y_1 \end{array} \right) - \mathbb{P} \left(\begin{array}{c} x_0 \text{---} y_0 \\ \downarrow \text{---} \uparrow \\ x_1 \text{---} y_1 \end{array} \right) \right]. \quad (6.2.54)$$

Recall that the arrows in the events show the direction that the loop is traversed. From this we can finally deduce that

$$\langle S_x^1 S_x^3 S_y^1 S_y^3 \rangle_{\Lambda, \beta} = \frac{1}{4} \left[-(-1)^{\|x-y\|} \mathbb{P}(x_0=y_0) + \mathbb{P} \left(\begin{array}{c} x_0 \text{---} y_0 \\ \text{---} x_1 \text{---} y_1 \end{array} \right) + \mathbb{P} \left(\begin{array}{c} x_0 \text{---} y_0 \\ \uparrow \text{---} \downarrow \\ x_1 \text{---} y_1 \end{array} \right) - \mathbb{P} \left(\begin{array}{c} x_0 \text{---} y_0 \\ \downarrow \text{---} \uparrow \\ x_1 \text{---} y_1 \end{array} \right) \right]. \quad (6.2.55)$$

Now we note that the last two probabilities are equal (swap y_0 and y_1).

The correlations d) and e) follow easily using the same techniques and considerations as above. \square

For the $\tilde{H}_{\tilde{\Lambda}}^{(2)}$ model the factor $z_{x_i, y_j}(\sigma, \omega)$ does not play a role (it is equal to one in all cases). There are no spin flips at bars, making several aspects simpler. We will require the following identity, it is easy to prove

$$\langle R_x^3 R_y^3 \rangle_{\tilde{\Lambda}, \beta}^{(2)} = \mathbb{P}(x_0=y_0). \quad (6.2.56)$$

From this we can easily obtain some bounds on these correlations that are potentially very difficult to obtain without the loop model.

Corollary 6.2.4. *For $i, j = 1, 2, 3$, $x \neq y$, $i \neq j$ and Λ bipartite*

$$\mathbf{a)} \quad \langle (S_x^i)^2 (S_y^i)^2 \rangle_{\Lambda, \beta} - \langle (S_x^3)^2 \rangle_{\Lambda, \beta} \langle (S_y^3)^2 \rangle_{\Lambda, \beta} \leq \frac{1}{18} + \frac{3}{4} (-1)^{\|x-y\|} \langle S_x^i S_y^i \rangle_{\Lambda, \beta}$$

$$\mathbf{b)} \quad \langle S_x^i S_x^j S_y^i S_y^j \rangle_{\Lambda, \beta} \leq \frac{1}{4} ((-1)^{\|x-y\|} - 1) \langle S_x^i S_y^i \rangle_{\Lambda, \beta}$$

$$\mathbf{c)} \quad \langle S_x^i S_x^j S_y^i S_y^j \rangle_{\Lambda, \beta} \leq \frac{1}{4} ((-1)^{\|x-y\|} + 1) \langle S_x^i S_y^i \rangle_{\Lambda, \beta}$$

$$\mathbf{d)} \quad \langle S_x^i S_x^j S_y^i S_y^j \rangle_{\Lambda, \beta} \begin{cases} \geq 0 & \text{if } \|x-y\| \text{ is odd} \\ \leq 0 & \text{if } \|x-y\| \text{ is even} \end{cases}$$

$$\mathbf{e)} \quad \langle S_x^i S_x^j S_y^i S_y^j \rangle_{\Lambda, \beta} \begin{cases} \leq 0 & \text{if } \|x-y\| \text{ is odd} \\ \geq 0 & \text{if } \|x-y\| \text{ is even} \end{cases}$$

Proof. All inequalities are immediate from Proposition 6.2.3 when we note that $E\left[\begin{smallmatrix} x_0 & y_0 \\ \perp & \perp \\ x_1 & y_1 \end{smallmatrix}\right]$ is a sub-event of $E[x_0 - x_1]$ and $E\left[\begin{smallmatrix} x_0 & \perp & y_0 \\ \perp & \perp & \perp \\ x_1 & \perp & y_1 \end{smallmatrix}\right]$ is a sub-event of $E[x_0 - y_0]$. \square

Other inequalities of interest involve correlations between nearest neighbour points. Equation (29) in [106] allows us to obtain the following bound in the ground state ($\beta \rightarrow \infty$)

$$\mathbb{P}(0_0 - e_{1_0}) \geq \frac{1}{d} \frac{2J_2 - 3J_1}{4J_2 - 3J_1}. \quad (6.2.57)$$

Now looking at Proposition 6.2.3 b) for $\|x - y\| = 1$ (say $x = 0, y = e_1$) we see that if $J_1 = 0$ then the event $\mathbb{P}(0_0 - e_{1_0})$ puts us into the case of one of the last two probabilities. Ignoring the first probability (as it is difficult to control) we obtain (for $J_2 > 0 = J_1$)

$$\langle (S_0^3)^2 (S_{e_1}^3)^2 \rangle_{\Lambda, \beta} - \langle (S_0^3)^2 \rangle_{\Lambda, \beta} \langle (S_{e_1}^3)^2 \rangle_{\Lambda, \beta} \geq -\frac{1}{36} + \frac{1}{8d}. \quad (6.2.58)$$

This bound is positive for $d \leq 4$, however it was not sufficient to deduce nematic order Theorem 6.2.12. A lower bound on $\rho(e_1)$ in terms of $\mathbb{P}(0_0 - e_{1_0})$ can be deduced.

Proposition 6.2.5. *For $J_2 > 0$*

$$\rho(e_1) \geq \frac{-J_1}{3J_2} + \frac{2}{9} - \left(\frac{-J_1}{J_2} + \frac{1}{2} \right) \mathbb{P}(0_0 - e_{1_0}). \quad (6.2.59)$$

Proof. We use that $\lim_{\beta \rightarrow \infty} \langle H_{\Lambda_L}^{J_1, J_2} \rangle_{\beta} \leq \langle \psi, H_{\Lambda_L}^{J_1, J_2} \psi \rangle$ for any state ψ . The expectation of $H_{\Lambda_L}^{J_1, J_2}$ can be calculated as

$$\begin{aligned} \langle H_{\Lambda_L}^{J_1, J_2} \rangle_{\beta} &= -d|\Lambda_L| \langle J_1 \mathbf{S}_x \cdot \mathbf{S}_y + J_2 (\mathbf{S}_x \cdot \mathbf{S}_y)^2 \rangle_{\beta} \\ &= -d|\Lambda_L| \left(-3J_1 \mathbb{P}(0_0 - e_{1_0}) + 3J_2 \left(\rho(e_1) + \frac{4}{9} \right) + \frac{3}{2} J_2 \mathbb{P}\left(\begin{smallmatrix} 0_0 & \perp & e_{1_0} \\ \perp & \perp & \perp \\ 0_1 & \perp & e_{1_1} \end{smallmatrix}\right) \right). \end{aligned} \quad (6.2.60)$$

Now we define a state $\psi_{\text{Néel}} = \otimes_{x \in \Lambda_L} |(-1)^x\rangle$ and find

$$\langle \psi_{\text{Néel}}, H_{\Lambda_L}^{J_1, J_2} \psi_{\text{Néel}} \rangle = -d|\Lambda_L| (-J_1 + 2J_2). \quad (6.2.61)$$

The result follows from using the bound $\mathbb{P}\left(\begin{smallmatrix} 0_0 & \perp & e_{1_0} \\ \perp & \perp & \perp \\ 0_1 & \perp & e_{1_1} \end{smallmatrix}\right) \leq \mathbb{P}(0_0 - e_{1_0})$. \square

6.2.6 Occurrence of macroscopic loops

Setting and results

We take the cubic lattice in \mathbb{Z}^d with side length L , denoted Λ_L , with periodic boundary conditions. The edge set, \mathcal{E}_L , will consist of pairs of nearest neighbour lattice points. Precisely

$$\Lambda_L = \left\{ -\frac{L}{2} + 1, \dots, \frac{L}{2} \right\}^d, \quad (6.2.62)$$

$$\mathcal{E}_L = \{\{x, y\} \subset \Lambda_L \mid \|x - y\| = 1 \text{ or } |x_i - y_i| = L - 1 \text{ for some } i = 1, \dots, d\}. \quad (6.2.63)$$

For the main theorem we need to introduce two integrals, they come about due to similar considerations as in [58]

$$I_d = \frac{1}{(2\pi)^d} \int_{[-\pi, \pi]^d} \left(\frac{1}{d} \sum_{i=1}^d \cos k_i \right)_+ \sqrt{\frac{\varepsilon(k + \pi)}{\varepsilon(k)}} dk, \quad (6.2.64)$$

$$K_d = \frac{1}{(2\pi)^d} \int_{[-\pi, \pi]^d} \sqrt{\frac{\varepsilon(k + \pi)}{\varepsilon(k)}} dk. \quad (6.2.65)$$

Here $(\cdot)_+$ denotes the positive part and $\varepsilon(k) = 2 \sum_{i=1}^d (1 - \cos(k_i))$.

Theorem 6.2.6. *Let $d \geq 3$ and $J_1 \leq 0 \leq J_2$, there is a β_0 such that for $\beta > \beta_0$ and L even there is a $c = c(J_1, J_2, d, \beta) > 0$ such that*

$$\liminf_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \mathbb{P}(0_0 - x_0) \geq c. \quad (6.2.66)$$

More precisely we obtain two possibilities for this constant, c :

$$\liminf_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \mathbb{P}(0_0 - x_0) \geq \liminf_{L \rightarrow \infty} \begin{cases} \sqrt{\mathbb{P}(0_0 - e_{1_0})} \left(\sqrt{\mathbb{P}(0_0 - e_{1_0})} - I_d \sqrt{\frac{1}{4} - \frac{J_2}{J_1}} \right) + o\left(\frac{1}{\beta}\right), \\ 1 - K_d \sqrt{\mathbb{P}(0_0 - e_{1_0})} \sqrt{\frac{1}{4} - \frac{J_2}{J_1}} + o\left(\frac{1}{\beta}\right). \end{cases} \quad (6.2.67)$$

Note we have already taken a $\liminf_{L \rightarrow \infty}$ for the integrals I_d, K_d but we do not write their discrete version here for brevity, the origin of their discrete versions is at the end of this section. Showing that there is a positive lower bound for (6.2.67) is sufficient to prove the theorem. It can be seen from the proof that a positive lower bound will exist for L large enough, however it is the infinite volume limit that we are really interested in. Positivity of this lower bound implies the occurrence of macroscopic loops and hence implies Néel order for those values of J_1 and J_2 in the spin-1 system.

Of course we see that for $-J_1 + J_2 > 0$ the positivity of the lower bound doesn't depend on the value of $J_1^2 + J_2^2$, only on the ratio $-J_1/J_2$. This means there corresponds an angle, measured from the J_1 axis, such that for angles less than this we have proved the existence of macroscopic loops. The bound is positive for large enough β if

$$\sqrt{\mathbb{P}(0_0 - e_{1_0})} < \frac{1}{K_d} \sqrt{\frac{-4J_1}{-J_1 + 4J_2}} \text{ or } \sqrt{\mathbb{P}(0_0 - e_{1_0})} > I_d \sqrt{\frac{1}{4} - \frac{J_2}{J_1}}. \quad (6.2.68)$$

One of these is certainly satisfied if $I_d K_d < (-4J_1)/(-J_1 + 4J_2)$. A table of values of I_d and K_d for various d is presented Section 6.2.1 and in [111]. If $J_1^2 + J_2^2 = 1$ this is the case in $d = 3$ for $J_1 < -0.42$, $d = 4$ for $J_1 < -0.28$ and $d = 5$ for $J_1 < -0.22$.

A similar theorem (Theorem 6.2.12) concerning nematic order (corresponding to correlation b) in 6.2.3) can be proved using the same methods. Unfortunately showing that one of the lower bounds obtained was positive proved difficult due to the seemingly unavoidable issue of bounding more complicated connection probabilities from below.

In [70] the theorem is proved by appealing to previous literature and using the loop model when required. The theorem can also be achieved by just using the loop model. The proof will be laid out as follow. Firstly reflection positivity will be proved for the loop model. From this we obtain an infrared bound for a correlation function related to $\mathbb{P}(0_0 - e_{1_0})$. We will then use the Falk-Bruch inequality to transfer this bound to a bound on the Fourier transform of $\mathbb{P}(0_0 - e_{1_0})$. We work with this model as the lack of spin flips at bars makes it possible to prove reflection positivity and obtain the required infrared bound.

Reflection positivity for the random loop model

We first introduce some new notation for readability. The aim is to follow the approach in [111] hence notation will be largely consistent where possible. First, for $t \in [0, \beta]$ and $x \in \Lambda_L$ we denote the probability that the point $(0_0, 0) \in \tilde{\Lambda}_L \times [0, \beta]$ is connected to the point (x_0, t) by $\kappa(x, t)$, when $t = 0$ we will abbreviate this to $\kappa(x)$. We define the Fourier and inverse Fourier transform as follows

$$\hat{\kappa}(k, t) = \sum_{x \in \Lambda_L} e^{-ik \cdot x} \kappa(x, t), \quad (6.2.69)$$

$$\kappa(x, t) = \frac{1}{L^d} \sum_{k \in \Lambda_L^*} e^{ik \cdot x} \hat{\kappa}(k, t). \quad (6.2.70)$$

Here $\Lambda_L^* = \left\{ k \in \frac{2\pi}{L} \mathbb{Z}^d \mid -\pi < k_n \leq \pi, n = 1, \dots, d \right\}$ is the dual lattice to Λ_L .

Recall the definition of a space-time spin configuration $\sigma : \tilde{\Lambda}_L \times [0, \beta] \rightarrow \{-1/2, 1/2\}$. We will work with $\tilde{H}_{\tilde{\Lambda}_L}^2$ for the remainder of this section as we are currently interested in loops (so no spin flips at bars). These results automatically transfer to results about long-range order in the spin models. We also introduce real vector fields $\mathbf{v} = (v_{x_i})_{x \in \Lambda_L}$ that act on sites of $\tilde{\Lambda}_L$ (but with values that only depend on $x \in \Lambda_L$, not on $i \in \{0, 1\}$). More precisely \mathbf{v} is a function $\tilde{\Lambda}_L \rightarrow \mathbb{R}$ such that $v_{x_0} = v_{x_1}$ for every $x \in \Lambda_L$. Now we define a new partition function

$$Z(\mathbf{v}) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma^{(2)}(\xi)} \exp \left\{ -(-2J_1) \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta dt \left[(\sigma_{x_i, t} - \sigma_{y_j, t})(v_{x_i} - v_{y_j}) + \frac{1}{4}(v_{x_i} - v_{y_j})^2 \right] \right\}. \quad (6.2.71)$$

Notice that $Z(0) = Z_{\tilde{\Lambda}, \beta}^{(2)}$. We write v_{x_i} even though there is no dependence on i as it will be convenient to define an inner product on $\tilde{\Lambda}_L$ (6.2.81) to avoid chasing extra factors of 2 in calculations. We can also write this as

$$Z(\mathbf{v}) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma^{(2)}(\xi)} \exp \left\{ -(-2J_1) \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta dt \left[(\sigma_{x_i, t} + \frac{1}{2}v_{x_i} - \sigma_{y_j, t} - \frac{1}{2}v_{y_j})^2 - (\sigma_{x_i, t} - \sigma_{y_j, t})^2 \right] \right\}. \quad (6.2.72)$$

In order to prove reflection positivity for this partition function we must introduce reflections in a concrete way, it turns out that they can be simply indexed. For $i \in \{1, \dots, d\}$ and $l \in \{\frac{1}{2}, \frac{3}{2}, \dots, L - \frac{1}{2}\}$ let $R_{i, l}$ be the reflection $\tilde{\Lambda}_L \rightarrow \tilde{\Lambda}_L$ across edges associated to $\{x, y\} \in \mathcal{E}$ for $x_i = l - \frac{1}{2}$, $y_i = l + \frac{1}{2}$. Recall that sites $x_0, x_1 \in \tilde{\Lambda}_L$ play identical roles in the random loop model and we consider them as having the same spatial coordinates. We also define the parts of $\tilde{\Lambda}_L$ to the ‘left’ and ‘right’ of the plane of reflection as the set of points in $\tilde{\Lambda}_L$ associated to the following subsets of Λ_L

$$\Lambda_L^{(1)} = \left\{ x \in \Lambda_L \mid x_i = l - \frac{L}{2}, \dots, l - \frac{1}{2} \right\}, \quad \Lambda_L^{(2)} = \left\{ x \in \Lambda_L \mid x_i = l + \frac{1}{2}, \dots, l + \frac{L}{2} \right\}. \quad (6.2.73)$$

We can then write the field as $\mathbf{v} = (\mathbf{v}^{(1)}, \mathbf{v}^{(2)})$ where $\mathbf{v}^{(i)} = \mathbf{v}|_{\tilde{\Lambda}_L^{(i)}}$. Also write $R\mathbf{v}^{(1)}$ for the field $(R\mathbf{v}^{(1)})_x = v_{R^x}^{(1)}$, $x \in \tilde{\Lambda}_L^{(1)}$ and define $R\mathbf{v}^{(2)}$ similarly. Note that if $x \in \Lambda^{(1)}$ then $Rx \in \Lambda^{(2)}$. Now we can state and prove the property of reflection positivity.

Lemma 6.2.7.

$$Z(\mathbf{v}^{(1)}, \mathbf{v}^{(2)})^2 \leq Z(\mathbf{v}^{(1)}, R\mathbf{v}^{(1)})Z(R\mathbf{v}^{(2)}, \mathbf{v}^{(2)}) \quad (6.2.74)$$

Proof. We want to split the assignment of intensities ι into ι' and ι'' such that $\iota = \iota' + \iota''$ in a helpful way. ι'' will consist of single bar events where the spin value at time $t-$ and $t+$ are the same at each of the four sites associated to it.

$$\iota'' \left(\left\{ \frac{a' \ a}{a' \ a} \ \frac{a \ b}{a \ b} \right\} \right) = -2J_1 \quad (6.2.75)$$

ι' makes up the remaining events in ι

$$\iota' \left(\left\{ \frac{a' a}{a' c} \frac{a b}{c b} \right\}_{a \neq c} \right) = -2J_1, \quad \iota' \left(\left\{ \frac{a' a}{c' c} \frac{a a'}{c c'} \right\}_{a' \neq c'} \right) = J_2, \quad \iota' \left(\left\{ \frac{b a}{b c} \frac{a b}{c b} \right\} \right) = J_2. \quad (6.2.76)$$

Here it may be helpful to interpret these intensities slightly differently. One way is to interpret the point process as above with the understanding that events obtained from above specifications by switching ‘0’ and ‘1’ sites occur with the same intensity. This switching of sites plays the role of the crosses. Another interpretation is that a bar event at (x, y, t) always connects x_1 and y_0 , how the bar effects the loop structure then depends on the number of crosses that have occurred in the preceding vertical segment. Now using Lemma 2.2 of [111] we have

$$Z(\mathbf{v}) = \int \rho_{\iota'}(d\xi') \int \rho_{\iota''}(d\xi'') \sum_{\sigma \in \Sigma^{(2)}(\xi' \cup \xi'')} \exp \left\{ -(-2J_1) \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta dt \left[(\sigma_{x_i, t} - \sigma_{y_j, t})(v_{x_i} - v_{y_j}) + \frac{1}{4}(v_{x_i} - v_{y_j})^2 \right] \right\}. \quad (6.2.77)$$

We can now make use of the way we split the intensities in ι' and ι'' . If $F : \Sigma \rightarrow \mathbb{R}$ is a function on space-time spin configurations then

$$\int \rho_{\iota''}(d\xi'') \sum_{\sigma \in \Sigma^{(2)}(\xi' \cup \xi'')} F(\sigma) = \sum_{\sigma \in \Sigma^{(2)}(\xi')} F(\sigma) \int \rho_{\iota''}(d\xi'') \prod_{(x_i, y_j, t) \in \xi''} \delta_{\sigma_{x_i, t}, \sigma_{y_j, t}}. \quad (6.2.78)$$

This is because all that the function F ‘sees’ at ι'' events is that $\sigma_{x_i, t} = \sigma_{y_j, t}$ for a pair of sites joined by a bar. Here (x, y, t) is a point where an event of type (6.2.75) occurs. We also have for ξ' and $\sigma \in \Sigma^{(2)}(\xi')$ that

$$\int \rho_{\iota''}(d\xi'') \prod_{(x_i, y_j, t) \in \xi''} \delta_{\sigma_{x_i, t}, \sigma_{y_j, t}} = \exp \left\{ -(-2J_1) \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta dt (1 - \delta_{\sigma_{x_i, t}, \sigma_{y_j, t}}) \right\}. \quad (6.2.79)$$

Using $1 - \delta_{\sigma_{x_i, t}, \sigma_{y_j, t}} = (\sigma_{x_i, t} - \sigma_{y_j, t})^2$ with (6.2.78) and (6.2.79) gives

$$Z(\mathbf{v}) = \int \rho_{\iota'}(d\xi') \sum_{\sigma \in \Sigma^{(2)}(\xi')} \exp \left\{ -(-2J_1) \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta dt \left(\sigma_{x_i, t} + \frac{1}{2}v_{x_i} - \sigma_{y_j, t} - \frac{1}{2}v_{y_j} \right)^2 \right\}. \quad (6.2.80)$$

This can now be treated as in [111] as the measure $\rho_{\iota'}$ is reflection symmetric. This can be seen by noting that for a reflection through edges any event of ι' associated to an edge $\{x, y\}$ crossed by the reflection plane is symmetric with respect to swapping of the sites x_0, x_1 with the sites y_0, y_1 (recall that the sites x_0 and x_1 play equivalent roles). \square

Lemma 6.2.8. $Z(\mathbf{v})$ is maximised by $\mathbf{v} \equiv \mathbf{0}$.

Proof. See [13, 35, 43, 111] for details. Showing maximisers exist is simple. We can fix the field value at 0_0 to be 0 and take $\mathbf{v}^{(n)}$ such that $v_{0_0}^{(n)} = 0$ and $\sup_{x_i} |v_{x_i}^{(n)}| \rightarrow \infty$ as $n \rightarrow \infty$, note that $Z(\mathbf{v}^{(n)}) \rightarrow 0$ for any such $\mathbf{v}^{(n)}$. Hence we can take the maximum on a compact set, as $Z(\mathbf{v})$ is continuous and positive maximisers exist.

The proof that the maximiser is given by $\mathbf{v} \equiv \mathbf{0}$ is easy. Take an arbitrary maximising field, \mathbf{v} , by Lemma 6.2.7 the field $(\mathbf{v}^{(1)}, R\mathbf{v}^{(1)})$ is also a maximising field with $v_{x_i} = v_{(Rx)_i}$ for each $x_i \in \tilde{\Lambda}_L^{(1)}$. Notice that if we repeat this procedure then after $\log_2(|\Lambda_L|)$ we will have a maximising field that is constant. Now we note that the value of $Z(\mathbf{v})$ for a constant field does not depend on the value of that constant, hence we can take the constant $\mathbf{v} \equiv 0$. \square

Infrared bound for the correlation function

From the preceding section we can obtain an infrared bound (IRB) on the correlation function. First we define the inner product and discrete Laplacian on $\tilde{\Lambda}_L$. For \mathbf{v} and \mathbf{v}' fields on $\tilde{\Lambda}_L$ we define their inner product, and the discrete Laplacian as

$$(\mathbf{v}, \mathbf{v}') = \sum_{x_i \in \tilde{\Lambda}_L} \bar{v}_{x_i} v'_{x_i} \quad (6.2.81)$$

$$(\Delta \mathbf{v})_{x_i} = \sum_{y_j: \{x_i, y_j\} \in \tilde{\mathcal{E}}_L} (v_{y_j} - v_{x_i}) \quad (6.2.82)$$

Lemma 6.2.9. For $k \in \Lambda_L^* \setminus \{0\}$

$$\tilde{\kappa}(k, 0) =: \int_0^\beta dt \hat{\kappa}(k, t) \leq \frac{1}{(-2J_1)\varepsilon(k)} \quad (6.2.83)$$

where $\varepsilon(k) = 2 \sum_{i=1}^d (1 - \cos k_i)$.

Proof. To begin we see

$$Z(\mathbf{v}) = \int \rho(d\omega) \sum_{\sigma \in \Sigma^{(2)}(\omega)} \exp \left\{ (-2J_1) \left(\int_0^\beta (\sigma_{\cdot, t}, \Delta v) dt + \frac{\beta}{4} (v, \Delta v) \right) \right\}. \quad (6.2.84)$$

As usual we choose our field to be given by $v_{x_i} = \cos(k \cdot x)$ where $x_i = (x, i)$ and expand around $v = 0$ to second order. We will make use of the identity $-\Delta \mathbf{v} = \varepsilon(k)\mathbf{v}$ for this particular choice of \mathbf{v} . Let $\eta > 0$ be a (small) parameter. Now

$$Z(\eta \mathbf{v}) = Z(\mathbf{0}) + \int \rho(d\omega) \sum_{\sigma \in \Sigma^{(2)}(\omega)} \frac{\eta^2 (-2J_1)^2 \varepsilon(k)^2}{2} \int_0^\beta dt \int_0^\beta dt' (\sigma_{\cdot, t}, \mathbf{v})(\sigma_{\cdot, t'}, \mathbf{v}) - \frac{\eta^2}{4} (-2J_1) \beta \varepsilon(k) (\mathbf{v}, \mathbf{v}) + O(\eta^4). \quad (6.2.85)$$

Collecting terms gives

$$Z(0) \left(1 + 2\eta^2 J_1^2 \varepsilon(k)^2 \beta \int_0^\beta dt \mathbb{E} [(\sigma_{\cdot,0}, \mathbf{v})(\sigma_{\cdot,t}, \mathbf{v})] - \frac{\eta^2}{2} (-J_1) \beta \varepsilon(k) (\mathbf{v}, \mathbf{v}) \right) + O(\eta^4). \quad (6.2.86)$$

We can calculate the expectation quite easily.

$$\begin{aligned} \mathbb{E} [(\sigma_{\cdot,0}, \mathbf{v})(\sigma_{\cdot,t}, \mathbf{v})] &= \sum_{x_i, z_n \in \tilde{\Lambda}_L} \cos(k \cdot x) \cos(k \cdot (x - z)) \overbrace{\mathbb{E} [\sigma_{0,0} \sigma_{z_n,t}]}^{\frac{1}{4} \hat{k}(z,t)} \\ &= \sum_{x_i \in \tilde{\Lambda}_L} \frac{1}{2} \cos^2(k \cdot x) \hat{k}(k, t) \\ &= \frac{1}{2} (\mathbf{v}, \mathbf{v}) \hat{k}(k, t). \end{aligned} \quad (6.2.87)$$

On the second line we have used that $\cos \theta = \operatorname{Re} (e^{i\theta})$. Finally we have

$$Z(\eta \mathbf{v}) = Z(0)(\mathbf{v}, \mathbf{v}) \left(1 + \eta^2 J_1^2 \beta \varepsilon(k)^2 \int_0^\beta dt \hat{k}(k, t) - \frac{\eta^2}{2} (-J_1) \beta \varepsilon(k) \right) + O(\eta^4). \quad (6.2.88)$$

From the Gaussian domination inequality $Z(\mathbf{v}) \leq Z(\mathbf{0})$ we know the bracket is bounded by 1 for small enough η , hence rearranging gives

$$\int_0^\beta dt \hat{k}(k, t) \leq \frac{1}{(-2J_1) \varepsilon(k)}. \quad (6.2.89)$$

□

The next step is to transfer this infrared bound to $\hat{k}(k, 0)$. We will need the Falk-Bruch inequality.

$$\frac{1}{2} \langle A^* A + A A^* \rangle_{\tilde{\Lambda}_L, \beta}^{(2)} \leq \frac{1}{2} \sqrt{(A, A)_{Duh}^{(2)}} \sqrt{\langle [A^*, [\tilde{H}_{\tilde{\Lambda}_L}^{(2)}, A]] \rangle_{\tilde{\Lambda}_L, \beta}^{(2)}} + \frac{1}{\beta} (A, A)_{Duh}^{(2)}. \quad (6.2.90)$$

Where $(\cdot, \cdot)_{Duh}^{(2)}$ is the Duhamel inner product

$$(A, B)_{Duh}^{(2)} = \frac{1}{Z_{\tilde{\Lambda}_L, \beta}^{(2)}} \int_0^\beta ds \operatorname{Tr} A^* e^{-s \tilde{H}_{\tilde{\Lambda}_L}^{(2)}} B e^{-(\beta-s) \tilde{H}_{\tilde{\Lambda}_L}^{(2)}}. \quad (6.2.91)$$

We will use this inequality with $A = \hat{R}_k^3 = \sum_{x \in \Lambda_L} e^{-ik \cdot x} R_x^3$ (and hence $A^* = \hat{R}_{-k}^3$). The main

task is calculating the double commutator. It is simple to show

$$[\hat{R}_{-k}^3, [\hat{H}_{\tilde{\Lambda}_L}^2, \hat{R}_k^3]] = \sum_{x,y:\{x,y\} \in \mathcal{E}_L} [R_x^3 + \cos(k(x-y))R_y^3, [2J_1 \mathcal{S}_{x,y}^{(2)} - J_2 \mathcal{D}_{x,y}^{(2)}, R_x^3]]. \quad (6.2.92)$$

We need to calculate some the expectations of these double commutators. To begin we define new operators $\mathcal{S}_{x,y}^{33}$ and $\mathcal{D}_{x,y}^{33}$ by their matrix elements,

$$\langle a', b' | \otimes \langle c', d' | \mathcal{S}_{x,y}^{33} | a, b \rangle \otimes | c, d \rangle = (b - b')^2 \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'}, \quad (6.2.93)$$

$$\langle a', b' | \otimes \langle c', d' | \mathcal{D}_{x,y}^{33} | a, b \rangle \otimes | c, d \rangle = (a - a' + b - b')^2 \delta_{a,d} \delta_{b,c} \delta_{a',d'} \delta_{b',c'}. \quad (6.2.94)$$

We have the following result

Lemma 6.2.10.

$$\mathcal{S}_{x,y}^{33} = -[R_x^3, [\mathcal{S}_{x,y}^{(2)}, R_x^3]] = -[R_y^3, [\mathcal{S}_{x,y}^{(2)}, R_x^3]], \quad (6.2.95)$$

$$\mathcal{D}_{x,y}^{33} = -[R_x^3, [\mathcal{D}_{x,y}^{(2)}, R_x^3]] = -[R_y^3, [\mathcal{D}_{x,y}^{(2)}, R_x^3]]. \quad (6.2.96)$$

Proof. The proof is tedious (and somewhat messy). The propensity for making mistakes is high, hence one of the calculations will be done explicitly.

$$[R_x^3, [\mathcal{S}_{x,y}^{(2)}, R_x^3]] = \underbrace{2R_x^3 \mathcal{S}_{x,y}^{(2)} R_x^3}_1 - \underbrace{\mathcal{S}_{x,y}^{(2)} (R_x^3)^2}_2 - \underbrace{(R_x^3)^2 \mathcal{S}_{x,y}^{(2)}}_3. \quad (6.2.97)$$

1. $2\langle a', b' | \otimes \langle c', d' | R_x^3 \mathcal{S}_{x,y}^{(2)} R_x^3 | a, b \rangle \otimes | c, d \rangle$
 $= 2(a+b) \langle a', b' | \otimes \langle c', d' | \sum_{\alpha, \beta, \gamma, \delta} R_x^3 | \alpha, \beta \rangle \otimes | \gamma, \delta \rangle \langle \alpha, \beta | \otimes \langle \gamma, \delta | \mathcal{S}_{x,y}^{(2)} | a, b \rangle \otimes | c, d \rangle$
 $= 2(a+b) \langle a', b' | \otimes \langle c', d' | \sum_{\beta} R_x^3 | a, \beta \rangle \otimes | \beta, d \rangle \delta_{b,c}$
 $= 2(a+b)(a' + b') \delta_{a,b'} \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'}.$
2. $-\langle a', b' | \otimes \langle c', d' | \mathcal{S}_{x,y}^{(2)} (R_x^3)^2 | a, b \rangle \otimes | c, d \rangle = -(a+b)^2 \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'}.$
3. $-\langle a', b' | \otimes \langle c', d' | (R_x^3)^2 \mathcal{S}_{x,y}^{(2)} | a, b \rangle \otimes | c, d \rangle = -(a' + b')^2 \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'}.$

(6.2.98)

For 3 we have used the same method as for 1. Combining these gives the result. \square

Now to calculate the expectation of the double commutator we require $\langle \mathcal{S}_{0,e_1}^{33} \rangle_{\tilde{\Lambda}_L, \beta}^{(2)}$ and $\langle \mathcal{D}_{0,e_1}^{33} \rangle_{\tilde{\Lambda}_L, \beta}^{(2)}$. Again we need a small lemma for this calculation.

Lemma 6.2.11.

$$\langle \mathcal{S}_{0,e_1}^{33} \rangle_{\tilde{\Lambda}_L, \beta}^{(2)} = \mathbb{P}(0_0 - e_{1_0}), \quad (6.2.99)$$

$$\langle \mathcal{D}_{0,e_1}^{33} \rangle_{\tilde{\Lambda}_L, \beta}^{(2)} \leq 8\mathbb{P}(0_0 - e_{1_0}), \quad (6.2.100)$$

Remark. We could calculate $\langle \mathcal{D}_{0,e_1}^{33} \rangle_{\tilde{\Lambda}_L, \beta}^{(2)}$ exactly. However it involves probabilities of the kind seen in Section 6.2.5 (and even more that have not been seen). Many of these terms are hard to bound other than by $\mathbb{P}(0_0 - e_{1_0})$ and hence we would end up with a much bigger multiple of $\mathbb{P}(0_0 - e_{1_0})$ than we do here. Of course if we could bound these complicated probabilities in theory the result could be improved, as could many results here.

Proof. For the first equality we let ω be a realisation of ρ and $\omega \cup b_0$ be the realisation where a single bar on edge $\{0_1, e_{1_0}\}$ has been added at $t = 0$. Then

$$\begin{aligned} \langle \mathcal{S}_{0,e_1}^{33} \rangle_{\tilde{\Lambda}_L, \beta}^{(2)} &= \frac{1}{Z_{\tilde{\Lambda}_L, \beta}^{(2)}} \int \rho(d\omega) \sum_{\sigma \in \Sigma^{(2)}(\omega \cup b_0)} (\sigma_{0_1,0+} - \sigma_{0_1,0-})^2 \\ &= \frac{1}{Z_{\tilde{\Lambda}_L, \beta}^{(2)}} \int \rho(d\omega) (\chi(0_{1+} e_{1_0}) + \chi(0_0 - e_{1_0})) \sum_{\sigma \in \Sigma^{(2)}(\omega \cup b_0)} (\sigma_{0_1,0+} - \sigma_{0_1,0-})^2. \end{aligned} \quad (6.2.101)$$

Here $\chi(E)$ is the indicator function of the event E . Note that a bar added between disjoint loops merges them and adding a bar within a loop splits it. The integral over $E [0_0 - e_{1_0}]$ with a bar added between $(0_1, 0)$ and $(e_{1_0}, 0)$, this forces $\sigma_{0_1,0+} = \sigma_{0_1,0-}$ so this contributes nothing. The second term is over $E [0_{1+} e_{1_0}]$ with the same bar added. The sum becomes

$$\sum_{\sigma \in \Sigma^{(2)}(\omega \cup b_0)} (\sigma_{0_1,0+} - \sigma_{0_1,0-})^2 = 2^{|\mathcal{L}(\omega)|-1} \sum_{a,b=-1/2}^{1/2} (a-b)^2 = 2^{|\mathcal{L}(\omega)|}. \quad (6.2.102)$$

Hence we have the first result. For the second result let $\omega \cup d_0$ be the realisation with an extra double bar on edge $\{0, e_1\}$ at $t = 0$ joining point 0_0 to e_{1_1} and point 0_1 to e_{1_0} . Then

$$\begin{aligned} \langle \mathcal{D}_{0,e_1}^{33} \rangle_{\tilde{\Lambda}_L, \beta}^{(2)} &= \frac{1}{Z_{\tilde{\Lambda}_L, \beta}^{(2)}} \int \rho(d\omega) \sum_{\sigma \in \Sigma^{(2)}(\omega \cup d_0)} (\sigma_{0_0,0+} - \sigma_{0_0,0-} + \sigma_{0_1,0+} - \sigma_{0_1,0-})^2 \\ &= \frac{1}{Z_{\tilde{\Lambda}_L, \beta}^{(2)}} \int \rho(d\omega) (\chi(0_{1+} e_{1_0}) + \chi(0_0 - e_{1_0})) \sum_{\sigma \in \Sigma^{(2)}(\omega \cup d_0)} (\sigma_{0_0,0+} - \sigma_{0_0,0-} + \sigma_{0_1,0+} - \sigma_{0_1,0-})^2 \end{aligned} \quad (6.2.103)$$

It can be seen (either by looking at the appropriate loop pictures or otherwise) that for $\omega \in E [0_0 - e_{1_0}]$, the sum can be bounded by looking at the four sites $0_0, 0_1, e_{1_0}, e_{1_1}$. We

consider whether they are in one, two or three different loops as follows

$$\sum_{\sigma \in \Sigma^{(2)}(\omega \cup d_0)} (\sigma_{0_0,0+} - \sigma_{0_0,0-} + \sigma_{0_1,0+} - \sigma_{0_1,0-})^2 \leq \begin{cases} 12 \cdot 2^{|\mathcal{L}(\omega)|-1} & \text{one loop} \\ 16 \cdot 2^{|\mathcal{L}(\omega)|-2} & \text{two loops} \\ 2 \cdot 2^{|\mathcal{L}(\omega)|-3} & \text{three loops.} \end{cases} \quad (6.2.104)$$

Noting that the four sites being in one, two or three separate loops are disjoint events we can bound the integral over $E [0_0-e_{1_0}]$ by the most likely event giving a bound of $6\mathbb{P}(0_0-e_{1_0})$.

As for the integral over $E [0_{1+}-e_{1_0}]$, the same considerations result in a bound of $2\mathbb{P}(0_0-e_{1_0})$. In this case the sites can be in four loops but then adding a double bar makes the sum equal to zero. In the case of three or two loops with the sum none zero we are in $\omega \in E [0_i-e_{1_j}]$ for some $(i, j) \neq (1, 0)$. The result follows. \square

Finally we can use these results to see

$$\begin{aligned} \langle [\hat{R}_{-k}^3, [\tilde{H}_{\tilde{\Lambda}_L}^{(2)}, \hat{R}_k^3]] \rangle_{\tilde{\Lambda}_L, \beta}^{(2)} &= \sum_{x, y: \{x, y\} \in \mathcal{E}_L} (1 + \cos(k \cdot (x - y))) (-2J_1 \mathcal{S}_{x, y}^{33} + J_2 \mathcal{D}_{x, y}^{33}) \\ &\leq |\Lambda_L| (-2J_1 + 8J_2) \mathbb{P}(0_0-e_{1_0}) \varepsilon(k + \pi). \end{aligned} \quad (6.2.105)$$

The first inequality used Lemma 6.2.10 and the inequality used Lemma 6.2.11. We also have

$$\langle \widehat{R}_0^3, \widehat{R}_x^3 \rangle_{Duh}^{(2)}(k) = \tilde{\kappa}(k, 0). \quad (6.2.106)$$

From this we have the bound

$$\langle \widehat{R}_0^3, \widehat{R}_x^3 \rangle_{\tilde{\Lambda}_L, \beta}^{(2)}(k) \leq \frac{\sqrt{\mathbb{P}(0_0-e_{1_0})}}{2} \sqrt{\frac{-2J_1 + 8J_2}{-2J_1}} \sqrt{\frac{\varepsilon(k + \pi)}{\varepsilon(k)}} + \frac{1}{\beta} \frac{1}{(-2J_1)\varepsilon(k)} \quad (6.2.107)$$

Now we use the identity

$$\frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \mathbb{P}(0_0-x_0) = \kappa(y) - \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^* \setminus \{0\}} e^{iky} \hat{\kappa}(k) \quad (6.2.108)$$

with $y = 0$ and $y = e_i$. For the second choice we use the sum rule in [58], more precisely we use (6.2.108) and the identity

$$\sum_{k \in \Lambda_L^* \setminus \{0\}} \cos(k_1) \hat{\kappa}(k) = \sum_{k \in \Lambda_L^* \setminus \{0\}} \hat{\kappa}(k) \left(\frac{1}{d} \sum_{i=1}^d \cos(k_i) \right) \leq \sum_{k \in \Lambda_L^* \setminus \{0\}} \hat{\kappa}(k) \left(\frac{1}{d} \sum_{i=1}^d \cos(k_i) \right)_+. \quad (6.2.109)$$

This gives the result.

6.2.7 Nematic order for $J_1 \leq 0 \leq J_2$ - an initial result

The loop model was effective in giving an explicit region where macroscopic loops (and Néel order for the corresponding spin system) occur. There remains part of the quadrant $J_1 \leq 0 \leq J_2$ where long-range order has not been shown. The aim of this section is to prove an analogous result to that of the previous section with the aim to eventually be able to prove long-range order in the remainder of the quadrant. The result in [69] suggests the possibility of showing *nematic order* for $|J_1|$ sufficiently small. Nematic order is expected to be weaker than Néel order. Much of the argument is the same as in Section 6.2.6 however the proof of reflection positivity is slightly more involved. We use the following notation,

$$\begin{aligned} \rho(x) &= \langle (S_0^3)^2 (S_x^3)^2 \rangle_{\Lambda_L, \beta}^2 - \langle (S_0^3)^2 \rangle_{\Lambda_L, \beta}^2 \langle (S_x^3)^2 \rangle_{\Lambda_L, \beta}^2 \\ &= -\frac{1}{36} + \frac{1}{4} \mathbb{P} \left(\begin{array}{c} 0_0 \text{---} x_0 \\ | \text{---} | \\ 0_1 \text{---} x_1 \end{array} \right) + \frac{1}{2} \mathbb{P} \left(\begin{array}{c} 0_0 \text{---} x_0 \\ \pm \text{---} \pm \\ 0_1 \text{---} x_1 \end{array} \right) + \frac{1}{4} \mathbb{P} \left(\begin{array}{c} 0_0 \text{---} x_0 \\ \text{---} \times \text{---} \\ 0_1 \text{---} x_1 \end{array} \right). \end{aligned} \quad (6.2.110)$$

This is a function of probabilities of sites being connected at time $t = 0$. The corresponding event for the connections being between $(0, 0)$ and (x, t) is denoted $\rho(x, t)$. We can see from the proof of Proposition 6.2.3 that $\rho(x)$ is the same if we take expectations in $\langle \cdot \rangle_{\Lambda_L, \beta}^{(1)}$ or $\langle \cdot \rangle_{\Lambda_L, \beta}^{(2)}$. The main theorem of this section is the following:

Theorem 6.2.12. *Let $d \geq 3$ and $J_1 \leq 0 \leq J_2$, for L even we have two bounds*

$$\liminf_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \rho(x) \geq \liminf_{L \rightarrow \infty} \begin{cases} \frac{2}{9} - \sqrt{\mathbb{P}(0_0 \text{---} e_{1_0})} \sqrt{\frac{-2J_1 + \frac{9}{4}J_2}{4J_2}} K_d + o\left(\frac{1}{\beta}\right), \\ \rho(e_1) - \sqrt{\mathbb{P}(0_0 \text{---} e_{1_0})} \sqrt{\frac{-2J_1 + \frac{9}{4}J_2}{4J_2}} I_d + o\left(\frac{1}{\beta}\right). \end{cases} \quad (6.2.111)$$

It is difficult to give a satisfactory bound on $\rho(e_1)$. But as for Néel order we reason as follows. The sum is certainly positive for β large enough if

$$\sqrt{\mathbb{P}(0_0 \text{---} e_{1_0})} < \frac{2}{9K_d} \sqrt{\frac{4J_2}{-2J_1 + \frac{9}{4}J_2}} \quad \text{or} \quad \sqrt{\mathbb{P}(0_0 \text{---} e_{1_0})} < \frac{\rho(e_1)}{I_d} \sqrt{\frac{4J_2}{-2J_1 + \frac{9}{4}J_2}}. \quad (6.2.112)$$

Combining Proposition 6.2.5 with the second bound of (6.2.112) we have the sufficient condition of

$$\mathbb{P}(0_0 \text{---} e_{1_0}) + \left(\frac{I_d}{-2J_1 + J_2} \right) \sqrt{J_2 \left(-2J_1 + \frac{9}{4}J_2 \right)} \sqrt{\mathbb{P}(0_0 \text{---} e_{1_0})} - \frac{2}{9} \left(\frac{-3J_1 + 2J_2}{-2J_1 + J_2} \right) \leq 0. \quad (6.2.113)$$

This is a quadratic inequality in $\sqrt{\mathbb{P}(0_0 \text{---} e_{1_0})}$. For $d = 3$ the largest root is bounded below by 0.5 for all values of $J_1 \leq 0 \leq J_2$ on the unit circle. We then see that a modest upper

bound on $\sqrt{\mathbb{P}(0_0 - e_{1_0})}$ should yield nematic order, however finding such a bound seems quite difficult. The rest of this section is dedicated to the proof of Theorem 6.2.12.

To begin we define a partition function dependent on external fields, \mathbf{v} , as in Section 6.2.6

$$Z(\mathbf{v}) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma^{(2)}(\xi)} \exp \left\{ -J_2 \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta (\sigma_{x_0, t} \sigma_{x_1, t} - \sigma_{y_0, t} \sigma_{y_1, t})(v_{x_i} - v_{y_j}) + \frac{1}{4}(v_{x_i} - v_{y_j})^2 dt \right\} \quad (6.2.114)$$

we can also write this as

$$Z(\mathbf{v}) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma^{(2)}(\xi)} \exp \left\{ -J_2 \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta dt \left[\left(\sigma_{x_0, t} \sigma_{x_1, t} + \frac{v_{x_i}}{2} - \sigma_{y_0, t} \sigma_{y_1, t} - \frac{v_{y_j}}{2} \right)^2 - (\sigma_{x_0, t} \sigma_{x_1, t} - \sigma_{y_0, t} \sigma_{y_1, t})^2 \right] \right\}. \quad (6.2.115)$$

Hopefully the reader can forgive this clash of notation with the partition function on fields introduced in Section 6.2.6. The partition function in Section 6.2.6 will not appear or be used in this section. The partition function (6.2.114) will play the same role in this section and the prospect of yet more new notation was not appealing.

Lemma 6.2.13. *For any reflection, R , across edges*

$$Z(\mathbf{v}_1, \mathbf{v}_2)^2 \leq Z(\mathbf{v}_1, R\mathbf{v}_1)Z(R\mathbf{v}_2, \mathbf{v}_2) \quad (6.2.116)$$

Proof. We note here that

$$(\sigma_{x_0, t} \sigma_{x_1, t} - \sigma_{y_0, t} \sigma_{y_1, t})^2 = 1 - \delta_{\sigma_{x_0, t} \sigma_{x_1, t}, \sigma_{y_0, t} \sigma_{y_1, t}}. \quad (6.2.117)$$

Recalling the proof of reflection positivity previously this suggests that we should split the intensities of the Poisson point process as follows.

$$\iota' \left(\left\{ \frac{b \ a \ a \ b}{b \ a \ a \ b} \right\} \right) = J_2 \quad (6.2.118)$$

ι' makes up the remaining events in ι

$$\iota' \left(\left\{ \frac{b \ a \ a \ b}{b \ c \ c \ b} \right\}_{a \neq c} \right) = J_2, \quad \iota' \left(\left\{ \frac{a' \ a \ a \ b}{a' \ c \ c \ b} \right\} \right) = -2J_1, \quad \iota' \left(\left\{ \frac{a' \ a \ a \ a'}{c' \ c \ c \ c'} \right\}_{a' \neq c'} \right) = J_2. \quad (6.2.119)$$

Again there are two possible interpretations of how the bars are incorporated. Now if F is

a function on space-time spin configurations then given a realisation ξ' of $\rho_{l'}$

$$\int \rho_{l''}(\mathrm{d}\xi'') \sum_{\sigma \in \Sigma^{(2)}(\xi' \cup \xi'')} F(\sigma) = \sum_{\sigma \in \Sigma^{(2)}(\xi')} F(\sigma) \int \rho_{l''}(\mathrm{d}\xi'') \prod_{(x,y,t) \in \xi''} \delta_{\sigma_{x_i,t}, \sigma_{y_j,t}} \delta_{\sigma_{x_n,t}, \sigma_{y_m,t}} \quad i \neq n, j \neq m \quad (6.2.120)$$

The product of delta functions incorporates the requirement that two sets of bars occur between sites x and y at time t . It can be checked that

$$\delta_{\sigma_{x_i,t}, \sigma_{y_j,t}} \delta_{\sigma_{x_n,t}, \sigma_{y_m,t}} = \delta_{\sigma_{x_0,t} \sigma_{x_1,t}, \sigma_{y_0,t} \sigma_{y_1,t}} - \delta_{\sigma_{x_0,t}, -\sigma_{y_0,t}} \delta_{\sigma_{x_1,t}, -\sigma_{y_1,t}} \delta_{\sigma_{x_0,t}, \sigma_{x_1,t}}. \quad (6.2.121)$$

If we use this to rewrite (6.2.120) we can see that the second term on the right hand side is not a double bar event, hence when multiplying out the product only the first term survives. This means

$$\int \rho_{l''}(\mathrm{d}\xi'') \sum_{\sigma \in \Sigma^{(2)}(\xi' \cup \xi'')} F(\sigma) = \sum_{\sigma \in \Sigma^{(2)}(\xi')} F(\sigma) \int \rho_{l''}(\mathrm{d}\xi'') \prod_{(x,y,t) \in \xi''} \delta_{\sigma_{x_0,t} \sigma_{x_1,t}, \sigma_{y_0,t} \sigma_{y_1,t}}. \quad (6.2.122)$$

Given ξ' and $\sigma \in \Sigma(\xi')$

$$\int \rho_{l''}(\mathrm{d}\xi'') \prod_{(x,y,t) \in \xi''} \delta_{\sigma_{x_0,t} \sigma_{x_1,t}, \sigma_{y_0,t} \sigma_{y_1,t}} = \exp \left\{ -J_2 \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta \mathrm{d}t (1 - \delta_{\sigma_{x_0,t} \sigma_{x_1,t}, \sigma_{y_0,t} \sigma_{y_1,t}}) \right\}. \quad (6.2.123)$$

Now it can be seen that the identity that informed the splitting of the intensities was a useful one. Combining what we have as before we obtain

$$Z(\mathbf{v}) = \int \rho_{l'}(\mathrm{d}\xi') \sum_{\sigma \in \Sigma^{(2)}(\xi')} \exp \left\{ -J_2 \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta \mathrm{d}t \left(\sigma_{x_0,t} \sigma_{x_1,t} + \frac{v_{x_i}}{2} - \sigma_{y_0,t} \sigma_{y_1,t} - \frac{v_{y_j}}{2} \right)^2 \right\}. \quad (6.2.124)$$

We are now in the same situation as we were for the previous proof of reflection positivity. It is again standard to complete the proof by introducing extra fields, the reader is encouraged to consult [111] for further details. \square

From this it follows that $Z(\mathbf{v}) \leq Z(\mathbf{0})$ for any field \mathbf{v} as previously. Now we want an IRB, for this we have the following lemma.

Lemma 6.2.14. *For $k \in \Lambda_L^* \setminus \{0\}$ and $J_2 > 0$*

$$\int_0^\beta \mathrm{d}t \hat{\rho}(k, t) \leq \frac{1}{J_2 \varepsilon(k)} \quad (6.2.125)$$

Proof. One extra observation is required. We see that we can write

$$Z(\mathbf{v}) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma^{(2)}(\xi)} \exp \left\{ -J_2 \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta dt \left[((\sigma_{x_0, t} \sigma_{x_1, t} - \alpha) - (\sigma_{y_0, t} \sigma_{y_1, t} - \alpha))(v_{x_i} - v_{y_j}) + \frac{1}{4}(v_{x_i} - v_{y_j})^2 \right] \right\} \quad (6.2.126)$$

We then follow precisely the proof of Lemma 6.2.9 and see that if we take $\alpha = -\frac{1}{12}$ we obtain the result. \square

This time when we use Falk-Bruch we take $A = \mathcal{F}((R_x^3)^2 - \frac{2}{3})(k)$, where $\mathcal{F}(g)$ denotes the Fourier transform of g . The double commutator calculation is similar to before,

$$\left\langle A^*, [\tilde{H}_{\Lambda_L}^{(2)}, A] \right\rangle_{\beta, \Lambda}^{(2)} = - \sum_{x, y: \{x, y\} \in \tilde{\mathcal{E}}_L} [(R_x^3)^2 + \cos k(x-y)(R_y^3)^2, [-2J_1 \mathcal{S}_{x, y}^{(2)} + J_2 \mathcal{D}_{x, y}^{(2)}, (R_x^3)^2]]. \quad (6.2.127)$$

Now we define operators that will give our double commutators. Recall the operator $\mathcal{S}_{x, y}^{33}$ and define $Q_{x, y}^{(1)}$ and $Q_{x, y}^{(2)}$ by

$$\langle a', b' | \otimes \langle c', d' | Q_{x, y}^{(1)} | a, b \rangle \otimes | c, d \rangle = 4ad(b - b')^2 \delta_{a, a'} \delta_{d, d'} \delta_{b, c} \delta_{b', c'} \quad (6.2.128)$$

$$\langle a', b' | \otimes \langle c', d' | Q_{x, y}^{(2)} | a, b \rangle \otimes | c, d \rangle = 4(ab - a'b')^2 \delta_{a, d} \delta_{b, c} \delta_{a', d'} \delta_{b', c'} \quad (6.2.129)$$

The relation between these operators and the double commutator is given by the following lemma.

Lemma 6.2.15.

$$\mathcal{S}_{x, y}^{33} = - [(R_x^3)^2, [\mathcal{S}_{x, y}^{(2)}, (R_x^3)^2]] \quad (6.2.130)$$

$$Q_{x, y}^{(1)} = - [(R_y^3)^2, [\mathcal{S}_{x, y}^{(2)}, (R_x^3)^2]] \quad (6.2.131)$$

$$Q_{x, y}^{(2)} = - [(R_x^3)^2, [\mathcal{D}_{x, y}^{(2)}, (R_x^3)^2]] = - [(R_y^3)^2, [\mathcal{D}_{x, y}^{(2)}, (R_x^3)^2]] \quad (6.2.132)$$

Proof. The proof is essentially the same as that of Lemma 6.2.10, we calculate the matrix elements of the double commutator and see that they are the same. The only slightly surprising result is that $[(R_x^3)^2, [\mathcal{S}_{x, y}^{(2)}, (R_x^3)^2]] \neq [(R_y^3)^2, [\mathcal{S}_{x, y}^{(2)}, (R_x^3)^2]]$ so the proof will be presented.

$$\begin{aligned} & [(R_y^3)^2, [\mathcal{S}_{x, y}^{(2)}, (R_x^3)^2]] \\ &= \underbrace{(R_y^3)^2 \mathcal{S}_{x, y}^{(2)} (R_x^3)^2}_1 + \underbrace{(R_x^3)^2 \mathcal{S}_{x, y}^{(2)} (R_y^3)^2}_2 - \underbrace{(R_y^3)^2 (R_x^3)^2 \mathcal{S}_{x, y}^{(2)}}_3 - \underbrace{\mathcal{S}_{x, y}^{(2)} (R_x^3)^2 (R_y^3)^2}_4 \end{aligned} \quad (6.2.133)$$

$$\begin{aligned}
1. \quad & \langle a', b' | \otimes \langle c', d' | (R_x^3)^2 S_{x,y}^{(2)} (R_x^3)^2 | a, b \rangle \otimes | c, d \rangle \\
& = \delta_{a,b} \langle a', b' | \otimes \langle c', d' | \sum_{\alpha, \beta, \gamma, \delta} (R_y^3)^2 | \alpha, \beta \rangle \otimes | \gamma, \delta \rangle \langle \alpha, \beta | \otimes \langle \gamma, \delta | S_{x,y}^{(2)} | a, b \rangle \otimes | c, d \rangle \\
& = \delta_{a,b} \langle a', b' | \otimes \langle c', d' | \sum_{\beta} (R_y^3)^2 | a, \beta \rangle \otimes | \beta, d \rangle \delta_{b,c} \\
& = \delta_{a,b} \delta_{c',d'} \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'}, \\
2. \quad & \langle a', b' | \otimes \langle c', d' | (R_x^3)^2 S_{x,y}^{(2)} (R_y^3)^2 | a, b \rangle \otimes | c, d \rangle = \delta_{c,d} \delta_{a',b'} \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'}, \\
3. \quad & -\langle a', b' | \otimes \langle c', d' | (R_x^3)^2 (R_x^3)^2 S_{x,y}^{(2)} | a, b \rangle \otimes | c, d \rangle = -\delta_{a',b'} \delta_{c',d'} \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'}, \\
4. \quad & -\langle a', b' | \otimes \langle c', d' | S_{x,y}^{(2)} (R_x^3)^2 (R_y^3)^2 | a, b \rangle \otimes | c, d \rangle = -\delta_{a,b} \delta_{c,d} \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'}.
\end{aligned} \tag{6.2.134}$$

This gives matrix elements of

$$-(\delta_{a,b} - \delta_{a',b'}) (\delta_{c,d} - \delta_{c',d'}) \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'} = -4ad(b-b')^2 \delta_{a,a'} \delta_{d,d'} \delta_{b,c} \delta_{b',c'}. \tag{6.2.135}$$

The other equality follow in the same way. \square

We need the expectations of these operators. they are easily calculated using the same considerations as in Section 6.2.6.

Lemma 6.2.16.

$$\langle Q_{x,y}^{(1)} \rangle_{\tilde{\Lambda}_{L,\beta}}^{(2)} \leq \mathbb{P}(0_0 - e_{1_0}), \tag{6.2.136}$$

$$\langle Q_{x,y}^{(1)} \rangle_{\tilde{\Lambda}_{L,\beta}}^{(2)} \leq \frac{9}{4} \mathbb{P}(0_0 - e_{1_0}). \tag{6.2.137}$$

Proof. The first inequality is obvious as $4ad(b-b')^2 \leq (b-b')^2$ which puts us in the case of $S_{x,y}^{33}$. For the second integral we use the same method as when calculating $\langle \mathcal{D}_{0,e_1}^{33} \rangle_{\tilde{\Lambda}_{L,\beta}}^{(2)}$.

$$\langle Q_{x,y}^{(2)} \rangle_{\tilde{\Lambda}_{L,\beta}}^{(2)} = \frac{1}{Z_{\tilde{\Lambda}_{L,\beta}}^2} \int \rho(d\bar{\omega}) \sum_{\sigma \in \Sigma^{(2)}(\bar{\omega} \cup d_0)} 4(\sigma_{0_0,0+} \sigma_{0_1,0+} - \sigma_{0_0,0-} \sigma_{0_1,0-})^2. \tag{6.2.138}$$

We look at the cases $\omega \in E[0_0 - e_{1_0}]$ and $\omega \notin E[0_0 - e_{1_0}]$. For the cases of $0_0, 0_1, e_{1_0}, e_{1_1}$ being in 1,2,3 or 4 different loops we look at the possible ways of forming the loops (which sites are connected and what order they are connected in). Then we can add the double bars and see which spins are necessarily equal and which can be different. We then bound the sum in each of these cases. If $\omega \in E[0_0 - e_{1_0}]$ the biggest contribution is the case of two loops with two of the sites $0_0, 0_1, e_{1_0}, e_{1_1}$ each, adding the double bar puts each term in the sum in a different loop giving a bound of $2 \cdot 2^{|\mathcal{L}(\omega)|}$. In the case $\omega \notin E[0_0 - e_{1_0}]$ the largest contribution is the case of three loops with 0_0 and e_{1_1} connected, the sum is $\frac{1}{4} 2^{|\mathcal{L}(\omega)|}$. Adding these cases and recalling that $\mathbb{P}(x_i - y_j)$ does not depend on i or j gives the result. \square

Combining these gives us a bound on the double commutator

$$\left\langle \left[\widehat{(R_x^3)^2}(-k), [\tilde{H}_{\tilde{\Lambda}_L}^{(2)}, \widehat{(R_x^3)^2}(k)] \right] \right\rangle_{\beta, \Lambda}^{(2)} \leq |\Lambda_L| (-2J_1 + \frac{9}{4}J_2) \mathbb{P}(0_0 - e_{1_0}) \varepsilon(k + \pi). \quad (6.2.139)$$

We have the identity $\mathcal{F}((R_0^3)^2 - \frac{2}{3}, (R_x^3)^2 - \frac{2}{3})_{Duh}^2(k) = \int_0^\beta dt \hat{\rho}(k, t)$. Then Falk-Bruch gives

$$\mathcal{F} \left\langle \left((R_0^3)^2 - \frac{2}{3} \right) \left((R_x^3)^2 - \frac{2}{3} \right) \right\rangle_{\tilde{\Lambda}_L, \beta}^{(2)} \leq \frac{\sqrt{\mathbb{P}(0_0 - e_{1_0})}}{2} \sqrt{\frac{-2J_1 + \frac{9}{4}J_2}{J_2}} \sqrt{\frac{\varepsilon(k + \pi)}{\varepsilon(k)}} + \frac{1}{\beta} \frac{1}{J_2 \varepsilon(k)}. \quad (6.2.140)$$

Using this with (6.2.108) as before we obtain two bounds in the theorem.

6.2.8 Néel order via space-time reflection positivity

We now use the method of space-time reflection positivity first used in [17] for the quantum Ising model and also used on loop models in [111]. The main difference is that the fields we introduced to obtain infrared bounds in previous results will now also depend on time (i.e. $t \in [0, \beta]$). We begin by introducing two integrals that will be needed for the statement of the main theorem,

$$K'_d = \frac{1}{(2\pi)^d} \int_{[\pi, \pi]^d} \sqrt{\frac{d}{\varepsilon(k)}} dk, \quad (6.2.141)$$

$$I'_d = \frac{1}{(2\pi)^d} \int_{[\pi, \pi]^d} \sqrt{\frac{1}{d\varepsilon(k)}} \left(\sum_{i=1}^d \cos k_i \right)_+ dk. \quad (6.2.142)$$

The main theorem of this section is then:

Theorem 6.2.17. *Let $L(0_0, 0)$ denote the length of the loop containing $(0_0, 0)$. For L even there is a β_0 such that for $\beta > \beta_0$ there is a $c = c(J_1, J_2, d, \beta) > 0$ such that*

$$\liminf_{L \rightarrow \infty} \mathbb{E} \left[\frac{L(0_0, 0)}{\beta |\Lambda_L|} \right] \geq c. \quad (6.2.143)$$

More precisely, for β large enough we obtain two possibilities for this constant, c :

$$\liminf_{L \rightarrow \infty} \mathbb{E} \left[\frac{L(0_0, 0)}{\beta |\Lambda_L|} \right] \geq \liminf_{L \rightarrow \infty} \left\{ \begin{array}{l} 2 - 2 \sqrt{\frac{(J_2 - 2J_1) \mathbb{P}[0_0 - e_{1_0}]}{(-J_1)}} K'_d \left(1 + o\left(\frac{1}{\beta}\right) \right) \\ 2 \sqrt{\mathbb{P}[0_0 - e_{1_0}]} \left(\sqrt{\mathbb{P}[0_0 - e_{1_0}]} - \sqrt{\frac{(J_2 - 2J_1)}{(-J_1)}} I'_d \left(1 + o\left(\frac{1}{\beta}\right) \right) \right) \end{array} \right\}. \quad (6.2.144)$$

For the explicit dependence on β see (6.2.178) and (6.2.181). As for Theorem 6.2.6 it is sufficient to prove there is a positive lower bound for (6.2.144). There is a positive bound if

$$\sqrt{\mathbb{P}[0_0 - e_{1_0}]} < \frac{1}{K'_d} \sqrt{\frac{(-J_1)}{(J_2 - 2J_1)}} \quad \text{or} \quad \sqrt{\mathbb{P}[0_0 - e_{1_0}]} > I'_d \sqrt{\frac{(J_2 - 2J_1)}{(-J_1)}}. \quad (6.2.145)$$

One of these inequalities is satisfied if

$$I'_d K'_d \leq \frac{(-J_1)}{(J_2 - 2J_1)}. \quad (6.2.146)$$

This is the case for $d = 3$ if $J_1 < -0.22$ with $J_1^2 + J_2^2 = 1$ which is an improvement on Section 6.2.6. The proof of this theorem comprises the rest of this section.

We now consider fields depending on space and time $\mathbf{v} : \tilde{\Lambda}_L \times [0, \beta]_{per} \rightarrow \mathbb{R}$ such that $v_{x_0, t} = v_{x_1, t}$ for every $x \in \Lambda_L$ and $t \in [0, \beta]$. Define a partition function

$$Z(\mathbf{v}) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ -(-2J_1) \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta dt [(\sigma_{x_i, t} - \sigma_{y_j, t})(v_{x_i, t} - v_{y_j, t}) + \frac{1}{4}(v_{x_i, t} - v_{y_j, t})^2] \right. \\ \left. + \sum_{x_i \in \tilde{\Lambda}_L} \int_0^\beta \left[a \sigma_{x_i, t} \frac{\partial^2 v_{x_i, t}}{\partial t^2} - b \left(\frac{\partial v_{x_i, t}}{\partial t} \right)^2 \right] \right\}, \quad (6.2.147)$$

where a and b are constants to be chosen later. We consider only \mathbf{v} 's that are twice differentiable with respect to t and such that $\left| \frac{\partial v_{x_i, t}}{\partial t} \right| \leq c_0$ for every x_i, t . Denote the set of all such fields by \mathcal{V}_{c_0} .

Lemma 6.2.18. $\forall \mathbf{v} \in \mathcal{V}_{c_0} \exists \mathbf{v}^* \in \mathcal{V}_{c_0}$ depending on t but not on x_i such that $Z(\mathbf{v}) \leq Z(\mathbf{v}^*)$.

Proof. The proof is the same as in Lemma 6.2.7, note that the sum over $x_i \in \tilde{\Lambda}_L$ plays no role and is easily reflected. \square

We want that the field $\mathbf{0}$ (i.e. $v_{x_i, t} = 0 \forall x_i, t$) is a maximiser. From the previous lemma we need only consider fields constant in space. To prove the result we need to consider reflections in time, the proof is more involved than previously.

Lemma 6.2.19. If $b > 2a^2 d(J_2 - 2J_1) \kappa(e_1)$ then $\exists c_0 > 0$ such that $Z(\mathbf{v}) \leq Z(\mathbf{0}) \forall \mathbf{v} \in \mathcal{V}_{c_0}$.

Proof. For N even we define

$$Z_N(\mathbf{v}) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ -\frac{N}{\beta} \sum_{x_i \in \tilde{\Lambda}_L} \sum_{t \in \frac{\beta}{N} \{1, \dots, N\}} \left[a(\sigma_{x_i, t + \frac{\beta}{N}} - \sigma_{x_i, t})(v_{t + \frac{\beta}{N}} - v_t) + b(v_{t + \frac{\beta}{N}} - v_t)^2 \right] \right\} \quad (6.2.148)$$

where we have written $v_{x_i,t} = v_t$ as \mathbf{v} is constant in space and have discretised the derivatives. We have the relation

$$\lim_{N \rightarrow \infty} Z_N(\mathbf{v}) = Z(\mathbf{v}). \quad (6.2.149)$$

We can reflect horizontally in the lines $t = \frac{\beta}{N}n$ for $n = 1, \dots, N$. Using Cauchy-Schwarz gives

$$Z_N(\mathbf{v}^{(1)}, \mathbf{v}^{(2)})^2 \leq Z_N(\mathbf{v}^{(1)}, R\mathbf{v}^{(1)})Z(R\mathbf{v}^{(2)}, \mathbf{v}^{(2)}) \quad (6.2.150)$$

where $\mathbf{v}^{(1)}$ and $\mathbf{v}^{(2)}$ are the parts of the field above and below the reflection plane, respectively. This gives a maximiser of the form

$$v_t^* = (-1)^{\frac{N}{\beta}t} \frac{c}{N}, \quad (6.2.151)$$

where $|c| \leq c_0 \frac{N}{2}$. We want to show that $c = 0$, we first use this \mathbf{v}^*

$$Z_N(\mathbf{v}^*) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ -\frac{4bc^2|\tilde{\Lambda}_L|}{\beta} - \frac{2ac}{\beta} \sum_{x_i \in \tilde{\Lambda}_L} \sum_{t \in \frac{\beta}{N}\{1, \dots, N\}} (-1)^{\frac{N}{\beta}t} (\sigma_{x_i, t + \frac{\beta}{N}} - \sigma_{x_i, t}) \right\}. \quad (6.2.152)$$

When integrating over the realisation, ξ , of ρ_t we can replace an event $(x, y, t) \in \xi$ by $\frac{1}{2}$ an event at t and $\frac{1}{2}$ an event at $t + \frac{\beta}{N}$, this gives

$$Z_N(\mathbf{v}^*) = e^{-\frac{4bc^2|\tilde{\Lambda}_L|}{\beta}} \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \prod_{(x,y,t) \in \xi} \prod_{i \neq j} \frac{1}{2} \left(\exp \left\{ \frac{2ac}{\beta} (\sigma_{x_i, t + \frac{\beta}{N}} + \sigma_{y_j, t + \frac{\beta}{N}} - \sigma_{x_i, t} - \sigma_{y_j, t}) \right\} \right. \\ \left. + \exp \left\{ -\frac{2ac}{\beta} (\sigma_{x_i, t + \frac{\beta}{N}} + \sigma_{y_j, t + \frac{\beta}{N}} - \sigma_{x_i, t} - \sigma_{y_j, t}) \right\} \right) + O\left(\frac{1}{N}\right). \quad (6.2.153)$$

The $O\left(\frac{1}{N}\right)$ term corresponds to realisation where two transitions occur at the same edge in a time interval $[t, t + \frac{\beta}{N}]$. At a single bar the factor is

$$\frac{1}{2} \left(\exp \left\{ \frac{2ac}{\beta} (\sigma_{x_1, t + \frac{\beta}{N}} + \sigma_{y_0, t + \frac{\beta}{N}} - \sigma_{x_1, t} - \sigma_{y_0, t}) \right\} + \exp \left\{ -\frac{2ac}{\beta} (\sigma_{x_1, t + \frac{\beta}{N}} + \sigma_{y_0, t + \frac{\beta}{N}} - \sigma_{x_1, t} - \sigma_{y_0, t}) \right\} \right) \\ = \exp \left\{ \frac{8a^2c^2}{\beta^2} (\sigma_{x_1, t + \frac{\beta}{N}} - \sigma_{x_1, t})^2 + O(c^4) \right\}. \quad (6.2.154)$$

The factor at double bars is

$$\exp \left\{ \frac{8a^2c^2}{\beta^2} (\sigma_{x_0, t + \frac{\beta}{N}} - \sigma_{x_0, t})^2 + O(c^4) \right\} \exp \left\{ \frac{8a^2c^2}{\beta^2} (\sigma_{x_1, t + \frac{\beta}{N}} - \sigma_{x_1, t})^2 + O(c^4) \right\} \\ = \exp \left\{ \frac{8a^2c^2}{\beta^2} \left((\sigma_{x_0, t + \frac{\beta}{N}} - \sigma_{x_0, t})^2 + (\sigma_{x_1, t + \frac{\beta}{N}} - \sigma_{x_1, t})^2 \right) + O(c^4) \right\}. \quad (6.2.155)$$

Note that for a single bar joining x and y in interval $[t, t + \frac{\beta}{N}]$ we have $\sigma_{x_0, t + \frac{\beta}{N}} = \sigma_{x_0, t}$

(assuming only one bar occurs) meaning we can use the factor for double bars at every event in ξ , hence we have

$$Z_N(\mathbf{v}^*) = e^{-\frac{4bc^2|\tilde{\Lambda}_L|}{\beta}} \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ \frac{8a^2c^2}{\beta^2} \sum_{(x,y,t) \in \xi} \left((\sigma_{x_0,t+\frac{\beta}{N}} - \sigma_{x_0,t})^2 + (\sigma_{x_1,t+\frac{\beta}{N}} - \sigma_{x_1,t})^2 \right) + O(c^4) \right\} + O\left(\frac{1}{N}\right) \quad (6.2.156)$$

We now want to expand the exponential into terms that can be dealt with. Let A be the event that an event occurs on edge $\{0, e_1\}$ in time interval $[0, \frac{\beta}{N}]$ we have

$$Z_N(\mathbf{v}^*) = Z_N(\mathbf{0}) \left[1 - \frac{4bc^2}{\beta} |\tilde{\Lambda}_L| \right] + \frac{8a^2c^2}{\beta^2} |\mathcal{E}| N \int_A \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \left((\sigma_{0_0, \frac{\beta}{N}} - \sigma_{0_0,0})^2 + (\sigma_{0_1, \frac{\beta}{N}} - \sigma_{0_1,0})^2 \right) + O(c^4) + O\left(\frac{1}{N}\right), \quad (6.2.157)$$

here we have used space-time translation invariance. Now let $\xi \cup b_0$ be the realisation, ξ , of ρ_t with an extra bar (single or double) at $\{0, e_1\} \times \{0\}$, then

$$\begin{aligned} & \lim_{N \rightarrow \infty} \frac{1}{Z_N(\mathbf{0})} \frac{N}{\beta} \int_A \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \left((\sigma_{0_0, \frac{\beta}{N}} - \sigma_{0_0,0})^2 + (\sigma_{0_1, \frac{\beta}{N}} - \sigma_{0_1,0})^2 \right) \\ &= (J_2 - 2J_1) \lim_{N \rightarrow \infty} \frac{1}{Z_N(\mathbf{0})} \frac{N}{\beta} \int_{E[0_1 - e_{1_0}]} \rho_t(d\xi) \mathbb{1}_{[(0_0,0) \neq (0_0,0+)] \cup [(0_1,0) \neq (0_1,0+)]} (\xi \cup b_0) \\ & \quad \sum_{\sigma \in \Sigma(\xi \cup b_0)} \left((\sigma_{0_0, \frac{\beta}{N}} - \sigma_{0_0,0})^2 + (\sigma_{0_1, \frac{\beta}{N}} - \sigma_{0_1,0})^2 \right) \\ &= 2(J_2 - 2J_1) \mathbb{P}[0_0 - e_{1_0}]. \end{aligned} \quad (6.2.158)$$

Here we calculate the sum under the condition $[(0_0,0) \neq (0_0,0+)] \cup [(0_1,0) \neq (0_1,0+)]$ as follows

$$\begin{aligned} & \sum_{\sigma \in \Sigma(\xi \cup b_0)} \left((\sigma_{0_0, \frac{\beta}{N}} - \sigma_{0_0,0})^2 + (\sigma_{0_1, \frac{\beta}{N}} - \sigma_{0_1,0})^2 \right) \\ & \leq 2^{|\mathcal{L}(\xi)|-1} \sum_{a,b,c,d=-\frac{1}{2}}^{\frac{1}{2}} \left((a-b)^2 + (c-d)^2 \right) \\ & = 2 \cdot 2^{|\mathcal{L}(\xi)|}. \end{aligned} \quad (6.2.159)$$

Inserting this into (6.2.157) gives

$$Z_N(\mathbf{v}^*) \leq Z_N(\mathbf{0}) \left[1 - \frac{4bc^2}{\beta} |\tilde{\Lambda}_L| + \frac{16a^2c^2}{\beta} |\mathcal{E}| (J_2 - 2J_1) \kappa(e_1) \right] + O(c^4) + O\left(\frac{1}{N}\right). \quad (6.2.160)$$

We see from this that $c = 0$ is a local maximiser if $b > 2a^2d(J_2 - 2J_1)\kappa(e_1)$. \square

We now use this lemma to obtain an infrared bound. We first introduce the space-time

Fourier transform of $\kappa(x, t)$,

$$\tilde{\kappa}(k, \tau) = \sum_{x \in \Lambda_L} \int_0^\beta dt e^{-ik \cdot x - i\tau t} \kappa(x, t). \quad (6.2.161)$$

We have the following inequality.

Lemma 6.2.20. *If $b > 2a^2 d(J_2 - 2J_1)\kappa(e_1)$ assume c_0 is such that $Z(\mathbf{v}) \leq Z(\mathbf{0}) \forall \mathbf{v} \in \mathcal{V}_{c_0}$ then for $(k, \tau) \neq (0, 0)$*

$$\tilde{\kappa}(k, \tau) \leq \frac{(-2J_1)\varepsilon(k) + 4b\tau^2}{((-2J_1)\varepsilon(k) + a\tau^2)^2}. \quad (6.2.162)$$

Proof. Unsurprisingly we choose $v_{x_i, t} = \cos(k \cdot x + \tau t)$ then for $\eta > 0$

$$\begin{aligned} Z(\eta \mathbf{v}) &= \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ (-2J_1) \int_0^\beta dt \left[\eta(\sigma_{\cdot, t}, \Delta v_{\cdot, t}) + \frac{1}{4} \eta^2(v_{\cdot, t}, \Delta v_{\cdot, t}) \right] \right. \\ &\quad \left. + \sum_{x_i \in \tilde{\Lambda}_L} \int_0^\beta dt \left[a\eta \sigma_{x_i, t} \frac{\partial^2 v_{x_i, t}}{\partial t^2} + b\eta^2 v_{x_i, t} \frac{\partial^2 v_{x_i, t}}{\partial t^2} \right] \right\}, \end{aligned} \quad (6.2.163)$$

where we have used the identity $(f, -\Delta g) = \sum_{\{x, y\} \in \mathcal{E}} (f_x - f_y)(g_x - g_y)$. Using that $-\Delta \mathbf{v} = \varepsilon(k) \mathbf{v}$ and $-\frac{\partial^2 \mathbf{v}}{\partial t^2} = \tau^2 \mathbf{v}$ we have

$$\begin{aligned} Z(\eta \mathbf{v}) &= \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ - \int_0^\beta dt \left[\eta((-2J_1)\varepsilon(k) + a\tau^2)(\sigma_{\cdot, t}, v_{\cdot, t}) \right. \right. \\ &\quad \left. \left. + \frac{1}{4} \eta^2((-2J_1)\varepsilon(k) + 4b\tau^2)(v_{\cdot, t}, v_{\cdot, t}) \right] \right\} \\ &= \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \left(1 + \frac{1}{2} \eta^2((-2J_1)\varepsilon(k) + a\tau^2)^2 \int_0^\beta dt \int_0^\beta dt' (\sigma_{\cdot, t}, v_{\cdot, t})(\sigma_{\cdot, t'}, v_{\cdot, t'}) \right. \\ &\quad \left. - \frac{1}{4} \eta^2((-2J_1)\varepsilon(k) + 4b\tau^2) \int_0^\beta dt (v_{\cdot, t}, v_{\cdot, t}) \right) + O(\eta^4). \end{aligned} \quad (6.2.164)$$

We can calculate in the same way as in previous sections to obtain

$$(\sigma_{\cdot, t}, v_{\cdot, t})(\sigma_{\cdot, t'}, v_{\cdot, t'}) = \sum_{x_i, y_j \in \tilde{\Lambda}_L} \cos(k \cdot x + \tau t) \cos(k \cdot y + \tau t) \sigma_{x_i, t} \sigma_{y_j, t'}, \quad (6.2.165)$$

and

$$\frac{1}{Z(\mathbf{0})} \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \sigma_{x_i, t} \sigma_{y_j, t'} = \frac{1}{4} \kappa(y - x, t' - t). \quad (6.2.166)$$

Finally

$$\begin{aligned}
& \int_0^\beta dt \int_0^\beta dt' \sum_{x_i, y_j \in \tilde{\Lambda}_L} \cos(k \cdot x + \tau t) \cos(k \cdot y + \tau t) \kappa(y - x, t' - t) \\
&= \int_0^\beta dt \int_0^\beta dt'' \sum_{x_i, z_j \in \tilde{\Lambda}_L} \cos(k \cdot x + \tau t) \cos(k \cdot (x + z) + \tau(t + t'')) \kappa(z, t'') \\
&= \int_0^\beta dt \sum_{x_i \in \tilde{\Lambda}_L} \cos(k \cdot x + \tau t) \operatorname{Re} e^{ik \cdot x + i\tau t} \sum_{z_j \in \tilde{\Lambda}_L} \int_0^\beta dt'' e^{ik \cdot z + i\tau t''} \kappa(z, t'') \\
&= \int_0^\beta dt \sum_{x_i \in \tilde{\Lambda}_L} \cos(k \cdot x + \tau t)^2 \times 2 \underbrace{\tilde{\kappa}(-k, -\tau)}_{\tilde{\kappa}(k, \tau)}
\end{aligned} \tag{6.2.167}$$

Putting this together we get

$$\begin{aligned}
Z(\eta \mathbf{v}) = Z(\mathbf{0}) \left[1 + \frac{1}{4} \eta^2 ((-2J_1)\varepsilon(k) + a\tau^2)^2 \tilde{\kappa}(k, \tau) \int_0^\beta dt (v_{\cdot, t}, v_{\cdot, t}) \right. \\
\left. - \frac{1}{4} \eta^2 ((-2J_1)\varepsilon(k) + 4b\tau^2) \int_0^\beta dt (v_{\cdot, t}, v_{\cdot, t}) \right] + O(\eta^4).
\end{aligned} \tag{6.2.168}$$

From this we know from the previous lemma that for $\eta > 0$ small enough

$$((-2J_1)\varepsilon(k) + a\tau^2)^2 \tilde{\kappa}(k, \tau) \leq ((-2J_1)\varepsilon(k) + 4b\tau^2). \tag{6.2.169}$$

The result follows. \square

Now we want to optimise over a and b to obtain the best bound possible. We first take $b > 2a^2 d(J_2 - 2J_1)\kappa(e_1)$ for $a \geq 0$ and optimise over a , first we differentiate

$$\begin{aligned}
& \frac{\partial}{\partial a} \frac{(-2J_1)\varepsilon(k) + 8da^2(J_2 - 2J_1)\kappa(e_1)\tau^2}{((-2J_1)\varepsilon(k) + a\tau^2)^2} \\
& \frac{16da(J_2 - 2J_1)\kappa(e_1)}{((-2J_1)\varepsilon(k) + a\tau^2)^2} - \frac{2\tau^2((-2J_1)\varepsilon(k) + 8da^2(J_2 - 2J_1)\kappa(e_1)\tau^2)}{((-2J_1)\varepsilon(k) + a\tau^2)^3}.
\end{aligned} \tag{6.2.170}$$

There is a minimum at

$$a = \frac{1}{8d(J_2 - 2J_1)\kappa(e_1)}, \tag{6.2.171}$$

note that taking $a = 0$ gives the bound $((-2J_1)\varepsilon(k))^{-1}$, taking a as in (6.2.171) gives a strict improvement:

$$\tilde{\kappa}(k, \tau) \leq \frac{1}{(-2J_1)\varepsilon(k) + \frac{\tau^2}{8d(J_2 - 2J_1)\kappa(e_1)}}. \tag{6.2.172}$$

We now use a Fourier identity to obtain the bounds of the theorem. To begin

$$\begin{aligned}
\hat{\kappa}(k, 0) &= \frac{1}{\beta} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z}} \tilde{\kappa}(k, \tau) \\
&\leq \frac{1}{\beta} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z}} \frac{1}{(-2J_1)\varepsilon(k) + \frac{\tau^2}{8d(J_2-2J_1)\kappa(e_1)}} \\
&= \frac{1}{\beta} \sum_{n \in \mathbb{Z}} \frac{1}{(-2J_1)\varepsilon(k) + \frac{(2\pi)^2 n^2}{8\beta^2 d(J_2-2J_1)\kappa(e_1)}} \\
&= \frac{1}{\beta} \sum_{n \in \mathbb{Z}} \frac{\frac{8\beta^2 d(J_2-2J_1)\kappa(e_1)}{(2\pi)^2}}{\frac{8\beta^2 d(J_2-2J_1)(-2J_1)\varepsilon(k)\kappa(e_1)}{(2\pi)^2} + n^2}.
\end{aligned} \tag{6.2.173}$$

Now use the identity

$$\sum_{n \in \mathbb{Z}} \frac{1}{c^2 + n^2} = \frac{\pi}{c} \coth(\pi c), \tag{6.2.174}$$

after some cancellation we have

$$\hat{\kappa}(k, 0) \leq \sqrt{\frac{2d(J_2 - 2J_1)\kappa(e_1)}{(-2J_1)\varepsilon(k)}} \coth(\beta \sqrt{2d(J_2 - 2J_1)(-2J_1)\kappa(e_1)\varepsilon(k)}). \tag{6.2.175}$$

For the first bound in Theorem 6.2.17 we calculate

$$\begin{aligned}
1 = \kappa(0, 0) &= \frac{1}{\beta|\Lambda_L|} \sum_{k \in \Lambda_L^*} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z}} \tilde{\kappa}(k, \tau) \\
&= \frac{1}{\beta|\Lambda_L|} \tilde{\kappa}(0, 0) + \frac{1}{\beta|\Lambda_L|} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z} \setminus \{0\}} \tilde{\kappa}(0, \tau) + \frac{1}{\beta|\Lambda_L|} \sum_{k \in \Lambda_L^* \setminus \{0\}} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z}} \tilde{\kappa}(k, \tau)
\end{aligned} \tag{6.2.176}$$

Let $L(0_0, 0)$ denote the length of the loop containing the point $(0_0, 0)$. The first term is given by

$$\frac{1}{\beta|\Lambda_L|} \tilde{\kappa}(0, 0) = \frac{1}{2} \mathbb{E} \left[\frac{L(0_0, 0)}{\beta|\Lambda_L|} \right], \tag{6.2.177}$$

(recalling that sites x_0 and x_1 are equivalent). The second term vanishes in the limit $|\Lambda_L| \rightarrow \infty$ and we can bound the third term using (6.2.175). Putting this together and taking the limit $|\Lambda_L| \rightarrow \infty$ gives

$$\begin{aligned}
&\lim_{|\Lambda_L| \rightarrow \infty} \mathbb{E} \left[\frac{L(0_0, 0)}{\beta|\Lambda_L|} \right] \\
&\geq 2 - 2 \sqrt{\frac{2d(J_2 - 2J_1)\kappa(e_1)}{(-2J_1)}} \frac{1}{(2\pi)^d} \int_{[-\pi, \pi]^d} dk \frac{\coth(\beta \sqrt{2d(J_2 - 2J_1)(-2J_1)\kappa(e_1)\varepsilon(k)})}{\varepsilon(k)}.
\end{aligned} \tag{6.2.178}$$

The cotangent $\rightarrow 1$ as $\beta \rightarrow \infty$, hence

$$\lim_{\beta \rightarrow \infty} \lim_{|\Lambda_L| \rightarrow \infty} \mathbb{E} \left[\frac{L(0_0, 0)}{\beta |\Lambda_L|} \right] \geq 2 - 2 \sqrt{\frac{2(J_2 - 2J_1)\kappa(e_1)}{(-2J_1)}} K'_d. \quad (6.2.179)$$

For the second bound we note

$$\kappa(e_1) = \frac{1}{\beta |\Lambda_L|} \sum_{k \in \Lambda_L^*} \sum_{\tau \in \frac{2\pi}{\beta} \mathbb{Z}} \tilde{\kappa}(k, \tau) \frac{1}{d} \sum_{i=1}^d \cos k_i. \quad (6.2.180)$$

The same considerations give

$$\begin{aligned} & \lim_{|\Lambda_L| \rightarrow \infty} \mathbb{E} \left[\frac{L(0_0, 0)}{\beta |\Lambda_L|} \right] \\ & \geq 2\kappa(e_1) - 2 \sqrt{\frac{2d(J_2 - 2J_1)\kappa(e_1)}{(-2J_1)}} \frac{1}{d(2\pi)^d} \int_{[-\pi, \pi]^d} dk \frac{\coth(\beta \sqrt{2d(J_2 - 2J_1)\kappa(e_1)\varepsilon(k)})}{\varepsilon(k)} \left(\sum_{i=1}^d \cos k_i \right)^+. \end{aligned} \quad (6.2.181)$$

Taking the limit $\beta \rightarrow \infty$ gives the second bound

$$\lim_{\beta \rightarrow \infty} \lim_{|\Lambda_L| \rightarrow \infty} \mathbb{E} \left[\frac{L(0_0, 0)}{\beta |\Lambda_L|} \right] \geq 2 \sqrt{\mathbb{P}[0_0 - e_{1_0}]} \left(\sqrt{\mathbb{P}[0_0 - e_{1_0}]} - \sqrt{\frac{(J_2 - 2J_1)}{-J_1}} I'_d \right). \quad (6.2.182)$$

This completes the proof.

6.2.9 Nematic order via space-time reflection positivity - an initial result

We now use the method of space-time reflection positivity to study the nematic correlation function (6.2.110). Recall the integrals in (6.2.141) and the correlation $\rho(x, t)$ (6.2.110) then for the space-time Fourier transform,

$$\tilde{\rho}(k, \tau) = \sum_{x \in \Lambda_L} \int_0^\beta dt e^{-ik \cdot x - i\tau t} \rho(x, t), \quad (6.2.183)$$

we have the following theorem.

Theorem 6.2.21. *For β large enough*

$$\lim_{\beta \rightarrow \infty} \liminf_{L \rightarrow \infty} \frac{1}{\beta |\Lambda_L|} \tilde{\rho}(0, 0) \geq \liminf_{L \rightarrow \infty} \begin{cases} \frac{2}{9} - 2 \sqrt{\frac{(J_2 - 2J_1)\kappa(e_1)}{J_2}} K'_d \left(1 + o\left(\frac{1}{\beta}\right) \right) \\ \rho(e_1) - 2 \sqrt{\frac{(J_2 - 2J_1)\kappa(e_1)}{J_2}} I'_d \left(1 + o\left(\frac{1}{\beta}\right) \right). \end{cases} \quad (6.2.184)$$

For the explicit dependence on β see (6.2.208). The proof of the theorem incorporates the methods used in sections 6.2.7 and 6.2.8.

For a field $\mathbf{v} : \tilde{\Lambda}_L \times [0, \beta]_{per} \rightarrow \mathbb{R}$ such that $v_{x_0, t} = v_{x_1, t}$ for every $x \in \Lambda_L$ and $t \in [0, \beta]$ define the partition function

$$Z(\mathbf{v}) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ -(-2J_1) \sum_{\{x_i, y_j\} \in \tilde{\mathcal{E}}_L} \int_0^\beta dt [(\sigma_{x_0, t} \sigma_{x_1, t} - \sigma_{y_0, t} \sigma_{y_1, t})(v_{x_i, t} - v_{y_j, t}) + \frac{1}{4}(v_{x_i, t} - v_{y_j, t})^2] \right. \\ \left. + \sum_{x_i \in \tilde{\Lambda}_L} \int_0^\beta \left[a \left(\sigma_{x_0, t} \sigma_{x_1, t} - \frac{1}{12} \right) \frac{\partial^2 v_{x_i, t}}{\partial t^2} - b \left(\frac{\partial v_{x_i, t}}{\partial t} \right)^2 \right] \right\}, \quad (6.2.185)$$

where a and b are constants (chosen later). We consider only \mathbf{v} 's that are twice differentiable with respect to t with $\left| \frac{\partial v_{x_i, t}}{\partial t} \right| \leq c_0$ for every x_i, t . Denote the set of all such fields by \mathcal{V}_{c_0} .

Lemma 6.2.22. $\forall \mathbf{v} \in \mathcal{V}_{c_0} \exists \mathbf{v}^* \in \mathcal{V}_{c_0}$ depending on t but not on x_i such that $Z(\mathbf{v}) \leq Z(\mathbf{v}^*)$.

Proof. The proof is the same as Proposition 6.2.13, the sum over $x_i \in \tilde{\Lambda}_L$ plays no role. \square

Lemma 6.2.23. If $b > 4a^2 d(J_2 - 2J_1) \kappa(e_1)$ then $\exists c_0 > 0$ such that $Z(\mathbf{v}) \leq Z(\mathbf{0}) \forall \mathbf{v} \in \mathcal{V}_{c_0}$.

Proof. The proof is similar to Lemma 6.2.19. First we discretise in time, noting we need only consider fields constant in space, let N be even and define

$$Z_N(\mathbf{v}) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ -\frac{N}{\beta} \sum_{x_i \in \tilde{\Lambda}_L} \sum_{t \in \frac{\beta}{N} \{1, \dots, N\}} \left[a (\sigma_{x_0, t+\frac{\beta}{N}} \sigma_{x_1, t+\frac{\beta}{N}} - \sigma_{x_0, t} \sigma_{x_1, t}) (v_{t+\frac{\beta}{N}} - v_t) - b (v_{t+\frac{\beta}{N}} - v_t)^2 \right] \right\}. \quad (6.2.186)$$

Then again $\lim_{N \rightarrow \infty} Z_N(\mathbf{v}) = Z(\mathbf{v})$. Reflecting horizontally in lines $t = \frac{\beta}{N} n$ for $n = 1, \dots, N$ and using Cauchy-Schwarz gives $Z_N(\mathbf{v}^{(1)}, \mathbf{v}^{(2)}) \leq Z_N(\mathbf{v}^{(1)}, R\mathbf{v}^{(1)}) Z_N(R\mathbf{v}^{(2)}, \mathbf{v}^{(2)})$. Hence we have a maximiser of the form

$$\mathbf{v}_t^* = (-1)^{\frac{N}{\beta} t} \quad |c| \leq c_0 \frac{N}{2}. \quad (6.2.187)$$

The aim is to show that $c = 0$. Inserting this \mathbf{v}^* into Z_N gives

$$Z_N(\mathbf{v}^*) = \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ -\frac{4bc^2 |\tilde{\Lambda}_L|}{\beta} - \frac{4ac}{\beta} \sum_{x \in \Lambda_L} \sum_{t \in \frac{\beta}{N} \{1, \dots, N\}} (-1)^{\frac{N}{\beta} t} (\sigma_{x_0, t+\frac{\beta}{N}} \sigma_{x_1, t+\frac{\beta}{N}} - \sigma_{x_0, t} \sigma_{x_1, t}) \right\}. \quad (6.2.188)$$

Note we have replaced the sum over $x_i \in \tilde{\Lambda}_L$ with twice the sum over $x \in \Lambda_L$. When integrating over a realisation, ξ , of ρ_t we can replace an event $(x, y, t) \in \xi$ by $\frac{1}{2}$ an event at t and $\frac{1}{2}$ an event at $t + \frac{\beta}{N}$, this gives

$$Z_N(\mathbf{v}^*) = e^{-\frac{4bc^2 |\tilde{\Lambda}_L|}{\beta}} \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \prod_{(x, y, t) \in \xi} \frac{1}{2} \left(\exp \left\{ \frac{4ac}{\beta} (\sigma_{x_0, t+\frac{\beta}{N}} \sigma_{x_1, t+\frac{\beta}{N}} + \sigma_{y_0, t+\frac{\beta}{N}} \sigma_{y_1, t+\frac{\beta}{N}} - \sigma_{x_0, t} \sigma_{x_1, t} - \sigma_{y_0, t} \sigma_{y_1, t}) \right\} \right. \\ \left. + \exp \left\{ -\frac{4ac}{\beta} (\sigma_{x_0, t+\frac{\beta}{N}} \sigma_{x_1, t+\frac{\beta}{N}} + \sigma_{y_0, t+\frac{\beta}{N}} \sigma_{y_1, t+\frac{\beta}{N}} - \sigma_{x_0, t} \sigma_{x_1, t} - \sigma_{y_0, t} \sigma_{y_1, t}) \right\} \right) + O\left(\frac{1}{N}\right). \quad (6.2.189)$$

The $O\left(\frac{1}{N}\right)$ term is for realisations where two events occur on the same edge in a time interval $[t, t + \frac{\beta}{N}]$. At double bars we calculate the factor as

$$\exp\left\{\frac{32a^2c^2}{\beta^2}(\sigma_{x_0,t+\frac{\beta}{N}}\sigma_{x_1,t+\frac{\beta}{N}} - \sigma_{x_0,t}\sigma_{x_1,t})^2 + O(c^4)\right\} \quad (6.2.190)$$

At single bars we calculate the factor as

$$\begin{aligned} & \exp\left\{\frac{8a^2c^2}{\beta^2}(\sigma_{x_0,t} + \sigma_{y_1,t})^2(\sigma_{x_1,t+\frac{\beta}{N}} - \sigma_{x_1,t})^2 + O(c^4)\right\} \\ & \leq \exp\left\{\frac{8a^2c^2}{\beta^2}(\sigma_{x_1,t+\frac{\beta}{N}} - \sigma_{x_1,t})^2 + O(c^4)\right\} \\ & \leq \exp\left\{\frac{32a^2c^2}{\beta^2}(\sigma_{x_0,t})^2(\sigma_{x_0,t} + \sigma_{y_1,t})^2(\sigma_{x_1,t+\frac{\beta}{N}} - \sigma_{x_1,t})^2 + O(c^4)\right\} \\ & = \exp\left\{\frac{32a^2c^2}{\beta^2}(\sigma_{x_0,t+\frac{\beta}{N}}\sigma_{x_1,t+\frac{\beta}{N}} - \sigma_{x_0,t}\sigma_{x_1,t})^2 + O(c^4)\right\} \end{aligned} \quad (6.2.191)$$

where the last line used that $\sigma_{x_0,t+\frac{\beta}{N}} = \sigma_{x_0,t}$ at a single bar (assuming only one bar occurs in the time interval). Hence

$$Z_N(\mathbf{v}^*) \leq e^{-\frac{4bc^2|\tilde{\Lambda}_L|}{\beta}} \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp\left\{\frac{32a^2c^2}{\beta^2}(\sigma_{x_0,t+\frac{\beta}{N}}\sigma_{x_1,t+\frac{\beta}{N}} - \sigma_{x_0,t}\sigma_{x_1,t})^2 + O(c^4)\right\} + O\left(\frac{1}{N}\right). \quad (6.2.192)$$

Let A denote the event that an event occurs on edge $\{0, e_1\}$ on time interval $\left[0, \frac{\beta}{N}\right]$, expanding the exponentials gives

$$\begin{aligned} Z_N(\mathbf{v}^*) \leq Z_N(\mathbf{0}) \left[1 - \frac{4bc^2}{\beta}|\tilde{\Lambda}_L|\right] + \frac{32a^2c^2}{\beta^2}|\mathcal{E}_L|N \int_A \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} (\sigma_{x_0,t+\frac{\beta}{N}}\sigma_{x_1,t+\frac{\beta}{N}} - \sigma_{x_0,t}\sigma_{x_1,t})^2 \\ + O(c^4) + O\left(\frac{1}{N}\right). \end{aligned} \quad (6.2.193)$$

Now let $\xi \cup b_0$ be the realisation, ξ , of ρ_t with an extra event at $\{0, e_1\} \times \{0\}$, then

$$\begin{aligned} & \lim_{N \rightarrow \infty} \frac{1}{Z_N(\mathbf{v})} \frac{N}{\beta} \int_A \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} (\sigma_{x_0,t+\frac{\beta}{N}}\sigma_{x_1,t+\frac{\beta}{N}} - \sigma_{x_0,t}\sigma_{x_1,t})^2 \\ & = (J_2 - 2J_1) \lim_{N \rightarrow \infty} \frac{1}{Z_N(\mathbf{v})} \frac{N}{\beta} \int_{E[0_1 - e_{1_0}]} \rho_t(d\xi) \mathbb{1}_{[(0_0,0) \neq (0_0,0+)] \cup [(0_1,0) \neq (0_1,0+)]}(\xi \cup b_0) \\ & \quad \sum_{\sigma \in \Sigma(\xi)} (\sigma_{x_0,t+\frac{\beta}{N}}\sigma_{x_1,t+\frac{\beta}{N}} - \sigma_{x_0,t}\sigma_{x_1,t})^2 \\ & \leq (J_2 - 2J_1) \mathbb{P}[0_0 - e_{1_0}]. \end{aligned} \quad (6.2.194)$$

Where we used the bound

$$\sum_{\sigma \in \Sigma(\xi)} (\sigma_{x_0, t + \frac{\beta}{N}} \sigma_{x_1, t + \frac{\beta}{N}} - \sigma_{x_0, t} \sigma_{x_1, t})^2 \leq 2^{|\mathcal{L}(\xi)|-1} \sum_{a, b, c, d = -\frac{1}{2}}^{\frac{1}{2}} (ab - cd)^2 = 2^{|\mathcal{L}(\xi)|}. \quad (6.2.195)$$

Inserting this we have

$$Z_N(\mathbf{v}^*) \leq Z_N(\mathbf{0}) \left[1 - \frac{4bc^2}{\beta} |\tilde{\Lambda}_L| \frac{32a^2c^2}{\beta} |\mathcal{E}| (J_2 - 2J_1) \kappa(e_1) \right] + O(c^4) + O\left(\frac{1}{N}\right) \quad (6.2.196)$$

and note that $c = 0$ is a local maximum if $b > 4a^2d(J_2 - 2J_1)\kappa(e_1)$. \square

Now we want to derive an infrared bound, we have the following lemma.

Lemma 6.2.24. *If $b > 2a^2d(J_2 - 2J_1)\kappa(e_1)$ assume c_0 is such that $Z(\mathbf{v}) \leq Z(\mathbf{0}) \forall \mathbf{v} \in \mathcal{V}_{c_0}$ then for $(k, \tau) \neq (0, 0)$*

$$\tilde{\rho}(k, \tau) \leq \frac{J_2 \mathcal{E}(k) + 4b\tau^2}{(J_2 \mathcal{E}(k) + a\tau^2)^2} \quad (6.2.197)$$

Proof. As usual for these proofs we choose field \mathbf{v} with $v_{x_i, t} = \cos(k \cdot x + \tau t)$. Now $-\Delta \mathbf{v} = \mathcal{E}(k)$ and $-\frac{\partial^2 \mathbf{v}}{\partial t^2} = \tau^2 \mathbf{v}$. Now for $\eta > 0$

$$\begin{aligned} Z(\eta \mathbf{v}) &= \int \rho_i(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ J_2 \int_0^\beta dt [\eta(\sigma_{\cdot, 0, t} \sigma_{\cdot, 1, t}, \Delta \mathbf{v}_t) + \frac{1}{4} \eta^2(\mathbf{v}_t, \Delta \mathbf{v}_t)] \right. \\ &\quad \left. + \sum_{x_i \in \tilde{\Lambda}_L} \int_0^\beta dt \left[a\eta \left(\sigma_{x_0, t} \sigma_{x_1, t} - \frac{1}{12} \right) \frac{\partial^2 v_{x_i, t}}{\partial t^2} + b\eta^2 v_{x_i, t} \frac{\partial^2 v_{x_i, t}}{\partial t^2} \right] \right\} \\ &= \int \rho_i(d\xi) \sum_{\sigma \in \Sigma(\xi)} \exp \left\{ - \int_0^\beta dt [(\eta J_2 \mathcal{E}(k) + a\eta\tau^2)(\sigma_{\cdot, 0, t} \sigma_{\cdot, 1, t}, \mathbf{v}_t) + \left(\frac{1}{4} \eta^2 J_2 \mathcal{E}(k) + b\eta^2 \tau^2 \right) (\mathbf{v}_t, \mathbf{v}_t)] \right\} \\ &= \int \rho_i(d\xi) \sum_{\sigma \in \Sigma(\xi)} \left(1 + \frac{1}{2} \eta^2 (J_2 \mathcal{E}(k) + a\tau^2)^2 \int_0^\beta dt \int_0^\beta dt' (\sigma_{\cdot, 0, t} \sigma_{\cdot, 1, t}, \mathbf{v}_t) (\sigma_{\cdot, 0, t'} \sigma_{\cdot, 1, t'}, \mathbf{v}_{t'}) \right. \\ &\quad \left. - \frac{1}{4} \eta^2 (J_2 \mathcal{E}(k) + 4b\tau^2) \int_0^\beta dt (\mathbf{v}_t, \mathbf{v}_t) \right) + O(\eta^4). \end{aligned} \quad (6.2.198)$$

Some calculation is required to deal with the double integral.

$$\begin{aligned} &\left(\sigma_{\cdot, 0, t} \sigma_{\cdot, 1, t} - \frac{1}{12}, \mathbf{v}_t \right) \left(\sigma_{\cdot, 0, t'} \sigma_{\cdot, 1, t'} - \frac{1}{12}, \mathbf{v}_{t'} \right) \\ &= \sum_{x_i, y_j \in \tilde{\Lambda}_L} \cos(k \cdot x + \tau t) \cos(k \cdot y + \tau t') \left(\sigma_{x_0, t} \sigma_{x_1, t} - \frac{1}{12} \right) \left(\sigma_{y_0, t'} \sigma_{y_1, t'} - \frac{1}{12} \right), \end{aligned} \quad (6.2.199)$$

we further have

$$\begin{aligned}
& \frac{1}{Z(\mathbf{0})} \int \rho_t(d\xi) \sum_{\sigma \in \Sigma(\xi)} \left(\sigma_{x_0,t} \sigma_{x_1,t} - \frac{1}{12} \right) \left(\sigma_{y_0,t'} \sigma_{y_1,t'} - \frac{1}{12} \right) \\
&= \frac{1}{144} - \frac{1}{6} \mathbb{E}[\sigma_{0,t} \sigma_{0_1,t}] + \mathbb{E}[\sigma_{x_0,t} \sigma_{x_1,t} \sigma_{y_0,t'} \sigma_{y_1,t'}] \\
&= -\frac{1}{144} + \frac{1}{4} \left(\rho(y-x, t'-t) + \frac{1}{36} \right) \\
&= \frac{1}{4} \rho(y-x, t'-t).
\end{aligned} \tag{6.2.200}$$

Putting this together we have

$$\begin{aligned}
& \frac{1}{Z(\mathbf{0})} \int \rho_t(d\xi) \int_0^\beta dt \int_0^\beta dt' \sum_{\sigma \in \Sigma(\xi)} \left(\sigma_{\cdot_0,t} \sigma_{\cdot_1,t} - \frac{1}{12}, \mathbf{v}_t \right) \left(\sigma_{\cdot_0,t'} \sigma_{\cdot_1,t'} - \frac{1}{12}, \mathbf{v}_{t'} \right) \\
&= \frac{1}{4} \int_0^\beta dt \int_0^\beta dt' \sum_{x_i, y_j \in \bar{\Lambda}_L} \cos(k \cdot x + \tau t) \cos(k \cdot y + \tau t') \rho(y-x, t'-t) \\
&= \frac{1}{4} \int_0^\beta dt \int_0^\beta dt'' \sum_{x_i, z_j \in \bar{\Lambda}_L} \cos(k \cdot x + \tau t) \cos(k \cdot (x+z) + \tau(t+t'')) \rho(z, t'') \\
&= \frac{1}{4} \int_0^\beta dt \sum_{x_i \in \bar{\Lambda}_L} \cos(k \cdot x + \tau t) \operatorname{Re} e^{ik \cdot x + i\tau t} \sum_{z_j \in \bar{\Lambda}_L} \int_0^\beta dt'' e^{ik \cdot z + i\tau t''} \rho(z, t'') \\
&= \frac{1}{4} \int_0^\beta dt \sum_{x_i \in \bar{\Lambda}_L} \cos(k \cdot x + \tau t) \times 2 \underbrace{\tilde{\rho}(-k, -\tau)}_{\tilde{\rho}(k, \tau)} \\
&= \frac{1}{2} \tilde{\rho}(k, \tau) \int_0^\beta dt d(\mathbf{v}_t, \mathbf{v}_t).
\end{aligned} \tag{6.2.201}$$

From this we have

$$Z(\eta \mathbf{v}) = Z(\mathbf{0}) \left[1 + \frac{1}{4} \eta^2 (J_2 \varepsilon(k) + a\tau^2)^2 \tilde{\rho}(k, \tau) \int_0^\beta dt d(\mathbf{v}_t, \mathbf{v}_t) - \frac{1}{4} \eta^2 (J_2 \varepsilon(k) + 4b\tau^2) \int_0^\beta dt d(\mathbf{v}_t, \mathbf{v}_t) \right] + O(\eta^4). \tag{6.2.202}$$

We know from Lemma 6.2.23 that for η small enough

$$\frac{1}{4} (J_2 \varepsilon(k) + a\tau^2)^2 \tilde{\rho}(k, \tau) \leq \frac{1}{4} (J_2 \varepsilon(k) + 4b\tau^2), \tag{6.2.203}$$

the result follows. \square

Now we optimise a and b . We take $b = 4a^2 d(J_2 - 2J_1) \kappa(e_1)$ and

$$a = \frac{1}{16d(J_2 - 2J_1) \kappa(e_1)}. \tag{6.2.204}$$

With a small calculation we now have the bound

$$\tilde{\rho}(k, \tau) \leq \frac{1}{J_2 \varepsilon(k) + \frac{\tau^2}{16d(J_2 - 2J_1)\kappa(e_1)}}. \quad (6.2.205)$$

We relate this to $\hat{\rho}(k, 0)$ with some more calculation

$$\begin{aligned} \hat{\rho}(k, 0) &= \frac{1}{\beta} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z}} \tilde{\rho}(k, \tau) \\ &\leq \frac{1}{\beta} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z}} \frac{1}{J_2 \varepsilon(k) + \frac{\tau^2}{16d(J_2 - 2J_1)\kappa(e_1)}} \\ &= \frac{1}{\beta} \sum_{n \in \mathbb{Z}} \frac{\frac{16\beta^2 d(J_2 - 2J_1)\kappa(e_1)}{(2\pi)^2 n^2}}{\frac{16\beta^2 d(J_2 - 2J_1)\kappa(e_1)}{(2\pi)^2 n^2} + n^2}. \end{aligned} \quad (6.2.206)$$

Now we use the identity

$$\sum_{n \in \mathbb{Z}} \frac{1}{c^2 + n^2} = \frac{\pi}{c} \coth(\pi c), \quad (6.2.207)$$

after calculation we have

$$\hat{\rho}(k, 0) \leq 2 \sqrt{\frac{d(J_2 - 2J_1)\kappa(e_1)}{J_2 \varepsilon(k)}} \coth\left(\beta \sqrt{4d(J_2 - 2J_1)J_2 \kappa(e_1) \varepsilon(k)}\right). \quad (6.2.208)$$

Now we are ready to derive the first bound in Theorem 6.2.21,

$$\begin{aligned} \frac{2}{9} = \rho(0, 0) &= \frac{1}{\beta|\Lambda_L|} \sum_{k \in \Lambda_L^*} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z}} \tilde{\rho}(k, \tau) \\ &= \frac{1}{\beta|\Lambda_L|} \tilde{\rho}(0, 0) + \frac{1}{\beta|\Lambda_L|} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z} \setminus \{0\}} \tilde{\rho}(0, \tau) + \frac{1}{\beta|\Lambda_L|} \sum_{k \in \Lambda_L^* \setminus \{0\}} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z}} \tilde{\rho}(k, \tau). \end{aligned} \quad (6.2.209)$$

The second term vanishes as $|\Lambda_L| \rightarrow \infty$, the third term can be bounded using (6.2.208).

Hence

$$\lim_{\beta \rightarrow \infty} \lim_{|\Lambda_L| \rightarrow \infty} \frac{1}{\beta|\Lambda_L|} \tilde{\rho}(0, 0) \geq \frac{2}{9} - 2 \sqrt{\frac{(J_2 - 2J_1)\kappa(e_1)}{J_2}} K'_d. \quad (6.2.210)$$

The second bound follows in the same way from the identity

$$\rho(e_1, 0) = \frac{1}{\beta|\Lambda_L|} \sum_{k \in \Lambda_L^*} \sum_{\tau \in \frac{2\pi}{\beta}\mathbb{Z}} \tilde{\rho}(k, \tau) \frac{1}{d} \sum_{i=1}^d \cos k_i. \quad (6.2.211)$$

Chapter 7

Dilute spin systems

7.1 Setting for a quenched spin system

We begin by introducing the setting for quenched spin systems, both quantum and classical. In keeping with the general theme of this thesis we will consider a quenched Heisenberg model, we can easily generalise to other models. Experimentally speaking the quenched system is more physically relevant than its annealed counterpart. Theoretically there should not be a substantial difference between quenched and annealed, although techniques in this thesis will find the annealed system much more amenable. Results for quenched systems are out of reach using the techniques presented here due to reflection positivity not holding. Nevertheless we present the quenched setting to demonstrate that dilution can be realised mathematically in several ways.

Let (Λ, \mathcal{E}) be a finite graph with vertices Λ and edges \mathcal{E} . We call a subset, $\Omega \subset \Lambda$, a partition and note that $\Omega \cup \Omega^c = \Lambda$. Ω will correspond to occupied sites and its complement Ω^c to vacant sites. If Ω is a strict subset of Λ we call it a random partition or a random system. We now look at the classical and quantum case separately.

7.1.1 A classical quenched system

For a fixed partition Ω we define Hamiltonian

$$H_{\Lambda}^{cl}(\Omega, u, h) = -2 \sum_{\langle x, y \rangle} (S_x^1 S_y^1 + u S_x^2 S_y^2 + S_x^3 S_y^3) - h \sum_{x \in \Omega} S_x^3 \quad (7.1.1)$$

where $(S_x^1, S_x^2, S_y^3) \in \mathbb{S}^2$ is a classical spin at $x \in \Lambda$ and the first sum is over edges $\{x, y\} \in \mathcal{E}$ such that $x, y \in \Omega$. Recall that $u = 1$ corresponds to the Heisenberg ferromagnet. Then the partition function and Gibbs states are given by

$$Z_\Lambda^{cl}(\Omega, u, h, \beta) = \int d\mathbf{S}_\Lambda e^{-\beta H_\Lambda^{cl}(\Omega, u, h)}, \quad \langle \cdot \rangle_{\Lambda, \Omega, u, h, \beta}^{cl} = \frac{1}{Z_\Lambda^{cl}(\Omega, u, h, \beta)} \int d\mathbf{S}_\Lambda \cdot e^{-\beta H_\Lambda^{cl}(\Omega, u, h)}, \quad (7.1.2)$$

where $d\mathbf{S}_\Lambda$ is the Haar measure on $(\mathbb{S}^2)^\Lambda$ with $\int d\mathbf{S}_\Lambda = 1$. The aim is to assign a probability $P(\Omega)$ to each partition, Ω . In addition to the averaging $\langle \cdot \rangle_{\Lambda, \Omega, u, h, \beta}^{cl}$ we take an average over partitions. For a function g on partitions define

$$\langle\langle g \rangle\rangle_\Lambda = \sum_{\Omega \subset \Lambda} P(\Omega) g(\Omega). \quad (7.1.3)$$

For example we could take $g(\Omega) = \langle f \rangle_{\Lambda, \Omega, u, h, \beta}^{cl}$ for some function, f , of spins. One natural candidate for P is $P(\Omega) = p^{|\Omega|}(1-p)^{|\Lambda|-|\Omega|}$ with $p \in [0, 1]$, equivalent to a Bernoulli(p) variable at each $x \in \Lambda$.

7.1.2 A quantum quenched system

The setting for quantum systems is much the same as for classical systems. For fixed $\Omega \subset \Lambda$ define

$$H_\Lambda^{qu}(\Omega, u, h) = -2 \sum_{\langle x, y \rangle} (S_x^1 S_y^1 + u S_x^2 S_y^2 + S_x^3 S_y^3) - h \sum_{x \in \Omega} S_x^3 \quad (7.1.4)$$

where now (S_x^1, S_x^2, S_y^3) is a spin- S operator at $x \in \Lambda$ for $S \in \frac{1}{2}\mathbb{N}$ and the first sum is over edges $\{x, y\} \in \mathcal{E}$ such that $x, y \in \Omega$. $u = 1$ corresponds to the Heisenberg ferromagnet and, if (Λ, \mathcal{E}) is bipartite, $u = -1$ is unitarily equivalent to the Heisenberg antiferromagnet. The partition function and Gibbs states are

$$Z_\Lambda^{qu}(\Omega, u, h, \beta) = \text{Tr} e^{-\beta H_\Lambda^{qu}(\Omega, u, h)}, \quad \langle \cdot \rangle_{\Lambda, \Omega, u, h, \beta}^{qu} = \frac{1}{Z_\Lambda^{qu}(\Omega, u, h, \beta)} \text{Tr} \cdot e^{-\beta H_\Lambda^{qu}(\Omega, u, h)}, \quad (7.1.5)$$

where the trace is over $\otimes_{x \in \Lambda} \mathbb{C}^{2S+1}$. Again we can average over $\Omega \subset \Lambda$ according to some probability distribution P ,

$$\langle\langle g \rangle\rangle_\Lambda = \sum_{\Omega \subset \Lambda} P(\Omega) g(\Omega). \quad (7.1.6)$$

For g a function on partitions. Another candidate for P can be defined for a fixed n by

$$P(\Omega) = \begin{cases} \left(\binom{|\Lambda|}{n} \right)^{-1} & \text{if } |\Omega| = n \\ 0 & \text{else.} \end{cases} \quad (7.1.7)$$

7.2 Setting for an annealed spin system

In this section we introduce a specific annealed system that we will work with in the next section. We only introduce the quantum system. The classical case is very similar, as for the quenched case.

We work on a graph consisting of a bipartite lattice, Λ_L ,

$$\Lambda_L = \left\{ -\frac{L}{2} + 1, \dots, \frac{L}{2} \right\}^d, \quad (7.2.1)$$

with $L \in \mathbb{N}$ and periodic boundary conditions together with the set of nearest neighbour edges, \mathcal{E}_L . Each site has an occupation number, $n_x \in \{0, 1\}$.

Let S^1, S^2 and S^3 denote the usual spin- S matrices on \mathbb{C}^{2S+1} for $S \in \frac{1}{2}\mathbb{N}$ and let $\mathbf{S} = (S^1, S^2, S^3)$. Denote $S_x^i = S^i \otimes \mathbb{1}_{\Lambda_L \setminus \{x\}}$. We take the algebra \mathcal{A}_{Λ_L} of observables of all functions $A : \{0, 1\}^{\Lambda_L} \rightarrow \mathcal{M}_{\Lambda_L}$ where \mathcal{M}_{Λ_L} is the C^* -algebra of linear operators acting on the space $\otimes_{x \in \Lambda_L} \mathbb{C}^{2S+1}$. The Hamiltonian of the system $H_L = H_L^u(\mathbf{n}, \mu)$ is then

$$H_L = -2 \sum_{\langle x, y \rangle} n_x n_y \left(S_x^1 S_y^1 + u S_x^2 S_y^2 + S_x^3 S_y^3 \right) - \mu \sum_{x \in \Lambda_L} n_x, \quad (7.2.2)$$

for $u, \mu \in \mathbb{R}$ and $|u| \leq 1$. The case $u = 1$ is the Heisenberg ferromagnet, $u = 0$ is the XY model and $u = -1$ is unitarily equivalent to the Heisenberg antiferromagnet. We have partition function and Gibbs states given by

$$Z_L(\beta) = \sum_{\mathbf{n}} \text{Tr} e^{-\beta H_L}, \quad (7.2.3)$$

$$\langle \cdot \rangle_{\beta} = \frac{1}{Z_L(\beta)} \sum_{\mathbf{n}} \text{Tr} \cdot e^{-\beta H_L}. \quad (7.2.4)$$

7.3 Long-range order for an annealed quantum spin system

The aim of this section is to prove a phase transition occurs for some values of β and μ in the model (7.2.2). We have reflection positivity for this model (Lemma (7.3.2)). It should come as no surprise that Néel order can be recovered for this model for μ and β large enough. What is perhaps more surprising is the occurrence of the more interesting staggered states in Section 7.4.

Theorem 7.3.1. *For $S \in \frac{1}{2}\mathbb{N}$, L even, $d \geq 3$, and $u \in [-1, 0]$ we have the bounds*

$$\liminf_{L \rightarrow \infty} \frac{1}{L^d} \sum_{x \in \Lambda_L} (-1)^{\|x\|} \langle n_0 S_0^3 n_x S_x^3 \rangle_\beta \geq \liminf_{L \rightarrow \infty} \begin{cases} \frac{S(S+1)\langle n_0 \rangle_\beta}{3} - \frac{S}{(2\pi)^d} \int_{[-\pi, \pi]^d} dk \sqrt{\frac{d}{\varepsilon(k)}} + o\left(\frac{1}{\beta}\right) \\ \langle n_0 S_0^3 n_{e_1} S_{e_1}^3 \rangle_\beta - \frac{S\sqrt{d}}{(2\pi)^d} \int_{[\pi, \pi]^d} dk \sqrt{\frac{1}{\varepsilon(k)}} \left(\frac{1}{d} \sum_{i=1}^d \cos k_i \right)_+ + o\left(\frac{1}{\beta}\right) \end{cases} \quad (7.3.1)$$

For μ large enough the first bound will be positive for large enough S or d . For example if $d = 3$ the first bound is positive for $S \geq \frac{3}{2}$.

7.3.1 Proof of Néel order

To begin let $\mathbf{v} = (v_x)_{x \in \Lambda_L}$ with $v_x \in \mathbb{R}$ be a real valued field on Λ_L . We define a new Hamiltonian and partition function using this field,

$$H(\mathbf{v}) = H_L - \sum_{x \in \Lambda_L} (\Delta \mathbf{v})_x n_x S_x^3. \quad (7.3.2)$$

$$Z(\mathbf{v}) = \sum_{\mathbf{n}} \text{Tr} e^{-\beta H(\mathbf{v})}. \quad (7.3.3)$$

A calculation shows that

$$\begin{aligned} H(\mathbf{v}) = & \sum_{\{x,y\} \in \mathcal{E}_L} \left((n_x S_x^1 - n_y S_y^1)^2 + (\sqrt{u} n_x S_x^2 - \sqrt{u} n_y S_y^2)^2 + \left(n_x S_x^3 + \frac{n_x v_x}{2} - n_y S_y^3 - \frac{n_y v_y}{2} \right)^2 \right) \\ & - \frac{1}{4} \sum_{\{x,y\} \in \mathcal{E}_L} (n_x v_x - n_y v_y)^2 - \underbrace{2d \sum_{x \in \Lambda_L} n_x \left((S_x^1)^2 + u(S_x^2)^2 + (S_x^3)^2 \right)}_{C_{\Lambda_L}} - \mu \sum_{x \in \Lambda_L} n_x. \end{aligned} \quad (7.3.4)$$

We then define

$$H'(\mathbf{v}) = H(\mathbf{v}) + \frac{1}{4} \sum_{\{x,y\} \in \mathcal{E}_L} (n_x v_x - n_y v_y)^2 + C_{\Lambda_L}, \quad (7.3.5)$$

$$Z'(\mathbf{v}) = \sum_{\mathbf{n}} \text{Tr} e^{-\beta H'(\mathbf{v})}. \quad (7.3.6)$$

Let R be a reflection through edges in \mathcal{E}_L , then R uniquely determines $\Lambda_1, \Lambda_2 \subset \Lambda_L$ such that $\Lambda_1 \cup \Lambda_2 = \Lambda_L$, $\Lambda_1 \cap \Lambda_2 = \emptyset$ with $R\Lambda_1 = \Lambda_2$. We can write a field on Λ_L as $\mathbf{v} = (\mathbf{v}_1, \mathbf{v}_2)$ where $\mathbf{v}_i = \mathbf{v}|_{\Lambda_i}$. Given a reflection R we define $\mathfrak{h} = \mathcal{A}_{\Lambda_1} \cong \mathcal{A}_{\Lambda_2}$, then $H'(\mathbf{v})$ is an operator on $\mathfrak{h} \otimes \mathfrak{h}$. Reflection positivity for $Z'(\mathbf{v})$ is as follows.

Lemma 7.3.2. *Let $u \leq 0$. For any reflection, R , across edges we have*

$$Z'(\mathbf{v}_1, \mathbf{v}_2)^2 \leq Z'(\mathbf{v}_1, R\mathbf{v}_1)Z'(\mathbf{v}_2, R\mathbf{v}_2). \quad (7.3.7)$$

Proof. Let R be a reflection across edges. To begin write

$$f(n_x, n_y, \mathbf{S}_x, \mathbf{S}_y) = \left((n_x S_x^1 - n_y S_y^1)^2 + (\sqrt{u} n_x S_x^2 - \sqrt{u} n_y S_y^2)^2 + \left(n_x S_x^3 + \frac{n_x v_x}{2} - n_y S_y^3 - \frac{n_x v_x}{2} \right)^2 \right). \quad (7.3.8)$$

Denote by \mathcal{E}_i the set of edges with both end points in Λ_i , denote by $\{x_i, y_i\}$, $i = 1, \dots, k$ the edges crossing the reflection plane. Then using Trotter's formula we have

$$\begin{aligned} & \left| \sum_{\mathbf{n}} \text{Tr} \exp \left\{ -\beta \left(\sum_{\{x,y\} \in \mathcal{E}_1 \cup \mathcal{E}_2} f(n_x, n_y, \mathbf{S}_x, \mathbf{S}_y) + \sum_{i=1}^k f(n_{x_i}, n_{y_i}, \mathbf{S}_{x_i}, \mathbf{S}_{y_i}) \right) \right\} \right|^2 \\ &= \lim_{m \rightarrow \infty} \left| \sum_{\mathbf{n}} \text{Tr} \left(\exp \left\{ -\frac{\beta}{m} \sum_{\{x,y\} \in \mathcal{E}_1 \cup \mathcal{E}_2} f(n_x, n_y, \mathbf{S}_x, \mathbf{S}_y) \right\} \exp \left\{ -\frac{\beta}{m} \sum_{i=1}^k f(n_{x_i}, n_{y_i}, \mathbf{S}_{x_i}, \mathbf{S}_{y_i}) \right\} \right)^m \right|^2 \end{aligned} \quad (7.3.9)$$

Now we use the identity

$$e^{-M^2} = \int_{-\infty}^{\infty} \frac{ds}{2\sqrt{\pi}} e^{-\frac{s^2}{4}} e^{isM} \quad (7.3.10)$$

to obtain

$$\begin{aligned}
& \lim_{m \rightarrow \infty} \left| \sum_{\mathbf{n}} \int \mathrm{d}\nu(s_1^n) \dots \mathrm{d}\nu(s_{3km}^n) \mathrm{Tr}_{\mathfrak{g} \otimes \mathfrak{b}} \prod_{j=1}^m \exp \left\{ -\frac{\beta}{m} \sum_{(x,y) \in \mathcal{E}_1 \cup \mathcal{E}_2} f(n_x, n_y, \mathbf{S}_x, \mathbf{S}_y) \right\} \right. \\
& \prod_{l=1}^k \left(\exp \left\{ i s_{3lj}^n \sqrt{\frac{\beta}{m}} (n_{x_l} S_{x_l}^1 - n_{y_l} S_{y_l}^1) \right\} \exp \left\{ i s_{3(l+1)j}^n \sqrt{\frac{\beta}{m}} (\sqrt{u} n_{x_l} S_{x_l}^2 - \sqrt{u} n_{y_l} S_{y_l}^2) \right\} \right. \\
& \left. \exp \left\{ i s_{3(l+2)j}^n \sqrt{\frac{\beta}{m}} \left(n_{x_l} S_{x_l}^3 + \frac{n_{x_l} v_{x_l}}{2} - n_{y_l} S_{y_l}^3 - \frac{n_{y_l} v_{y_l}}{2} \right) \right\} \right)^2 \\
& = \lim_{m \rightarrow \infty} \left| \left[\sum_{\mathbf{n}} \int \mathrm{d}\nu(s_1^n) \dots \mathrm{d}\nu(s_{3km}^n) \mathrm{Tr}_{\mathfrak{b}} \prod_{j=1}^m \exp \left\{ -\frac{\beta}{m} \sum_{(x,y) \in \mathcal{E}_1} f(n_x, n_y, \mathbf{S}_x, \mathbf{S}_y) \right\} \right. \right. \\
& \left. \prod_{l=1}^k \exp \left\{ i s_{3lj}^n \sqrt{\frac{\beta}{m}} n_{x_l} S_{x_l}^1 \right\} \exp \left\{ i s_{3(l+1)j}^n \sqrt{\frac{\beta}{m}} \sqrt{u} n_{x_l} S_{x_l}^2 \right\} \exp \left\{ i s_{3(l+2)j}^n \sqrt{\frac{\beta}{m}} \left(n_{x_l} S_{x_l}^3 + \frac{n_{x_l} v_{x_l}}{2} \right) \right\} \right] \\
& \left[\sum_{\mathbf{n}} \int \mathrm{d}\nu(s_1^n) \dots \mathrm{d}\nu(s_{3km}^n) \mathrm{Tr}_{\mathfrak{b}} \prod_{j=1}^m \exp \left\{ -\frac{\beta}{m} \sum_{(x,y) \in \mathcal{E}_2} f(n_x, n_y, \mathbf{S}_x, \mathbf{S}_y) \right\} \right. \\
& \left. \prod_{l=1}^k \exp \left\{ -i s_{3lj}^n \sqrt{\frac{\beta}{m}} n_{y_l} S_{y_l}^1 \right\} \exp \left\{ -i s_{3(l+1)j}^n \sqrt{\frac{\beta}{m}} \sqrt{u} n_{y_l} S_{y_l}^2 \right\} \exp \left\{ -i s_{3(l+2)j}^n \sqrt{\frac{\beta}{m}} \left(n_{y_l} S_{y_l}^3 + \frac{n_{y_l} v_{y_l}}{2} \right) \right\} \right] \right|^2.
\end{aligned} \tag{7.3.11}$$

Where we have used that \mathcal{E}_1 and \mathcal{E}_2 are disjoint and that $\mathrm{Tr} A \otimes B = \mathrm{Tr} A \mathrm{Tr} B$. Using the Cauchy-Schwarz inequality and tracing the previous steps backwards for each product coming from Cauchy-Schwarz we obtain the result. \square

The property of Gaussian domination is then

$$Z'(\mathbf{v}) \leq Z'(\mathbf{0}) \iff Z(\mathbf{v}) \leq \sum_{\mathbf{n}} \mathrm{Tr} e^{-\beta H'(\mathbf{0})} e^{-\frac{\beta}{4}(\mathbf{n}\mathbf{v}, \mathbf{n}\Delta\mathbf{v})}. \tag{7.3.12}$$

We used $\mathbf{n}\mathbf{v}$ as shorthand for the field given by $(n\nu)_x = n_x v_x$. This inequality can easily be proved, starting from a field maximising field \mathbf{v} , apply reflections continually until the field is constant. From reflection positivity this field is also a maximiser, as $Z'(\mathbf{v})$ has the same value for any constant field we may take the constant zero. Note that we used that we sum over all possible configurations of \mathbf{n} in the definition of $Z'(\mathbf{v})$.

We use Gaussian domination to prove an infrared bound. We first make a preliminary definition. We define a Duhamel correlation function, $(\cdot, \cdot)_{Duh}^{\mathbf{n}}$ for this system as

$$(A, B)_{Duh}^{\mathbf{n}} = \frac{1}{Z_L(\beta)} \sum_{\mathbf{n}} \frac{1}{\beta} \int_0^\beta \mathrm{d}s \mathrm{Tr} A e^{-sH_L} B^* e^{-(\beta-s)H_L}. \tag{7.3.13}$$

We have the following lemma.

Lemma 7.3.3. For $k \in \Lambda_L^*$

$$\mathcal{F}\left((n_0 S_0^3, n_x S_x^3)_{Duh}^{\mathbf{n}}\right)(k) \leq \frac{1}{2\beta\varepsilon(k)}. \quad (7.3.14)$$

Proof. We choose $v_x = \cos(k \cdot x)$ for $k \in \Lambda_L^*$. For this choice of field we have that $\Delta \mathbf{v} = -\varepsilon(k)\mathbf{v}$ for $\varepsilon(k) = 2 \sum_{i=1}^d (1 - \cos k_i)$. Let $\eta > 0$ be a (small) parameter. From a Taylor expansion we have

$$Z(\eta \mathbf{v}) = Z(\mathbf{0}) + \frac{1}{2} \left(\Delta \mathbf{v}, \frac{\partial^2 Z(\mathbf{v})}{\partial(\Delta \mathbf{v})_x \partial(\Delta \mathbf{v})_y} \Big|_{\Delta \mathbf{v}=\mathbf{0}} (\Delta \mathbf{v}) \right) + O(\eta^4). \quad (7.3.15)$$

We can calculate the derivative

$$\frac{\partial^2 Z(\mathbf{v})}{\partial(\Delta \mathbf{v})_x \partial(\Delta \mathbf{v})_y} \Big|_{\Delta \mathbf{v}=\mathbf{0}} = \beta \frac{\partial}{\partial(\Delta \mathbf{v})_x} \sum_{\mathbf{n}} \text{Tr } n_x S_x^3 e^{-\beta H(\mathbf{v})} \Big|_{\Delta \mathbf{v}=\mathbf{0}} = \beta^2 (n_x S_x^3, n_y S_y^3)_{Duh}^{\mathbf{n}} Z(\mathbf{0}). \quad (7.3.16)$$

The second inequality relies on the Duhamel formula. Using this we have

$$\begin{aligned} Z(\eta \mathbf{n}) &= Z(\mathbf{0}) + \frac{1}{2} \eta \varepsilon(k)^2 \beta^2 \sum_{x, y \in \Lambda_L} \cos(k \cdot x) \cos(k \cdot y) (n_x S_x^3, n_y S_y^3)_{Duh}^{\mathbf{n}} Z(\mathbf{0}) + O(\eta^4) \\ &= Z(\mathbf{0}) \left(1 + \frac{1}{2} \eta^2 \varepsilon(k)^2 \beta^2 \mathcal{F}\left((n_0 S_0^3, n_x S_x^3)_{Duh}^{\mathbf{n}}\right)(k) \sum_{x \in \Lambda_L} \cos^2(k \cdot x) \right) + O(\eta^4). \end{aligned} \quad (7.3.17)$$

Here we have used the translation invariance of $(n_x S_x^3, n_y S_y^3)_{Duh}^{\mathbf{n}}$. Also we have

$$e^{-\frac{1}{4}\beta(\mathbf{nv}, \mathbf{n}\Delta \mathbf{v})} = e^{\frac{1}{4}\beta\varepsilon(k) \sum_x n_x \cos^2(k \cdot x)}. \quad (7.3.18)$$

From Gaussian domination we can consider the η^2 terms and see that for η small enough

$$\frac{1}{2} \eta^2 \varepsilon(k)^2 \beta^2 \mathcal{F}\left((n_0 S_0^3, n_x S_x^3)_{Duh}^{\mathbf{n}}\right)(k) \sum_{x \in \Lambda_L} \cos^2(k \cdot x) \leq \frac{1}{4} \eta^2 \beta \varepsilon(k) \sum_{x \in \Lambda_L} \cos^2(k \cdot x). \quad (7.3.19)$$

The result follows. \square

We now use the Falk-Bruch inequality to transfer this infrared bound to the correlation $\langle n_0 S_0^3 n_x S_x^3 \rangle_\beta$.

$$\frac{1}{2} \langle A^* A + A A^* \rangle_\beta \leq \frac{1}{2} \sqrt{\langle A, A \rangle_{Duh}^{\mathbf{n}}} \sqrt{\langle [A^*, [H, A]] \rangle_\beta} + \langle A, A \rangle_{Duh}^{\mathbf{n}}. \quad (7.3.20)$$

We take $A = \mathcal{F}(n_x S_x^3)(k)$ and $H = \beta H_L$. A simple calculation shows

$$[A^*, [H, A]] = 4\beta \sum_{\{x,y\} \in \mathcal{E}} \left((1 - u \cos(k \cdot (x - y))) n_x S_x^1 n_y S_y^1 + (u - \cos(k \cdot (x - y))) n_x S_x^2 n_y S_y^2 \right). \quad (7.3.21)$$

From this we have

$$\langle [A^*, [H, A]] \rangle_\beta = 4\beta |\Lambda_L| \varepsilon_u(k) \quad (7.3.22)$$

where

$$\varepsilon_u(k) = \sum_{i=1}^d \left((1 - u \cos k_i) \langle n_0 S_0^1 n_{e_i} S_{e_i}^1 \rangle_\beta + (u - \cos k_i) \langle n_0 S_0^2 n_{e_i} S_{e_i}^2 \rangle_\beta \right). \quad (7.3.23)$$

It is easy to show that $\varepsilon_u(k) \leq 4S^2 d$. We now have from Falk-Bruch

$$\mathcal{F} \left(\langle n_0 S_0^3 n_x S_x^3 \rangle_\beta \right) (k) \leq \sqrt{\frac{\varepsilon_u(k)}{2\varepsilon(k)}} + \frac{1}{2\beta\varepsilon(k)} \quad (7.3.24)$$

From this we obtain two bounds by expanding the Fourier transform around the points 0 and e_1 respectively. These bounds are

$$\frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \langle n_0 S_0^3 n_x S_x^3 \rangle_\beta \geq \begin{cases} \frac{1}{3} S(S+1) \langle n_0 \rangle_\beta - \frac{S\sqrt{2d}}{|\Lambda_L|} \sum_{k \in \Lambda_L^* \setminus \{0\}} \left(\sqrt{\frac{1}{2\varepsilon(k)}} + \frac{1}{2\beta\varepsilon(k)} \right) \\ \langle n_0 S_0^3 n_{e_1} S_{e_1}^3 \rangle_\beta - \frac{S\sqrt{2d}}{|\Lambda_L|} \sum_{k \in \Lambda_L^* \setminus \{0\}} \left(\sqrt{\frac{1}{2\varepsilon(k)}} + \frac{1}{2\beta\varepsilon(k)} \right) \left(\frac{1}{d} \sum_{i=1}^d \cos k_i \right)_+ \end{cases} \quad (7.3.25)$$

where $(\cdot)_+$ denotes the positive part. Taking limits $L \rightarrow \infty$ and then $\beta \rightarrow \infty$ gives

$$\lim_{\beta \rightarrow \infty} \lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \langle n_0 S_0^3 n_x S_x^3 \rangle_\beta \geq \begin{cases} \frac{1}{3} S(S+1) \langle n_0 \rangle_\beta - \frac{S\sqrt{d}}{(2\pi)^d} \int_{[-\pi, \pi]^d} \sqrt{\frac{1}{\varepsilon(k)}} \\ \langle n_0 S_0^3 n_{e_1} S_{e_1}^3 \rangle_\beta - \frac{S\sqrt{d}}{(2\pi)^d} \int_{[\pi, \pi]^d} \sqrt{\frac{1}{\varepsilon(k)}} \left(\frac{1}{d} \sum_{i=1}^d \cos k_i \right)_+ \end{cases} \quad (7.3.26)$$

this completes the proof.

7.4 Staggered long-range order for diluted quantum spin models

7.4.1 Introduction

In this section we study annealed site diluted quantum lattice spin systems, including the XY model with spin $\frac{1}{2}$ and the Heisenberg antiferromagnet with spin $S \geq \frac{1}{2}$. We find regions of the parameter space where, in spite of being a priori favourable for a densely occupied state, phases with staggered occupancy occur at low temperatures.

Two quantum spin models (the XY model with spin $\frac{1}{2}$ and the Heisenberg antiferromagnet) on the hypercubic lattice \mathbb{Z}^d ($d \geq 2$) with the annealed site dilution are considered. The models are formulated in terms of the Hamiltonian

$$H = -\frac{1}{S^2} \sum_{\langle x,y \rangle} n_x n_y (S_x^1 S_y^1 + u S_x^2 S_y^2 + S_x^3 S_y^3 - S(S+1)) - \mu \sum_{\mathbf{x}} n_{\mathbf{x}} - \kappa \sum_{\langle x,y \rangle} n_x n_y. \quad (7.4.1)$$

Here S_x^i 's are the standard spin- S operators acting on the site \mathbf{x} and $n_{\mathbf{x}}$ is the occupancy number indicating presence or absence ($n_{\mathbf{x}} = 1$ or $n_{\mathbf{x}} = 0$) of a particle at the site \mathbf{x} . The parameters μ and κ are the chemical potential and the interaction parameter for the particle occupancy. The XY model with spin- $\frac{1}{2}$ is obtained by the choosing $(S, u) = (\frac{1}{2}, 0)$ while $S \geq \frac{1}{2}$ and $u = -1$ yields the Heisenberg antiferromagnet.

The main claim concerns the existence of a staggered long range order characterised by the presence of two distinct states (in the thermodynamic limit) with preferential occupation of either the even or the odd sublattice. Indeed, it will be proven that such states occur in a region of parameters μ and κ , at intermediate inverse temperatures, β .

The existence of such states can be viewed as a demonstration of an “effective entropic repulsion” caused by the interaction of quantum spins leading to an impactful restriction of the “available phase space volume”. As a result, occupation of adjacent sites might turn out to be unfavourable—it results in an effective repulsion between particles in nearest neighbour sites and as a result eventually leads to a staggered order. It is easy to understand that this is the case for the annealed site diluted Potts model with large number of spin states q [23] where this effect is indeed caused by a pure entropic repulsion: two nearest neighbour occupied sites contribute the Boltzmann factor $q + q(q-1)e^{-\beta}$ which is at low temperatures much smaller than the factor q^2 obtained from two next nearest neighbour spins that are free to take all possible spin values entirely independently. Actually, the same is true—even though less obvious—in the case of diluted models with classical continuous

spins [24]. Our results constitute an extension of similar claims to a quantum situation.

To get a control on effective repulsion, we rely on a standard tool—the chessboard estimates which follow from reflection positivity. The classical references on this topic are [35, 39, 41, 42, 43] with a recent review [13]. For our case the treatment in [16] is especially useful. In particular, we use the setting from [16, Section 3.3] for an efficient formulation of the long range order in terms of coexistence of the corresponding infinite-volume KMS states.

While we are restricting ourselves only to the case $u = 0, -1$, the models with $-1 < u < 0$ are also covered by reflection positivity, hence results might be extended to this region. However, one would require bounds on the expectation of certain occupancy configurations (see Lemmas 7.4.5-7.4.8), that seem harder to achieve than in the cases $u = 0, -1$.

We introduce the models and state the main result in Section 7.4.2. The proof is deferred to Section 7.4.3.

7.4.2 Setting and Main Results

For a fixed *even* $L \in \mathbb{N}$, we consider the *torus* $\mathbb{T}_L = \mathbb{Z}^d / L\mathbb{Z}^d$ consisting of L^d sites that can be identified with the set $\{-L/2 + 1, -L/2 + 2, \dots, L/2 - 1, L/2\}^d$. On the torus \mathbb{T}_L we take the *algebra* \mathfrak{A}_L of *observables* of all functions $A : \{0, 1\}^{\mathbb{T}_L} \rightarrow \mathcal{M}_L$ where \mathcal{M}_L is the C^* -algebra of linear operators acting on the space $\otimes_{x \in \mathbb{T}_L} \mathbb{C}^{2S+1}$ with $S \in \frac{1}{2}\mathbb{N}$ (complex $(2S + 1)^{|\mathbb{T}_L|}$ -dimensional matrices).

A particular example of an observable is the Hamiltonian $H_L \in \mathfrak{A}_L$ of the form (7.4.1) with the periodic boundary conditions (on the torus \mathbb{T}_L),

$$H_L(n) = -\frac{1}{S^2} \sum_{\langle x, y \rangle \in \mathbb{E}_L} n_x n_y \left(S_x^1 S_y^1 + u S_x^2 S_y^2 + S_x^3 S_y^3 - S(S + 1) \right) - \mu \sum_{x \in \mathbb{T}_L} n_x - \kappa \sum_{\langle x, y \rangle \in \mathbb{E}_L} n_x n_y. \quad (7.4.2)$$

Here, \mathbb{E}_L is the set of all edges connecting nearest neighbour sites in the torus \mathbb{T}_L and (S^1, S^2, S^3) are the spin- S matrices. The Gibbs state on the torus is given by

$$\langle \cdot \rangle_{L, \beta} = \frac{1}{Z_L(\beta)} \sum_n \text{Tr} \cdot e^{-\beta H_L} \quad (7.4.3)$$

with $Z_L(\beta) = \sum_n \text{tr} e^{-\beta H_L}$. Infinite volume states of a quantum spin system are formulated in terms of KMS states, an analog of DLR states for classical systems. Let us briefly recall this notion in the form to be used in our situation. Here we follow closely the treatment

from [16] which can be consulted for a more detailed discussion of KMS states in a setting similar to ours. Let \mathfrak{A} denote the C^* algebra of quasilocal observables,

$$\mathcal{A} = \overline{\mathcal{A}_0}, \quad \text{where} \quad \mathcal{A}_0 = \bigcup_{\Lambda \text{ finite}} \mathcal{A}_\Lambda, \quad (7.4.4)$$

where the overline denotes the norm-closure. We define the *time evolution operators* $\alpha_t^{(L)}$ acting on $A \in \mathfrak{A}_L$ and for any $t \in \mathbb{R}$ as

$$\alpha_t^{(L)}(A) = e^{itH_L} A e^{-itH_L}. \quad (7.4.5)$$

It is well known that for a local operator $A \in \mathcal{A}_0$ we can expand $\alpha_t^{(L)}(A)$ as a series of commutators,

$$\alpha_t^{(L)}(A) = \sum_{m \geq 0} \frac{(it)^m}{m!} [H_L, [H_L, \dots, [H_L, A] \dots]]. \quad (7.4.6)$$

The map $t \rightarrow \alpha_t^{(L)}$ extends to all $t \in \mathbb{C}$ [56, Theorem III.3.6] and for $A \in \mathcal{A}_0$, as $L \rightarrow \infty$, $\alpha_t^{(L)}(A)$ converges in norm to a one-parameter family of operators $\alpha_t(A)$ on \mathfrak{A} uniformly on compact subsets of \mathbb{C} (one can consult the proof, for example, in [93] and see that the same proof structure works in this case). A state $\langle \cdot \rangle_\beta$ on \mathfrak{A} (a positive linear functional ($\langle A \rangle_\beta \geq 0$ if $A \geq 0$) such that $\langle \mathbb{1} \rangle_\beta = 1$) is called a KMS state (or is said to satisfy the KMS condition) with a Hamiltonian H at an inverse temperature β , if we have

$$\langle AB \rangle_\beta = \langle \alpha_{-i\beta}(B)A \rangle_\beta \quad (7.4.7)$$

for the above defined family of operators α_t at imaginary values $t = -i\beta$. One can see that the Gibbs state (7.4.3) satisfies the KMS condition for the finite volume time evolution operator.

A special class of *observables* are classical events $\mathbb{1}_{\mathcal{F}} I$ obtained as a product of the identity $I \in \mathcal{M}_L$ with the indicator $\mathbb{1}_{\mathcal{F}}$ of an occupation event $\mathcal{F} \subset \{0, 1\}^{\mathbb{T}_L}$. Often we will consider (classical) block events depending only on the occupation configuration on the block-cube of 2^d sites, $C = \{0, 1\}^d \subset \mathbb{T}_L$. Namely, the events of the form $\mathcal{E} \times \{0, 1\}^{\mathbb{T}_L \setminus C}$ where $\mathcal{E} \subset \{0, 1\}^C$. We will refer to these events directly as block events \mathcal{E} and use a streamlined notation $\langle \mathcal{E} \rangle_{L, \beta}$ (resp. $\langle \mathcal{E} \rangle_\beta$) instead of $\langle \mathbb{1}_{\mathcal{E} \times \{0, 1\}^{\mathbb{T}_L \setminus C}} I \rangle_{L, \beta}$ (resp. $\langle \mathbb{1}_{\mathcal{E} \times \{0, 1\}^{\mathbb{T}_L \setminus C}} I \rangle_\beta$).

In particular, to characterise the long-range order states mentioned above, we introduce the block events $\mathcal{G}^e = \{\mathbf{n}^e\}$ and $\mathcal{G}^o = \{\mathbf{n}^o\}$ where \mathbf{n}^e and \mathbf{n}^o are the even and the odd staggered configurations on C : $\mathbf{n}_x^e = 1$ iff \mathbf{x} is an even site in C and $\mathbf{n}_x^e = 1$ iff \mathbf{x} is an odd site in C . Notice that the sets \mathcal{G}^e and \mathcal{G}^o are disjoint. The main result for the quantum system with Hamiltonian (7.4.2) can now be stated as follows.

Theorem 7.4.1. *Let $u = -1$ and $S \geq \frac{1}{2}$ or $u = 0$ and $S = \frac{1}{2}$. For each case there exists $\mu_0 > 0$ and a function κ_0 (both depending on u, S , and d) that is positive on $(0, \mu_0)$ and such that for any $\mu > 0$, $\kappa < \max(\kappa_0(\mu), 0)$, and any $0 < \varepsilon < \frac{1}{2}$, there exists $\beta_0 = \beta_0(\mu, \kappa, \varepsilon)$ such that for any $\beta > \beta_0$ there exist two distinct KMS states, $\langle \cdot \rangle_\beta^e$ and $\langle \cdot \rangle_\beta^o$, that are staggered,*

$$\langle \mathcal{G}^e \rangle_\beta^e \geq 1 - \varepsilon \text{ and } \langle \mathcal{G}^o \rangle_\beta^o \geq 1 - \varepsilon. \quad (7.4.8)$$

The proof of this theorem is the content of Section 7.4.3. For the technical estimates, we will restrict ourselves to the two-dimensional case $d = 2$. The proof in higher dimensions employing the same methods is straightforward but rather cumbersome. For $d = 2$ we construct the function κ_0 explicitly.

Notice that the claim is true for any negative κ . This is not so surprising, negative κ triggers antiferromagnetic staggered order at low temperatures. More interesting is the case, established by the theorem, when this happens for positive κ where it is a demonstration of an effective entropic repulsion stemming from the quantum spin.

7.4.3 Proof of Theorem 7.4.1

Reflection Positivity for the Annealed Quantum Model

Consider now a splitting of the torus \mathbb{T}_L into 2 disjoint halves, $\mathbb{T}_L = \mathbb{T}_L^+ \cup \mathbb{T}_L^-$, separated by a pair of planes; say, $P_1 = \{(-1/2, x_2, \dots, x_d)$ and $P_2 = \{(L/2 - 1/2, x_2, \dots, x_d), x_2, \dots, x_d \in \mathbb{R}$. We introduce a reflection $\theta : \mathbb{T}_L \rightarrow \mathbb{T}_L$ defined by $\theta(x) = (-(x_1 + 1), x_2, \dots, x_d)$.¹ Any such reflection (parallel P_1 and P_2 of distance $L/2$ in arbitrary half-integer position and orthogonal to any coordinate axis) will be called *reflections through planes between the sites* or simply *reflections* (we will not use the other reflections through planes on the sites that are useful for classical models).

Further, consider two subalgebras $\mathfrak{A}_L^+, \mathfrak{A}_L^- \subset \mathfrak{A}_L$ living on the sets $\mathbb{T}_L^+, \mathbb{T}_L^-$, respectively. Namely, we define \mathfrak{A}_L^+ as a set of all operator-valued functions $A : \{0, 1\}^{\mathbb{T}_L^+} \rightarrow \mathcal{M}_L^+$, where \mathcal{M}_L^+ is the set of all operators of the form $A^+ \otimes I$ acting on the subspace $\otimes_{x \in \mathbb{T}_L^+} \mathbb{C}^{2S+1}$ and I is the identity on the complementary space $\otimes_{x \in \mathbb{T}_L^-} \mathbb{C}^{2S+1}$. Similarly for \mathfrak{A}_L^- .

The reflection θ can be naturally elevated to an involution $\theta : \mathfrak{A}_L^+ \rightarrow \mathfrak{A}_L^-$ acting on \mathcal{M}_L^+ in a

¹Notice that on the torus, the reflection with respect to P_1 is identical with that with respect to P_2 (just notice that $|x_1 - (-1/2)| = |y_1 - (-1/2)|$ with $x_1 \neq y_1$ implies $y_1 = -(x_1 + 1)$, while $|x_1 - (L/2 - 1/2)| = |y_1 - (L/2 - 1/2)|$ with $x_1 \neq y_1$ implies $y_1 = -(x_1 + L + 1)$ and $-(x_1 + 1) = -(x_1 + L + 1) \pmod{L}$).

properly parametrized basis as $\theta(A_+ \otimes I) = I \otimes A_+$ and reflecting the configuration \mathbf{n} ,

$$(\theta A)(\theta \mathbf{n}) = \theta(A(\mathbf{n})). \quad (7.4.9)$$

Finally, we say that a state $\langle \cdot \rangle$ on \mathfrak{A}_L is reflection positive with respect to θ if for any $A, B \in \mathfrak{A}_L^+$ we have

$$\langle A\theta B \rangle = \overline{\langle B\theta A \rangle} \quad (7.4.10)$$

and

$$\langle A\theta A \rangle \geq 0. \quad (7.4.11)$$

Here, \bar{A} denotes the complex conjugation of the matrix A . The standard consequence of the reflection positivity is the Cauchy-Schwartz inequality

$$\langle A\theta B \rangle^2 \leq \langle A\theta A \rangle \langle B\theta B \rangle \quad (7.4.12)$$

for any $A, B \in \mathfrak{A}_L^+$.

In our situation of an annealed diluted quantum model, we are dealing with the state

$$\langle A \rangle_{L,\beta} = \frac{\sum_{\mathbf{n} \in \{0,1\}^{\mathbb{T}_L}} \text{Tr } A(\mathbf{n}) e^{-\beta H_L(\mathbf{n})}}{\sum_{\mathbf{n} \in \{0,1\}^{\mathbb{T}_L}} \text{Tr } e^{-\beta H_L(\mathbf{n})}} \quad (7.4.13)$$

for any $A \in \mathfrak{A}_L$ and with the Hamiltonian $H_L \in \mathfrak{A}_L$ of the form (7.4.2). The standard proof of reflection positivity may be extended to this case.

Lemma 7.4.2. *The state $\langle \cdot \rangle_{L,\beta}$ is reflection positive for any θ through planes between the sites and any $\mu, \kappa \in \mathbb{R}$, $\beta \geq 0$, and any $u \leq 0$.*

Proof. The equality (7.4.10) is immediate. For (7.4.11) we first write the Hamiltonian H_L in the form $H_L(\mathbf{n}, \theta \mathbf{m}) = J(\mathbf{n}) + \theta \overline{J(\mathbf{m})} - \sum_{\alpha} D_{\alpha}(\mathbf{n}) \theta \overline{D_{\alpha}(\mathbf{m})}$ for any $\mathbf{n}, \mathbf{m} \in \{0,1\}^{\mathbb{T}_L^+}$ where $J \in \mathfrak{A}_L^+$ consists of all terms of the Hamiltonian with (both) sites in \mathbb{T}_L^+ and $D_{\alpha} \overline{\theta D_{\alpha}}$, with $D_{\alpha} \in \mathfrak{A}_L^+$ indexed by α , are representing the terms containing the sites adjacent to both sides to the reflection plane.

Notice that to have a correct negative sign with the terms $D_{\alpha} \overline{\theta D_{\alpha}}$, we need the condition $u \leq 0$. Indeed, if $\{x, y\}$ is an edge crossing the reflection plane the corresponding D_{α} 's are $\frac{1}{S^2} n_x S_x^1$, $\frac{1}{S^2} i \sqrt{-u} n_x S_x^2$, $\frac{1}{S^2} n_x S_x^3$. Recalling that in the standard basis $\overline{iS^2} = iS^2$, we need $u \leq 0$. Note that the term $\sum_{\langle x,y \rangle} n_x n_y (\kappa - S(S+1)/S^2)$ is simply a constant times the identity for each \mathbf{n} and can be bounded by $\pm d |\mathbb{T}_L| |\kappa - S(S+1)/S^2|$, hence we can pull it out of the trace and the sum as a constant and ignore it, as we do for the remainder of the proof. For

the claim (7.4.11) we need to show that

$$\sum_{\mathbf{n}, \mathbf{m} \in \{0,1\}^{\mathbb{T}_L^+}} \text{Tr} A(\mathbf{n}) \overline{\theta A(\mathbf{m})} e^{-\beta H_L(\mathbf{n}, \theta \mathbf{m})} \geq 0 \quad (7.4.14)$$

for any $A \in \mathfrak{A}_L^+$. Adapting the standard proof, see e.g. [39, Theorem 2.1], by Trotter formula we get

$$e^{-\beta H_L(\mathbf{n}, \theta \mathbf{m})} = \lim_{k \rightarrow \infty} \left(e^{-\frac{\beta}{k} J(\mathbf{n})} e^{-\frac{\beta}{k} \overline{\theta J(\mathbf{m})}} \left[1 + \frac{\beta}{k} \sum_{\alpha} D_{\alpha}(\mathbf{n}) \overline{\theta D_{\alpha}(\mathbf{m})} \right] \right)^k =: \lim_{k \rightarrow \infty} F_k(\mathbf{n}, \mathbf{m}). \quad (7.4.15)$$

The needed claim will be verified once show that

$$\sum_{\mathbf{n}, \mathbf{m} \in \{0,1\}^{\mathbb{T}_L^+}} \text{Tr} \left(A(\mathbf{n}) \overline{\theta A(\mathbf{m})} F_k(\mathbf{n}, \mathbf{m}) \right) \geq 0 \quad (7.4.16)$$

for all k . Indeed, proceeding exactly in the same way as in the proof of Theorem 2.1 in [39], we can conclude that for each $\mathbf{n}, \mathbf{m} \in \{0,1\}^{\mathbb{T}_L^+}$ the operator $F_k(\mathbf{n}, \mathbf{m})$ can be written as a sum of terms of the form $F_k^{(\ell)}(\mathbf{n}) \theta F_k^{(\ell)}(\mathbf{m})$, where $F_k^{(\ell)} \in \mathfrak{A}_L^+$. Each such term yields

$$\begin{aligned} & \sum_{\mathbf{n}, \mathbf{m} \in \{0,1\}^{\mathbb{T}_L^+}} \text{Tr} (A(\mathbf{n}) \overline{\theta A(\mathbf{m})} F_k^{(\ell)}(\mathbf{n}) \theta F_k^{(\ell)}(\mathbf{m})) = \\ & = \sum_{\mathbf{n}, \mathbf{m} \in \{0,1\}^{\mathbb{T}_L^+}} \text{Tr} (A(\mathbf{n}) F_k^{(\ell)}(\mathbf{n}) \overline{\theta (A F_k^{(\ell)})}(\mathbf{m})) = \left| \sum_{\mathbf{n} \in \{0,1\}^{\mathbb{T}_L^+}} \text{Tr} (A(\mathbf{n}) F_k^{(\ell)}(\mathbf{n})) \right|^2 \geq 0 \end{aligned} \quad (7.4.17)$$

completing thus the proof. \square

Chessboard estimates

Consider \mathbb{T}_L partitioned into $(L/2)^d$ disjoint $2 \times 2 \times \dots \times 2$ blocks $C_{\mathbf{t}} \subset \mathbb{T}_L$ labeled by vectors $\mathbf{t} \in \mathbb{T}_{L/2}$ with $2\mathbf{t}$ denoting the position of their lower left corner. Clearly, $C_{\mathbf{t}} = C + 2\mathbf{t}$ with $C_{\mathbf{0}} = C$.

If $\mathbf{t} \in \mathbb{T}_{L/2}$ with $|\mathbf{t}| = 1$, we let $\theta_{\mathbf{t}}$ be the reflection with respect to the plane between C and $C_{\mathbf{t}}$ corresponding to \mathbf{t} . Further, if \mathcal{E} is a block event, $\mathcal{E} \subset \{0,1\}^C$, we let $\vartheta_{\mathbf{t}}(\mathcal{E}) \subset \{0,1\}^{C_{\mathbf{t}}}$ be the correspondingly reflected event, $\mathbf{n} \in \mathcal{E}$ iff $\theta_{\mathbf{t}} \mathbf{n} \in \vartheta_{\mathbf{t}}(\mathcal{E})$. For other \mathbf{t} 's in $\mathbb{T}_{L/2}$ we define $\vartheta_{\mathbf{t}}(\mathcal{E})$ by a sequence of reflections (note that the result does not depend on the choice of sequence leading from C to $C_{\mathbf{t}}$). If all coordinates of \mathbf{t} are even this simply results in the translation by $2\mathbf{t}$.

Chessboard estimates are formulated in terms of a mean value of a homogenised pattern

based on a block event \mathcal{E} disseminated throughout the lattice,

$$q_{L,\beta}(\mathcal{E}) := \left(\left\langle \prod_{t \in \mathbb{T}_{L/2}} \vartheta_t(\mathcal{E}) \right\rangle_{L,\beta} \right)^{(2/L)^d}. \quad (7.4.18)$$

If $u \leq 0$, $\mathcal{E}_1, \dots, \mathcal{E}_m$ are block events, and $\mathbf{t}_1, \dots, \mathbf{t}_m \in \mathbb{T}_{L/2}$ are distinct, we get, by a standard repeated use of reflection positivity, the chessboard estimates

$$\left\langle \prod_{j=1}^m \vartheta_{\mathbf{t}_j}(\mathcal{E}_j) \right\rangle_{L,\beta} \leq \prod_{j=1}^m \left(\left\langle \prod_{t \in \mathbb{T}_{L/2}} \vartheta_t(\mathcal{E}_j) \right\rangle_{L,\beta} \right)^{(2/L)^d} = \prod_{j=1}^m q_{L,\beta}(\mathcal{E}_j). \quad (7.4.19)$$

Note that we have chosen to split \mathbb{T}_L into $2 \times 2 \times \dots \times 2$ blocks with the bottom left corner of the basic block C at the origin $(0, 0, \dots, 0)$. If we had instead replaced the basic block C by its shift $C + \mathbf{e}$ by the unit vector $\mathbf{e} = (1, 0, \dots, 0)$, the same estimate would hold with the new partition with all blocks shifted by \mathbf{e} . We will use this fact in the sequel.

The proof of the useful property of subadditivity of the function $q_{L,\beta}$ for classical systems [13, Lemma 5.9] can be also directly extended to our case.

Lemma 7.4.3. *If $\mathcal{E}, \mathcal{E}_1, \mathcal{E}_2, \dots$ are events on B such that $\mathcal{E} \subset \cup_k \mathcal{E}_k$, then*

$$q_{L,\beta}(\mathcal{E}) \leq \sum_k q_{L,\beta}(\mathcal{E}_k). \quad (7.4.20)$$

Proof. Using subadditivity of $\langle \cdot \rangle_{L,\beta}$, we get

$$q_{L,\beta}(\mathcal{E})^{(L/2)^d} = \left\langle \prod_{t \in \mathbb{T}_{L/2}} \vartheta_t(\mathcal{E}) \right\rangle_{L,\beta} \leq \sum_{(k_t)} \left\langle \prod_{t \in \mathbb{T}_{L/2}} \vartheta_t(\mathcal{E}_{k_t}) \right\rangle_{L,\beta} \quad (7.4.21)$$

Using now the chessboard estimate

$$\left\langle \prod_{t \in \mathbb{T}_{L/2}} \vartheta_t(\mathcal{E}_{k_t}) \right\rangle_{L,\beta} \leq \prod_{t \in \mathbb{T}_{L/2}} q_{L,\beta}(\mathcal{E}_{k_t}), \quad (7.4.22)$$

we get

$$q_{L,\beta}(\mathcal{E})^{(L/2)^d} \leq \sum_{(k_t)} \prod_{t \in \mathbb{T}_{L/2}} q_{L,\beta}(\mathcal{E}_{k_t}) = \prod_{t \in \mathbb{T}_{L/2}} \left(\sum_k q_{L,\beta}(\mathcal{E}_k) \right) = \left(\sum_k q_{L,\beta}(\mathcal{E}_k) \right)^{(L/2)^d}. \quad (7.4.23)$$

□

Let us introduce the set \mathcal{B} of bad configurations, $\mathcal{B} = \{0, 1\}^C \setminus (\mathcal{G}^c \cup \mathcal{G}^o)$, and use $\tau_{\mathbf{r}}$ to denote the shift by $\mathbf{r} \in \mathbb{T}_L$. The proof of the existence of two distinct KMS states is based

on the following lemma.

Lemma 7.4.4. *There exists a function κ_0 as stated in Theorem 7.4.1 such that for any $\varepsilon > 0$, $\mu > 0$ and $\kappa < \kappa_0(\mu)$ there exists β_0 such that for any $\beta > \beta_0$, any L sufficiently large, and any distinct $t_1, t_2 \in \mathbb{T}_L$,*

$$\langle \mathcal{B} \rangle_{L,\beta} < \varepsilon, \quad (7.4.24)$$

$$\langle \tau_{2t_1}(\mathcal{G}^\varepsilon) \cap \tau_{2t_2}(\mathcal{G}^0) \rangle_{L,\beta} < \varepsilon. \quad (7.4.25)$$

Deferring its proof to the next section, we show here how it implies Theorem 7.4.1.

Proof of Theorem 7.4.1 given Lemma 7.4.4. We closely follow the proof of Lemma 4.5 and Proposition 3.9 in [16]. Define

$$\mathbb{T}_L^{\text{front}} = \{x \in \mathbb{T}_L : -\lfloor L/4 - 1/2 \rfloor \leq x_1 \leq \lceil L/4 - 1/2 \rceil\}. \quad (7.4.26)$$

We denote by $\mathfrak{A}_L^{\text{front}}$ the algebra of observables localised in $\mathbb{T}_L^{\text{front}}$.

Let $\Delta_M \subset \mathbb{T}_{L/2}$ be a $M \times M$ block of sites on the “back” of $\mathbb{T}_{L/2}$ ($\text{dist}(0, \Delta_M) \geq L/4 - M$). Then for a block event \mathcal{E} depending only on the occupancy in C define

$$\rho_{L,M}(\mathcal{E}) = \frac{1}{|\Delta_M|} \sum_{t \in \Delta_M} \tau_{2t}(\mathcal{E}). \quad (7.4.27)$$

If $\langle \mathcal{E} \rangle_{L,\beta} \geq c$ for all $L \gg 1$ for a constant $c > 0$ then we can define a new state on $\mathfrak{A}_L^{\text{front}}$, by

$$\langle \cdot \rangle_{L,M;\beta} = \frac{\langle \rho_{L,M}(\mathcal{E}) \cdot \rangle_{L,\beta}}{\langle \rho_{L,M}(\mathcal{E}) \rangle_{L,\beta}}. \quad (7.4.28)$$

We claim that if $\langle \cdot \rangle_\beta$ is a weak limit of $\langle \cdot \rangle_{L,M;\beta}$ as $L \rightarrow \infty$ and then $M \rightarrow \infty$ then $\langle \cdot \rangle_\beta$ is a KMS state at inverse temperature β invariant under translations by $2t$ for $t \in \mathbb{T}_L$.

Indeed translation invariance comes from the spatial averaging in $\rho_{L,M}(\mathcal{E})$. As in [16] we need to show that $\langle \cdot \rangle_\beta$ satisfies the KMS condition (7.4.7). For an observable A on the ‘front’ of the torus, $\mathbb{T}_L^{\text{front}}$, we have

$$[\alpha_t^{(L)}(A), \rho_{L,M}(\mathcal{E})] \rightarrow 0 \text{ as } L \rightarrow \infty \quad (7.4.29)$$

in norm topology uniformly for t in compact subsets of \mathbb{C} . Using this and (7.4.7) for the finite volume Gibbs states we have that for A, B bounded operators on the “front” of the torus

$$\langle \rho_{L,M}(\mathcal{E})AB \rangle_{L,\beta} = \langle \rho_{L,M}(\mathcal{E})\alpha_{-i\beta}^{(L)}(A)B \rangle_{L,\beta} + o(1) \text{ as } L \rightarrow \infty. \quad (7.4.30)$$

Because $\alpha_{-i\beta}^{(L)}(B) \rightarrow \alpha_{-i\beta}(B)$ as $L \rightarrow \infty$ in norm we have that $\langle \cdot \rangle_{L,M;\beta}$ converges as $L \rightarrow \infty$ and then $M \rightarrow \infty$ to a KMS state at inverse temperature β .

The proof of Theorem 7.4.1 follows by taking $\mathcal{E} = \mathcal{G}^e$ or $\mathcal{E} = \mathcal{G}^o$ as we know both staggered occupations have the same expectation we can define a state $\langle \cdot \rangle_{L,M;\beta}^e$, using Lemma 7.4.4 we conclude that $\langle \rho_{L,M}(\mathcal{G}^e) \rangle_{L,\beta}$ is uniformly positive and hence

$$\langle \tau_{2t}(\mathcal{G}^e) \rangle_{L,M;\beta}^e \geq 1 - \varepsilon, \quad (7.4.31)$$

for any $t \in \mathbb{T}_L^{\text{front}}$ (if $M \ll L/2$) and similarly for $\langle \cdot \rangle_{L,M;\beta}^o$. If ε is small enough then the right-hand side of this inequality will be greater than $1/2$, hence in the thermodynamic limit \mathcal{G}^e will dominate. \square

To prove Lemma 7.4.4 we use a version of Peierls' argument hinging on chessboard estimates.

Peierls argument

For a given occupation configuration, consider the event $\tau_{2t_1}(\mathcal{G}^e) \cap \tau_{2t_2}(\mathcal{G}^o)$ that the blocks C_{t_1} and C_{t_2} have different staggered configurations described by \mathcal{G}^e and \mathcal{G}^o respectively. The idea is to show the existence of a contour separating the points t_1 and t_2 and to use chessboard estimates to show that occurrence of such a contour is improbable.

Consider the set of all blocks (labeled by) $t \in \mathbb{T}_{L/2}$ such that a translation of the even staggered configuration $\tau_{2t}(\mathcal{G}^e)$ is occurring on it. Let $\Delta \subset \mathbb{T}_{L/2}$ be its connected component containing t_1 . Consider the component $\bar{\Delta} \subset \mathbb{T}_{L/2}$ of Δ^c containing t_2 . The set of edges γ of the graph $\mathbb{T}_{L/2}$ between vertices of $\bar{\Delta}$ and its complement $\bar{\Delta}^c$ is a minimal cutset of Δ . Informally, γ is a contour between Δ with all its holes except the one containing t_2 filled up and the remaining component containing t_2 — *a contour separating t_1 and t_2* . The standard fact is that the number of contours with a fixed number of edges $|\gamma| = n$ separating two vertices t_1 and t_2 is bounded by c^n with a suitable constant c .

Given a contour γ of length $|\gamma| = n$, there exists a coordinate direction such that there are at least n/d edges in γ aligned along this direction. Precisely half of them have their outer endpoint (the vertex in $\bar{\Delta}$) “on the left” of its inner endpoint, choosing (arbitrarily) the direction of the chosen coordinate axis (without loss of generality we can take for this the first coordinate axis) as e_1 , there are at least $n/(2d)$ edges $\{t, t + e_1\}$ such that $t \in \bar{\Delta}$ and $t + e_1 \in \Delta$.

Now, the crucial claim is that with each contour we can associate at least $1/2$ of the $n/(2d)$

bad blocks (with a configuration from $\vartheta_{2t}(\mathcal{B})$), all belonging to a given fixed partition: either to our original partition of \mathbb{T}_L labelled by $\mathbb{T}_{L/2}$ or to a new partition of \mathbb{T}_L with the basic block C shifted by a unit vector from \mathbb{T}_L in direction \mathbf{e}_1 . Indeed, any block corresponding to an outer vertex t above is either bad or, if not, it has to be a translation $\tau_{2t}(\mathcal{G}^o)$ of the odd staggered configuration (being the even staggered configuration would be in contradiction with the assumption that Δ is a component of the set of blocks with even staggered configuration). However, then the block shifted by a unit vector in \mathbb{T}_L in direction \mathbf{e}_1 features an odd staggered configuration on its left-hand half and an even staggered configurations on its right-hand half, i.e., a configuration that belongs to the properly shifted set \mathcal{B} (here it is helpful that the set \mathcal{B} is invariant with respect to the reflection through the middle plane of the block).

We use $S(\gamma)$ to denote this collection of at least $|\gamma|/(4d)$ bad blocks associated with contour γ . Given that, according to the construction above, all blocks from $S(\gamma)$ belong to the same partition (either the original one or a shifted one), we can use the chessboard estimate based on the the corresponding partition to bound the probability that all blocks of a given set $S(\gamma)$ are bad by

$$\left\langle \prod_{t \in S(\gamma)} \vartheta_t(\mathcal{B}) \right\rangle_{L,\beta} \leq q_{L,\beta}(\mathcal{B})^{|S(\gamma)|}. \quad (7.4.32)$$

As a result, assuming that $q_{L,\beta}(\mathcal{B}) \leq 1$ (we will later show it can be made arbitrarily small), the expectation of the event $\tau_{2t_1}(\mathcal{G}^e) \cap \tau_{2t_2}(\mathcal{G}^o)$ is bounded by

$$\left\langle \tau_{2t_1}(\mathcal{G}^e) \cap \tau_{2t_2}(\mathcal{G}^o) \right\rangle_{L,\beta} \leq \sum_{\gamma \text{ separating } t_1 \text{ and } t_2} q_{L,\beta}(\mathcal{B})^{|\gamma|/(4d)} 2^{|\gamma|/(2d)+1}. \quad (7.4.33)$$

Here, $2^{|\gamma|/(2d)+1}$ is the bound on the number of sets $S(\gamma)$ associated with the contour γ once the direction \mathbf{e}_1 is chosen.

This leads to the final bound

$$\left\langle \tau_{2t_1}(\mathcal{G}^e) \cap \tau_{2t_2}(\mathcal{G}^o) \right\rangle_{L,\beta} \leq \sum_{n=4}^{\infty} 2(4q_{L,\beta}(\mathcal{B})^{n/(4d)})c^n. \quad (7.4.34)$$

We now see that Lemma 7.4.4 will hold if $q_{L,\beta}(\mathcal{B})$ can be made arbitrarily small by tuning the parameters of the model correctly. Hence we turn our attention to this.

For the remaining technical part of this section we restrict ourselves to the *two-dimensional case*.

For $d = 2$, the set \mathcal{B} consists of 14 configurations that can be classified into five events

according to the number of sites in C that are occupied, $\mathcal{B} = \mathcal{B}^{(0)} \cup \mathcal{B}^{(1)} \cup \mathcal{B}^{(2)} \cup \mathcal{B}^{(3)} \cup \mathcal{B}^{(4)}$. Here, $\mathcal{B}^{(0)}$ and $\mathcal{B}^{(4)}$ consist of a single configuration (empty and full, respectively) and $\mathcal{B}^{(1)}, \mathcal{B}^{(2)}, \mathcal{B}^{(3)}$ consist each of 4 configurations related by symmetries. Notice that the event $\mathcal{B}^{(2)}$ has precisely two occupied sites at neighbouring positions (excluding the configurations \mathbf{n}^e and \mathbf{n}^o).

By subadditivity we can bound $q_{L,\beta}(\mathcal{B})$ by the sum of expectations of homogenised patterns based on the fourteen configurations from \mathcal{B} disseminated throughout the lattice by reflections. Of course, in view of the symmetries, we can consider only 5 configurations $\mathbf{n}^{(k)}, k = 0, 1, \dots, 4$, one from each event $\mathcal{B}^{(k)}, k = 0, 1, \dots, 4$.

We use $Z_L^{(k)}(\beta)$ to denote the corresponding quantities

$$Z_L^{(k)}(\beta) = q_{L,\beta}(\{\mathbf{n}^{(k)}\})^{(L/2)^2} Z_L(\beta), \quad (7.4.35)$$

for $k \in \{0, 1, \dots, 4\}$. For notational consistency we also denote the contribution of staggered configurations on \mathbb{T}_L as $Z_L^e(\beta)$ and $Z_L^o(\beta)$.

Lemma 7.4.5. *For any $u, \mu, \kappa \in \mathbb{R}$ with $|u| \leq 1$ we have*

$$Z_L^{(0)}(\beta) = (2S + 1)^{L^2}, \quad (7.4.36)$$

$$Z_L^e(\beta) = Z_L^o(\beta) = e^{\frac{1}{2}\beta\mu L^2} (2S + 1)^{L^2}. \quad (7.4.37)$$

Proof. It follows immediately from the observation that in these cases there are no interactions between spins at neighbouring sites. \square

Obtaining bounds for the remaining disseminated configurations is more difficult and will be done separately for the two considered types of quantum spin models. First we prove estimates for the antiferromagnetic case.

Lemma 7.4.6. *For $u = -1$ (the antiferromagnet) and any $\mu, \kappa \in \mathbb{R}$ we have*

$$Z_L^{(1)}(\beta) \leq (2S + 1)^{L^2} \exp\left\{\beta L^2\left(\frac{\mu}{4} + \frac{\kappa}{4} - \frac{1}{8S}\right)\right\}, \quad (7.4.38)$$

$$Z_L^{(2)}(\beta) \leq (2S + 1)^{L^2} \exp\left\{\beta L^2\left(\frac{\mu}{2} + \frac{3\kappa}{4} - \frac{1}{2S}\right)\right\}, \quad (7.4.39)$$

$$Z_L^{(3)}(\beta) \leq (2S + 1)^{L^2} \exp\left\{\beta L^2\left(\frac{3\mu}{4} + \frac{5\kappa}{4} - \frac{7}{8S}\right)\right\}, \quad (7.4.40)$$

$$Z_L^{(4)}(\beta) \leq (2S + 1)^{L^2} \exp\left\{\beta L^2\left(\mu + 2\kappa - \frac{3}{2S}\right)\right\}. \quad (7.4.41)$$

Proof. We present the proof for $Z_L^{(4)}(\beta)$ and $Z_L^{(3)}(\beta)$, the other two inequalities follow by a simpler application of the same method. First, using the unitary operator $U = \prod_{x \in \mathbb{T}_L^e} e^{i\pi S_x^2}$,

we get

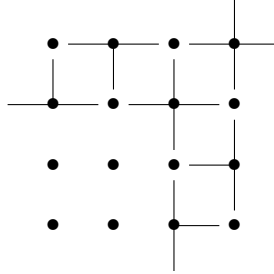
$$Z_L^{(4)}(\beta) = \exp\left\{\beta L^2\left(\mu + 2\kappa - \frac{2S(S+1)}{S^2}\right)\right\} \text{Tr} \exp\left\{-\frac{\beta}{S^2} \sum_{\langle x,y \rangle} \mathbf{S}_x \cdot \mathbf{S}_y\right\}. \quad (7.4.42)$$

For a site \mathbf{x}_0 consider its four nearest neighbours $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4$. The operator $-\sum_{\langle x,y \rangle} \mathbf{S}_x \cdot \mathbf{S}_y$ can be written as a sum of $L^2/2$ operators of the form of $B_{\mathbf{x}_0}^{(4)} := -\mathbf{S}_{\mathbf{x}_0} \cdot (\sum_{k=1}^4 \mathbf{S}_{\mathbf{x}_k})$ summing over \mathbf{x}_0 on the even sublattice. According to [35, Theorem C.2], the largest eigenvalue of each operator $B_{\mathbf{x}_0}^{(4)}$ is $S(4S + 1)$. As a result, we get the bound

$$\text{Tr} \exp\left\{-\frac{\beta}{S^2} \sum_{\langle x,y \rangle} \mathbf{S}_x \cdot \mathbf{S}_y\right\} \leq (2S + 1)^{L^2} \exp\left\{\beta L^2 \frac{4S+1}{2S}\right\}. \quad (7.4.43)$$

Combining with the prefactor, the inequality follows.

For $Z_L^{(3)}(\beta)$ we follow the same procedure combining, however, operators $B_{\mathbf{x}_0}^{(\ell)} := -\mathbf{S}_{\mathbf{x}_0} \cdot (\sum_{k=1}^{\ell} \mathbf{S}_{\mathbf{x}_k})$, with $\ell = 1, 2, 3, 4$ neighbours of \mathbf{x}_0 . Note that a dissemination of a block of three occupied and one unoccupied site throughout the lattice via reflections yields a pattern where 1/4 of the 2×2 blocks are empty and the remaining blocks are full, with the empty blocks evenly spaced throughout the lattice. Thus there are $5L^2/4$ edges with both end sites occupied and we can tile these edges by $L^2/8$ copies of each of the operators $B_{\mathbf{x}_0}^{(\ell)}$, $\ell = 1, 2, 3, 4$. Observe that $(4 + 3 + 2 + 1)L^2/8 = 5L^2/4$ yields the correct number of edges. Nevertheless a tiling yielding the claimed bound uses $L^2/8$ operators $B_{\mathbf{x}_0}^{(4)}$ and $L^2/4$ operators $B_{\mathbf{x}_0}^{(3)}$ arranged in each 16×16 cell as shown below.



The inequality follows by using the claim [35, Theorem C.2] that the largest eigenvalue of the operator $B_{\mathbf{x}_0}^{(\ell)}$ is $S(\ell S + 1)$. Collecting the terms we get the claimed bound.

The pattern of $Z_L^{(2)}(\beta)$ consists of alternating double lines of occupied and unoccupied sites resulting in tiling with $L^2/4$ operators of the form $B_{\mathbf{x}_0}^{(3)}$ whose largest eigenvalue is $S(3S + 1)$.

The bound for $Z_L^{(1)}(\beta)$ is also straightforward with $L^2/4$ edges and $L^2/8$ of operators $B_{\mathbf{x}_0}^{(2)}$ whose largest eigenvalue is $S(2S + 1)$. Notice that tiling with $L^2/4$ of operators $B_{\mathbf{x}_0}^{(1)}$ would be also possible, but would lead to a bigger bound. \square

The corresponding inequalities for the spin- $\frac{1}{2}$ XY model are as follows.

Lemma 7.4.7. *For the quantum XY model ($u = 0$) with $S = \frac{1}{2}$ and any $\mu, \kappa \in \mathbb{R}$,*

$$Z_L^{(1)}(\beta) \leq 2^{L^2} \exp\left\{\beta L^2\left(\frac{\mu}{4} + \frac{\kappa}{4} + \frac{\sqrt{2}}{4} - 3\right)\right\}, \quad (7.4.44)$$

$$Z_L^{(2)}(\beta) \leq 2^{L^2} \exp\left\{\beta L^2\left(\frac{\mu}{2} + \frac{3\kappa}{4} - \frac{5}{4}\right)\right\}, \quad (7.4.45)$$

$$Z_L^{(3)}(\beta) \leq 2^{L^2} \exp\left\{\beta L^2\left(\frac{3\mu}{4} + \frac{5\kappa}{4} + \frac{\sqrt{6-11}}{4}\right)\right\}, \quad (7.4.46)$$

$$Z_L^{(4)}(\beta) \leq 2^{L^2} \exp\left\{\beta L^2(\mu + 2\kappa + \sqrt{6} - 6)\right\}. \quad (7.4.47)$$

Proof. The calculation is straightforward using the same method as in Lemma 7.4.6 with operators $A_{x_0}^{(\ell)} := S_{x_0}^1(\sum_{k=1}^{\ell} S_{x_k}^1) + S_{x_0}^2(\sum_{k=1}^{\ell} S_{x_k}^2)$. Their largest eigenvalue according to [35, Theorem C.1] is $\frac{1}{2}\sqrt{m(m+1)}$ if $\ell = 2m$ and $\frac{1}{2}m$ if $\ell = 2m - 1$, i.e., $1/2$, $\sqrt{2}/2$, 1 , and $\sqrt{6}/2$ for the operators $A_{x_0}^{(1)}$, $A_{x_0}^{(2)}$, $A_{x_0}^{(3)}$, and $A_{x_0}^{(4)}$, respectively. \square

As a result, we are getting the following bounds on the expectations of the disseminated bad configurations $q_{L,\beta}(\{\mathbf{n}^{(k)}\})$ for $k = 0, 1, \dots, 4$.

Lemma 7.4.8. *Let $u, \mu, \kappa \in \mathbb{R}$. We have*

$$q_{L,\beta}(\{\mathbf{n}^{(0)}\}) \leq e^{-2\beta\mu}. \quad (7.4.48)$$

Further we have for $u = -1$ (the antiferromagnet),

$$q_{L,\beta}(\{\mathbf{n}^{(1)}\}) \leq \exp\left\{\beta\left(-\mu + \kappa - \frac{1}{2S}\right)\right\}, \quad (7.4.49)$$

$$q_{L,\beta}(\{\mathbf{n}^{(2)}\}) \leq \exp\left\{\beta\left(3\kappa - \frac{2}{S}\right)\right\}, \quad (7.4.50)$$

$$q_{L,\beta}(\{\mathbf{n}^{(3)}\}) \leq \exp\left\{\beta\left(\mu + 5\kappa - \frac{7}{2S}\right)\right\}, \quad (7.4.51)$$

$$q_{L,\beta}(\{\mathbf{n}^{(4)}\}) \leq \exp\left\{\beta\left(2\mu + 8\kappa - \frac{6}{S}\right)\right\}, \quad (7.4.52)$$

and for $u = 0$ and $S = \frac{1}{2}$ (the XY model),

$$q_{L,\beta}(\{\mathbf{n}^{(1)}\}) \leq \exp\left\{\beta(-\mu + \kappa + \sqrt{2} - 12)\right\}, \quad (7.4.53)$$

$$q_{L,\beta}(\{\mathbf{n}^{(2)}\}) \leq \exp\left\{\beta(3\kappa - 5)\right\}, \quad (7.4.54)$$

$$q_{L,\beta}(\{\mathbf{n}^{(3)}\}) \leq \exp\left\{\beta(\mu + 5\kappa + \sqrt{6} - 11)\right\}, \quad (7.4.55)$$

$$q_{L,\beta}(\{\mathbf{n}^{(4)}\}) \leq \exp\left\{\beta(2\mu + 8\kappa - 4(6 - \sqrt{6}))\right\}. \quad (7.4.56)$$

Proof. All the estimates follow from the previous lemmas using

$$q_{L,\beta}(\{\mathbf{n}^{(k)}\}) = \left(\frac{Z_L^{(k)}(\beta)}{Z_L(\beta)} \right)^{(2/L)^2} \leq \left(\frac{Z_L^{(k)}(\beta)}{2Z_L^\epsilon(\beta)} \right)^{(2/L)^2}. \quad (7.4.57)$$

□

Further, using subadditivity (Lemma 7.4.3) we have

$$q_{L,\beta}(\mathcal{B}) \leq q_{L,\beta}(\{\mathbf{n}^{(0)}\}) + 4 \sum_{k=1}^3 q_{L,\beta}(\{\mathbf{n}^{(k)}\}) + q_{L,\beta}(\{\mathbf{n}^{(4)}\}). \quad (7.4.58)$$

From Lemma 7.4.8 we can see that if we choose $\mu > 0$ and κ sufficiently small, the upper bounds on the disseminated events can simultaneously be made arbitrarily small by choosing β sufficiently large.

More precisely, we see that there exists $\mu_0 > 0$ and a function κ_0 that is positive on $(0, \mu_0)$ such that if $\mu > 0$, $\kappa < \max(\kappa_0(\mu), 0)$, and $\epsilon > 0$, there exists $\beta_0(\mu, \kappa, \epsilon)$ such that the claims of the Lemma 7.4.4 and thus also Theorem 7.4.1 are valid for any $\beta \geq \beta_0$.

Explicit expressions for the function κ_0 are

$$\kappa_0(\mu) = \min\left(\frac{2}{3S}, \frac{1}{2S} + \mu, \frac{7}{10S} - \frac{\mu}{5}, \frac{3}{4S} - \frac{\mu}{4}\right) \quad (7.4.59)$$

for the case of an antiferromagnet ($u = -1$) with spin S and

$$\kappa_0(\mu) = \min\left(\frac{5}{3}, \frac{6-\sqrt{6}}{2} - \frac{\mu}{4}\right) \quad (7.4.60)$$

for the case of XY model with spin $1/2$.

7.5 The spin-1 Bose-Hubbard model

In this section we look at a model of itinerant particles on a lattice that possess a spin. More specifically we look at Bosons with a spin-1 degree of freedom. We will introduce a probabilistic representation of the spin-1 Bose-Hubbard model that should be familiar from Chapter 6. This allows us to present off-diagonal and spin correlations in terms of probabilities in this representation. Note that because particles are free to move on the lattice the site spin correlation will have a dependency on the presence of a particle at each site.

7.5.1 Setting

We work on lattice, $\Lambda \subset \mathbb{Z}^d$, with a set of edges, \mathcal{E} . We consider a collection of N itinerant spin-1 particles on the lattice. We denote by x_i the position of the i^{th} particle and by Δ_i its Laplacian. The spin- S operators on \mathbb{C}^{2S+1} are denoted by S^1, S^2, S^3 with S_i^k denoting the spin operator S^k acting on the i^{th} particle and $\mathbf{S} = (S^1, S^2, S^3)$.

The state space is given by $\mathcal{H} = P_{\text{sym}} \otimes_{i=1}^N (l^2(\Lambda) \otimes \mathbb{C}^3)$ where P_{sym} is the projection onto the symmetric subspace. The Hamiltonian is given by

$$H(J_1, J_2, V) = - \sum_{i=1}^N \Delta_i - \frac{1}{2} \sum_{i \neq j} \delta_{x_i, x_j} (J_1 \mathbf{S}_i \cdot \mathbf{S}_j + J_2 (\mathbf{S}_i \cdot \mathbf{S}_j)^2 - 2J_2) + V \sum_{\substack{i \neq j \neq k \\ k \neq i}} \delta_{x_i, x_j} \delta_{x_j, x_k}. \quad (7.5.1)$$

Note that the structure of the spin operators in $H(J_1, J_2, V)$ means that we need only symmetrise in space variables and not in spin variables. Later we will take the limit $V \rightarrow \infty$ to impose the constraint of having at most two particles per site. The partition function and Gibbs states for inverse temperature $\beta > 0$ are given by

$$Z_\beta(J_1, J_2, V) = \text{Tr}_{\mathcal{H}} P_{\text{sym}} e^{-\beta H(J_1, J_2, V)}, \quad (7.5.2)$$

$$\langle \cdot \rangle_\beta^{J_1, J_2, V} = \frac{1}{Z_\beta(J_1, J_2, V)} \text{Tr}_{\mathcal{H}} P_{\text{sym}} \cdot e^{-\beta H(J_1, J_2, V)}. \quad (7.5.3)$$

We will derive a probabilistic representation of this system that will allow us to recast off-diagonal and spin correlations in terms of probabilities.

7.5.2 A probabilistic representation

To begin we note that

$$Z_\beta(J_1, J_2, V) = \frac{1}{N!} \sum_{\pi} \sum_{x_1, \dots, x_N} \langle x_{\pi(1)} \dots x_{\pi(N)} | \text{Tr}_{\mathbb{C}^{3N}} e^{-\beta H(J_1, J_2, V)} | x_1 \dots x_N \rangle. \quad (7.5.4)$$

Where π is a permutation on N letter and x_i is a possible position for the i^{th} particle. Now denote a configuration of positions $(x_1^j, \dots, x_N^j) = \omega^j$ then using Trotter's formula we have

$$\begin{aligned}
& Z_\beta(J_1, J_2, V) \\
&= \lim_{M \rightarrow \infty} \frac{1}{N!} \text{Tr}_{\mathbb{C}^{3N}} \sum_{\pi} \sum_{x_1, \dots, x_N} \left\langle x_{\pi(1)} \dots x_{\pi(N)} \left| \left(\prod_{i=1}^N e^{\frac{\beta}{M} \Delta_i} e^{\frac{\beta}{2M} \sum_{i \neq j} (J_1 \mathbf{S}_i \cdot \mathbf{S}_j + J_2 (\mathbf{S}_i \cdot \mathbf{S}_j)^2 - 2J_2)} \right)^M \right| x_1 \dots x_N \right\rangle \\
&= \lim_{M \rightarrow \infty} \frac{1}{N!} \text{Tr}_{\mathbb{C}^{3N}} \sum_{\pi} \sum_{\omega^1, \dots, \omega^M} \prod_{j=1}^M \left\langle \pi(\omega^j) \left| \prod_{i=1}^N \left(1 + \frac{\beta}{M} \Delta_i \right) e^{\frac{\beta}{2M} \sum_{i \neq j} (J_1 \mathbf{S}_i \cdot \mathbf{S}_j + J_2 (\mathbf{S}_i \cdot \mathbf{S}_j)^2 - 2J_2)} \right| \omega^{j+1} \right\rangle. \\
&= \frac{1}{N!} \sum_{\pi} \sum_{x_1, \dots, x_N} \int^* d\omega_1 \dots d\omega_N \\
& \quad \text{Tr}_{\mathbb{C}^{3N}} \exp \left\{ \frac{1}{2} \sum_{x \in \Lambda} \int_0^\beta dt \sum_{i: \omega_i(t)=x} \sum_{\substack{j \neq i \\ \omega_j(t)=x}} (J_1 \mathbf{S}_i \cdot \mathbf{S}_j + J_2 (\mathbf{S}_i \cdot \mathbf{S}_j)^2 - 2J_2) - V \sum_{\substack{i \neq j \neq k \\ k \neq i}} \delta_{\omega_i(t), \omega_j(t)} \delta_{\omega_j(t), \omega_k(t)} \right\}. \tag{7.5.5}
\end{aligned}$$

with the understanding that $\omega^{M+1} \equiv \omega^1$. Here \int^* denotes the integral over random walks $\omega_i, i = 1, \dots, N$ such that $\{\omega_i(0)\}_{i=1}^N = \{\omega_i(\beta)\}_{i=1}^N = \{x_1, \dots, x_N\}$. Taking the limit $V \rightarrow \infty$ will introduce the constraint that at most two walks can occupy a site at the same time. Denote by χ_E the indicator that there are at most two walks at any $(x, t) \in \Lambda \times [0, \beta]$. We then have

$$\begin{aligned}
& \lim_{V \rightarrow \infty} Z_\beta(J_1, J_2, V) \\
&= \frac{1}{N!} \sum_{\pi} \sum_{x_1, \dots, x_N} \int^* d\omega_1 \dots d\omega_N \chi_E \\
& \quad \text{Tr}_{\mathbb{C}^{3N}} \exp \left\{ \frac{1}{2} \sum_{x \in \Lambda} \int_0^\beta dt \sum_{i: \omega_i(t)=x} \sum_{\substack{j \neq i \\ \omega_j(t)=x}} (J_1 \mathbf{S}_i \cdot \mathbf{S}_j + J_2 (\mathbf{S}_i \cdot \mathbf{S}_j)^2 - 2J_2) \right\}. \tag{7.5.6}
\end{aligned}$$

Denote $\lim_{V \rightarrow \infty} Z_\beta(J_1, J_2, V) = Z_\beta(J_1, J_2)$.

7.5.3 Off diagonal correlations

Off diagonal correlations involve walks that start at x and end at y , with the understanding that we use periodic boundary conditions on $[0, \beta]$. We denote by $\sigma(x)$ the off diagonal correlation between sites 0 and x and by $Z_\beta(J_1, J_2; \omega_{0,x})$ the partition function $Z_\beta(J_1, J_2)$

conditioned to include a walk joining sites 0 and x . We can write this as

$$Z_\beta(J_1, J_2; \omega_{0,x}) = \frac{1}{N!} \sum_\pi \sum_{x_1, \dots, x_N} \int_{0 \leftrightarrow x} d\omega_1 \dots d\omega_N \chi_E \text{Tr}_{\mathbb{C}^{3N}} \exp \left\{ \frac{1}{2} \sum_{x \in \Lambda} \int_0^\beta dt \sum_{i: \omega_i(t)=x} \sum_{\substack{j \neq i \\ \omega_j(t)=x}} (J_1 \mathbf{S}_i \cdot \mathbf{S}_j + J_2 (\mathbf{S}_i \cdot \mathbf{S}_j)^2 - 2J_2) \right\} \quad (7.5.7)$$

then

$$\sigma(x) = \frac{Z_\beta(J_1, J_2; \omega_{0,x})}{Z_\beta(J_1, J_2)}. \quad (7.5.8)$$

We can also think of $\sigma(x)$ as the probability of a walk joining 0 and x in the system weighted by the spin interactions in $H(J_1, J_2)$, i.e. write $\sigma(x) = \hat{\mathbb{P}}(0 \longleftrightarrow x)$.

7.5.4 Spin correlations

We now expand the trace over \mathbb{C}^{3N} as in [111] to obtain a different probabilistic representation suitable for representing spin correlations as probabilities of events. We first define two operators. Let $|a\rangle$ denote the eigenvector of S^3 with eigenvalue a , $S^3|a\rangle = a|a\rangle$. Further we denote $|a, b\rangle = |a\rangle \otimes |b\rangle$, then we define T_{ij}, P_{ij} , operators on $\mathbb{C}^3 \otimes \mathbb{C}^3$ as

$$T_{ij}|a, b\rangle = |b, a\rangle \quad P_{ij} = \sum_{a,b=-S}^S (-1)^{a-b} |a, -a\rangle \langle b, -b|. \quad (7.5.9)$$

P_{ij} has matrix elements $\langle a, b|P_{ij}|c, d\rangle = (-1)^{a-c} \delta_{a,-b} \delta_{c,-d}$, also $\frac{1}{3}P_{ij}$ is the projector onto the spin singlet. We can show the following relations

$$J_1 \mathbf{S}_i \cdot \mathbf{S}_j + J_2 (\mathbf{S}_i \cdot \mathbf{S}_j)^2 = J_2 + J_1 T_{ij} + (-J_1 + J_2) P_{ij}. \quad (7.5.10)$$

Then we have

$$\begin{aligned}
Z_\beta(J_1, J_2) &= \frac{1}{N!} \sum_{\pi} \sum_{x_1, \dots, x_N} \int^* d\omega_1 \dots d\omega_N \chi_E \text{Tr}_{\mathbb{C}^{3N}} \exp \left\{ \frac{1}{2} \sum_{x \in \Lambda} \int_0^\beta dt \sum_{\substack{i: \omega_i(t)=x \\ j \neq i}} \sum_{\omega_j(t)=x} (J_1 T_{ij} + (-J_1 + J_2) P_{ij} - J_2) \right\} \\
&= \frac{1}{N!} \sum_{\pi} \sum_{x_1, \dots, x_N} \int^* d\omega_1 \dots d\omega_N \chi_E \lim_{M \rightarrow \infty} \\
&\quad \text{Tr}_{\mathbb{C}^{3N}} \left(\prod_{x \in \Lambda} \exp \left\{ \frac{1}{2M} \int_0^\beta dt \sum_{\substack{i: \omega_i(t)=x \\ j \neq i}} \sum_{\omega_j(t)=x} (J_1 T_{ij} + (-J_1 + J_2) P_{ij} - J_2) \right\} \right)^M \\
&= \lim_{M \rightarrow \infty} \frac{1}{N!} \sum_{\pi} \sum_{x_1, \dots, x_N} \int^* d\omega_1 \dots d\omega_N \chi_E \\
&\quad \text{Tr}_{\mathbb{C}^{3N}} \left(\prod_{x \in \Lambda} \left[1 + \int_0^\beta dt \sum_{\substack{i: \omega_i(t)=x \\ j \neq i}} \sum_{\omega_j(t)=x} \left(\frac{1}{2M} (J_1 T_{ij} + (-J_1 + J_2) P_{ij}) - \frac{J_2}{M} \right) \right] \right)^M
\end{aligned} \tag{7.5.11}$$

where we have used Trotter's formula. We now expand the trace

$$\begin{aligned}
Z_\beta(J_1, J_2) &= \lim_{M \rightarrow \infty} \frac{1}{N!} \sum_{\pi} \sum_{x_1, \dots, x_N} \int^* d\omega_1 \dots d\omega_N \chi_E \\
&\quad \sum_{\sigma^1, \dots, \sigma^M} \prod_{j=1}^M \left\langle \sigma^j \left| \prod_{x \in \Lambda} \left[1 + \int_0^\beta dt \sum_{\substack{i: \omega_i(t)=x \\ j \neq i}} \sum_{\omega_j(t)=x} \left(\frac{1}{2M} (J_1 T_{ij} + (-J_1 + J_2) P_{ij}) - \frac{J_2}{M} \right) \right] \right| \sigma^{j+1} \right\rangle.
\end{aligned} \tag{7.5.12}$$

As before we have the understanding that $\sigma^{M+1} \equiv \sigma^1$. As in [111] the sum over σ^i 's gives an integral over a Poisson point process on intervals $\{x\} \times [t_1, t_2] \subset \Lambda \times [0, \beta]$ that have two walks present. Events are crosses and double bars of intensity J_1 and $J_2 - J_1$ respectively.

$$Z_\beta(J_1, J_2) = \frac{1}{N!} \sum_{\pi} \sum_{x_1, \dots, x_N} \int^* d\omega_1 \dots d\omega_N d\rho(\omega) \chi_E \sum_{\sigma^1, \dots, \sigma^m} \langle \sigma^1 | R_{i_1 j_1} | \sigma^2 \rangle \dots \langle \sigma^m | R_{i_m j_m} | \sigma^1 \rangle, \tag{7.5.13}$$

where ρ is the measure associated to the Poisson point process described above and the $R_{ij} = R_{ij}(\omega)$ are either T_{ij} "crosses" or P_{ij} "double bars" ordered by time of occurrence over all intervals where two walks overlap, each realisation has $m = m(\omega)$ events.

From this we can define a set of loops, $\mathcal{L}(\omega)$, from a realisation, ω , of N random walks on Λ together with the Poisson point process of crosses and double bars on overlapping walks. The loops can be rigorously defined in analogy to [2, 70, 81, 107, 111], they are best understood pictorially.

We now want to introduce space-time spin configurations. For realisation ω of N random walks and the Poisson point process a space-time spin configuration compatible with ω is a

piecewise constant function $\sigma : \text{supp}(\omega) \rightarrow \{-1, 0, 1\}$ that is constant on vertical segments of each loop and flips sign on crossing a bar, where $\text{supp}(\omega)$ is the support of the random walks $\omega^1, \dots, \omega^N$. We see that for the product in (7.5.13) to differ from zero $\sigma^1, \dots, \sigma^m$ must follow the same rules. This means that if we denote by $\Sigma(\omega)$ the set of all compatible spin configurations for ω we have

$$\sum_{\Sigma(\omega)} 1 = 3^{|\mathcal{L}(\omega)|}. \quad (7.5.14)$$

This gives us

$$Z_\beta(J_1, J_2) = \frac{1}{N!} \sum_{\pi} \sum_{x_1, \dots, x_N} \int^* d\omega_1 \dots d\omega_N d\rho(\omega) \chi_E 3^{|\mathcal{L}(\omega)|}, \quad (7.5.15)$$

using this we can use the same expansion to obtain spin correlations between particles. We begin by defining the total spin operator at site $x \in \Lambda$ by

$$S_x^3 = \sum_{i=1}^N S_i^3 \delta_{x_i, x}. \quad (7.5.16)$$

Let $x, y \in \Lambda$ with $x \neq y$, using the same expansion as previously we can obtain

$$\begin{aligned} \langle S_x^3 S_y^3 \rangle_\beta^{J_1, J_2} &= \sum_{i \neq j=1}^N \frac{1}{N!} \sum_{\pi} \sum_{x_1, \dots, x_N} \int_{i \leftrightarrow j}^* d\omega_1 \dots d\omega_N d\rho(\omega) \chi_E \sum_{\sigma \in \Sigma(\omega)} \sigma_i \sigma_j \delta_{x_i, x} \delta_{x_j, y}. \\ &= \sum_{i \neq j=1}^N \frac{2}{3} (\mathbb{P}[E_{xy}^+] - \mathbb{P}[E_{xy}^-]) \\ &= \frac{N(N-1)}{3} (\mathbb{P}[E_{xy}^+] - \mathbb{P}[E_{xy}^-]) \end{aligned} \quad (7.5.17)$$

where E_{xy}^+ is the event that sites x and y both contain a particle at time $t = 0$ and are joined by a loop with the same vertical direction at both sites. E_{xy}^- is the same event except that the vertical directions are opposite. Similarly we have

$$\langle (S_x^3)^2 (S_y^3)^2 \rangle_\beta^{J_1, J_2} - \langle (S_x^3)^2 \rangle_\beta^{J_1, J_2} \langle (S_y^3)^2 \rangle_\beta^{J_1, J_2} = \frac{N(N-1)}{9} \mathbb{P}[E_{xy}], \quad (7.5.18)$$

where $E_{xy} = E_{xy}^+ = E_{xy}^-$ is the event that sites x and y both contain a particle at time $t = 0$ and are joined by a loop.

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