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# Dynamics and Stability of Critical Spin Liquids

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## Abstract

Quantum fluctuations can dramatically change the low-temperature properties of matter. This is illustrated clearly in quantum spin liquids — novel phases of frustrated magnets which do not order in the ground state, but instead exhibit a rich array of quantum effects. These include exotic fractionalized spin excitations, emergent gauge fields, and long-range entanglement. However, despite over fifty years passing since their first proposal on the triangular lattice, conclusive experimental observation remains outstanding. Many challenges remain unresolved. On the one hand, experiments are faced with a multitude of complicating factors which disrupt the apparently fragile quantum states. On the other, more fundamental theoretical challenges remain which restrict their description fine-tuned (soluble) models. Both of these challenges are underscored by recent experimental and numerical advances which point towards strongly-coupled, gapless states. These may be highly sensitive to perturbations as well as particularly hard to model.

In this Thesis, we make predictions for the dynamics and stability of a class of critical quantum spin liquids on the triangular lattice. These critical spin liquids are especially difficult to study theoretically because they have no well-defined non-interacting limit. Nonetheless, we show how a careful treatment of interactions between the emergent fractionalised particles can lead to concrete predictions for the stability and dynamics of the paradigmatic  $J_1$ – $J_2$  Heisenberg model. We apply our approach to interpret recent numerical and experimental measurements. In the former case, we obtain quantitative results for the dynamical spin structure factor and phase diagram compatible with comprehensive numerical efforts. In the case of experiment, we use our model to discuss recent evidence for spin-liquid behaviour in ytterbium delafossite materials  $\text{KYSe}_2$  and  $\text{NaYSe}_2$ . Going beyond pure spin models, we investigate the stability of gapless spin liquids against small perturbations that are necessarily present in experiments. In this context, we find that a wide class of spin liquids with emergent  $\text{U}(1)$  gauge fields are unstable upon infinitesimal coupling to the lattice, using a combination of complementary field-theoretical and numerical methods. Specifically, we study the  $\text{U}(1)$  Dirac spin liquid as well as deconfined quantum critical points. The latter are a proposed class of phase transitions with emergent symmetries beyond the Landau paradigm. The instability of these models represent the first examples of a weak-coupling Peierls instability in two dimensions. We then study in detail the effects of dynamical, quantum phonons in stabilising the spin-disordered ground state.

The results of this Thesis provide a theoretical step forward towards understanding the nature and stability of gapless quantum spin liquid states. Our advances in describing the dynamics of spin liquids can be applied to a wide class of commonly-employed parton-mean-field theories, and highlight the urgency in understanding the influence of disorder, competing interactions, and other degrees of freedom which may act to relieve the magnetic frustration.

## Kurzzusammenfassung

Quantenfluktuationen können die Tieftemperatureigenschaften von Materie grundlegend verändern, wie das Beispiel der Quantenspinflüssigkeiten deutlich zeigt. Quantenspinflüssigkeiten sind neuartige Phasen frustrierter Magnete, die im Grundzustand keine Ordnung aufweisen, dafür aber eine Vielzahl von Quanteneffekten. Dazu gehören exotische fraktionierte Spinanregungen, emergente Eichfelder und weitreichende Verschränkung. Obwohl seit ihrer konzeptioneller Entdeckung auf dem Dreiecksgitter mehr als fünfzig Jahre vergangen sind, steht eine schlüssige experimentelle Beobachtung noch aus. Viele Herausforderungen bleiben ungelöst. Einerseits sind die Experimente mit einer Vielzahl von komplizierenden Faktoren konfrontiert, die die fragilen Quantenzustände stören. Andererseits bestehen nach wie vor grundlegendere theoretische Herausforderungen, die ihre Beschreibung auf fein abgestimmte (lösbare) Modelle beschränken. Beide Herausforderungen werden durch die jüngsten experimentellen und numerischen Fortschritte unterstrichen, die auf stark gekoppelte, lückenlose Zustände hindeuten. Diese können sehr empfindlich auf Störungen reagieren und besonders schwer zu beschreiben sein.

In dieser Arbeit machen wir Vorhersagen für die Dynamik und Stabilität einer Klasse von kritischen Quantenspinflüssigkeiten auf dem Dreiecksgitter. Diese kritischen Spinflüssigkeiten sind theoretisch besonders schwierig zu untersuchen, da sie keinen nicht wechselwirkenden Limes haben. Dennoch zeigen wir, wie eine sorgfältige Behandlung der Wechselwirkungen zwischen den entstehenden fraktionierten Teilchen zu konkreten Vorhersagen über die Stabilität und Dynamik des paradigmatischen  $J_1$ – $J_2$  Heisenberg-Modells führen kann. Wir wenden unseren Ansatz an, um neuere numerische und experimentelle Messungen zu analysieren. Zunächst erarbeiten wir quantitative Ergebnisse für den dynamischen Spinstrukturfaktor und das Phasendiagramm, die mit umfassenden numerischen Bemühungen vereinbar sind. Wir verwenden unser Modell, um jüngste Beweise für Spinflüssigkeitsverhalten in den Ytterbium-Delafossit-Materialien  $\text{KYSe}_2$  und  $\text{NaYSe}_2$  zu interpretieren. Über reine Spinmodelle hinausgehend, untersuchen wir die Stabilität von kritischen Spinflüssigkeiten gegenüber kleinen Störungen, die in Experimenten zwangsläufig vorhanden sind. In diesem Zusammenhang stellen wir fest, dass eine breite Klasse von Quantenspinflüssigkeiten mit emergenten  $U(1)$ -Eichfeldern bei infinitesimaler Kopplung an das Gitter instabil ist, wobei wir eine Kombination aus komplementären feldtheoretischen und numerischen Methoden verwenden. Insbesondere untersuchen wir die  $U(1)$ -Dirac-Spinflüssigkeit sowie dekonfinierte quantenkritische Punkte, eine Klasse von Phasenübergängen mit emergenten Symmetrien jenseits des Landau-Paradigmas. Die Instabilität dieser Modelle ist das erste Beispiel für eine Peierls-Instabilität bei kleiner Kopplung in zwei Dimensionen. Anschließend untersuchen wir im Detail die Auswirkungen dynamischer Quantenphononen auf die Stabilisierung des spingestörten Grundzustands.

Die Ergebnisse dieser Arbeit stellen einen Schritt zum Verständnis der Natur und Stabilität von kritischen Quantenspinflüssigkeitszuständen dar. Unsere Fortschritte bei der Beschreibung der Dynamik von Quantenspinflüssigkeiten lassen sich auf eine breite Klasse gängiger Parton-Molekularfeldzuständen anwenden und unterstreichen die Notwendigkeit, den Einfluss von Unordnung, konkurrierenden Wechselwirkungen und anderen Freiheitsgraden zu verstehen, die möglicherweise die magnetische Frustration aufheben können.



## Publications

The work presented in this Thesis represents my own original work. Many results have previously been included in the following manuscripts:

- U. F. P. Seifert\*, J. Willsher\*, M. Drescher, F. Pollmann, and J. Knolle, *Spin-Peierls instability of the  $U(1)$  Dirac spin liquid*, [Nature Communications](#) **15**, 7110 (2024).
- D. Hofmeier\*, J. Willsher\*, U. F. P. Seifert, and J. Knolle, *Spin-Peierls instability of deconfined quantum critical points*, [Physical Review B](#) **110**, 125130 (2024).
- F. Ferrari\*, J. Willsher\*, U. F. P. Seifert, R. Valentí, and J. Knolle, *Stability of algebraic spin liquids coupled to quantum phonons* (2024), [arXiv:2410.16376](#).
- J. Willsher and J. Knolle, *Dynamics and stability of  $U(1)$  spin liquids beyond mean-field theory* (2025), [arXiv:2503.13831](#).

Here, \* indicates joint first authorship, listed alphabetically. Where projects were undertaken collaboratively, I contributed significantly to all stages of the analytical progress, including performing calculations, conceptualising the projects, and interpreting numerical results. I also contributed to the following experimental work which is included in Chapter 4:

- A. O. Scheie, M. Lee, K. Wang, P. Laurell, E. S. Choi, D. Pajerowski, Q. Zhang, J. Ma, H. D. Zhou, S. Lee, S. M. Thomas, M. O. Ajeesh, P. F. S. Rosa, A. Chen, V. S. Zapf, M. Heyl, C. D. Batista, E. Dagotto, J. E. Moore, and D. A. Tennant, *Spectrum and Low-Energy Gap in Triangular Quantum Spin Liquid  $\text{NaYbSe}_2$*  (2024), [arxiv:2406.17773](#).

I developed a theoretical model used in the interpretation of data, to appear in a future version of this preprint. I would like to also acknowledge several ongoing collaborations which have influenced this Thesis. In particular, I include unpublished results obtained in collaboration with F. Ferrari, D. Hofmeier, M. Knap, A. Romen, and A. Scheie. I additionally contributed to the following journal articles during my PhD, which do not appear in this Thesis, but are listed for completeness:

- T. Hodson, J. Willsher, and J. Knolle, *One-dimensional long-range Falikov-Kimball model: Thermal phase transition and disorder-free localization*, [Physical Review B](#) **104**, 045116 (2021).
- S.-W. Liu, J. Willsher, T. Bilitewski, J.-J. Li, A. Smith, K. Christensen, R. Moessner, and J. Knolle, *Butterfly effect and spatial structure of information spreading in a chaotic cellular automaton*, [Physical Review B](#) **103**, 094109 (2021).
- J. Willsher, S.-W. Liu, R. Moessner, and J. Knolle, *Measurement-induced phase transition in a chaotic classical many-body system*, [Physical Review B](#) **106**, 024305 (2022).
- J. Willsher, H.-K. Jin, and J. Knolle, *Magnetic excitations, phase diagram, and order-by-disorder in the extended triangular-lattice Hubbard model*, [Physical Review B](#) **107**, 064425 (2023).
- J. Habel, A. Mook, J. Willsher, and J. Knolle, *Breakdown of chiral edge modes in topological magnon insulators*, [Physical Review B](#) **109**, 024441 (2024).



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## 1.1 Motivation

Every discipline has its own rules. In high-energy physics, the dynamics of electrons and the electromagnetic field are described by quantum electrodynamics (QED). This theory is a set of rules for the behaviour of charged matter, which is able to produce some of the most accurate predictions in all of physics. It describes the electron as a fundamental particle with spin-1/2 and a magnetic moment slightly above two (Schwinger, 1948) — the latter prediction agrees with experiment up to twelve significant figures (Fan *et al.*, 2023). It achieves an astonishing level of accuracy almost unparalleled in physics (Guellati-Khelifa, 2023).

In condensed matter we do *low-energy physics*. While also often interested in the electron, we study its collective behaviour within materials at relatively low temperatures. The rich complexity of QED is hidden from us at these scales, where the appropriate description of electron interactions is through the Coulomb potential. Going even further, we can form whole theories based on semiclassical models of electrons, such as the Drude theory of resistivity. Moving away from fundamental physics, the *status quo* is to form simplified models which are ignorant to the details of a more fundamental theory. But in this case, ignorance is a sign of wisdom. The ability to abstract the relevant details from a fundamental theory to produce a collective description of complex phenomena is the key to describing the richness of different branches of science. By forming models of non-fundamental theories, we may describe a rich world of phenomenology.

Phenomenology can be fundamental too, in a way. Thermodynamics is an incredible theory which was constructed without any microscopic models in mind. Based on its own set of fundamental rules, it describes the flow of heat and limits of performing work. Statistical mechanics and later quantum physics came only after these rules had been developed, serving to explain and confirm their predictions (Hoddeson *et al.*, 1992). However, there are some examples where progress has led to an upset in our understanding (Kuhn, 1970). Nernst's heat theorem is a form of the third law of thermodynamics, which states that the entropy of a system approaches zero as you cool it to zero temperature. This law requires that any gaseous or liquid state orders as it cools, meaning matter enters a regular state at zero temperature with no residual entropy density. Does everything freeze at zero temperature? Surprisingly it doesn't. There is a class of magnets — so called frustrated magnets — where local magnetic constraints lead to a macroscopic number of low-energy states. This, in turn, prohibits magnetic ordering since there is no obvious ground state to fall into. We will describe shortly how this behaviour emerges in simple classical models, which leads to disordered states at zero temperatures. This apparent violation of the third law provides the starting point for adding quantum effects, where the behaviour can become even more exotic.

Modern condensed matter physics exists at the intersection of fundamental physics and

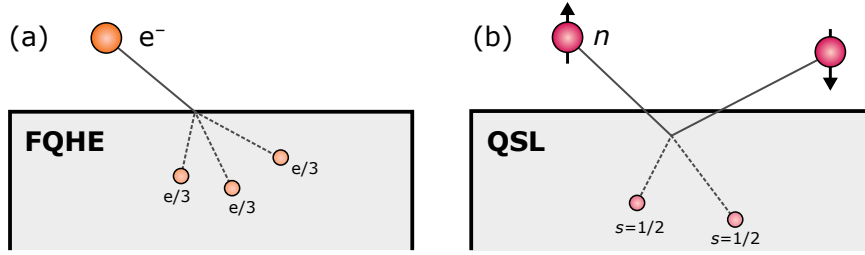


**Figure 1.1:** *Archetypal examples of fractionalisation.* (a) The electron charge  $e$  fractionalises into three quasiparticles with fractional charge  $e/3$  in the  $\nu = 1/3$  fractional quantum Hall effect (FQHE). (b) The spin  $S = 1$  spin flip excitation caused by scattering a neutron fractionalises into two  $S = 1/2$  spinons in a quantum spin liquid (QSL).

phenomenology. It is, at heart, the study of a macroscopic number of strongly interacting degrees of freedom (on the order of  $10^{22}$ ), and predicting their emergent properties and collective behaviours. It was put succinctly by one of the pioneers of the last century: *More is different* (Anderson, 1972). A collection of particles can be thought of as more than a sum of its parts. If this is the case, how do we begin to understand what sort of physics can emerge? As Anderson discussed, the most powerful organising principle that we have is Landau’s symmetry-based approach (Landau and Lifshitz, 1980). In this framework, we may classify the zoo of possible phases using their symmetries. The system has a global symmetry which may be successively partially broken by phase transitions into ordered phases. This theory describes, for example, a ferromagnet as an ordered phase since it breaks the rotational invariance of the vacuum (picking a direction to point its magnetic field). By heating it above the Curie–Weiss temperature, this state restores the full symmetry of the vacuum when it becomes a paramagnet. In this case, thermal fluctuations destroy any local magnetic order. The two phases are distinguished by an order parameter, a *local* measure of how magnetic the material is. This is the key tenet of the Landau paradigm: order is something that we can locally probe.

Landau’s theory is not only successful at describing what types of states can exist, but also at describing, in broad terms, what properties they must have. Stepping into the quantum description of magnetism, we can understand the ferromagnet as a state formed when local magnetic moments interact in such a way which makes them want to align. When this magnetic state spontaneously breaks continuous rotational symmetry, there must be a corresponding *quasiparticle* called a magnon in its spectrum. This magnon represents a fluctuation of the magnetic order, and is guaranteed to be gapless in the case described above.

Again, nature has surprises for us. Beyond Landau, we have discovered that there may be different phases which are not distinguished purely by symmetry. A foundational example of this is the fractional quantum Hall effect (Tsui *et al.*, 1982; von Klitzing, 2017). The backdrop for this state is a 2D electron gas in a strong magnetic field. The electrons form macroscopically degenerate Landau levels with a filling fraction determined by the magnetic field strength. For certain fields, which represent rational fillings  $\nu = 1/3, 1/5$ , etc., the interactions of the electrons dominate and a surprising behaviour emerges. We get a new phase of matter where the fundamental charge is not  $e$ , as guaranteed by electromagnetism,

but can be for example  $e/3$ . Figure 1.1 depicts this scenario of the electron *fractionalising* into three quasiholes, and splitting the unit of charge along with it. This is a case where the emergent quasiparticle is not a result of a symmetry being broken within Landau’s paradigm. Instead, there is a new type of *topological* order which cannot be measured locally (Wen, 1991). They are phases with high quantum entanglement and where the order is only evident in global properties. In the case of the fractional quantum Hall effect the most pronounced consequence of the topological order is a ground state degeneracy which depends on the topology of the underlying manifold, as well as protected chiral edge states. This new type of order opens the door for new phases of matter beyond symmetry breaking (Wen, 2004).

Quantum spin liquids are a phase of quantum magnets where the local magnetic moments do not order at zero temperature, choosing instead to remain in a *liquid* state. They emerge from the highly-degenerate ground states of frustrated magnets, where quantum fluctuations lead to the formation of long-range entanglement, much like the fractional quantum Hall effect (Kalmeyer and Laughlin, 1987). Quantum spin liquids are a paradigmatic example of *spin fractionalisation*. Figure 1.1 shows how the fundamental spin flip excitation splits into two spin-1/2 particles, presented here as a neutron generating a pair of fermionic ‘spinon’ particles. This phase of matter also goes beyond Landau’s paradigm — the many exotic properties cannot be described in general terms by symmetry breaking, since the state is fully symmetric (Wen, 2002). The physics of these disordered magnets is instead determined by emergent gauge theories. We will show soon that fractionalising spins necessarily introduces a gauge degree of freedom. The universal physics of quantum spin liquids is dominated by *emergent gauge fields*. Quantum magnets can host phases of matter that are truly more than a sum of their parts.

This Thesis studies in detail a recent proposal that a quantum spin liquid on a triangular lattice antiferromagnet hosts an *emergent quantum electrodynamics*. In this model, the spins fractionalise into fermionic spinons which behave like electrons coupled to an emergent photon. The resulting theory looks exactly like that of QED in two dimensions — the fundamental model of electrons interacting through the electromagnetic field (McGreevy, 2019). It is a truly surprising prediction, so let us summarise: We take the high-energy theory of quantum electrodynamics, and place its main character, the electron, on a triangular lattice. These spin-1/2 degrees of freedom interact via the exchange interactions, a low-energy manifestation of the spin-statistics theorem.<sup>1</sup> Instead of being able to work with a simpler toy model when we cool the system down, we are faced with an emergent analogue which appears to be described by exactly the same equations! Somehow, the low-energy physics recreates the high-energy. If more is different, then it would be ironic if more also turns out to be the same.

This observation has led many to ask, *how fundamental is fundamental physics?* Some even postulate that the equations which govern our universe could be emergent themselves (’t Hooft, 1999, 2007; Wen, 2004; Volovik, 2009). Indeed the greatest problem of modern high-energy physics is to understand the UV-completion of the respective theories. That means, even though we understand the equations at play in our universe at the energy scales

<sup>1</sup>Not to mention the many levels of abstraction involved in the formation of atoms, the crystal that leads to a lattice of magnetic ions, the formation of effective spin-1/2 moments, etc. The phenomenology spans chemistry, materials science, atomic and nuclear physics, and condensed matter.

we can observe (to some very good accuracy), how do they emerge from a more fundamental theory? In condensed matter models we have access to this UV theory. In the case of spin liquids, it is nothing but our spin Hamiltonian. We can heat our magnet to high temperatures and perform an experiment on it just as well as at low temperatures. We can fire neutrons or X-rays to probe its fast dynamics without building a particle accelerator.<sup>2</sup> By probing at different scales and understanding the ways in which physics can emerge, we can understand the relation between the universal and lattice-scale physics.

The goals of the work at hand are to understand better the mechanisms of this type of emergence in condensed matter physics. How can gauge fields emerge in magnets? What are the signatures of fractionalisation in this context? Is it robust? There seem to be key differences between fundamental and non-fundamental physics. In the rest of this Chapter, we will introduce the non-fundamental aspects. With a view to describing emergent quantum electrodynamics, we introduce classical and quantum spin liquids. Throughout we keep in mind this goal; QED has massless photons, and so we use examples of critical (or massless) states.

## 1.2 Frustrated magnetism

### Triangular lattice Ising model

Frustration is a consequence of not getting what you want. When we anthropomorphise a spin and say that it is frustrated, we mean that a local magnetic constraint cannot be satisfied globally. We can go further and say that frustration can lead to dramatic results (Balents, 2010).

Constraints emerge in classical and quantum systems by way of interactions. Whereas ferromagnetic interactions lead to an alignment of spins, antiferromagnetic interactions prefer to have spins point in opposite directions. To make this more concrete, consider the Hamiltonian of Ising spins

$$H = J \sum_{\langle ij \rangle} S_i S_j, \quad (1.1)$$

where  $S_i = \pm 1$ . The sites  $\langle ij \rangle$  are nearest neighbours on the lattice. For ferromagnetic  $J < 0$ , the lowest energy configuration is all spins pointing in the same direction: all up, or all down. For antiferromagnetic interactions  $J > 0$ , the result depends on geometry. Fig. 1.2 depicts the classical Ising model on the square and triangular lattices. In the case of the square lattice, it is possible to point each of the four neighbours of every spin in the opposing direction. Formally this is because the square lattice is *bipartite*. On the other hand, in the case of a triangular lattice, the spins cannot all be happy. Looking at an individual triangular plaquette in Fig. 1.2(a), we see that two of the sites can be occupied with satisfied, opposing, spin configurations. However the remaining third sites will always make one of their neighbours unhappy.

The *local* constraint of spins being oriented opposite to their neighbours cannot be satisfied *globally*. Not only is the ground state unhappy, but it is also massively degenerate. There

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<sup>2</sup>Without always building a particle accelerator. Many experiments require either a *small* particle accelerator or nuclear reactor.

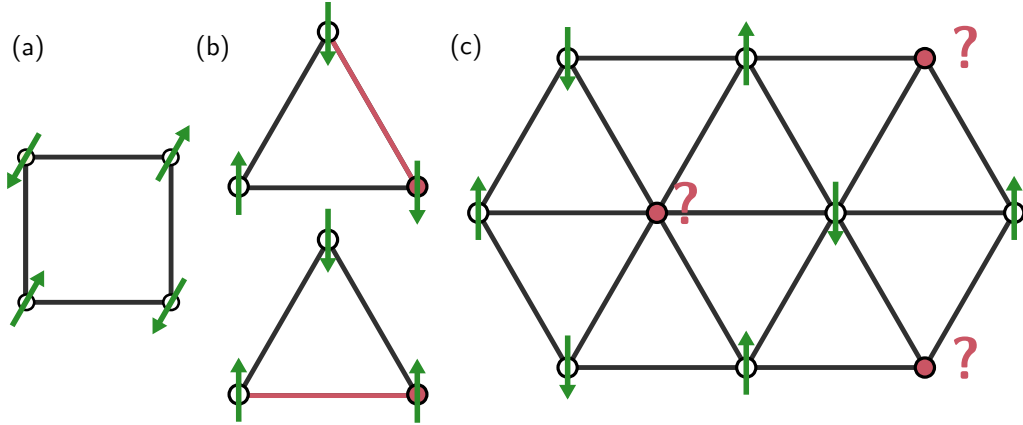


**Figure 1.2: Ising model on the square and frustrated triangular lattice.** In the antiferromagnetic Ising model, neighbouring spins want to anti-align. (a) On the square lattice, all spins can satisfy this constraint. (b) On a triangular plaquette, only two bonds can simultaneously satisfy this constraint. One remains frustrated. (c) The lowest energetic state when tiling the lattice, given the constraint to be in the ground state. The resulting energy is independent of the configuration of spins on one third of the sites.

are a macroscopic number of equally unsatisfied states. There is a simple configuration which demonstrates this, shown in Fig. 1.2(b). In a system with  $N$  sites, we are able to arrange two thirds in a satisfied configuration. However, the remaining  $N/3$  sites can be arbitrarily oriented, up or down. This means there are at least  $2^{N/3}$  possible states in the ground state. The consequence of this is a residual entropy density even at absolute zero, which is at least  $s_0 = k_B \log(2)/3 \approx 0.23 k_B$ . In fact, this model was studied by Wannier (1950) who showed that the exact number of states in the ground state is in fact much higher. There are many configurations not shown here that have the same energy. The result is a residual entropy of  $s_0 \approx 0.338 k_B$ . This residual entropy is an apparent violation of the third law of thermodynamics. This state at zero temperature has no spin order, leading us to call it a classical spin liquid.

Let us take a look at this model more quantitatively, following Chalker (2017). Our aim is to study its ground state properties and correlations. The ground-state sector of this model has a description in terms of a *height model*. The basic idea is outlined in Fig. 1.3. We can associate a field  $h_i$  with each site around a plaquette, which is defined as varying by +1 along a satisfied bond, and  $-2$  along a frustrated bond. Within the ground state, there must always be one frustrated bond around any plaquette, and so the height model returns to its original value (we say it is single-valued in the ground-state sector). Using this basic rule, we can start to differentiate different configurations in the ground state based on the behaviour of the height field. For this, define the average height field around a triangle as  $h(\mathbf{r}) = (h_1 + h_2 + h_3)/3$ . We show this in Fig. 1.3(b,c) for two possible configurations in the ground state. We distinguish the spins by their flippability. We call a spin flippable if we can flip it without changing the energy. The configuration with a flat height field is the *maximally-flippable* state. In this case,  $N/3$  spins can be flipped without increasing the

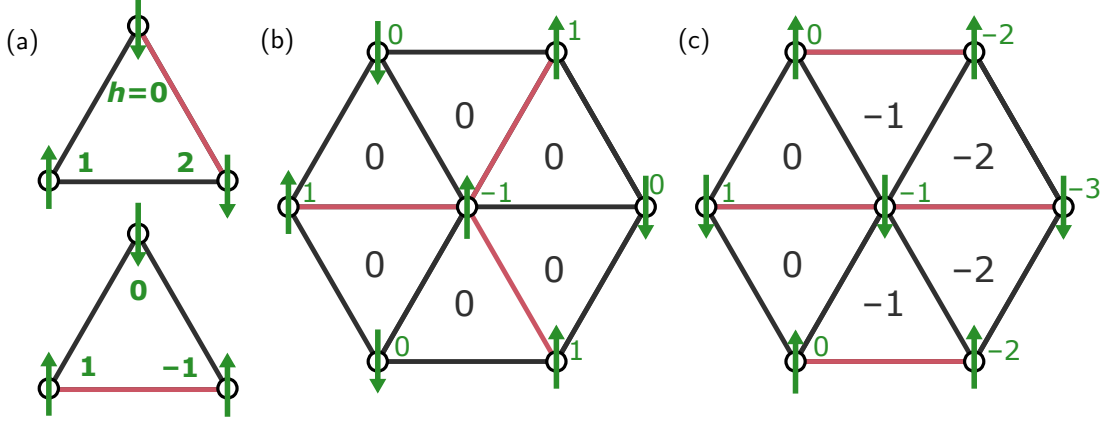


Figure 1.3: *Height-model description of the frustrated Ising model ground-state sector* (a) Height field on two plaquettes. (b) Maximally flippable state. (c) No flippable spins.

energy. On the other hand, the state with the maximal gradient of the height field has no flippable spins.

We can understand the difference using intuition from the dimer-model literature (Moessner and Sondhi, 2001a,b). The system prefers to be in states which are more flippable, since fluctuations around the ground state contribute higher entropy. This effect can be captured by assigning each configuration an entropic weight which is proportional to the gradient of the height field. This naturally prefers the flippable states with flat height-field configurations. To do this, we coarse grain the height field by considering  $h(\mathbf{r})$  as a function of continuous space. Next, we write down the entropic weight of a given configuration to lowest order

$$\mathcal{H}[h(\mathbf{r})] = \frac{K}{2} \int d^2\mathbf{r} |\nabla h(\mathbf{r})|^2. \quad (1.2)$$

The probability of the field having a given configuration can be written in terms of this weight as

$$P[h(\mathbf{r})] = \frac{1}{Z} e^{-\mathcal{H}[h(\mathbf{r})]}, \quad Z = \int \mathcal{D}h(\mathbf{r}) e^{-\mathcal{H}[h(\mathbf{r})]}. \quad (1.3)$$

We have produced an effective low-energy field theory, which describes the long-wavelength fluctuations. With this theory to hand, we have the tools to calculate some properties of the ground state.

We are interested in calculating correlation functions of spin operators using this formalism. Focusing on one spin at the top of the triangle, we write

$$S_i = \text{Re} e^{i\pi h(\mathbf{r}_i)/3}. \quad (1.4)$$

Given that our entropic weight (1.2) is completely independent of the value of  $h(\mathbf{r})$ , instead only depending on its gradient, we can say that  $h(\mathbf{r})$  must uniformly take all values between 0 and  $2\pi$ . This, in turn, implies that  $\langle S_i \rangle = 0$ , i.e. there is no average spin order<sup>3</sup>. Some

<sup>3</sup>If the entropic weight had a potential  $-m^2 \cos^2 h(\mathbf{r})$ , then this would immediately favour integer  $h$  configurations with  $\langle S_i \rangle = 1$ . This is not present in this model.

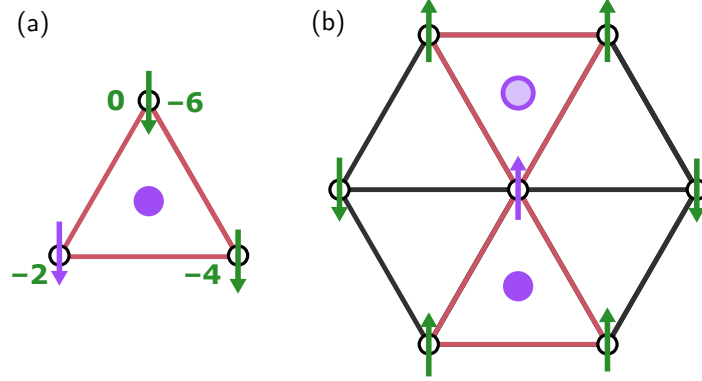


**Figure 1.4:** *Vortex configurations in the height model.* (a) A triangle with three frustrated bonds makes the height field non-single valued, shown as a purple vortex at the centre of the plaquette. (b) Flipping a spin takes us out of the ground state manifold. It introduces a vortex and anti-vortex configuration.

algebraic manipulations then show (Wen, 2004; Chalker, 2017)

$$\langle S_{\mathbf{r}} S_0 \rangle \sim \langle e^{(i\pi/3)[h_{\mathbf{r}} - h_0]} \rangle \sim e^{-\pi^2 \langle [h_{\mathbf{r}} - h_0]^2 \rangle / 18}. \quad (1.5)$$

This expresses the spin correlation function in terms of the height fields. We can write the entropic weight in momentum space

$$\mathcal{H}[h(\mathbf{r})] = \frac{K}{2} \int d^2 \mathbf{k} |h(\mathbf{q})|^2, \quad (1.6)$$

and then the correlator is an integral over the momentum-space Green's function

$$\langle [h_{\mathbf{r}} - h_0]^2 \rangle = \frac{1}{2\pi^2 K} \int d^2 \mathbf{k} |\mathbf{k}|^{-2} (1 - e^{i\mathbf{k} \cdot \mathbf{r}}) \simeq \log |\mathbf{r}| / (\pi K). \quad (1.7)$$

Together, we find the spin-spin correlation function is a power law (Blote and Hilborst, 1982)

$$\langle S_{\mathbf{r}} S_0 \rangle \sim |\mathbf{r}|^{-\pi/(18K)}. \quad (1.8)$$

We have a *critical phase*, where the spin correlations are algebraic. This signals that there are long-range correlations within the ground state manifold, a direct consequence of the massively degenerate state.

The height field mapping is only valid in the ground state manifold. If we want to consider excitations that go beyond this, we will see that the height field becomes non-single valued. For example, consider flipping a spin on the triangle in Fig. 1.3(a) such that there are three unfrustrated bonds on a plaquette. This configuration is shown in Fig. 7.2(a). On such a triangle, the height field winds by  $-6$ . We call this a vortex configuration. Whenever a spin is flipped out of the ground-state manifold in this way, it introduces a vortex and an anti-vortex, shown in Fig. 7.2(b). This configuration has energy  $4J$  above the ground state manifold.

Once created, the vortices can move on the lattice freely without incurring any additional energy cost (Chalker, 2017). They interact only through an entropic contribution, which scales logarithmically in their separation as  $\log(r)$ . This is our first example of fractionalisation: the physics of a spin flip is controlled by the dynamics of a vortex-anti-vortex pair interacting with a weak potential. Remarkably, this  $\log(r)$  dependence mediated by the disordered background behaves just like the Coulomb interaction in two dimensions!

This is a classical spin liquid. Adding quantum fluctuations on top of this highly degenerate state will produce rich physics. Many states we encounter will share aspects with this model. Namely, we will study critical models with algebraic correlations and fractionalised excitations, albeit in a more involved quantum setting.

### Triangular lattice Heisenberg model

Now we turn to Heisenberg's model on the same triangular lattice. The Hamiltonian is given by

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = J \sum_i \left( S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right), \quad (1.9)$$

where  $\vec{S}_i^\alpha$  are the  $\alpha = x, y, z$  spin components. How does frustration manifest in this model? Before understanding the quantum model, we can first look at the classical one. In this classical limit, the spin operators can be treated as continuous vectors with length  $S \ll 1$ . We can then rewrite the Hamiltonian as follows

$$H = \frac{J}{2} \sum_{\Delta} \vec{S}_{\Delta}^2 + (\text{const.}), \quad (1.10)$$

where  $\vec{S}_{\Delta} = \vec{S}_1 + \vec{S}_2 + \vec{S}_3$  is the sum of the three spins around an upwards-pointing triangular plaquette. Eq. (1.10) tells us that the classical energy is minimised when  $|\vec{S}_{\Delta}| = 0$ , and there is no net magnetic moment on each triangle. This is achieved with the configuration shown in Fig. 1.5, called the 120-degree ordered state. The effect of frustration in this case is to create a new form of *non-collinear order*.

What is the nature of the quantum ground state? Far away from the classical regime, we can expect strong corrections due to quantum fluctuations. One key effect of such fluctuations is to suppress the magnitude of the order parameter. This means the expectation value of the spin amplitude is less than the size of the underlying spin  $|\langle S_z \rangle| < S$ , (Kittel, 1963). We will focus on the pure quantum limit,  $S = 1/2$ . Here, we investigate the possibility that  $|\langle S_z \rangle| = 0$  and we have a quantum spin liquid state.

Anderson (1973) proposed exactly this when he wrote down the first quantum spin liquid wave function for the triangular lattice Heisenberg model. This so-called resonating valence bond (RVB) state is a spin-liquid wavefunction formed by a massive superposition of local singlets on bonds. These singlets  $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$  have  $S = 0$ , and naturally form a basis for a spin-zero ground state (Lacroix *et al.*, 2011; Savary and Balents, 2016). The long-range entanglement and topological nature of the phase comes from the massive quantum superposition of product states formed by tiling the lattice with valence bonds. This naturally leads to analogy with the dimer models that we saw in the case of the Ising model height-field representation, and indeed this has been a fruitful line of research (Rokhsar and Kivelson,

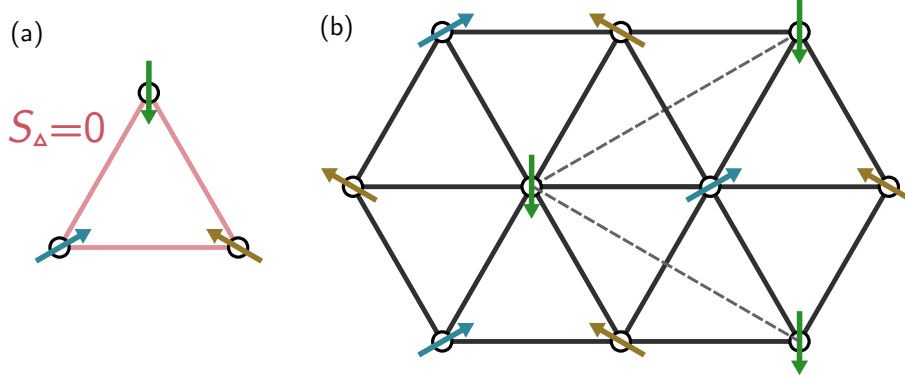


**Figure 1.5:** *Frustrated Heisenberg model on the triangular lattice.* (a) For classical Heisenberg spins, the most energetically favourable state is a 120-degree ordered state. Each bond is equally frustrated. (b) The resulting state tiles the lattice with a three site unit cell. Grey dashed lines highlight two next-nearest neighbour bonds.

1988; Moessner and Sondhi, 2001a). Just as we saw in the Ising case, the idea of fractionalisation appears automatically by considering a spin-flip excitation. In the basis of these dimers, the local spin-1 excitation is to form a triplet  $|\uparrow\downarrow\rangle + |\uparrow\downarrow\rangle$ . Just as we saw that vortices can be separated without an energy cost, the triplet dimer can be viewed as two spin-1/2 *fractionalised* particles which are also able to hop across the lattice (by way of reconfiguring dimers).

Anderson’s gapped spin-liquid ground state unfortunately turned out to be incorrect in the context of its original proposal. The ground state of the triangular lattice Heisenberg model is a 120-degree ordered state. The aforementioned  $1/S$  corrections do act to suppress the ordering moment, but only to  $\langle S_z \rangle = 0.239$  (Jolicoeur and Le Guillou, 1989). Modern numerical simulations also confirm that there is magnetic order (Iqbal *et al.*, 2016). However, fifty years later, the same triangular-lattice Heisenberg model is still being investigated as a potential candidate model to realise a QSL (Song *et al.*, 2019).

The necessary component is just *additional frustration*. So far we have been relying on the natural geometric frustration of the triangular lattice. For the Heisenberg model this is apparently not enough to destroy the order. It is possible to further frustrate the 120-degree state further by way of additional exchange frustration. The only necessary ingredient in our Heisenberg model is a next-nearest neighbour antiferromagnetic exchange,  $J_2 > 0$ . We can see from Fig. 1.5(b) that the next-nearest neighbour bonds connect sites on the same sublattice in the 120-degree ordered phases. Tuning an antiferromagnetic exchange on this bond will act to frustrate this ordered state even further.

A classical analysis by Jolicoeur *et al.* (1990) showed that above  $J_2/J_1 = 1/8$ , the state prefers to form a different type of magnetic order. This can be understood as ‘stripe’ magnetic order (Chubukov and Jolicoeur, 1992), where there is a 2-site unit cell. At the point  $J_2/J_1 = 1/8$ , there are many different types of magnetically ordered states which have the same energy. We call this the maximally frustrated point. A non-linear spin-wave calculation using the  $1/S$  expansion tantalisingly shows that the 120-degree order is pushed to zero before this

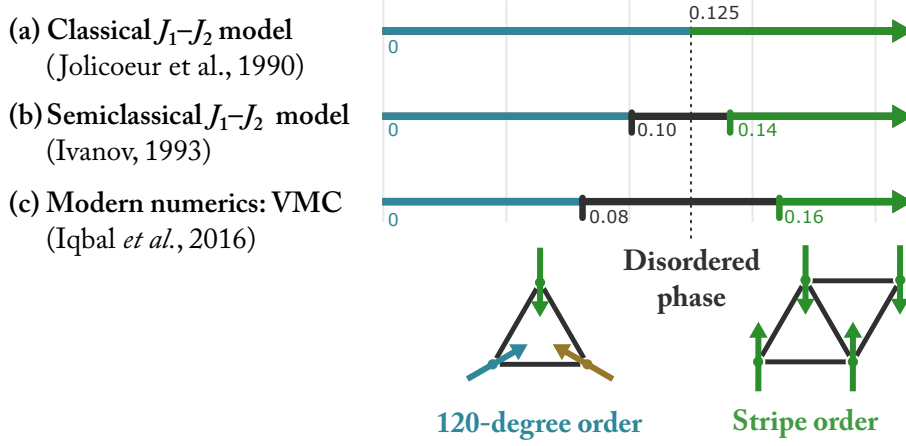


**Figure 1.6:** *Phase diagram of the  $J_1$ - $J_2$  Heisenberg model on the triangular lattice.* Review of the classical energy crossover point, semiclassical, and modern numerical results for the phase diagram. (a) Classical phase diagram of the model; first-order transition from 120-degree to stripe magnetic order at  $J_2/J_1 = 1/8$  (Jolicoeur *et al.*, 1990). (b) Semiclassical phase diagram; quantum fluctuations suppress the sublattice magnetisation to zero in an intermediate disordered phase (Ivanov, 1993). (c) Modern numerical approaches show a spin liquid around the classically maximally-frustrated point. Results here found using variational Monte Carlo (VMC) (Iqbal *et al.*, 2016).

maximally frustrated point. The stripe order is equally suppressed above it. This suggests that there might be some sort of spin-disordered phase in the range 0.1–0.14 (Ritchey *et al.*, 1990; Ivanov, 1993). Finally, we turn to modern numerical approaches which show an even more extended spin-liquid regime (Iqbal *et al.*, 2016). Figure 1.6 summarises these different approaches. Although Anderson was wrong about the  $J_2 = 0$  spin liquid, there is a modern-day consensus that there should be a spin liquid emerging in this model around the  $1/8$  point. It is our aim to investigate the nature and stability of exactly this phase.

### Fractionalisation: Stability and signatures

How do we define a spin liquid in practice? The first attempt can be to use the *negative definition*: it is a ground state of a frustrated magnet which does not show any spontaneous symmetry breaking, meaning the correlation functions of spin order parameters must satisfy

$$\langle \vec{S}_r \cdot \vec{S}_0 \rangle \rightarrow 0 \quad (1.11)$$

as we take the distance  $|\mathbf{r}| \rightarrow \infty$  (Lacroix *et al.*, 2011). In practice, the absence of any magnetic order means we should not see any magnetic Bragg peaks or any signs of a low-temperature phase transition in the specific heat. However often these conditions are difficult to prove, due to lack of data or insufficient resolution. There are also facts of life, such as disorder, which can obscure things further. See the reviews by Knolle and Moessner (2019); Broholm *et al.* (2020) for a more thorough discussion of this subject. We therefore add the following *positive condition*: spin liquids are spin-disordered ground states with deconfined,

fractional excitations. The presence of emergent, fractionalised quasiparticles is the defining feature that directs our attention to work on quantum spin liquids.

The field of spin liquids bifurcated in its early days into two tracks, as it was put by Moessner and Sondhi (2001a). There were those studying the original short-range RVB state, with its gapped excitations (Anderson, 1973; Rokhsar and Kivelson, 1988), including later the successful description on the triangular lattice in terms of dimer models (Moessner and Sondhi, 2001a,b, 2002). Then there was the other school, which investigated *gapless* quantum spin liquids with valence bonds on all length scales (Anderson, 1987; Baskaran *et al.*, 1987; Baskaran and Anderson, 1988).<sup>4</sup> These gapless models are studied using fractionalised fermions coupled to emergent gauge theories. This results in a strongly interacting theory, as one would expect for a gapless state. When these interactions lead to the fermions confining, i.e. sticking back together, it signals we took the wrong basis to describe the state (Mudry and Fradkin, 1994a,b). In this case where fractional particles confine, we are talking about a conventional magnet.

On the other hand, when the fractionalised excitations do not confine, we can get exciting new physics. This is the picture that resembles the fractional quantum Hall effect and is drawn in Fig. 1.1. We consider a theory of *spinons* as the fermionic fractionalised constituents of spins. Explicitly, we can define the spins in terms of Abrikosov fermions

$$\vec{S}_i = \frac{1}{2} f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta}, \quad (1.12)$$

where we must constrain that there is only one fermion per site. The physical spin degree of freedom is split into two *spinons*. The operator  $f_{i\uparrow}^\dagger$  corresponds to creating a spin-up fermion, and  $f_{i\downarrow}^\dagger$  to spin-down. This representation naturally introduces a gauge degree of freedom into the system. For example, it is possible to rotate each fermion by a phase  $f_i \rightarrow e^{i\theta_i} f_i$  and the spin  $\vec{S}_i$  in Eq. (1.12) is left invariant. This gauge degree of freedom is critical to understanding the resulting phase. Taking a lesson from fundamental physics, we know there are two types of behaviours that gauge theories can exhibit at long-wavelengths. Quantum chromodynamics is *confining*, meaning the charged fundamental fermions, quarks, cannot be observed on their own. The ‘hadrons’ that form from the confinement of spinons are nothing but regular magnetic quasiparticles, called magnons. On the other hand, quantum electrodynamics exists in our universe in a *deconfined*, or Coulomb phase. Formally it means the fundamental fermions, electrons, can be separated to infinity at finite energy cost. If our spinons are deconfined, then we have a true spin liquid.

The parton representation Eq. (1.12) is also the key to a modern classification of spin liquid states (Wen, 2002). Since disordered phases evade classification in Landau’s paradigm, they should be understood in terms of the type of emergent fermions and gauge fields. We mentioned in the Motivation that topological order is a useful tool to understand fractionalised phases. This intuition comes from the fact that the fractional quantum Hall state is an intrinsically topologically-ordered phase (Wen, 1991). It has the properties we mentioned before, such as a ground state degeneracy that depends on the character of the underlying manifold. However, this framework is applicable only to *gapped* phases. There exist ana-

<sup>4</sup>Work in this context was historically spurred on by parallel thinking about the cuprates.

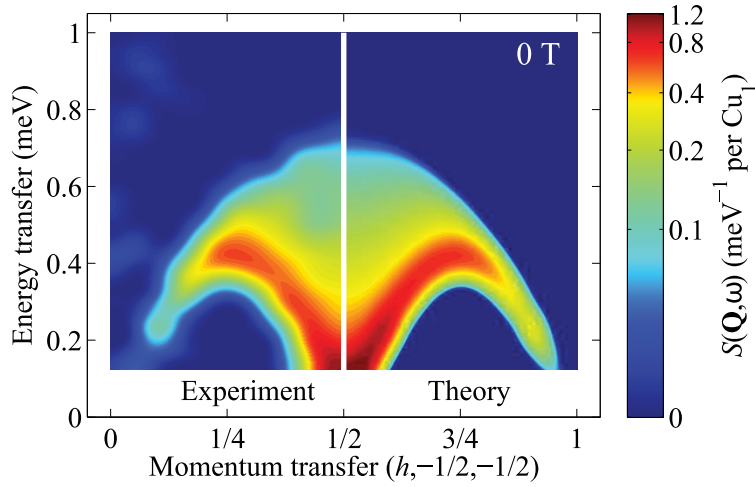


**Figure 1.7:** *Measured neutron scattering spectrum of a 1D spin chain compound.* Results are compared to a theoretical prediction based on spinon scattering. Figure adapted from Mourigal *et al.* (2013). Momenta are along the chain, in units of  $\pi$ .

logues of the FQHE state in spin liquids, called chiral spin liquids, but this does not apply to the gapless states that we consider here.

A more fundamental understanding comes from the ‘Lieb–Schultz–Mattis’ constraints (Lieb *et al.*, 2004; Oshikawa, 2000; Hastings, 2004). In the most terse formulation, these theorems state that a spin-1/2 system cannot have a topologically trivial, gapped, symmetric ground state. In practice, this leaves three possibilities for the ground state of a spin-1/2 quantum magnet (Chalker, 2017; Savary and Balents, 2016). First, the system can spontaneously break lattice symmetries, for example forming a valence bond solid state. In this case, the spins form local singlets and the unit cell is doubled. The system is gapped and is a symmetry-broken phase under Landau’s description. Second, the system can form a symmetric topologically non-trivial ground state. This state is also gapped, but instead of being classified within Landau’s paradigm, it has topological order. This leads to a finite ground state degeneracy. Third, the state can be critical. In this exotic scenario, the phase has gapless excitations which are in no way related to symmetry breaking. However it is still protected against small perturbations. One can think of this being due to the entangled ground state (Savary and Balents, 2016), or more formally through certain anomalies in the low-energy field theories (Cho *et al.*, 2017; Song *et al.*, 2020). There is also a recent understanding that these topologically ordered phases can be described through the lens of spontaneous symmetry breaking, only with more obscure ‘higher-form’ symmetries (McGreevy, 2023). In the case of emergent QED, it is a spontaneously broken 1-form symmetry that protects the gaplessness (Gaiotto *et al.*, 2015). In summary, gapless spin liquids enjoy a level of protection that trivial gapless states do not. It arises as a direct consequence of their fractionalisation and entanglement.

We must briefly mention an example of a well-understood state that fulfils many of these criteria. The spin-1/2 Heisenberg chain has a gapless ground state with critical correlations, and shows signatures of fractionalised excitations in neutron scattering. This is a

well-understood example of fractionalisation. Figure 1.7 shows neutron scattering data in this context compared to a theoretical prediction, adapted from the work of Mourigal *et al.* (2013). The broad continua seen above the momentum point  $\pi/2$  is a direct result of spin fractionalisation. When the inbound neutron excites two spinons, it has a range of possible energy and momentum states. These broad features appear in exact analytical calculations of the same response function, shown right in Fig. 1.7 using the Bethe Ansatz (Bethe, 1931). Exact results have recently been found in 2D (Knolle *et al.*, 2014a,b), but only in a non-interacting limit of Kitaev's honeycomb model.

Since the resurgence of interest into spin liquids at the turn of the century, there has been significant experimental effort put into the search for spin liquids. So far, there have been no definitive successful discoveries. One of the main challenges in the field is to make concrete predictions for the dynamics of quantum spin liquids beyond fine-tuned limits. This is necessary in order to have the same level of agreement as shown by 1D experiments which allow for claims of a discovery. In this Thesis, we make new predictions for the dynamics of the  $J_1$ – $J_2$  Heisenberg model, taking into account interactions between spinons and the emergent gauge fields. This provides a more realistic understanding of how fractionalisation might rear its head in experiment.

Another key goal of this Thesis is to understand the stability of 2D quantum spin liquids. Many of the aforementioned spin liquid candidates do not actually remain liquid down to zero temperature (Broholm *et al.*, 2020). We divide the concept of stability into four categories. Our knowledge must span all of these points in order to claim that a spin liquid might exist in experiment.

- i. Can we write down a QSL wavefunction? This is the most trivial definition of describing the state theoretically.
- ii. Is a QSL phase intrinsically stable? This means we have to make sure that the fractionalised excitations are deconfined. If instead we find that they prefer to confine, then it is a sign that we have actually described an ordered state in a more complicated basis.
- iii. Do spin models exist which realise a gapless QSL? Is the QSL a ground state of a toy Hamiltonian? We must also check that spin liquids are energetically preferred ground states of realistic spin models. In many cases, this is not the case. At this level it already becomes very challenging to make theoretical progress.
- iv. Finally, are QSLs resilient beyond simple toy models? Is fractionalisation robust to physical effects such as disorder, defects, competing interactions and spurious couplings? This point will be critical when trying to interpret experiments.

In this Thesis, we will look into a critical spin liquid which has been suggested to host an emergent form of QED, and work towards answering all of these points.

### 1.3 Peierls instability

Before we return to spin liquids, it is worth spending some time studying a simple critical state in one dimension. This is a half-filled band of free fermions. With a view to understanding the stability of similar (but much more complicated) states later on, we can ask if this

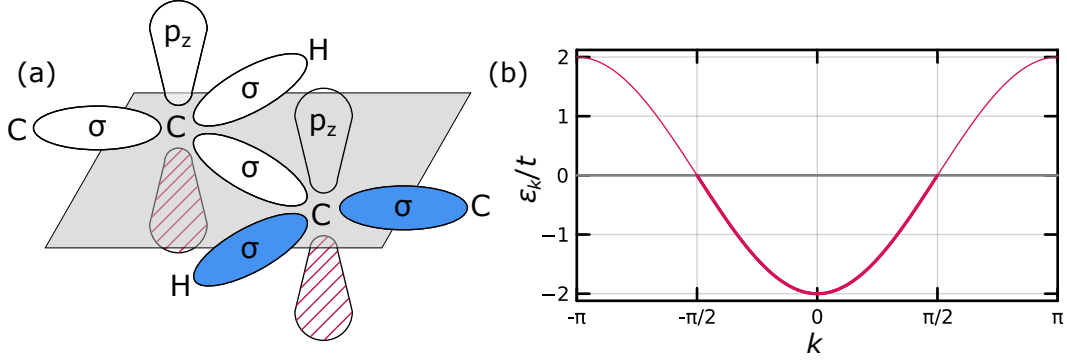


**Figure 1.8:** *Tight-binding model of the  $p_z$  electrons along a chain.* (a) Orbitals in the unit cell of polyacetylene. The in-plane  $\sigma$  bonds have a relative 120-degree angle and form the backbone of the chain. We write a tight-binding model for the electrons in the out-of-plane  $p_z$  orbitals. (b) Dispersion  $\varepsilon_k$  of the uniform chain, with occupied states below  $\varepsilon = 0$  highlighted with the bold line.

state is stable when coupled to other degrees of freedom. Peierls' theorem can be succinctly summarised as follows: a chain of equally spaced ions with odd numbers of free fermions per site is unstable for any infinitesimal coupling to the lattice (Peierls, 1996).

To prove his theorem, we can use a very simple tight binding model of free electrons to describe the bands of polyacetylene (Su *et al.*, 1979; Heeger *et al.*, 1988). This is a polymer of acetylene with a unit cell  $C_2H_2$ . The covalent backbone of the chain is formed by carbon-carbon and carbon-hydrogen bonds with a relative 120-degree angle in the plane. The remaining  $p_z$  orbital is half-filled, with one electron on each site. We show this unit cell in Fig. 1.8(a). This lends itself naturally to a simple tight-binding model, where the Hamiltonian of the  $p_z$ -electrons  $c_i$  are given by their kinetic energy

$$H = -t \sum_{i,\sigma=\pm} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}). \quad (1.13)$$

The hopping can be understood as an overlap of the out-of-plane  $p_z$  orbitals, and is therefore naturally dependent on the carbon-carbon bond length. We model this through the overlap of exponentially decaying orbitals, as

$$t_{ij} = t_0 e^{-g|x_i - x_j|}, \quad (1.14)$$

and define  $t_{ij} = t$  when  $x_i - x_j = a$  in the case where all carbon atoms are equally spaced with separation  $a$  in their equilibrium position. Diagonalising this Hamiltonian in momentum space, we find

$$H = -t \sum_k c_{k\sigma}^\dagger (e^{ika} + e^{-ika}) c_{k\sigma} = \sum_k \varepsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} \quad (1.15)$$

with energies  $\varepsilon_k = -2t \cos(ka)$ . This dispersion is plotted in Fig. 1.8(b). The system has two half-filled bands, meaning the Fermi surface is at  $k_F = \pm\pi/2$ . The band is metallic, with a high density of states at the Fermi level, and is a simple critical phase.

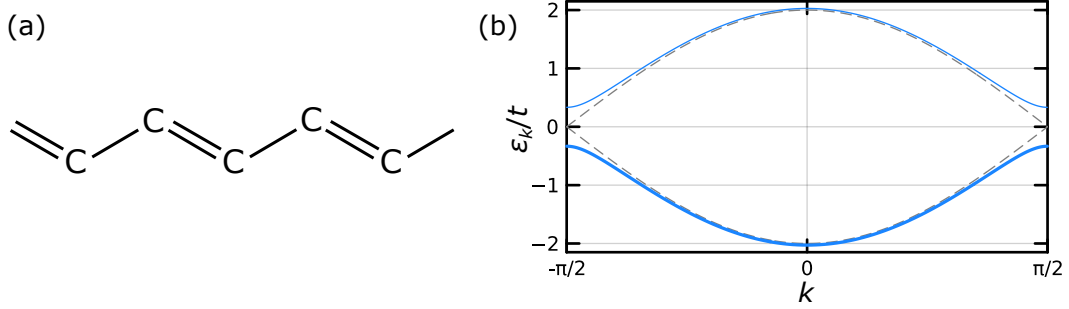


**Figure 1.9:** *Electronic structure of polyacetylene* (a) Peierls state of polyacetylene, shown in chemist's notation. The double bonds show where the electrons are localised. (b) Band structure with a gap  $\delta t = t/3$ .

However, experiments show that polyacetylene is an insulator with alternating strong and weak bonds, which also alternate in length (Heeger *et al.*, 1988). This is depicted in Fig. 1.9(a). There is nothing wrong with our tight-binding model of the  $p_z$  orbitals, but we must consider the effect of dimerising the chain. Taking an alternating displacement  $u_i = (-1)^i \delta u$  means the bond lengths change  $a \pm 2\delta u$ . This affects the overlap of the  $p_z$  orbitals, changing the hopping integrals to

$$t \rightarrow t(1 \mp 2g\delta u), \quad (1.16)$$

using a small- $\delta u$  expansion of Eq. (1.14). Here, we see that the constant  $g$  quantifies the electron-lattice coupling. It measures the extent to which the hopping is dependent upon the bond length.

What effect does this distortion have on the spectrum? Before doing an explicit calculation, note that the distortion has a 2-site unit cell and hence the lattice wavevector  $k = \pi/2$ . It is therefore commensurate with the Fermi wavevector for a half-filled band of fermions, and so we expect this to generally open a gap and transform the metal into an insulator. The doubled unit cell folds the Brillouin zone and opens gaps at the Fermi level. Explicitly, the energy becomes

$$\epsilon_k = \pm 2t \sqrt{\delta t^2 + \cos^2(ka/2)}, \quad (1.17)$$

where  $\delta t = 2gt\delta u$ . This spectrum is plotted in Fig. 1.9(b). We see that a gap has opened up at the Fermi level. The tight-binding model on this dimerised lattice becomes insulating. The critical phase is lost and the correlations will decay exponentially.

What would make the lattice dimerise? It is natural to think that the ions would want to lie in a totally translationally-invariant configuration in order to minimise their potential energy. That is, we can write a simple model of potential energy cost in the Harmonic approximation as

$$E_{\text{elast}}[u_i] = \frac{\kappa}{2} \sum_i (u_i - u_{i+1})^2 \quad (1.18)$$

with lattice stiffness  $\kappa$ . We can write the effective lattice potential for our dimerisation pattern as  $E_{\text{elast}}(\delta u) = 2\kappa(\delta u)^2$ . However, because the lower band is occupied, the dimerisa-

tion lowers the overall energy of the tight-binding electrons. We can understand the spontaneous dimerisation of polyacetylene as a competition of this potential energy cost and the electronic energy gain due to the opening of a band gap. We quantify the potential energy cost to the bonding electrons, and the energy gain of the band-delocalised electrons as follows. Expand the dispersion (1.17) around the Fermi surface and calculate the change in ground state energy

$$\delta\epsilon = \int_0^\Lambda dk \left( ka/2 - \sqrt{(ka)^2/4 + (\delta t)^2} \right) \simeq (\delta t)^2 \log(\delta t/\Lambda) + \dots, \quad (1.19)$$

where we have introduced a lattice-scale cutoff  $\Lambda \sim 1/a$  as a momentum-regulator. The change in energy will be negative for small  $\delta t \ll \Lambda$ , representing an energy gain. Substituting  $\delta t = 2gt \delta u$ , we can write the overall potential of the lattice distortion parameter

$$E(\delta u) = 2\kappa (\delta u)^2 + (2gt \delta u)^2 \log(2gt \delta u/\Lambda), \quad (1.20)$$

$$= 2\delta u^2 \left[ \kappa + t^2 g^2 \log(\delta u/c) \right]. \quad (1.21)$$

We defined a lattice-scale constant  $c$  in this final step. Due to the appearance of the logarithm in this expression which diverges as  $\delta u \rightarrow 0$ , the energy gain *always out competes* the cost of static lattice distortion. A finite equilibrium dimerisation is developed, resulting in alternating strong and weak hopping amplitudes. This explains the dimerised, insulating behaviour seen in polyacetylene (Su *et al.*, 1979; Heeger *et al.*, 1988), shown in Fig. 1.9. The magnitude of this gap is exponentially small in the spin-lattice coupling; we can minimise Eq. (1.21) to find the equilibrium distortion

$$\delta u_0 = ce^{-K/(t^2 g^2)}. \quad (1.22)$$

The critical coupling strength at which the dimerisation occurs is  $g_c = 0$ , and the equilibrium gap scales as

$$\Delta = 2\delta t_0 = 4gt ce^{-K/(t^2 g^2)}. \quad (1.23)$$

For even an infinitesimal electron-lattice coupling  $g \ll 1$ , this gap will always be non-zero (albeit small).

We contrast this with the behaviour in higher dimensions. An instructive example in two-dimensions is graphene. It is a hexagonal lattice of carbon, shown in Fig. 1.10(a). The planar lattice is formed by the overlap of the three in-plane  $sp^2$  orbitals with those of neighbouring carbons [in 1D we occupied one of these bonds with hydrogen, cf. Fig. 1.8(a)]. Just as before, we can write a tight-binding model for the out-of-plane  $p_z$  orbitals and now we find a semi-metallic ground state with Dirac cones at low energy (Wallace, 1947; Semenoff, 1984). This means there is a gapless, linear dispersion for low-lying excitations at the corners of the Brillouin zone.

Does the same Peierls mechanism mean that graphene should spontaneously distort? The pairwise dimerisation of the hexagons forming the honeycomb lattice is called the Kekulé distortion. It modulates the hopping amplitudes in such a way to open a gap at the Fermi level of the Dirac spectrum (Hou *et al.*, 2007; Chamon *et al.*, 2008). This pattern and the dispersion of the low-lying excitations is shown in Fig. 1.10(b). However, the electronic

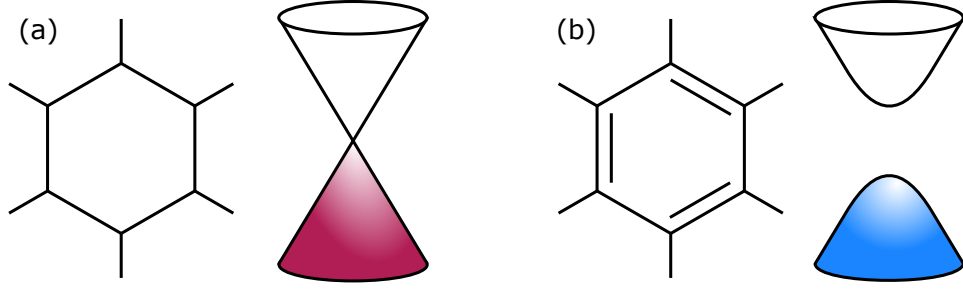


**Figure 1.10:** *Graphene's hexagonal lattice and low-energy dispersion.* (a) Regular hexagonal lattice of graphene, with Dirac dispersion at the corners of the Brillouin zone. (b) Kekulé distorted graphene, with gapped Dirac cones and spontaneous symmetry breaking. The lattice shows a small distortion and charge is localised on the shorter bonds around the hexagonal plaquettes.

energy gain from the resulting gapped spectrum in 2D is *not* logarithmically divergent as in 1D. To understand why, we can repeat the calculation above for the change in electronic energy  $\delta\epsilon$  given a specific lattice distortion  $\delta u$ . The gapped Dirac dispersion has the same form as above. The calculation for the energy gain can be formulated the same way, with the only difference being the measure  $\int dk k$  needed to integrate over momentum shells around the Dirac point. We evaluate

$$\delta\epsilon = \int_0^\Lambda dk k \left( ka - \sqrt{(ka)^2 + (\delta u)^2} \right) \simeq -\frac{3}{2}\Lambda (\delta u)^2 + (\delta u)^3 + \dots, \quad (1.24)$$

where we ignore higher-order terms in  $\delta u$ . We once again see an energy gain, but without a logarithmic correction. The leading potential for the distortion mode is then purely quadratic  $2(\delta u)^2[\kappa - cg^2]$ . Only when the coupling is large enough  $g > g_c$  does the hexagonal lattice spontaneously distort, where  $g_c = \sqrt{\kappa/c}$ . This means there is no instability at weak electron-lattice coupling. This reduced energy gain can be understood as being a direct result of the 2D density of states vanishing at the Dirac cone. This explains why graphene famously does not display this Kekulé distortion and has a semimetallic ground state.

Interestingly, if graphene is folded into a quasi-one-dimensional carbon nanotube, then this distortion can be observed (Chamon, 2000). Another way to engineer a Kekulé phase is to artificially increase the effective electron-lattice coupling  $g > g_c$ . This has been explored using an atom-trap platform (Hou *et al.*, 2007), surface disorder (Qu *et al.*, 2022), or lithium ion intercalation (Gutiérrez *et al.*, 2016; Bao *et al.*, 2021). Peierls' result is clearly highly dimensionally-dependent. Its universality in 1D is determined by its weak-coupling nature — the chain will be unstable independent of the exact value of microscopic couplings. We will return to this instability later in this Thesis in the context of 2D spin liquids. It turns out that it is also possible to find a generic weak-coupling instability in certain two-dimensional models.

## 1.4 Outline of the Thesis

In this Thesis, we tackle the aforementioned problems regarding the dynamics and stability of a quantum spin liquid on the triangular lattice. We investigate the U(1) Dirac quantum spin liquid, a critical gapless phase described by a conformal field theory. We emphasise throughout the connection to the better-understood 1D spin liquid states, which provides a fruitful perspective.

In Chapter 2, we introduce the theoretical descriptions of both the U(1) Dirac spin liquid, as well as its 1D Luttinger liquid sibling. In the context of the 1D model, we introduce the tools of bosonisation which will be useful throughout. In the 2D model, we focus on the use of parton mean-field theory to describe quantum spin liquid states. We also discuss recent developments that have led to the prediction that this is a stable phase of matter. Given this background [answering the tasks (i) and (ii) as listed above], we move on to the other challenges. The results of this Thesis are then organised into three parts:

In Chapter 3, we investigate the dynamics of this quantum spin liquid. Going beyond the mean-field results in the literature, we successfully incorporate interaction effects to produce predictions for the inelastic neutron scattering response. Through the methods we develop, we also form a framework to analytically predict the phase diagram of Heisenberg-type spin models. This is the first such analytical solution to the third problem (iii) highlighted above. By incorporating gauge fluctuations, we predict the nature of phase transitions to neighbouring phases. We then apply these results to the compounds NaYbSe<sub>2</sub> and KYbSe<sub>2</sub> in Chapter 4. We focus on interpreting neutron scattering data.

We move on in Chapter 5 to study the stability of the model to perturbations, problem (iv). We predict the U(1) Dirac quantum spin liquid has a spin-Peierls instability upon infinitesimal coupling to the lattice. We also investigate the stability of the model in the presence of dynamical phonons in Chapter 6. This approach allows us to predict the phase diagram of realistic spin-phonon models. This is backed up by rigorous numerical results for the triangular lattice Heisenberg model in both cases. We also use this as an opportunity to predict spectral signatures of fractionalisation in the phonons. This may also support the experimental search for spin liquids.

Finally, we turn to another related model in Chapter 7: deconfined quantum critical points. These are a proposed type of phase transition that go beyond the Landau paradigm. Discussing lattice distortions in this context, we provide another example of a spin-Peierls instability in two dimensions. We rigorously study the potential effects on lattice simulations.

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## Introduction

In this Chapter, we will review the background theory necessary for the rest of the Thesis. To do this, we will focus on three models with critical correlations and gapless excitations.

First, we will introduce the Luttinger liquid in one dimension. This will serve not only as a theoretical warm-up, but also as a recurring benchmark for our results in two dimensions.

Second, we will introduce quantum spin liquids in two dimensions using the Abrikosov fermion representation and parton mean-field theory. We will use the example of the proposed spin-liquid state in the square-lattice  $\pi$ -flux Ansatz. This serves as the context for us to derive a model of emergent quantum electrodynamics. We also introduce monopoles and will show how they lead to confinement.

Finally, we will introduce the quantum spin liquid at the centre of this Thesis: the Dirac spin liquid on the triangular lattice. We will discuss it from both a field-theoretic and numerical perspective. Finally, after the technical introduction, we end the Chapter by discussing the outstanding questions of the field.

## 2.1 Luttinger liquid in spin chains

Whereas spin liquids in two dimensions remain mysterious, we have a clear picture of spin fractionalisation in  $D = 1$ . This is in particular thanks to more advanced analytical tools available in lower dimensions. This includes an old picture of fractionalisation introduced by Jordan and Wigner (1928), bosonisation, and the renormalisation group.

### 2.1.1 Jordon–Wigner transformation & bosonisation

We begin by studying the following spin chain Hamiltonian,

$$\mathcal{H}_{\text{XXZ}} = \sum_i J \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right), \quad (2.1)$$

where each spin is a  $S = 1/2$  operator. This is often called the XXZ Hamiltonian, since the  $z$ -component of spin exchange is an independent parameter. In this model, spins interact with only their nearest neighbours through an antiferromagnetic exchange  $J$ . By tuning the anisotropy, we can smoothly go between the XY limit  $\Delta = 0$  to the Heisenberg model  $\Delta = 1$ . Our goal is to study its ground state properties and correlations as a function of this parameter. Returning to the spins themselves, we highlight that they obey the following bosonic spin algebra

$$[S_i^\alpha, S_j^\beta] = i\epsilon_{\alpha\beta\gamma} S_i^\gamma \delta_{ij}, \quad (2.2)$$

When on different sites  $i \neq j$ , they must commute  $[S_i^\alpha, S_j^\beta] = 0$ .

The problem is hard to solve in this form. We will find it insightful to write (2.1) in a series of different representations. First, transform spin operators so that we have

$$S_i^\pm = S_i^x \pm iS_i^y, \quad (2.3)$$

giving the Hamiltonian

$$\mathcal{H}_{\text{XXZ}} = \frac{1}{2} \sum_i J \left( S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + \Delta S_i^z S_{i+1}^z \right). \quad (2.4)$$

In the  $S^z$  basis, the eigenstates are  $|\pm \frac{1}{2}\rangle$ . The raising operator  $S^+$  satisfies  $S^+ |-\frac{1}{2}\rangle = |+\frac{1}{2}\rangle$  and annihilates  $|+\frac{1}{2}\rangle$ . We can see that there is a tempting mapping of the spin-half operators to spinless fermions (Giamarchi, 2003; Fradkin, 2013):

$$S_i^z \rightarrow c_i^\dagger c_i - \frac{1}{2}, \quad (2.5)$$

$$S_i^+ \rightarrow c_i^\dagger \quad S_i^- \rightarrow c_i. \quad (2.6)$$

This satisfies the necessary local commutation relations and represents the 2-dimensional Hilbert space through  $|+\frac{1}{2}\rangle \leftrightarrow |1\rangle$  and  $|-\frac{1}{2}\rangle \leftrightarrow |0\rangle$ . However there is a problem with this form of the mapping: it would result in spins at different sites anticommuting. To fix this, we modify Eq. (2.6) by adding a string to each  $S_i^\pm$  operator

$$S_i^+ \rightarrow c_i^\dagger (-1)^i e^{i\pi \sum_{n=-\infty}^i c_n^\dagger c_n}. \quad (2.7)$$

This is the Jordan–Wigner transform. The string is responsible for providing the extra minus sign needed to make sure the spins commute  $[S_i^\pm, S_j^\pm] = 0$  when  $i \neq j$  (Jordan and Wigner, 1928). We have effectively transmuted the statistics of the operators, with the downside that we have introduced non-local strings.

Let us now use this to find the ground state of our Hamiltonian (2.4). Despite the complex form of Eq. (2.7), we can show that the neighbour  $xy$ -exchange term becomes a simple hopping

$$S_i^+ S_{i+1}^- = -c_i^\dagger c_{i+1} e^{i\pi c_i^\dagger c_i} = -c_i^\dagger c_{i+1}. \quad (2.8)$$

The Hamiltonian therefore becomes

$$\mathcal{H}_{\text{XXZ}} = -t \sum_i \left( c_i^\dagger c_{i+1} + \text{h.c.} \right) + V \sum_i \left( c_i^\dagger c_i - \frac{1}{2} \right) \left( c_{i+1}^\dagger c_{i+1} - \frac{1}{2} \right). \quad (2.9)$$

We have defined the hopping  $t = J/2$  and the nearest-neighbour interaction  $V = J\Delta$  (Giamarchi, 2003). We can see some immediate and powerful consequences when  $\Delta = 0$ , which we call the XY spin Hamiltonian. In this limit, Eq. (2.9) is a free fermion model. The spectrum of the model is given by

$$\varepsilon_k = -2t \cos(k). \quad (2.10)$$

This is identical to the dispersion of the free fermions plotted in Fig. 1.8(b). The ground state has negative energy states  $\varepsilon_k < 0$  filled, meaning the Fermi surface is at  $k_F = \pm\pi/2$ . This is a half-filled band. Using Eq. (2.5) we find  $\langle c_i^\dagger c_i \rangle = 1/2$  implies  $\langle S_i^z \rangle = 0$ . This is our first fractionalised theory of a spin-disordered state. The excitations above the ground state are given by fermionic quasiparticles. What are the correlations of the spins? It is simple to show that

$$\langle S_0^z S_r^z \rangle = \langle c_0^\dagger c_0 c_r^\dagger c_r \rangle - \frac{1}{4} = |\langle c_0^\dagger c_r \rangle|^2, \quad (2.11)$$

which can then be evaluated by Fourier transforming to recover

$$\langle S_0^z S_r^z \rangle = \frac{1}{2} \delta_{0,r} - \frac{1}{\pi^2 r^2} \sin^2\left(\frac{\pi r}{2}\right). \quad (2.12)$$

At long distances, this is a power-law decay  $\sim 1/r^2$  with an alternating prefactor. The spin model therefore has algebraic correlations, and is a critical phase.

Our goal is now to describe the interacting model (2.9). In order to do this, we must undertake two more steps. First, we will coarse grain the lattice fermions and move to a continuum model. This will be a common procedure throughout this Thesis. Second, we will use *bosonisation* to map the interacting fermionic theory to another bosonic one. Bosonisation is a duality mapping that is possible in one dimension. We will show that it relies on writing a fermionic theory purely in terms of conserved bosonic currents, before forgetting about the fermions altogether (Mattis and Lieb, 1965; Coleman, 1975; Luther and Peschel, 1975). The resulting theory should describe the same physics in a more simple language. We highlight some very good textbooks which describe the nuances of this procedure in much more detail than we go into here (Giamarchi, 2003; Bruus *et al.*, 2004; Fradkin, 2013).

To proceed, we expand the dispersion  $\varepsilon_k$  in small- $k$  around the Fermi momentum  $k_F = \pi/2$ . To do this, we define the left- and right-moving fields

$$c_i^\dagger = e^{ik_F i} \psi_R(x) + e^{-ik_F i} \psi_L(x), \quad (2.13)$$

and then define the spinor

$$\psi(x) = \begin{pmatrix} \psi_R(x) \\ \psi_L(x) \end{pmatrix}. \quad (2.14)$$

The free part of the Hamiltonian at low energies can then be written as a Dirac equation

$$H_0 = v_F \sum_k k (\psi_{k,R}^\dagger \psi_{k,R} - \psi_{k,L}^\dagger \psi_{k,L}) = \int dx \psi^\dagger(x) i v_F \mu_3 \partial_x \psi(x). \quad (2.15)$$

Here, the Fermi velocity is simply  $v_F = J$ , and  $\mu_3$  is the  $z$ -Pauli matrix<sup>1</sup>. A key step is to define the currents associated with the left- and right-moving fermions

$$\rho_{R/L}(x) = \psi_{R/L}^\dagger(x) \psi_{R/L}(x). \quad (2.16)$$

<sup>1</sup>We use the notation  $\mu$  to highlight that this is in the chiral-spinor basis. In the spin basis we consistently use the notation  $\sigma$  for Pauli matrices

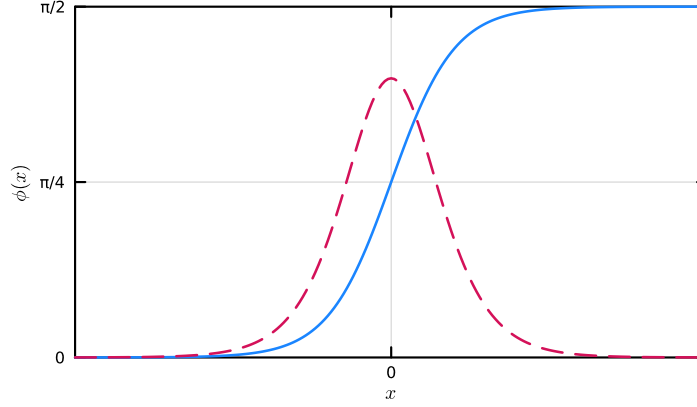


**Figure 2.1:** *Kink configuration of the bosonised field.* A fermion maps to a kink configuration in the bosonised field  $\phi(x)$ . The resulting fermion density is shown as the dashed line  $\rho_R(x) + \rho_L(x)$ .

Importantly, these currents commute with the Hamiltonian and represent conserved bosonic charges in the free Dirac theory. They are the key objects that we will leverage in the bosonisation mapping. A surprising result from Mattis and Lieb (1965) is that this fermionic theory can be written entirely in terms of the conserved currents<sup>2</sup>

$$H_0 = \pi v_F \int dx [\rho_R(x)^2 + \rho_L(x)^2] + \text{const.} \quad (2.17)$$

The final step of the bosonisation mapping is to introduce a dual bosonic field which takes over the role of the currents. We define the dual boson as follows

$$\partial_x \phi(x) = \pi [\rho_R(x) + \rho_L(x)], \quad (2.18)$$

meaning its gradient measures the total density of fermions (Sachdev, 2011). The action of the bosonised theory becomes

$$S_0 = \int dx d\tau \frac{1}{2\pi K} \left( v_F (\partial_x \phi)^2 + \frac{1}{v_F} (\partial_\tau \phi)^2 \right). \quad (2.19)$$

This is the Tomonaga–Luttinger liquid, where we call the parameter  $K = 1$  the Luttinger parameter (Tomonaga, 1950; Luttinger, 1963). This is the action of a free, massless, relativistic scalar field. It naturally has gapless excitations and algebraic correlations.

Next, we will add back interactions. We want to understand whether the ground state remains gapless. To do this, note that the original fermionic interaction term generates several different types of interactions in the low-energy field theory. The first type are the

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<sup>2</sup>Note that to derive this form of  $H_0$ , one must use the fact that the bosons do not trivially commute, but obey the Kac–Moody algebra. We spare the technical details here since we will not need anything more than the final form in this Thesis.

forward- and back-scattering interactions, which transfer momentum between R/L modes. They take the form

$$4V(\psi_R^\dagger \psi_R)(\psi_L^\dagger \psi_L) + V[(\psi_R^\dagger \psi_R)^2 + (\psi_L^\dagger \psi_L)^2]. \quad (2.20)$$

These can be represented in terms of the densities  $\rho_{R/L}$  and therefore act only to change the Luttinger parameter (2.19)

$$K = \sqrt{\frac{v_F + 3V/\pi}{v_F - V/\pi}}, \quad (2.21)$$

as well as the Fermi velocity  $v_F$  (not shown). The second type of interaction is the Umklapp scattering term, where two fermions with momentum difference  $2\pi$  scatter to the opposite chirality valley. It maps to the following operator in the bosonised form

$$-V(\psi_R^\dagger \psi_R^\dagger \psi_L \psi_L + \text{h.c.}) \longleftrightarrow \mu \cos(4\phi). \quad (2.22)$$

Taken all together, we write down our bosonised description of the interacting bosonic action (2.9)

$$S_{\text{SG}} = \int dx d\tau \left[ \frac{1}{2\pi K} ((\partial_x \phi)^2 + (\partial_\tau \phi)^2) - \mu \cos(4\phi) \right]. \quad (2.23)$$

We call this the Sine–Gordon model.<sup>3</sup> Let us think again about the types of excitations in this model. For a finite value of the interaction  $\mu > 0$ , the action is minimised by uniform field configurations  $\phi_0 = n\pi/2$ , with integer  $n$ . Consider a kink configuration  $\phi(x)$  which maps between two of these minima, shown in Fig. 2.1. This type of configuration is called a *soliton*. It maps between two different ground states  $\phi(x \rightarrow -\infty) = 0$  and  $\phi(x \rightarrow +\infty) = \pi/2$ , and can therefore not be removed purely by local fluctuations. Equation 2.18 tells us that this corresponds to a finite density of fermions, shown as a dashed line (Mandelstam, 1975). Therefore, we see that a localised fermion in our original theory corresponds to a non-local, solitonic, field configuration in the dual model.

## 2.1.2 Luttinger liquid phase

### Phase diagram

We have now performed several mappings: from spin a chain, to spinless fermions, and then to an interacting boson theory. We call this bosonic theory (2.23) the Sine–Gordon model, with bosonic field  $\phi(x)$ . It has a kinetic term with parameter  $K$ , and an interaction term  $\cos(4\phi)$ . We will now investigate the phases and correlations of this model.

The field configuration we drew before in Fig. 2.1 has a finite energy cost  $\mu$ . Therefore we see that if there is a finite value of the interaction  $\mu$  in the long-distance (IR) limit, there will be a spontaneous gap generated for the fermions (or dual soliton configurations). We then turn to the renormalisation group to understand the RG flow of this coupling and hence the stability of the gapless phase.

<sup>3</sup>This is “the sophomoric but unfortunately standard name” for this theory, as Coleman (1975) put it.

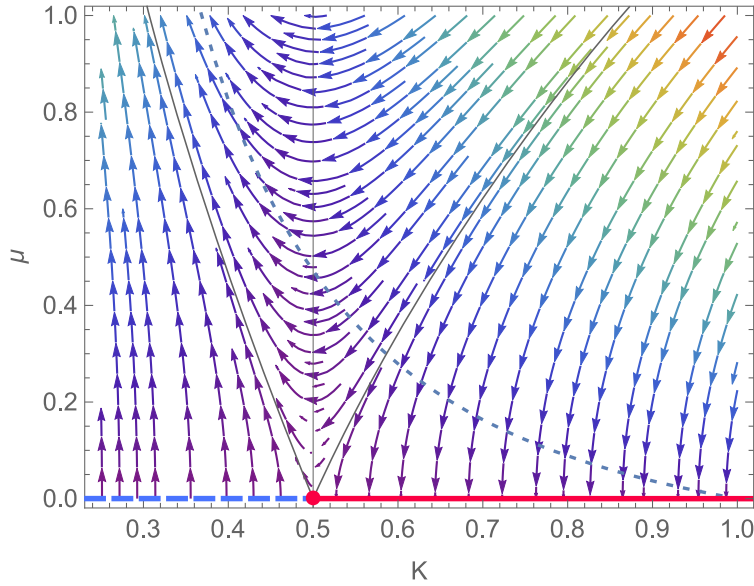


**Figure 2.2:** *Renormalisation group flow of the Sine-Gordon model.* RG flow equations Eq. (2.24) and (2.25). The line of fixed points with  $\mu = 0$  and  $1/2 \leq K \leq 1$  is the Luttinger liquid phase. For  $K < 1/2$ , the system flows to a Néel ordered phase.

To do this, we first write the renormalisation group (RG) equations, following (Giarmarchi, 2003):

$$\frac{dK}{ds} = \beta_K = -4K^2\mu^2, \quad (2.24)$$

$$\frac{d\mu}{ds} = \beta_\mu = (2 - 4K)\mu. \quad (2.25)$$

These are also called beta functions. These are calculated by successively integrating out high-momentum modes and evaluating the flow of the coupling constants. In real-space, we can think of this procedure as coarse-graining the microscopic details. The differential forms written here are called the beta functions, where  $s$  is the RG flow parameter. The bosonisation mapping defines lattice-scale (or ‘ultraviolet’, UV) couplings, which we call  $(\mu_0, K_0)$ . The long-distance physics, meaning the nature of the ground state and the correlation functions at distances much larger than the lattice spacing, will be governed instead by the fixed points of this RG flow  $(\mu_*, K_*)$ . Taking the long-distance, ‘infrared’ (IR), limit is equivalent to integrating these differential equations and taking  $s \rightarrow \infty$ .

The resulting flow equations are plotted in Fig. 2.2. We find three regimes with different fixed points. First, there is a line of fixed points with  $\mu = 0$  and  $K > 1/2$ . This is the Luttinger liquid phase. In this regime the beta function of  $\mu$ , Eq. (2.25), is negative. This means that we call  $\mu$  an *irrelevant* coupling. This is a technical term used in the RG literature, but describes accurately the physics: the interaction  $\cos(4\phi)$  does not drive the formation of a gap, but the system stays in a gapless Luttinger liquid phase. If we consider the point  $K = 0.75$  and add a small interaction  $\mu = 0.1$ , the flow diagram Fig. 2.2 shows us that the

coupling strength flows to zero. We call the point where the flow intersects the  $\mu = 0$  axis  $K_*$ , which is slightly reduced compared to the starting point  $K$ . The Luttinger liquid phase includes the  $K = 1, \mu = 0$  point we defined for the XY model. In this specific case, the UV model is a free theory and does not flow under RG (in other words, the Hamiltonian already lies on the line of fixed points). In the whole region  $1/2 < K < 1$  (for  $\mu$  below the separatrix), the resulting state is described by the free Hamiltonian (2.19), simply with a renormalised parameter  $K_*$ .

Next, for  $K < 1/2$  there is a sign change in Eq. (2.25). We see that for small  $\mu$ , the beta function becomes positive. This signals that the magnitude of the coupling  $\mu$  grows with RG flow. We call this a *relevant coupling* in the renormalisation group. Turning to the figure, we see that the coupling  $\mu \rightarrow \infty$  diverges when it is relevant. What is the physical consequence of this? To get an intuition, we can return to the action (2.23) with a finite  $\mu > 0$ . It has a classical minimum when its argument is  $\phi_0 = 0$ . Expanding around this point  $\phi = \delta\phi$ , we may write the potential for perturbations as

$$V[\delta\phi(x)] = 8\mu \delta\phi^2 - \mu + \dots \quad (2.26)$$

This explicitly produces a gap for the boson (Coleman, 1975). We conclude that in the regime  $K < 1/2$  where the coupling  $\mu$  is relevant, the bosonic excitations are now gapped. We will return to the nature of this phase imminently.

Finally, there is a line that separates the two phases. It intersects the horizontal axis  $\mu = 0$  at the point  $K = 1/2$ . The beta function for the coupling  $\mu$ , Eq. (2.25), is zero at this point, meaning the coupling  $\mu$  is marginal. This is the physically relevant point for the Heisenberg model. When the original spin model has no anisotropy  $\Delta = 1$  it has an additional SU(2) spin-rotation symmetry. In this case, the bosonisation mapping always places the UV theory  $(\mu_0, K_0)$  along the separatrix and the theory flows to  $K_* = 1/2$  in the IR limit.

Let us return to the nature of these different phases and ask how order parameters are represented in the Sine–Gordon theory. To do this, it will be useful to use the bosonisation dictionary once more. We define the order parameters of Néel order in the bosonised language as follows:

$$n_3 = (-1)^i S_i^z \leftrightarrow \cos(2\phi(x)) \quad (2.27)$$

We can define another order parameter which measures dimer order, or sometimes called valence-bond solid (VBS) order. This is a staggered dimerisation of the chain  $(-1)^i \vec{S}_i \cdot \vec{S}_{i+1}$ . In the bosonised language it is written:

$$v = (-1)^i \vec{S}_i \cdot \vec{S}_{i+1} \leftrightarrow \sin(2\phi(x)) \quad (2.28)$$

These two mappings are key to our analysis. They can be derived laboriously, or can be motivated more simply by observing how the relevant order parameters transform under lattice symmetries. We include these alongside the transformation of the bosonised field  $\phi(x)$  in Table 2.1. Using this mapping, we can identify the nature of the phase for  $K < 1/2$ . We saw in this limit that  $\mu \rightarrow +\infty$  and the field is pinned to a uniform value  $\phi_0 = 0$ . From this we see

$$\langle n_3 \rangle = \cos(0) \neq 0, \quad v = \sin(0) = 0; \quad (2.29)$$

i.e. it is a Néel ordered state. By adding more terms to the Hamiltonian, we can access different phases as well. We will return to this point in Chapter 7.

|        |               | $Z_2^z$         | $T_x$           | $\mathcal{I}$ | $\mathcal{T}$   |
|--------|---------------|-----------------|-----------------|---------------|-----------------|
| $\phi$ |               | $-\phi + \pi/2$ | $+\phi + \pi/2$ | $-\phi$       | $-\phi + \pi/2$ |
| $n_3$  | $\cos(2\phi)$ | —               | —               | +             | —               |
| $v$    | $\sin(2\phi)$ | +               | —               | —             | +               |
|        | $\cos(4\phi)$ | +               | +               | +             | +               |

Table 2.1: The symmetry properties of the field  $\phi$  under  $z$ -spin flip  $Z_2^z$ , as well as the external lattice symmetries: translation  $T_x$  and bond-inversion  $\mathcal{I}$  as is similarly obtained through bosonisation (Giamarchi, 2003). The order parameters are defined  $n_3 \sim \cos(2\phi)$  and  $v \sim \sin(2\phi)$ .

### Critical correlations

What is the nature of the state when  $K \geq 1/2$ ? Here, we expect a disordered state with  $\langle v \rangle = \langle n_3 \rangle = 0$ . This is because the phase  $\phi$  is completely free and will assume all values between 0 and  $2\pi$ . In the stable regime, we write the fixed-point action  $S_0$  as Eq. (2.19), but with Luttinger parameter  $K_*$  defined by the fixed point of the RG flow. Next, we can calculate correlation functions with respect to this free boson theory (Giamarchi, 2003). We use the following result

$$\langle [\phi(r) - \phi(0)]^2 \rangle_0 = K_* \log|r|. \quad (2.30)$$

Next, note that the functions  $\sin(n\phi)$  and  $\cos(n\phi)$  can be expressed as vertex functions  $V_n = e^{in\phi(x)}$ . These operators have correlation functions

$$\langle V_n^\dagger(r) V_n(0) \rangle = \langle e^{-in[\phi(r) - \phi(0)]} \rangle = e^{-(n^2/2) \langle [\phi(r) - \phi(0)]^2 \rangle_0} = |r|^{-n^2 K_*/2}. \quad (2.31)$$

This is the same calculation we performed in Section 1.2 in the context of the classical Ising model. Once again, we find *algebraic correlations* in this spin-disordered state. Explicitly for the case  $n = 2$ , we can calculate the correlations of Néel and VBS order

$$\langle n_3(r) n_3(0) \rangle \sim \langle v(r) v(0) \rangle \sim r^{-2K_*}. \quad (2.32)$$

Perhaps surprisingly, the exponent of decay is equal for both. In this context, we note that this agrees with the free-fermion result for the XY model. With  $K = 1$ , we get the dimension of the order parameters  $2\Delta = 2$  as seen in Eq. (2.12).

This Luttinger liquid phase is actually understood as a conformal field theory. This means all correlation functions will be described by exactly this sort of power-law behaviour. We identify the relevant exponents of the power-law correlation functions as  $-2\Delta$ , where  $\Delta$  is said to be the *scaling dimension* of the operator. In this case, we write  $\Delta_*(n) = n^2 K_*/4$ , where their correlation functions are governed by the exponent  $|r|^{-2\Delta_*}$ . These operators will generally represent observables in the lattice model. In our case  $n = 2$  are the order parameters, and  $n = 4$  corresponds to interactions in the Hamiltonian.

This scaling dimension  $\Delta = n^2 K/4$  of the operator  $\cos(n\phi)$  also controls the flow of the couplings under the renormalisation group. A relevant coupling is one where the scaling dimension is lower than the physical dimension  $\Delta < d$ . Irrelevant operators have  $\Delta > d$

and marginal  $\Delta = d$ . More formally, the generalisation of the beta function Eq. (2.25) to general couplings  $\mu_n$  would read

$$\frac{d\mu_n}{ds} = \beta_{\mu_n} = (2 - n^2 K/4)\mu_n = (2 - \Delta_n)\mu_n. \quad (2.33)$$

We can see that the coefficient of the leading term in the beta function is  $(d - \Delta)$ . For  $n = 2$ , the coupling  $\mu_2$  is *relevant* for all  $K < 2$ , i.e. the whole range of stability in Fig. 2.2. Why does this not also cause a transition to an ordered phase? The answer is because the operators  $\cos(2\phi)$  and  $\sin(2\phi)$  break lattice symmetries. If we want to construct new terms to add to the continuum action, we must restrict ourselves to ones which preserve the symmetry of the original spin model. As discussed, the  $\cos(4\phi)$  term is relevant and is explicitly produced in bosonisation by the Umklapp scattering processes. We can argue on general grounds that the  $\cos(8\phi)$  term is symmetry-allowed. However with scaling dimension  $16K$  it is only relevant below  $K < 1/8$ . For this reason, we do not write it in the action.

Finally, we will briefly comment that this formulation also allows the calculation of *dynamical* correlation functions. The susceptibility of spins for  $\omega > 0$  is (Meden and Schönhammer, 1992; Voit, 1993)

$$\chi(q, \omega + i\eta) = \frac{1}{[(q - \pi/2)^2 - \omega^2 - i\eta]^{1-K_*}}, \quad (2.34)$$

where we take the infinitesimal imaginary part to zero  $\eta \rightarrow 0+$ . This correlation function has an algebraic behaviour at low-frequencies at the momentum  $q = \pi/2$ . It diverges as  $S(\pi, \omega) \sim \omega^{-2K_*}$ . The continuum Luttinger liquid exponent controls the limiting behaviour at low energies. This critical, algebraic behaviour is a key feature of the Luttinger liquid which can be probed in neutron scattering experiments.

A non-trivial check of this critical behaviour is provided by measuring the temperature-dependence of the response. This should be controlled at low-energies by the same Luttinger-liquid exponents. Lake *et al.* (2005) performed a scaling collapse of this low-temperature spectral response in the Heisenberg antiferromagnetic chain material  $\text{KCuF}_3$ . They find a good scaling collapse controlled by exponent  $K_* = 1/2$ . We note that beyond the low-energy behaviour, the full spectral response of Heisenberg spin chains is actually understood. There is an exact analytic solution provided by the Bethe Ansatz (Bethe, 1931). Experimental work is able to find very good agreement with the full spectrum in this context (Mourigal *et al.*, 2013), as shown already in Fig. 1.7.

## 2.2 U(1) Dirac spin liquid part I: Square lattice

### 2.2.1 Parton construction

#### Abrikosov fermions

We will now review the description of quantum spin liquids as emergent gauge theories. This will provide the language to describe fractionalisation in 2D quantum spin liquids that we will rely on for the rest of this Thesis. For this introduction, we loosely follow the reviews of (Wen, 2004; Fradkin, 2013).

First, let us address a practical problem: how do we describe and categorise spin-disordered phases? Consider a general Heisenberg spin Hamiltonian with some antiferromagnetic exchanges  $J_{ij}$ ,

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j. \quad (2.35)$$

This can be formulated on any lattice with any series of short- and longer-range couplings. Any typical ordered state will be characterised by some non-zero spin expectation value

$$\langle \vec{S}_i \rangle \neq 0. \quad (2.36)$$

For example, a Néel state on the square lattice would have simply  $\langle S_i^z \rangle = m(-1)^{x+y}$ , where  $m$  measures the alternating sublattice magnetisation. A starting point for any effective model of Néel order comes in the form of an effective theory for this order parameter. Transitions between magnetic orders are written in terms of Landau–Ginzburg theory.

However, what if the spin order parameter is exactly zero? In this case, any attempt at an effective theory of the spins will trivially fail. To see this, imagine attempting a mean-field decoupling of Eq. (5.65). We find

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} \left( \vec{S}_i \cdot \langle \vec{S}_j \rangle + \langle \vec{S}_i \rangle \cdot \vec{S}_j - \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle \right). \quad (2.37)$$

In any state where  $\langle \vec{S}_i \rangle = 0$  everywhere, the Hamiltonian will vanish  $\mathcal{H} = 0$ .

The solution is to introduce an auxiliary representation. In most cases, this is simply redundant and acts purely to over-complicate the description. However for spin liquids it will provide the basis for understanding fractionalisation. Following Baskaran *et al.* (1987); Baskaran and Anderson (1988), we apply the Abrikosov fermion representation of our spin-1/2 degree of freedom

$$\vec{S}_i = \frac{1}{2} f_{i\alpha}^\dagger \vec{\sigma}^{\alpha\beta} f_{i\beta}. \quad (2.38)$$

These are charge neutral particles which obey the fermionic operator algebra

$$\{f_{i\alpha}^\dagger, f_{j\beta}\} = \delta^{(D)}(i-j)\delta_{\alpha\beta}, \quad \{f_{i\alpha}^\dagger, f_{j\beta}^\dagger\} = \{f_{i\alpha}, f_{j\beta}\} = 0. \quad (2.39)$$

Here, the spin indices  $\alpha, \beta$  take the values  $\uparrow, \downarrow$ . To see how this definition reproduces the spin algebra, write the operators

$$S_i^z = \frac{1}{2} (f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\downarrow}^\dagger f_{i\downarrow}), \quad (2.40)$$

$$S_i^+ = f_{i\uparrow}^\dagger f_{i\downarrow}, \quad S_i^- = f_{i\downarrow}^\dagger f_{i\uparrow}. \quad (2.41)$$

The states  $|\uparrow\rangle$  and  $|\downarrow\rangle$  have  $S^z$  eigenvalues  $\pm \frac{1}{2}$ . This shows clearly that we can identify the Hilbert spaces  $|+\frac{1}{2}\rangle \leftrightarrow |\uparrow\rangle$  and  $|-\frac{1}{2}\rangle \leftrightarrow |\downarrow\rangle$ . The problem is that we have introduced two new unphysical states by using the fermionic representation. The fermion states  $|0\rangle$  and  $|\uparrow\downarrow\rangle$ , i.e. the unoccupied and doubly-occupied states, have  $S^z$  eigenvalues 0 and 1. This is impossible for the original spin-1/2 system. The solution is to restrict the fermions to live within the subspace with only one particle per site. This single-occupancy constraint restricts

$$n_i = f_{i\alpha}^\dagger f_{i\alpha} = f_{i\uparrow}^\dagger f_{i\uparrow} + f_{i\downarrow}^\dagger f_{i\downarrow} = 1. \quad (2.42)$$

This must hold for all sites. An equivalent statement is that there are no sites with occupation zero or two

$$f_{i\uparrow}^\dagger f_{i\downarrow}^\dagger = f_{i\uparrow} f_{i\downarrow} = 0. \quad (2.43)$$

There is another feature of this fermionic representation of the spins that is important for our analysis. There is a gauge redundancy of the fractionalised description, given in Eq. (2.38). This consists of two parts. The first is a local U(1) phase rotation

$$f_{i\alpha} \rightarrow e^{i\theta_i} f_{i\alpha}. \quad (2.44)$$

The second is a particle-hole transformation, parameterised by an angle  $\phi$

$$f_{i\alpha} \rightarrow f_{i\alpha} \cos \phi_i + \alpha f_{i\bar{\alpha}}^\dagger \sin \phi_i. \quad (2.45)$$

We are working with an SU(2) gauge redundancy. To briefly make this explicit, we can rewrite the fermions into a doublet of SU(2)-gauge  $\Psi_i = \frac{1}{2}(f_{i\uparrow}, f_{i\downarrow}^\dagger)^T$ . Then, the two transformations act separately as  $\Psi_i \rightarrow e^{i\sigma_z \theta_i} \Psi_i$  and  $\Psi_i \rightarrow e^{i\sigma_y \phi_i} \Psi_i$ .

### Zeroth order mean-field theory

We can now apply this parton description to our first spin liquid state. We focus on the spin-half Heisenberg model on the square lattice

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j, \quad (2.46)$$

where  $J_{ij}$  is  $J_1$  on nearest-neighbour bonds. Transforming into the Abrikosov representation Eq. (2.38), we derive an interacting fermion theory

$$\begin{aligned} \mathcal{H}_{J_1 J_2} &= \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} \left( \frac{1}{2} f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta} \right) \cdot \left( \frac{1}{2} f_{j\alpha'}^\dagger \vec{\sigma}_{\alpha'\beta'} f_{j\beta'} \right) \\ &= \frac{1}{2} \sum_{\langle ij \rangle} J_{ij} \left( f_{i\alpha}^\dagger f_{i\beta} f_{j\beta}^\dagger f_{j\alpha} - \frac{1}{2} f_{i\alpha}^\dagger f_{i\alpha} f_{j\beta}^\dagger f_{j\beta} \right). \end{aligned} \quad (2.47)$$

In this final step, we used

$$\sigma_{\alpha\beta}^i \sigma_{\gamma\delta}^i = 2\delta_{\alpha\delta} \delta_{\beta\gamma} - \delta_{\alpha\beta} \delta_{\gamma\delta}. \quad (2.48)$$

Finally, using the anticommutation relations (2.39), we find

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} \left( f_{i\alpha}^\dagger f_{j\alpha} f_{j\beta}^\dagger f_{i\beta} + \frac{1}{2} n_i n_j - n_i \right). \quad (2.49)$$

The physical Hilbert space must be projected out by requiring one fermion per site. One can implement this at the level of the path integral using an auxiliary Lagrange multiplier field, as

$$Z = \int \mathcal{D}f \mathcal{D}f^\dagger \delta(f_{i\alpha}^\dagger f_{i\alpha} - 1) e^{-i \int dt \mathcal{H}} \quad (2.50)$$

$$= \int \mathcal{D}f \mathcal{D}f^\dagger \mathcal{D}a^0 e^{-i \int dt [\mathcal{H} + a_i^0 (f_{i\alpha}^\dagger f_{i\alpha} - 1)]}. \quad (2.51)$$

Therefore the final two terms in Eq. (2.49) evaluate to a constant which we can ignore from hereon. The effective Hamiltonian reads

$$\mathcal{H}[f_i, a_i^0] = -\frac{1}{2} \sum_{ij} J_{ij} f_{i\alpha}^\dagger f_{j\alpha} f_{j\beta}^\dagger f_{i\beta} + \sum_i a_i^0 (f_{i\alpha}^\dagger f_{i\alpha} - 1). \quad (2.52)$$

We have traded one difficult problem for another. The spin liquid Hamiltonian now takes the form of an interacting fermion theory with a constraint. The advantage is that we now have a way of performing mean-field theory on states with no spin order.

But what states can we produce if we are not allowed any spin order? The simplest answer is that we find a state with a finite expectation for the spinon hopping

$$\chi_{ij} = \langle f_{i\alpha}^\dagger f_{j\alpha} \rangle = \langle f_{i\uparrow}^\dagger f_{j\uparrow} + f_{i\downarrow}^\dagger f_{j\downarrow} \rangle. \quad (2.53)$$

Indeed it is possible that the four-spinon interaction could produce this state. Continuing in the path-integral language, let us decouple the interaction term in Eq. (2.52) with a Hubbard–Stratonovich transformation. This means we will introduce *yet another* fluctuating bosonic field. This gives the following action

$$\mathcal{H}[f_i, a_i^0, \chi_{ij}] = -\frac{1}{2} \sum_{ij} J_{ij} (\chi_{ij} f_{j\alpha}^\dagger f_{i\alpha} + \text{h.c.} - |\chi_{ij}|^2) + \sum_i a_i^0 (f_{i\alpha}^\dagger f_{i\alpha} - 1). \quad (2.54)$$

If we were to integrate out this field exactly, we would substitute the equation of motion for the boson  $\chi_{ij} = f_i^\dagger f_j$  into (2.54) to recover the four-fermion interaction (2.52). The parton mean-field theory comes instead from the saddle points of this theory (2.54) for both  $\chi_{ij}$  and  $a_i^0$  fields. This imposes  $\chi_{ij} = \langle f_i^\dagger f_j \rangle$  on average. Likewise, the saddle point in  $a_i^0$  defines a constant on-site chemical potential such that the important single-occupancy constraint is only imposed on average

$$\langle f_{i\alpha}^\dagger f_{i\alpha} \rangle = 1. \quad (2.55)$$

The advantage of the parton construction and mean-field theory then becomes clear. At this ‘zeroth-order’ level, we ignore all fluctuations of these fields  $\chi_{ij}$  and  $a_i^0$  (Wen, 1991, 2002). The interacting theory Eq. (2.52) is reduced to a quadratic fermionic hopping Hamiltonian, Eq. (2.54). However, this mean-field theory is totally uncontrolled. In order to believe any of the results, we must check the stability of the resulting phases to fluctuations.

We proceed by taking a mean-field Ansatz for the saddle point  $\chi_{ij}$ . This will define what type of spin liquid we generate. This consists of choosing a set of parameters for the hoppings and chemical potentials  $t_{ij}$  and  $\mu_i$ . The Hamiltonian is then

$$\mathcal{H}[f_i, \mu_i, \chi_{ij}] = - \sum_{ij} (t_{ij} f_{j\alpha}^\dagger f_{i\alpha} + \text{h.c.}) + \sum_i \mu_i f_{i\alpha}^\dagger f_{i\alpha}. \quad (2.56)$$

This form of the Hamiltonian can be explicitly diagonalised in momentum space to find the spectrum for the spinons. The parameters are defined self-consistently, with the hopping satisfying

$$t_{ij} = \frac{1}{2} J_{ij} \chi_{ij} = \frac{1}{2} J_{ij} \langle f_{i\alpha}^\dagger f_{j\alpha} \rangle, \quad (2.57)$$

and the chemical potential chosen to satisfy (2.55) on average.

This form of the mean-field Hamiltonian has a U(1) gauge symmetry. This becomes a dynamical gauge field in our new model. The hopping Ansatz can be decomposed into a magnitude and phase

$$t_{ij} = \bar{t}_{ij} e^{ia_{ij}}. \quad (2.58)$$

The gauge redundancy can be compensated by a shift of this phase of the hopping

$$f_{i\alpha} \rightarrow e^{i\theta_i} f_{i\alpha}, \quad (2.59)$$

$$a_{ij} \rightarrow a_{ij} + \theta_j - \theta_i. \quad (2.60)$$

This suggests that there will be gapless phase fluctuations of  $t_{ij}$  that could potentially destabilise the spin liquid. We will deal with this soon within first-order mean field theory. However, it is also worth noting already that the amplitude fluctuations of  $t_{ij}$  are always ignored! The justification for this is that they will be gapped excitations around the mean-field state (Wen, 2002). Foreshadowing a result in Chapter 3, we can say that this is not necessarily true beyond the saddle point approximation.

Parton mean-field theory is key to another important contribution: It is leveraged in Wen's classification of *symmetric* spin liquid states. In the standard Landau classification of phases, it is possible to categorise mean-field orders based on the symmetries of their order parameter. In practice, that means knowing which Hamiltonian symmetries — like lattice symmetries, SU(2) spin symmetry, etc. — are broken by the ground state. In spin liquids by definition, none of these symmetries are broken. The zoo of translationally-invariant spin-disordered states can be classified by the gauge symmetry that leaves the parton mean-field Ansatz invariant. This is called the invariant gauge group (IGG) and it determines much of the universal properties of a given spin liquid (Wen, 2002). A full classification of quantum orders comes from a more detailed understanding of the projective symmetry group (PSG). As we will shortly see, mean field Ansätze appear to break lattice symmetries like translation symmetry, but in fact do not if we accompany the lattice symmetry operations with a SU(2) transformation (we are always allowed to do this, since this is a redundancy in our parton description). We say in this case that the Ansatz realises the lattice symmetries *projectively*. Through the classification, Wen is able to predict what sort of spinon state (gapped, gapless, Dirac, etc.) is allowed with a given gauge group on a given lattice.

In this Thesis, we will exclusively focus on mean-field states that possess a U(1) gauge symmetry. That said, we will now briefly note that the class of  $\mathbb{Z}_2$  QSLs can be easily generated from this U(1) symmetric mean-field Hamiltonian (2.56) by adding more mean-field parameters that violate the U(1) symmetry. By doing this, we break the invariant gauge group from U(1) to  $\mathbb{Z}_2$ . A general Hamiltonian can be written as

$$\begin{aligned} \mathcal{H}[f_i, \mu_i, \zeta_i, \chi_{ij}, \Delta_{ij}] = & - \sum_{ij} \left[ t_{ij} f_{j\alpha}^\dagger f_{i\alpha} + \Delta_{ij} (f_{j\uparrow}^\dagger f_{i\downarrow}^\dagger - f_{j\downarrow}^\dagger f_{i\uparrow}^\dagger) + \text{h.c.} \right] \\ & + \sum_i \left[ \mu_i f_{i\alpha}^\dagger f_{i\alpha} + \zeta_i (f_{i\uparrow}^\dagger f_{i\downarrow}^\dagger - f_{i\downarrow}^\dagger f_{i\uparrow}^\dagger) + \text{h.c.} \right]. \end{aligned} \quad (2.61)$$

Here, the fermion bond-pairing terms  $\Delta_{ij} (f_{j\alpha}^\dagger f_{i\beta}^\dagger \epsilon^{\alpha\beta}) + \text{h.c.}$  break the gauge redundancy (2.59) down to a discrete subgroup  $f_{i\alpha} \rightarrow \pm f_{i\alpha}$ .

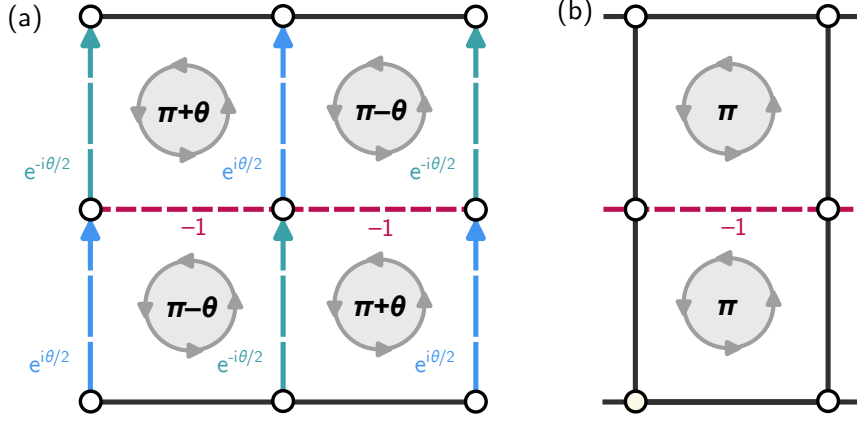


**Figure 2.3: Ansatzes on the square lattice.** (a) The staggered-flux Ansatz. Uniform hopping magnitude  $t$ , with phase  $\pm\phi = \pi - \theta$  through each square plaquette. (b) The uniform  $\pi$ -flux Ansatz. Uniform hopping magnitude, with phase  $\pi$  through each square plaquette. This is a special case of the staggered-flux Ansatz with  $\phi = \pi$ .

### Ansatz on the square lattice

We will now analyse several Ansatzes on the square lattice. The choice of Ansatz defines the type of spin liquid order. We consider states here with uniform hopping magnitude  $\bar{t}_{ij} = t$ , and varying phases. Although the hopping phases are gauge dependent, the plaquette fluxes are invariant under  $U(1)$  transformations (2.60). We define the flux on a square plaquette

$$W_{\square} = \sum_{ij \in \square} a_{ij}. \quad (2.62)$$

This represents the phase picked up by a spinon when hopping around the plaquette.

Let us define two related Ansatzes: the staggered-flux Ansatz, and the simpler uniform  $\pi$ -flux Ansatz. Firstly, the staggered-flux Ansatz is defined by the following choice of mean-field parameters

$$t_{i,i+y} = t \exp[i(-1)^{x+y}\theta/2], \quad t_{i,i+x} = (-1)^y t, \quad a_i^0 = 0. \quad (2.63)$$

We have taken the gauge as written by Song *et al.* (2019, 2020). This is shown in Fig. 2.3(a). We see that each plaquette has an alternating flux  $\pm\phi$ , where  $\phi = \pi - \theta$ . In the special case  $\theta = 0$ , we have a uniform  $\pi$ -flux state (Affleck and Marston, 1988). This Ansatz can be written as

$$t_{i,i+y} = t, \quad t_{i,i+x} = (-1)^y t, \quad a_i^0 = 0, \quad (2.64)$$

which is shown in Fig. 2.3(b).

Let us focus for now on the uniform  $\pi$ -flux Ansatz. It has a two-site unit cell, and therefore appears to have broken the lattice symmetries. Under translation in  $y$ , the  $x$ -hopping changes sign:

$$(t_{i,i+x}, t_{i,i+y}) = ((-1)^y t, t) \xrightarrow{i_y \rightarrow i_y + 1} (-t_{i,i+x}, t_{i,i+y}). \quad (2.65)$$

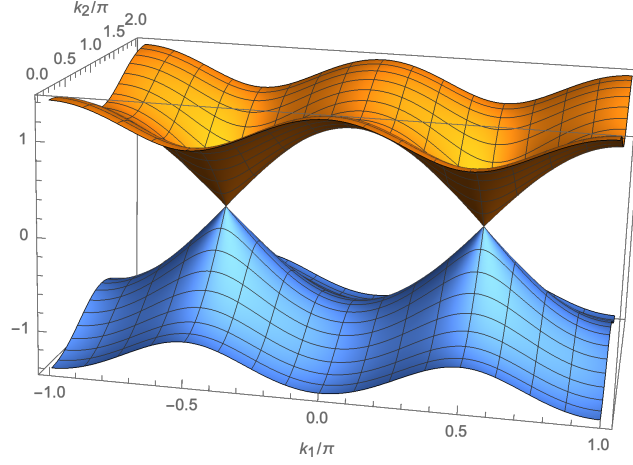


**Figure 2.4:** *Spectrum of spinons in the uniform  $\pi$ -flux Ansatz.* Dirac cones emerge at low energy with linear dispersion.

However this is not a different state. This change can be undone by a U(1) gauge transformation of the fermions

$$f_{i\alpha} \xrightarrow{i_y \rightarrow i_y + 1} (-1)^{i_x} f_{i\alpha}. \quad (2.66)$$

In terms of Eq. (2.59), this gauge transformation is  $\theta_i = i_x \pi$ . Together, the Hamiltonian for  $x$ -hopping transforms as

$$f_{i+x\alpha}^\dagger f_{i\alpha} t_{i,i+x} \xrightarrow{i_y \rightarrow i_y + 1} f_{i+x\alpha}^\dagger f_{i\alpha} t_{i,i+x}, \quad (2.67)$$

which is manifestly invariant.

What is the spectrum of the mean-field Hamiltonian defined by the  $\pi$ -flux state? We can diagonalise this quadratic Hamiltonian to calculate the dispersion of the spinons. We have a doubled unit cell in the  $y$ -direction with two sites in the unit cell. Moving to momentum space, we define the sublattice spinor

$$\psi_{\mathbf{k}}^\alpha = \begin{pmatrix} f_{\mathbf{k}\alpha,A} \\ f_{\mathbf{k}\alpha,B} \end{pmatrix}. \quad (2.68)$$

Here,  $A, B$  identify the sites at  $(0, 0)$  and  $(0, 1/2)$  offsets in terms of the lattice unit vectors  $\mathbf{a}_1 = \mathbf{x}$  and  $\mathbf{a}_2 = 2\mathbf{y}$ . We define the reciprocal lattice vectors  $\mathbf{q}_1 = (2\pi, 0)$  and  $\mathbf{q}_2 = (0, \pi)$ . The Hamiltonian in this basis reads

$$H = \sum_{\alpha} \sum_{\mathbf{k}} (\psi_{\mathbf{k}}^\alpha)^\dagger \begin{pmatrix} 2 \cos(k_1) & 1 + e^{ik_2} \\ 1 + e^{-ik_2} & -2 \cos(k_1) \end{pmatrix} \psi_{\mathbf{k}}^\alpha. \quad (2.69)$$

We define  $k_j = \mathbf{k} \cdot \mathbf{q}_j$  as the momenta in the reduced Brillouin zone. The eigenvalues are then

$$E_{\mathbf{k}} = \pm 2t \sqrt{\cos^2(k_1) + \cos^2(k_2/2)}, \quad (2.70)$$

where  $-\pi \leq k_{1,2} \leq \pi$ . We plot this dispersion in Fig. 2.4, showing two Dirac cones. These are at the momenta  $\mathbf{k} = \pm(\pi/2, \pi)$ . This is a gapless quantum spin liquid with Dirac dispersion. This surprising result implies that the low-energy excitations of our insulating magnet are gapless charge-neutral fermions. It is however *a priori* completely unclear whether this result holds beyond the zeroth-order mean field approximation. Most troublingly, we have ignored the fluctuations of a dynamical gauge field. This will be the focus of the next section.

### 2.2.2 First-order mean field theory

#### Continuum model

We will now consider the effects of gapless U(1) phase fluctuations of the mean-field order parameter  $\chi_{ij}$  on the stability of U(1) quantum spin liquid states. To do this, we will write down a continuum action for the  $\pi$ -flux state. Note that the uniform  $\pi$ -flux state actually has an additional particle-hole symmetry. In fact, this Ansatz actually preserves the whole SU(2) gauge redundancy of the Abrikosov fermion representation. Here, we will ignore this fact and only focus on the effect of U(1) gauge fluctuations<sup>4</sup>. We can write a low-energy theory for the fermions by expanding for small momenta away from the Dirac cones. Expanding the spinor matrix Eq. (2.69) about the Dirac points  $\pm\mathbf{Q} = (\pi/2, \pi)$ , we find

$$\sum_{\alpha} \sum_{\mathbf{k}'} (\psi_{\mathbf{k}' \pm \mathbf{Q}}^{\alpha})^{\dagger} [-2k'_1 \mu_3 + k'_2 \mu_2] \psi_{\mathbf{k}' \pm \mathbf{Q}}^{\alpha}. \quad (2.71)$$

Write as a spinor in real space (by Fourier transforming and rescaling the coordinates where necessary), then adding back the dynamics for the fermion, we have

$$\sum_{i=1}^4 \psi_i^{\dagger} (-i\partial_0 + \mu_3 \partial_1 + \mu_2 \partial_2) \psi_i. \quad (2.72)$$

Here, we find that each of the valleys (labelled  $\pm$ ) and spins ( $\alpha$ ) contribute an independent Dirac spinor  $\psi_i$  to this action with  $i = 1, 2, 3, 4$ . Defining the gamma matrices  $\{\gamma^0, \gamma^1, \gamma^2\} = \{i\mu^1, \mu^2, \mu^3\}$ , we get the action

$$\sum_{i=1}^4 \bar{\psi}_i i\gamma^{\mu} \partial_{\mu} \psi_i, \quad (2.73)$$

where  $\bar{\psi}_i = \psi_i^{\dagger} \gamma^0$ . We have therefore derived an effective Dirac equation from the Dirac cones of the spinon bands. The index  $i$  runs over the four fermion flavours  $N_f = 4$ . This comes from having two spins and two bands.

<sup>4</sup>In Wen's classification, the uniform  $\pi$ -flux state strictly falls into the class SU2Bn0: the SU(2)-Dirac states. The staggered-flux states on the other hand fall into the class U1Cn01n: the U(1)-Dirac states (Wen, 2002). The difference is historically important for understanding underdoped cuprates (Wen and Lee, 1996; Lee *et al.*, 1998, 2006). For the purposes of the work at hand, we can either choose to work with the uniform  $\pi$ -flux state and ignore this difference (Wen, 2004; Hermele *et al.*, 2004; Song *et al.*, 2020), or work instead with the staggered-flux Ansatz (Song *et al.*, 2019). These states have identical Dirac-like dispersions at low energy. For a more complete description of the  $\pi$ -flux state as a SU(2) gauge theory, see the works by Thomson and Sachdev (2018); Song *et al.* (2020).

Now let us include the effect of gauge fluctuations around their saddle point values. Taking the gauge (2.64), the hopping terms in the mean-field (2.56)  $\chi_{ij} f_{j\alpha}^\dagger f_{i\alpha}$  become

$$\chi_{i,i+x} = (-1)^{i_y} e^{-ia_{i,i+x}}, \quad (2.74)$$

$$\chi_{i,i+y} = e^{-ia_{i,i+y}}. \quad (2.75)$$

The link fields  $a_{i,i+\delta}$  are now the dynamical spatial components of a lattice gauge field (Marston and Affleck, 1989; Hermele *et al.*, 2004). We can now find the continuum description of this lattice gauge theory following Wen (2004). Here, the gauge field  $a^\mu(\mathbf{r})$  is composed of the spatial components and the scalar potential ( $a^0(\mathbf{r}), a^i(\mathbf{r})$ ). The lattice field is defined as a coarse-graining of the continuum field as follows:

$$a_i^0 = a^0(\mathbf{r}_i), \quad a_{ij}^i = \int_{\mathbf{r}_i}^{\mathbf{r}_j} d\mathbf{r}^i a_i(\mathbf{r}). \quad (2.76)$$

By defining the continuum field in this way, we fix the form of the gauge field in the continuum action. The fermion-gauge coupling in the lattice gauge theory becomes a minimally coupled U(1) gauge field in the continuum model. The only modification we need to make to our Dirac fermion action (2.73) is to replace the derivative  $\partial_\mu$  with the gauge-covariant one

$$D_\mu = \partial_\mu + ia_\mu. \quad (2.77)$$

The new minimally-coupled kinetic term is then  $\bar{\psi} i\gamma^\mu D_\mu \psi$ . This preserves the gauge-invariance of the fermions (2.59). To make this point explicit, the continuum gauge transformation now reads

$$\psi_i(x) \rightarrow e^{i\theta(x)} \psi_i(x), \quad (2.78)$$

$$a_\mu(x) \rightarrow a_\mu(x) - \partial_\mu \theta(x). \quad (2.79)$$

Finally, the gauge field does not have any intrinsic dynamics at the lattice scale (there was no kinetic term of the lattice electric field  $e_{ij}^2$ ). This means we do not immediately get a kinetic term  $(1/4e^2) f_{\mu\nu}^2$  in our coarse-grained version of the lattice gauge theory. However, since we are interested in the long-wavelength behaviour of this model, we can consider taking the continuum limit by perturbatively integrating out fermions. This generates dynamics for the gauge field (Rantner and Wen, 2001; Kim and Lee, 1999). The result of all of this work is surprising: the continuum description of a quantum magnet is exactly the action of quantum electrodynamics

$$\mathcal{L}_{\text{QED}_3} = - \sum_{i=1}^4 \bar{\psi}_i i\gamma^\mu (\partial_\mu - ia_\mu) \psi_i + \frac{1}{4e^2} f_{\mu\nu}^2. \quad (2.80)$$

However, the differences to the familiar quantum electrodynamics of electromagnetism will be drastic. QED behaves very differently in 2+1 dimensions. To see this, we can calculate the scaling dimension of the coupling strength  $e^2$  as a function of spacetime-dimension  $d = D + 1$ . First, note the dimension of the field  $[f_{\mu\nu}] = 2$ . In the familiar  $d = 4$ , we see that  $[e^2] = 0$ , and the coupling is marginally irrelevant. However in our  $d = 3$  model,  $[e^2] = 1$

and the coupling is relevant. This tells us that in the infrared limit we will flow to a *strongly-coupled fixed point*. The nature and stability of this fixed point is a challenge to understand, but will be decisive for the stability of our spin liquid. To distinguish, we call our model of the Dirac spin liquid QED<sub>3</sub> from hereon.

We recall that there are four flavours of fermions in this model. We will start writing the fermions  $\psi_i$  without an index, where we explicitly order the elements as follows

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} \psi_{+\uparrow} \\ \psi_{+\downarrow} \\ \psi_{-\uparrow} \\ \psi_{-\downarrow} \end{pmatrix}. \quad (2.81)$$

The Dirac action is invariant under SU(4) transformations  $\psi \rightarrow U\psi$ . We started out with only an SU(2) spin symmetry in our lattice model. When deriving the continuum form by expanding around two identical Dirac cones, we also introduced a SU(2) valley degree of freedom. Together, this SU(2)  $\times$  SU(2) is enhanced to a SU(4) flavour symmetry in our continuum theory model. The sixteen possible bilinears take the form

$$\bar{\psi} M_{ij} \psi = \bar{\psi} \sigma_i \tau_j \psi \quad (2.82)$$

where the matrix elements in the above basis are

$$\sigma^i \tau^j = \begin{pmatrix} (\tau^j)_{11} \sigma^i & (\tau^j)_{12} \sigma^i \\ (\tau^j)_{21} \sigma^i & (\tau^j)_{22} \sigma^i \end{pmatrix}. \quad (2.83)$$

We define the Pauli matrices for the spin indices to be  $\sigma^i$ , and those for valley indices to be  $\tau^i$ . In both cases the  $i = 0$  is the identity matrix. Remember that each of the Dirac spinors  $\psi_i = \psi_{\pm\alpha}$  has its own spinor index. We call these Pauli matrices  $\mu^i$ .

We want to answer the question of whether the U(1) Dirac spin liquid can be an intrinsically stable ground state. We have mapped our lattice model onto a continuum one, written in terms of a strongly coupled U(1) gauge theory with gapless Dirac fermions. The question of stability is now equivalent to asking if there is a stable gapless fixed point of continuum QED<sub>3</sub>. Our next challenge will be to determine whether the gauge field fluctuations spontaneously generate mass terms. We will show how this would drive the spin liquid into an ordered state.

### Mother of competing orders

The fermions transform as spinors of SU(4) in the irreducible representations **4**. Therefore the bilinears transform in a 16-dimensional representation of SU(4), which decomposes into two irreducible representations

$$\mathbf{16} = \mathbf{15} \oplus \mathbf{1}. \quad (2.84)$$

The singlet representation **1** contains the trivial mass term  $m = \bar{\psi}_i \psi_i$ . The other chiral masses  $M_{ij} = \sigma^i \tau^j$  (excluding  $i = j = 0$ ), all fall into the adjoint representation **15**. The singlet mass  $m$  can therefore be added to the action without breaking any symmetries of the

field theory. Does this mean that it will be spontaneously generated under RG flow? The answer is only yes if the mass is compatible with the symmetries of the original lattice model.

Given the understanding of how fermions transform projectively under the lattice symmetries (Wen, 2002), we can write down transformation rules for the continuum spinor fields too (Hermele *et al.*, 2005). Under translation  $T_x$  in the  $x$ -direction and time-reversal symmetry  $\mathcal{T}$ , we see

$$T_x : \psi \rightarrow i\mu^3 \sigma^2 \tau^3 \psi^*, \quad (2.85)$$

$$\mathcal{T} : \psi \rightarrow \mu^1 \tau^2 \psi^*. \quad (2.86)$$

What does this imply about the transformation of the various fermion bilinears? A calculation<sup>5</sup> then shows the following properties under time-reversal symmetry

$$\mathcal{T} : \bar{\psi} M_{ij} \psi \rightarrow \begin{cases} -\bar{\psi} M_{ij} \psi & j = 0, 2, \\ +\bar{\psi} M_{ij} \psi & j = 1, 3. \end{cases} \quad (2.87)$$

Therefore, we can see that the trivial mass  $m = \bar{\psi} \psi$  is odd under time-reversal symmetry. Therefore it is not compatible with our original lattice Hamiltonian and can be excluded from the effective action on symmetry grounds. In terms of spin operators, we can view this mass  $m$  as a constant spin-scalar chirality term  $\sim \vec{S}_i \cdot \vec{S}_j \times \vec{S}_k$ . Explicitly breaking time-reversal symmetry by adding such a perturbation to the spin model will create a finite mass  $m$  and destroy the conformal fixed point (see also Section 3.4).

Now we can investigate the transformation properties of the other fermion bilinears under lattice symmetries. Note that these cannot be added to the continuum action without explicitly breaking SU(4) symmetry. We split them into three types

$$(\vec{a})^i = \bar{\psi} M_{i0} \psi = \bar{\psi} \sigma^i \psi \quad i = 1, 2, 3, \quad (2.88)$$

$$b^j = \bar{\psi} M_{0j} \psi = \bar{\psi} \tau^j \psi \quad j = 1, 2, 3, \quad (2.89)$$

$$(\vec{n}^j)^i = \bar{\psi} M_{ij} \psi = \bar{\psi} \sigma^i \tau^j \psi \quad i, j = 1, 2, 3. \quad (2.90)$$

Looking at the vector  $\vec{b}^2$ , we can see how the components transform under  $x$ -translations (2.85):

$$T_x : (\vec{b}^2)^i = \bar{\psi} M_{i2} \psi \rightarrow -(\vec{b}^2)^i. \quad (2.91)$$

In fact considering all lattice symmetries, this continuum field transforms exactly like a coarse-grained Néel order parameter

$$\vec{N} = (-1)^{i_x + i_y} \vec{S}_i \longleftrightarrow \bar{\psi} \vec{\sigma} \tau^2 \psi. \quad (2.92)$$

Among the time-reversal-even operators, there are the spin-scalars  $b^{1,3}$  which can similarly be identified as VBS order parameters

$$v^x = (-1)^{i_x} \vec{S}_i \cdot \vec{S}_{i+x} \longleftrightarrow b^1 = \bar{\psi} \tau^1 \psi, \quad (2.93)$$

$$v^y = (-1)^{i_y} \vec{S}_i \cdot \vec{S}_{i+y} \longleftrightarrow b^3 = \bar{\psi} \tau^3 \psi. \quad (2.94)$$

<sup>5</sup>Some sources call it a simple calculation, but we avoid this wording.

This result motivated Hermele *et al.* (2005) to identify the Dirac QSL state as the ‘mother of many competing orders’. Spontaneous generation of different masses  $M_{ij}$  will induce different corresponding orders. Therefore, it could precipitate one of many competing orders by applying various perturbations to one fixed point. Through this mechanism, the spin liquid promises to explain the different competing states as respective instabilities. In this sense, even if the spin liquid is not intrinsically stable, we might be able to see its effects in organising the phase diagram of spin models. The full calculation of all mass transformations is also enlightening, showing many non-trivial orders in the other matrix elements of  $M_{ij}$ . The Néel and VBS orders are the most physically relevant, however.

What are the scaling dimensions of these operators? In the non-interacting theory, they are degenerate, with dimension  $\Delta_M = 2$ . They are relevant in the RG sense, meaning that if the coupling to the fermion masses are finite (and symmetry-allowed), then the coupling will grow in the IR and the fixed point will be gapped. Interactions with the gauge field act to lower this scaling dimension further. Since the particles  $\bar{\psi}$  and  $\psi$  are oppositely charged, the gauge interactions act to bind them together (Hermele *et al.*, 2005). To quantify this effect, Rantner and Wen (2002); Hermele *et al.* (2005) performed a large- $N_f$  expansion. This increases the number of fermion flavours from 4 to  $N_f$ , and consequently also the size of the gauge group to  $SU(N_f)$ . In practice, this is done to allow a controlled perturbative expansion, since the effect of the gauge field vanishes in the limit  $N_f \rightarrow \infty$ . The results read (Hermele *et al.*, 2005, 2007):

$$\Delta_M = 2 - \frac{64}{3\pi^2 N_f} + \dots, \quad (2.95)$$

$$\Delta_m = 2 + \frac{128}{3\pi^2 N_f} + \dots. \quad (2.96)$$

It happens that interactions with the gauge field also break the degeneracy between the singlet masses  $\Delta_m = [\bar{\psi}\psi]$  and the adjoint masses  $\Delta_M = [\bar{\psi}M_{ij}\psi]$ . For the physical value of  $N_f = 4$ , we find  $\Delta_M = 1.46$  and  $\Delta_m = 3.08$ .

A consequence of mapping order parameters to field-theoretic objects is that we can predict the correlation functions of spin observables. If we have a stable conformal fixed point in the IR limit, then the conformal data will predict the algebraic (power-law) correlation functions. Specifically, we find the antiferromagnetic and VBS correlations share the same exponent

$$\langle v_i^i v_j^i \rangle \sim \langle \vec{N}_i \cdot \vec{N}_j \rangle \sim |\mathbf{r}_i - \mathbf{r}_j|^{-2\Delta_M}. \quad (2.97)$$

This gives the state the name ‘critical’ or ‘algebraic spin liquid’. Although the name Dirac spin liquid has become more favoured in recent years, we highlight it in this Chapter because it makes particularly clear the connection to the Luttinger liquid.

One final condition for the stability of the conformal fixed point is the absence of any relevant four-fermion interactions. If these were relevant, they would quickly also lead to the dynamical generation of a mass and spontaneous symmetry breaking. Large- $N_f$  studies point to there being relevant 4-fermion interactions (Xu, 2008; Xu and Sachdev, 2008; Chester and Pufu, 2016a,b; Jian *et al.*, 2018). The stable case is supported by other analyses, which predict this symmetry breaking only happens for a lower number of fermion flavours  $N_{f,c} < 4$  (Appelquist *et al.*, 1988; Nash, 1989; Herbut, 2016; Pietro and Stamou, 2017). We

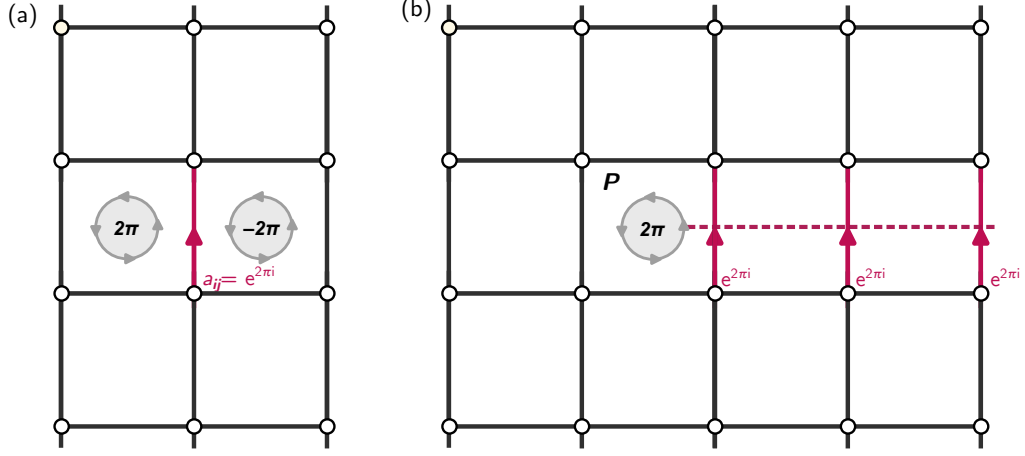


**Figure 2.5: Local monopole configuration on a lattice.** (a) A local large gauge transformation adds  $2\pi$  phase to a single bond. The neighbouring plaquettes have  $\pm 2\pi$  flux. This represents an identical state up to gauge transformations. (b) A string of such gauge transformations inserts a local monopole at  $P$ .

will therefore also assume no such dynamical mass generation due to interactions, and the presence of a stable conformal fixed point (Appelquist *et al.*, 1986; Karthik and Narayanan, 2016a).

### 2.2.3 Monopoles as instantons

#### Emergent $U(1)_{\text{topo}}$ symmetry

We have painted the picture above that the stability and correlations of the square-lattice algebraic spin liquid are governed by fermion bilinears. As we already did for the Sine-Gordon model in 1D, we studied the stability of the conformal fixed point by checking that there were no symmetry-allowed and relevant operators in the spectrum. As a reminder, we claim that if there is such an operator in the field theory that is allowed under lattice symmetries, it will be generated by the RG procedure. If this operator is relevant, its coupling will grow and take us away from the gapless fixed point.

Again recalling our 1D example, we saw that, beyond local bosonic excitations, there is another type of soliton excitation that is important for the physics. In Eq. (2.25) we see that the operator  $\cos(4\phi)$  is relevant for  $K < 1/2$ . In this section, we will show that  $\text{QED}_3$  also has operators of this nature, called monopoles. We will investigate them in this Section, and show that they are *strongly relevant*. We therefore conclude that they make the Dirac spin liquid unstable on the square lattice.

A key silent assumption when writing down a continuum theory is the smooth variation of the constituent fields. Most relevant is the coarse-graining of the gauge field, in equation (2.76). By assuming smooth configurations of the lattice gauge field, we ignore a class of allowed configurations. Consider the effect of shifting a single bond  $a_{ij}$  by  $2\pi Q$ . This acts

to add fluxes to the two neighbouring plaquettes

$$a_{ij} \rightarrow a_{ij} + 2\pi Q, \quad W_{\square} \rightarrow W_{\square} \pm 2\pi Q. \quad (2.98)$$

The sign is determined by the orientation of the bond  $ij$  around the plaquettes. We call this a *large gauge* transformation to highlight the fact that it is topologically distinct from local, smooth gauge transformations. The number  $Q$  must be an integer for the flux to change by a multiple of  $2\pi$ . This ensures that the action of adding a flux to a local plaquette is a pure gauge transformation. A charge moving around this bond in a loop which does not intersect the relevant bond will pick up an identical phase, independent of the flux  $2\pi Q$ .

Now a brief comment on the language used in the literature. The theory is often called *compact* QED<sub>3</sub> because these large gauge transformations are allowed. By this, we mean that the gauge field is compact in the sense that it lives on a circle  $a_{ij} \in [0, 2\pi)$ . This differs from the usual U(1) gauge field of electromagnetism which is a real number  $a(x) \in \mathbb{R}$ . Compact gauge theories naturally arise in lattice models, as described above. This will be what leads to the presence of monopole operators. These monopoles are much like the soliton operators which we saw in the Sine–Gordon model. There, the compact boson  $\phi$  displays a kink which jumps from one valley to another. In our case, it is a winding of the compact gauge field  $a_{ij}$  which represents a singular flux configuration called a monopole.

We can use this to construct a simple local magnetic monopole configuration, shown in Fig. 2.5. Taking a string of such gauge transformations along a line from infinity to the centre of the plaquette  $P$ , we construct a state where only  $W_P = 2\pi$  and  $W = 0$  everywhere else. The gauge field is discontinuous along the whole string, i.e. the configuration is not smooth. Such a string of discontinuity in the gauge field leads to a ‘Dirac monopole’ at  $P$ .

We can clearly see that we have neglected these configurations for  $a_{\mu}(x)$  in the continuum model. That is despite them being completely valid, gauge-equivalent states. Turning back to the continuum field theory, let us define an expression for the total magnetic flux (or monopole number)

$$Q = \frac{1}{2\pi} \int d^2x f_{12}, \quad (2.99)$$

where  $f_{\mu\nu} = \partial_{\mu}a_{\nu} - \partial_{\nu}a_{\mu}$ , and  $f_{12}$  is the magnetic flux density. We can define a current  $\mathcal{J}^{\mu}$  associated with this flux, such that Eq. (2.99) is the spatial integral of the charge density  $Q = \int d^2x \mathcal{J}^0$ . Explicitly,

$$\mathcal{J}^{\mu} = \frac{1}{4\pi} \epsilon^{\mu\nu\rho} \partial_{\nu}a_{\rho}. \quad (2.100)$$

Next, we take the divergence of (2.100) to give

$$\partial_{\mu}\mathcal{J}^{\mu} = \epsilon^{\mu\nu\rho} \partial_{\mu}\partial_{\nu}a_{\rho}(x) = 0, \quad (2.101)$$

when the field  $a_{\rho}(x)$  is a smooth function. This used the Bianchi identity of electromagnetism, or the fact that derivatives of an analytic function commute. This conservation law tells us that the monopole number is conserved in time  $Q = (\text{const})$ . This conservation law is a direct result of an emergent global topological symmetry, which we call  $U(1)_{\text{topo}}$ .

However, we argued above that this is not a real symmetry in the lattice gauge theory. Instead, we should allow our continuum model to break it, changing the flux number  $Q$  over time. We will correct the above conservation equation by adding a source for topological

charge  $\rho_m(x)$ , We motivate this by drawing the connection to the conserved electric charge current  $j^\nu = (1/e^2)\partial_\mu f^{\mu\nu}$ . The corresponding Gauss' laws in the presence of electric and magnetic charges read:

$$\partial_\mu \mathcal{J}^\mu = \rho_m(x), \quad \partial_\mu j^\mu = \rho_e(x). \quad (2.102)$$

For now, we will study the stability of a theory with no charges  $\rho_e = 0$ . This means investigating the stability of a pure compact U(1) gauge theory with no charged fermions. We will later return to the case relevant for QED<sub>3</sub> with  $N_f = 4$  charged spinons.

### Polyakov monopoles

Let us now investigate the consequences of allowing monopole operators which break  $U(1)_{\text{top}}$ . We will show that it causes confinement, the famous result from Polyakov (1977). To do this, it is insightful to change to another representation: perhaps surprisingly, electromagnetism in 2+1 dimensions has a dual formulation. We define the dual photon field  $\sigma(x)$  as follows (Polyakov, 1977)

$$\partial_\mu a_\nu(x) \longleftrightarrow \epsilon_{\mu\nu\rho} \partial^\rho \sigma(x). \quad (2.103)$$

Writing the kinetic term of electromagnetism as  $f_{\mu\nu} f^{\mu\nu} = (\epsilon^{\mu\nu\rho} f_{\mu\nu})^2$ , we see that the Maxwell action becomes the action of a free boson

$$\mathcal{L}_{\text{Maxwell}} = \frac{1}{e^2} f_{\mu\nu}^2 \longleftrightarrow \mathcal{L}_{\text{dual-Maxwell}} = \frac{e^2}{2} (\partial_\mu \sigma)^2. \quad (2.104)$$

The topological current (2.100) in this language becomes

$$\mathcal{J}^\mu = \frac{e^2}{(2\pi)^2} \partial^\mu \sigma. \quad (2.105)$$

The dual picture makes evident the nature of the topological symmetry: it acts as a shift on the dual photon

$$U(1)_{\text{topo}} : \quad \sigma(x) \rightarrow \sigma(x) + \beta, \quad (2.106)$$

for some global constant  $\beta$ . The operators which are charged under  $U(1)_{\text{topo}}$  can now be written

$$\mathcal{M}_Q(x) = e^{iQ\sigma(x)}. \quad (2.107)$$

These are the monopoles. They are local in dual electromagnetism, and related to the Maxwell electromagnetism (with a regular photon) via a non-local mapping (2.103). This also tells us that the field  $\sigma(x)$  should be understood modulo  $2\pi$  (Polyakov, 1987). That is to say, the configurations which differ by  $2\pi$  are physically equivalent, and the field  $\sigma(x)$  is a compact boson. Just like in the example of the Sine–Gordon model, there are soliton field configurations which take us between equivalent states that can be associated with a physical particle. In this case, solitons are monopoles in QED<sub>3</sub>.

Next, we can proceed to write down the partition function of the dual Maxwell theory in the presence of monopoles. Approximating the partition function as a dilute gas of  $N$  monopoles with positions  $z_i$ , we write

$$Z = \int \mathcal{D}\sigma(x) e^{-\frac{e^2}{2} \int d^3x (\partial_\mu \sigma)^2} \left[ \sum_{N=0}^{\infty} \frac{1}{N!} \left( \prod_{i=1}^N \int d^3z_i \right) \sum_Q e^{-S_0^Q} \mathcal{M}_Q(z_i) \right]. \quad (2.108)$$

The term  $S_0^Q = Q^2 S_0$  effectively measures the cost of inserting a charge- $Q$  monopole core. Next, we approximate further by only considering the contribution of single-charge monopoles. This allows us to reduce

$$\sum_{Q=\pm 1} e^{-S_0^Q} \mathcal{M}_Q(z_i) = e^{-S_0} \left( e^{i\sigma(z_i)} + e^{-i\sigma(z_i)} \right) = e^{-S_0} \cos(\sigma(z_i)). \quad (2.109)$$

Finally, we can simply resum the monopole gas partition function (2.108) to give an effective action

$$\mathcal{L}_{\text{Polyakov}} = \frac{e^2}{2} (\partial_\mu \sigma)^2 - e^{-S_0} \cos(\sigma). \quad (2.110)$$

Through the dual formulation, we have derived a Sine-Gordon like form of the dual photon. This motivates us to name the quantity  $y = e^{-S_0}$  the monopole fugacity, which is strongly relevant. This follows on the same grounds as Eq. (2.26), where we see now that a finite monopole density  $y$  leads here to a mass for the dual boson. One can also calculate correlation functions of the monopoles and show that their correlation functions are exponential in this phase (Polyakov, 1977, 1975, 1987). This exponential length scale tells us that they are confined.

### Fermions in a monopole background

Turning back to our model of continuum QED<sub>3</sub>, we can ask how the presence of gapless Dirac fermions changes Polyakov's results. We can express the resulting partition function in a mixed form (Shankar and Maciejko, 2021, 2024):

$$Z = \int \mathcal{D}\sigma(x) e^{-\frac{e^2}{2} \int d^3x (\partial_\mu \sigma)^2} \left[ \sum_{N=0}^{\infty} \frac{1}{N!} \left( \prod_{i=1}^N \int d^3z_i \right) \sum_{Q=\pm 1} e^{-S_0} \mathcal{M}_Q(z_i) \int \mathcal{D}\psi e^{-\int d^3x \bar{\psi} \gamma^\mu (\partial_\mu - iA_\mu^Q) \psi} \right]. \quad (2.111)$$

Here, the gauge field  $a$  is decomposed into an instanton background  $\mathcal{A}^Q$  and a smooth component. This smooth part is mapped to the dual photon  $\sigma$  and its fluctuations are included via the kinetic term  $(\partial_\mu \sigma)^2$ . The discontinuous part is the instanton background which provides a constant flux magnetic field  $2\pi Q$  for the Dirac fermions. We sum up over all instanton configurations  $Q$  in Eq. 2.111, where each monopole provides a background magnetic field  $\mathcal{A}^Q$ .

Fig. 2.6 shows the effect of such a  $2\pi$  background on a Dirac fermion (again in the  $Q = \pm 1$  sector). Each of the four Dirac cones are split into Landau levels. Each level has degeneracy  $4Q$ . We must always fulfil the constraint of one fermion per site in our parton theory in order to ensure gauge invariance. This now means that all negative levels are filled, and the zeroth Landau level must contain two fermion zero modes. Every flux insertion must then come with the creation of two fermion zero modes (Borokhov *et al.*, 2002). We will henceforth write the physical (gauge-invariant) monopoles within the QED<sub>3</sub> theory as

$$\Phi_a^\dagger(x) = c_i^\dagger c_j^\dagger \mathcal{M}(x). \quad (2.112)$$

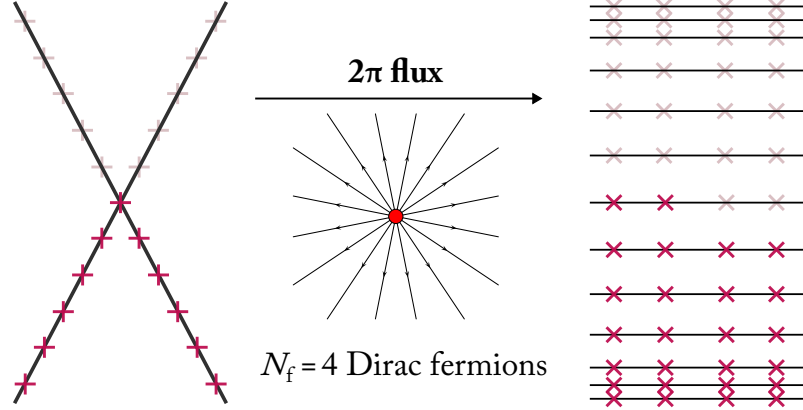


**Figure 2.6: Dirac Landau levels and the resulting fermion zero modes.** The effect of adding a  $2\pi$  flux background to the Dirac action is to split the spectrum into discrete Landau levels, each with degeneracy  $N_f$ . Gauge invariance requires that the zeroth Landau level is half-filled.

The indices of  $c_i^\dagger$  label which of the Dirac fermion's  $\psi_i$  zero modes are filled. Since there are  $\binom{4}{2} = 6$  ways of filling the zero modes, the index  $a = 1, \dots, 6$ .

We can directly use this picture to calculate the scaling dimension of the monopoles. This is thanks to a theorem from conformal field theory, called the state-operator correspondence. It tells us that the scaling dimension of a CFT primary operator (in this case a monopole) is equal to the free energy on a conformally-symmetric manifold (Borokhov *et al.*, 2002). The scaling dimension is then estimated by calculating the Casimir energy of  $N_f$  Dirac fermions in the background of a constant flux spread over the sphere  $S^2$ , shown in Fig. 2.6 (Borokhov *et al.*, 2002). The result, including next-order effects in  $N_f$  is (Pufu, 2014; Dyer *et al.*, 2013)

$$\Delta_\Phi = 0.265N_f - 0.0383. \quad (2.113)$$

In the case  $N_f = 4$ , this gives the scaling dimension  $\Delta_\Phi = 1.02$ . This is strongly relevant, far below  $d = 3$ , and is therefore likely to remain relevant also beyond the large- $N_f$  approximation. This result is supported by other CFT approaches, including ones which use insights from the conformal bootstrap (Chester and Pufu, 2016a; Albayrak *et al.*, 2022; He *et al.*, 2022). Finally, we note that quantum Monte Carlo simulations of lattice QED<sub>3</sub> also provide independent numerical evidence for these monopole scaling dimensions. Karthik and Narayanan (2019) find the monopole has a mild positive correction relative to the large- $N_f$  expansion. The results for  $N_f = 4$  give a scaling dimension in the range

$$\Delta_\Phi = 1.18\text{--}1.34. \quad (2.114)$$

We will refer to this range of values for the remainder of the Thesis. All approaches above consistently predict the scaling dimension to lie in the range  $1 < \Delta_\Phi < 3/2$ .

The six monopoles  $\Phi_a$  in the Dirac spin liquid transform as a vector of SO(6). For technical reasons on the square lattice<sup>6</sup>, this reducible six-dimensional SO(6) representation

<sup>6</sup>This relates back to an earlier detail we brushed under the rug. Because the staggered-flux state is continuously connected to the  $\pi$ -flux state with SU(2) symmetry, the fermion zero modes inherit SO(5) representations from that theory. QED<sub>3</sub> here is a Higgs descendent QCD<sub>3</sub> which must have a trivial monopole.

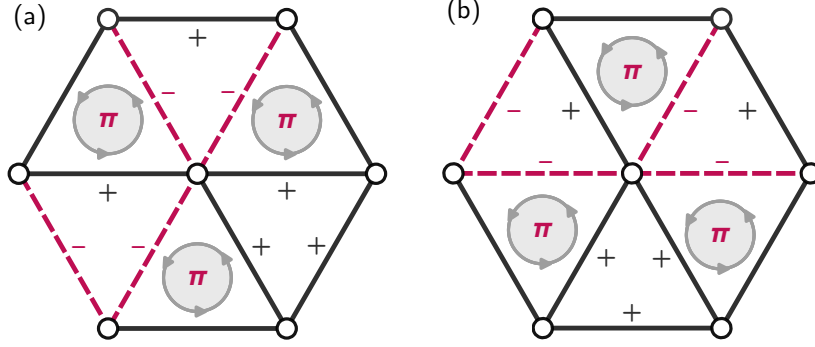


**Figure 2.7:** The  $\pi$ -flux Ansatz on the triangular lattice. (a,b) show two different gauges, and represent the same state.

must decompose into  $\text{SO}(5)$  representations (Wang *et al.*, 2017; Song *et al.*, 2020). The natural decomposition is  $\mathbf{6} = \mathbf{1} \oplus \mathbf{5}$ . The monopole in  $\mathbf{1}$  is trivial under the  $\text{SO}(6)$  symmetry and time-reversal even, which immediately implies that it can be added directly to the action:  $\mathcal{L}_{\text{sF}} = \mathcal{L} + \lambda(\Phi^\dagger + \text{h.c.})$ . This brief argument is substantiated by other approaches which predict explicitly that such a trivial monopole is present (Alicea, 2008; Song *et al.*, 2019).

Because the monopoles are symmetry-allowed and strongly relevant at  $N_f = 4$ , it leads to confinement by the Polyakov mechanism. This seals the fate of the Dirac spin liquid on the square lattice: it is *unstable at first-order mean-field theory*. Just as we saw in the continuum description of the XXZ chain in the regime  $K < 1/2$ , the spin liquid state is unstable. In both cases it was instanton events (monopoles and solitons) which led to this instability.

### 2.3 U(1) Dirac spin liquid part II: Triangular lattice

Now we turn to the main focus of this Thesis: the Heisenberg model on the triangular lattice. In particular, we return to the  $J_1$ - $J_2$  model from the Introduction

$$\mathcal{H}_{J_1 J_2} = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j. \quad (2.115)$$

We will now describe the model with a mean-field Ansatz and discuss how the best candidate state is also a Dirac spin liquid with  $\text{U}(1)$  gauge symmetry. We will then discuss two new breakthroughs that form the foundation of the results in this Thesis. First, the work by (Song *et al.*, 2019, 2020) which shows that the  $\text{U}(1)$  Dirac QSL is an intrinsically stable phase of matter on the triangular lattice at first-order mean field theory. Second, a growing body of numerical evidence that this phase describes the spin-disordered phase of the  $J_1$ - $J_2$  model.

#### 2.3.1 Emergent $\text{QED}_3$ on the triangular lattice

##### Zeroth-order mean-field theory: $\pi$ -flux Ansatz

Our starting point is once again to transform into the Abrikosov fermion representation and write down a zeroth-order mean-field Ansatz. On the triangular lattice, we will consider the

$\pi$ -flux state (Lu, 2016), depicted in Fig. 2.7. The Hamiltonian is given by

$$\mathcal{H}_0 = -t \sum_{\alpha} \sum_{\langle ij \rangle} t_{ij} (f_{j\alpha}^{\dagger} f_{i\alpha} + \text{h.c.}) . \quad (2.116)$$

The nearest-neighbour hoppings  $t_{ij} = \pm t$  produce alternating 0 and  $\pi$  fluxes through adjacent triangular plaquettes. In the gauge of Fig. 2.7(a), spinons hopping around upwards-pointing triangles enclose  $\pi$  flux and hence pick up a minus sign. Spinons hopping around the opposing triangles pick up no phase. The amplitude of the hopping is fixed self-consistently

$$t = J_1 |\langle f_{i\alpha}^{\dagger} f_{j\alpha} \rangle| / 2 , \quad (2.117)$$

where  $\langle ij \rangle$  lie on nearest-neighbour bonds. The mean-field Ansatz only has nearest-neighbour hoppings, and therefore only explicitly depends on the energy  $J_1$ . This is a U(1) symmetric Ansatz, meaning the mean-field Hamiltonian has a gapless gauge excitation. By writing  $t_{ij} = t e^{i a_{ij}}$ , we see that the U(1) gauge degree of freedom is given by  $f_{i\alpha}^{\dagger} \rightarrow e^{i \theta_i} f_{i\alpha}^{\dagger}$  and  $a_{ij} \rightarrow a_{ij} - \theta_i + \theta_j$ .

Although this Ansatz appears to break lattice symmetries, all physical quantities should be fully symmetric (Wen, 2002). Let us confirm this holds for our  $\pi$ -flux Ansatz. Taking the state shown in Fig. 2.7(b) and performing a  $C_6$  rotation about the central point, we recover the state Fig. 2.7(a). The action of this lattice symmetry transforms the Ansatz, but can be undone by an SU(2) gauge transformation. Specifically, consider the local particle hole transformation Eq. (2.45)

$$(f_{i\uparrow}, f_{i\downarrow})^T \rightarrow (f_{i\downarrow}^{\dagger}, -f_{i\uparrow})^T . \quad (2.118)$$

In the SU(2)-doublet notation, this takes  $\Psi \rightarrow i\sigma^2 \Psi$  (note that this is not a spinor transformation). The spin and direction of the kinetic terms is hereby swapped and the phase is inverted, i.e.  $f_{i\uparrow}^{\dagger} f_{j\uparrow} \rightarrow -f_{j\downarrow}^{\dagger} f_{i\downarrow}$ . Any process that hops a spinon along an odd number of bonds will hence pick up a minus sign. This effect indeed acts to swap the fluxes of the two upwards/downwards pointing plaquettes  $0 \leftrightarrow \pi$ . This gauge transform has hence been able to undo the apparent change of flux. We also note that this Ansatz appears to break translation symmetry, just as we saw for the  $\pi$ -flux state on the square lattice. In analogy with Eq. (2.66), this can equally be undone by a sign change that alternates on rows

$$f_{i\alpha} \xrightarrow{i_x \rightarrow i_x + 1} (-1)^{i_y} f_{i\alpha} . \quad (2.119)$$

The effect of this is to change the sign of all bonds, except the ones in the horizontal direction of the translation (two of the three bonds on each plaquette). This recovers exactly the original pattern.

Now let us find the spectrum of this mean-field theory at zeroth order. We construct our theory in terms of sublattice fermions  $f_{i,\alpha X}$  where  $X = A, B$  are the two sublattices, as shown in Fig. 2.8(a). The lattice unit vectors are

$$\mathbf{a}_1 = (2, 0) , \quad \mathbf{a}_2 = (1/2, \sqrt{3}/2) . \quad (2.120)$$

The relative offset of the two sites is  $\delta_{AB} = \mathbf{a}_1/2$ . Consequently, the reciprocal space is shown in Fig. 2.8(b), where the inverse lattice unit vectors are

$$\mathbf{q}_1 = \pi/a(1, -1/\sqrt{3}) , \quad \mathbf{q}_2 = (0, 4\pi/a\sqrt{3}) . \quad (2.121)$$

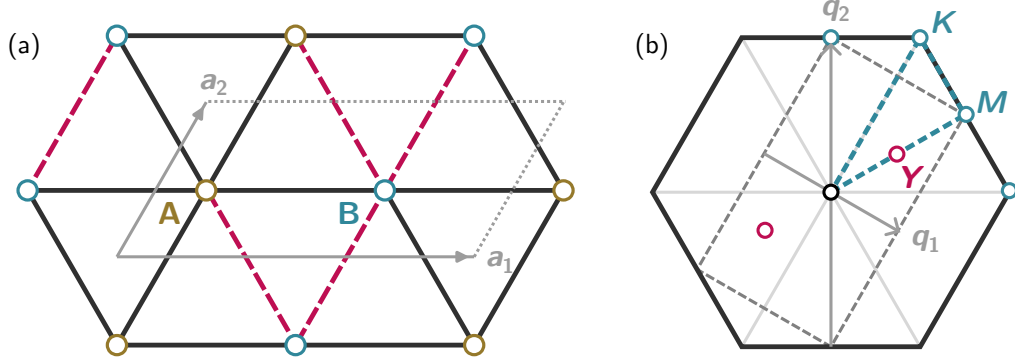


**Figure 2.8:** *Unit cell of the  $\pi$ -flux Ansatz on the triangular lattice.* (a) Doubled real-space unit cell with two sublattices  $A, B$ . Unit vectors labelled  $\mathbf{a}_{1,2}$ . (b) Reduced Brillouin zone with reciprocal lattice vectors  $\mathbf{q}_{1,2}$ . Gapless points  $\pm\mathbf{Y}$  highlighted in blue.

We define a basis of momenta  $\mathbf{k} = k_1\mathbf{q}_1 + k_2\mathbf{q}_2$  and the reduced Brillouin zone is drawn as the gray dashed rectangle. Now we transform to the momentum-space spinor representation  $\psi_{\mathbf{k}}^\alpha$  to find

$$\mathcal{H}_0 = -t \sum_{\alpha} \sum_{\mathbf{k}} (\psi_{\mathbf{k}}^\alpha)^\dagger H(\mathbf{k}) \psi_{\mathbf{k}}^\alpha. \quad (2.122)$$

where the Hamiltonian elements are given by

$$\begin{aligned} M(\mathbf{k})^{AA} &= -M_{\mathbf{k}}^{BB} = 2 \cos(k_2) \\ M(\mathbf{k})^{AB} &= 1 + e^{-ik_1} + e^{i(k_2-k_1)} - e^{-ik_2}, \end{aligned} \quad (2.123)$$

and where  $M(\mathbf{k})^{BA} = [M(\mathbf{k})^{AB}]^*$ . In the basis  $k_j = \mathbf{k} \cdot \mathbf{q}_j$ , the reduced Brillouin zone is spanned by  $-\pi \leq k_{1,2} \leq \pi$ . The eigenvalues of this matrix  $H(\mathbf{k})$  are

$$\varepsilon_{\mathbf{k}}^\pm = \pm 2t \sqrt{\cos^2(k_1/2) + \cos^2(k_2) + \sin^2(k_1/2 - k_2)} \quad (2.124)$$

with corresponding eigenvectors  $\alpha_{\mathbf{k}}^\pm$ . The Dirac cones of this spectrum are at the points  $\pm(\pi, \pi/2)$ , labelled as  $\pm\mathbf{Y}$  in Fig. 2.8(b). The bands are plotted in the original Brillouin zone in Fig. 2.9, showing that these points correspond to the points  $\mathbf{Y} = \mathbf{M}/2$ . The overall normalisation of this mean-field Hamiltonian is fixed self-consistently by evaluating

$$t = \frac{J_1}{2N} \sum_{\alpha\mathbf{k}} \langle (\psi_{\mathbf{k}}^\alpha)^\dagger \mu^1 \psi_{\mathbf{k}}^\alpha \rangle. \quad (2.125)$$

### First-order mean-field theory: Quantum numbers of monopoles

Once again, we must investigate the stability of this phase to gauge fluctuations in order to determine its intrinsic stability. We can expand the Hamiltonian (2.122) about the gapless Dirac points. Next, minimally coupling to the gauge field yields the QED<sub>3</sub> effective action

$$\mathcal{L}_{\text{QED}_3} = - \sum_{i=1}^4 \bar{\psi}_i i\gamma^\mu (\partial_\mu - ia_\mu) \psi_i + \frac{1}{4e^2} f_{\mu\nu}^2. \quad (2.126)$$

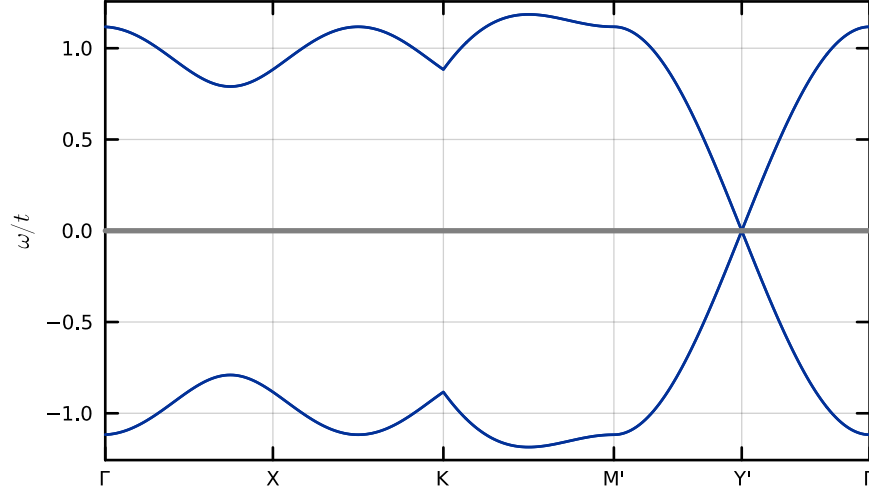


Figure 2.9: *Spinon bands of the Dirac spin liquid.*

where we now use the convention  $\{\gamma^0, \gamma^1, \gamma^2\} = \{i\mu^2, \mu^3, \mu^1\}$ . As in the square lattice case, note that the gauge field  $a_\mu$  is compact and so we should consider the effect of monopole configurations in the action. This theory has the same emergent SU(4) flavour symmetry group as before. We further note the presence of the topological U(1) symmetry. We will use the fact that the global symmetry group can be written

$$\text{SU}(4) \times \text{U}(1)_{\text{topo}} \simeq \text{SO}(6) \times \text{U}(1)_{\text{topo}} / \mathbb{Z}_2. \quad (2.127)$$

We can label all operators by their representations under these two groups:  $(\mathbf{d}, q)$ , where  $\mathbf{d}$  is a representation of SU(4) and  $q$  the charge of  $\text{U}(1)_{\text{topo}}$  (Zhang *et al.*, 2025). Just as before, we will initially ignore the effect of monopoles. This is equivalent to restricting to the operators that have charge-0 under  $\text{U}(1)_{\text{topo}}$ .

Similarly to the square lattice case, we can derive the transformations of the spinors under the projective lattice symmetries (Song *et al.*, 2019, 2020)

$$T_1 : \psi \rightarrow i\tau^2 \psi, \quad (2.128)$$

$$\mathcal{T} : \psi \rightarrow i\sigma^2 \tau^2 \mu^2 \psi. \quad (2.129)$$

This can be directly applied to calculate the corresponding transformation of fermion bilinears  $M_{ij} = \bar{\psi} \sigma^i \tau^j \psi$  on the triangular lattice. This is shown in Table 2.2. There are two classes of mass operators: inter-valley bilinears with momentum transfer  $\mathbf{M}$ , and intra-valley bilinears at the  $\Gamma$  point. The trivial mass  $m = \bar{\psi} \psi$  is once again time-reversal odd and does not transform under translations. We interpret it as a uniform spin-scalar chirality term. This is forbidden from being added to the action by time-reversal symmetry. Next, the adjoint mass elements  $b^j = \bar{\psi} \tau^j \psi$  and  $(n^j)^i = \bar{\psi} \sigma^i \tau^j \psi$  transform with momenta at the  $\mathbf{M}_j$  point and have the quantum numbers of VBS and stripe order parameters. These inter-valley bilinears

|          | $(T_1, T_2)$ | $R$       | $C_6$     | $\mathcal{T}$ |
|----------|--------------|-----------|-----------|---------------|
| $M_{00}$ | $(+, +)$     | $-$       | $+$       | $-$           |
| $M_{i0}$ | $(+, +)$     | $+$       | $-$       | $+$           |
| $M_{01}$ | $(-, -)$     | $+M_{03}$ | $-M_{02}$ | $+$           |
| $M_{02}$ | $(+, -)$     | $-M_{02}$ | $+M_{03}$ | $+$           |
| $M_{03}$ | $(-, +)$     | $+M_{01}$ | $+M_{01}$ | $+$           |
| $M_{i1}$ | $(-, -)$     | $-M_{i3}$ | $+M_{i2}$ | $-$           |
| $M_{i2}$ | $(+, -)$     | $+M_{i2}$ | $-M_{i3}$ | $-$           |
| $M_{i3}$ | $(-, +)$     | $-M_{i1}$ | $-M_{i1}$ | $-$           |

Table 2.2: Discrete symmetry transformations of fermion mass operators  $\bar{\psi} M_{ij} \psi$  (Song *et al.*, 2019, 2020). Translations  $T_j$  by lattice unit vectors  $\mathbf{b}_j$ ; reflection  $R$  in the vertical direction;  $C_6$  rotation; and time reversal  $\mathcal{T}$ . The relevant unit vectors of the real-space and reciprocal lattice are shown in Fig. 2.10.

have lattice momentum  $\mathbf{M}$  since they connect the two Dirac cones at  $\pm \mathbf{Y}$ , see Fig. 2.8(b). We can see that the gapless nature of the action is protected by lattice symmetries.

This was also true for the square lattice at the level of fermion bilinears, but was not true for monopoles. This led to an instability of the conformal fixed point. We must finally investigate the transformation properties of the monopoles under lattice symmetries on the triangular lattice (Song *et al.*, 2019, 2020). To do this, we will think about how the physical lattice symmetries are embedded within the enlarged symmetry group. The monopoles live in the representation  $(\mathbf{6}, 1)$ . That is, they are charge-1 under the  $U(1)_{\text{topo}}$ , and form a 6-dimensional vector under  $SU(4) \simeq SO(6)/\mathbb{Z}_2$ . The transformation properties of the monopoles will be fixed by the transformation of the fermion zero modes, Eq. (2.112). Depending on how the four zero modes are occupied with two spinful fermions will determine how the monopoles  $\Phi_a$  transform under lattice and spin symmetries.

Let us now briefly write down some example monopole wavefunctions on the triangular lattice and show that they transform as spin components  $S^i$  with  $i = 1, 2, 3$ . To do this, we must choose which fermion zero modes to fill in Eq. (2.112). The index  $i$  should not change under swapping valleys, and so our wavefunction should be symmetric under exchanging  $c_{+\alpha}^\dagger \leftrightarrow c_{-\alpha}^\dagger$ . Next, we want to construct states with a spin quantum number  $S = 1$  under the physical spin  $SO(3)$  symmetry. This can be done by filling the valleys  $|+, -\rangle$  as such

$$|\uparrow, \uparrow\rangle, \quad |\downarrow, \downarrow\rangle, \quad \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle). \quad (2.130)$$

We write the fermion zero mode wavefunctions (2.112) which generate these states in the form

$$(Z)^{\alpha\beta} c_{+\alpha}^\dagger c_{-\alpha}^\dagger \mathcal{M}(x), \quad (2.131)$$

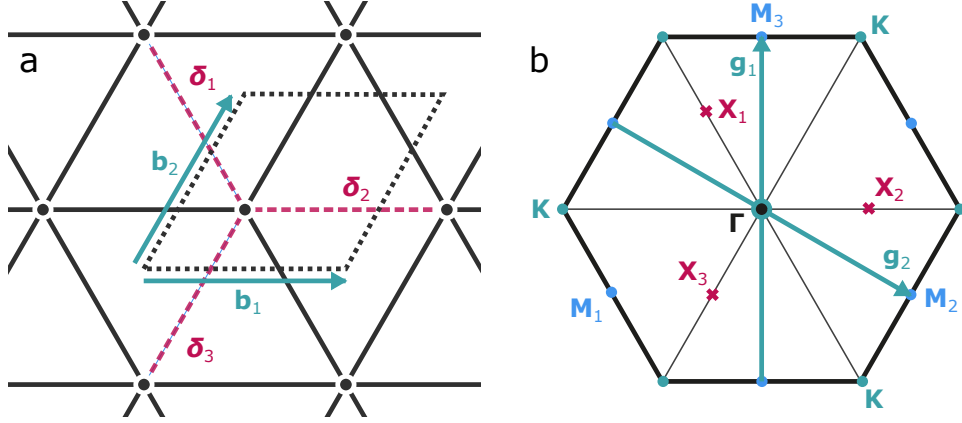


**Figure 2.10:** *Triangular lattice unit cell and reciprocal lattice.* (a) Lattice with unit vectors  $\mathbf{b}_j$  and nearest-neighbour bonds  $\delta_\alpha$  highlighted. (b) Reciprocal lattice with inverse lattice vectors  $\mathbf{g}_i$  and high-symmetry points in the Brillouin zone  $\mathbf{K}$  and  $\mathbf{M}_i$  labeled. The points  $\mathbf{X}_\alpha = -\mathbf{K}_\alpha/2$  are the momenta eigenvalues of gapless monopole excitations.

where the three matrices read

$$Z^+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad Z^- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad Z^3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (2.132)$$

Transforming to the basis of spin operators  $Z^{1,2} = (Z^+ \pm Z^-)/\sqrt{2}$ , we can write the physical spin-triplet monopoles

$$\mathcal{S}^i = (Z^i)^{\alpha\beta} c_{+\alpha}^\dagger c_{-\alpha}^\dagger \mathcal{M}(x), \quad (2.133)$$

Note that the matrices  $Z^i$  are nothing other than the spin-Pauli matrices multiplied by the antisymmetric matrix  $Z^i = \epsilon\sigma^i$ . We can also write down three monopoles with matrix elements  $Y^j = \epsilon\tau^j$  that are symmetric under spin rotations but form a triplet under  $\text{SO}(3)_{\text{valley}}$  (Song *et al.*, 2019). We call the corresponding spin-singlet monopoles  $\mathcal{D}^j$ . The two independent microscopic symmetries  $\text{SU}(2)_{\text{valley}}$  and  $\text{SU}(2)_{\text{spin}}$  are subgroups of the emergent  $\text{SU}(4)$ , and correspond to mutually commuting  $\text{SO}(3)_{\text{valley}}$  and  $\text{SO}(3)_{\text{spin}}$  subgroups of  $\text{SO}(6)$ . This lets us decompose  $\Phi_a$  into spin-singlet ( $a = 1, 2, 3$ ) and valley-singlet, spin-triplet components (4, 5, 6):

$$\Phi_a = \begin{pmatrix} \Phi_{1,2,3} \\ \Phi_{4,5,6} \end{pmatrix} = \begin{pmatrix} \vec{\mathcal{D}} \\ \vec{\mathcal{S}} \end{pmatrix}. \quad (2.134)$$

The valley-triplet components  $\mathcal{D}_\alpha$  transform under  $\text{SO}(3)_{\text{valley}}$ , and the spin-triplet components  $\mathcal{S}_\alpha$  under spin rotations.

There are also important discrete lattice symmetries of the triangular lattice. These are time-reversal symmetry  $\mathcal{T}$ , discrete translations  $T_{1,2}$  by the unit vectors  $\mathbf{b}_{1,2}$ , reflection  $R$  in the vertical direction, and  $C_6$  lattice rotation. The unit cell is drawn in Fig. 2.10(a). These discrete symmetries will act on the monopoles through some combination of  $\text{SO}(6)$  rotation and a  $\text{U}(1)_{\text{topo}}$  phase. The  $\text{SO}(6)$  rotation is dictated by action of the projective symmetries on the fermion zero modes. The additional phase can be interpreted as a Berry phase of

|                                        | $T_j$                                                 | $R$                   | $C_6$                         | $\mathcal{T}$                 |
|----------------------------------------|-------------------------------------------------------|-----------------------|-------------------------------|-------------------------------|
| $\mathcal{D}_1 = \Phi_1$               | $e^{-i\mathbf{X}_1 \cdot \mathbf{a}_j} \mathcal{D}_1$ | $-\mathcal{D}_3$      | $+\mathcal{D}_2^\dagger$      | $+\mathcal{D}_1^\dagger$      |
| $\mathcal{D}_2 = \Phi_2$               | $e^{-i\mathbf{X}_2 \cdot \mathbf{a}_j} \mathcal{D}_2$ | $+\mathcal{D}_2$      | $-\mathcal{D}_3^\dagger$      | $+\mathcal{D}_2^\dagger$      |
| $\mathcal{D}_3 = \Phi_3$               | $e^{-i\mathbf{X}_3 \cdot \mathbf{a}_j} \mathcal{D}_3$ | $-\mathcal{D}_1$      | $-\mathcal{D}_1^\dagger$      | $+\mathcal{D}_3^\dagger$      |
| $\mathcal{S}_\alpha = \Phi_{\alpha+3}$ | $e^{-i\mathbf{K} \cdot \alpha_j} \mathcal{S}_\alpha$  | $+\mathcal{S}_\alpha$ | $-\mathcal{S}_\alpha^\dagger$ | $-\mathcal{S}_\alpha^\dagger$ |

Table 2.3: Discrete symmetry transformations of monopole operators  $\Phi_a$  (Song *et al.*, 2019, 2020). Translations  $T_j$  by lattice unit vectors  $\mathbf{a}_j$ ; reflection  $R$  in the vertical direction;  $C_6$  rotation; and time reversal  $\mathcal{T}$ . The relevant unit vectors of the real-space and reciprocal lattice are shown in Fig. 2.10.

moving a charge on a background of flux (or alternatively, moving the monopole through the Dirac sea). The resulting transformations are shown in Table 2.3. The monopole quantum numbers were calculated by Song *et al.* (2019, 2020) using complementary numerical and spinon band topology-based analyses. The latter makes evident how non-trivial monopole quantum numbers follow from the distribution of gauge charges in the system's unit cell. The relevant inverse unit vectors and high-symmetry momenta are shown in Fig. 2.10(b). Importantly, we see that all of the monopoles transform under lattice symmetries. This is different to the case of the square lattice, where we claimed there is a trivial monopole in the  $SU(4)$  representation **1**. This trivial monopole could simply be added to the action, leading to Polakov confinement because it did not transform under lattice symmetries. The absence of such a trivial operator on the triangular lattice opens the door to the possibility of a stable Dirac spin liquid ground state.

Let us take a closer look at the symmetry properties in Table 2.3 and then use it to map the monopoles to lattice operators. The three spin-triplet monopoles  $\mathcal{S}_\alpha = \Phi_{\alpha+3}$ ,  $\alpha = 1, 2, 3$  transform identically as order parameters for antiferromagnetic 120-degree order. They are time-reversal odd, and transform under lattice translations with the momentum  $\mathbf{K}$ . The exact mapping between spin density and the spin-triplet monopoles, is given via

$$S_i^\alpha \simeq \text{Re}[i\mathcal{S}_\alpha(\mathbf{r}_i) e^{i\mathbf{K} \cdot \mathbf{r}_i}]. \quad (2.135)$$

Here, the components  $\alpha = 1, 2, 3$  denote the three  $SU(2)_{\text{spin}}$  components  $x, y, z$ . This mapping is defined up to a global multiplicative constant, not fixed by symmetry. We will call this constant  $\alpha_S$ , when necessary. We neglect possible multi-spin terms which may have the same transformation properties.

Next, the three valley-triplet, spin-singlet monopoles  $\mathcal{D}_\alpha = \Phi_\alpha$ ,  $\alpha = 1, 2, 3$  carry the same quantum numbers as order parameters of valence-bond solids. The phases they pick up under translations show that they have lattice momenta  $\mathbf{X}_\alpha = -\mathbf{K}_\alpha/2$ . These are shown in red in Fig. 2.10(a). We can identify the mapping between dimer order parameters  $D_a(\mathbf{r}_i)$  and spin-singlet monopoles, via

$$D_\alpha(\mathbf{r}_i) = \vec{S}_{\mathbf{r}_i} \cdot \vec{S}_{\mathbf{r}_i + \delta_\alpha} \simeq s_\alpha \text{Re}[\mathcal{D}_\alpha(\mathbf{r}_i) e^{i\mathbf{X}_\alpha \cdot \mathbf{r}_i}], \quad (2.136)$$

where we introduce the sign factors  $s_\alpha = +1, +1, -1$ . Note that the relative sign between  $\mathcal{D}_{1,2}$  and  $\mathcal{D}_3$  is due to the different  $\tau$  matrices appearing in the projective symmetry transfor-

mations of the fermions under translation (2.128) (Song *et al.*, 2020). The bonds  $\delta_\alpha$  identify three bond directions, as shown in Fig. 2.10(a). Again, this leading order mapping will be defined up to a constant, which we refer to as  $\alpha_{\mathcal{D}}$  when necessary.

The above analysis again lets us interpret the Dirac spin liquid as a mother, or unifying description, of competing orders (Hermele *et al.*, 2005; Song *et al.*, 2019). The competing order parameters are neatly encoded in the monopole operators. The correlations of these monopoles will once again lead to algebraic correlations of these order parameters in the spin liquid. Using the mappings (2.135), we can evaluate spin-spin correlation functions

$$\langle S_i^i S_j^{i'} \rangle \simeq \text{Re}[e^{i\mathbf{K} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle \mathcal{S}^i(\mathbf{r}_i)^\dagger \mathcal{S}^{i'}(\mathbf{r}_j) \rangle]. \quad (2.137)$$

Importantly, this correlation function is taken at equal times. We know from the CFT results that this correlation function is completely fixed as a power law,

$$\langle \mathcal{S}^i(\mathbf{r}_i)^\dagger \mathcal{S}^{i'}(\mathbf{r}_j) \rangle = \delta^{ii'} \langle \Phi^\dagger(\mathbf{r}_i) \Phi(\mathbf{r}_j) \rangle \sim \delta^{ii'} |\mathbf{r}_i - \mathbf{r}_j|^{-2\Delta_\Phi}, \quad (2.138)$$

where  $\Delta_\Phi$  is the monopole scaling dimension. We bring together Eqns. (2.137) and (2.138) to get

$$\langle S_i^z S_j^z \rangle \sim \text{Re} \left[ e^{i\mathbf{K} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|^{2\Delta_\Phi}} \right]. \quad (2.139)$$

The correlation function  $\langle S_i^z S_j^z \rangle$  is algebraic with an oscillating phase  $\cos(\mathbf{K} \cdot (\mathbf{r}_i - \mathbf{r}_j))$ . The same calculation follows for the dimer-dimer correlations via Eq. (2.136):

$$\langle D^\alpha(\mathbf{r}_i) D^\beta(\mathbf{r}_j) \rangle \simeq \text{Re}[e^{i\mathbf{X}_\alpha \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle \mathcal{D}^\alpha(\mathbf{r}_i)^\dagger \mathcal{D}^\beta(\mathbf{r}_j) \rangle]. \quad (2.140)$$

$$\sim \delta^{\alpha\beta} \text{Re} \left[ e^{i\mathbf{X}_\alpha \cdot (\mathbf{r}_i - \mathbf{r}_j)} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|^{2\Delta_\Phi}} \right] \quad (2.141)$$

Both the spin-spin and dimer-dimer correlation functions have power-law decays with a *universal* exponent. The equality of the exponent for both static correlators is a key prediction of the conformal field theory description of QED<sub>3</sub>. It is also a signature of the emergent SU(4) symmetry at low energies.

### Stability and conformal data

Let us now confirm that the state is stable on the triangular lattice. To do this rigorously, we must check that there are no relevant, symmetry-allowed perturbations. First, let us check that this is true for the monopoles. We have already shown that the  $q = 1$  monopoles satisfy this (this can be most trivially seen because they have finite lattice momentum). Now we can consider the  $q = 2, 3$  monopoles, which insert  $4\pi$  and  $6\pi$  of flux. First, note that the scaling dimensions in the large- $N_f$  expansion are given by (Pufu, 2014; Dyer *et al.*, 2013; Chester and Pufu, 2016a)

$$\Delta_\Phi = 0.265N_f - 0.038 \approx 1.02, \quad (2.142)$$

$$\Delta_{\Phi\Phi} = 0.673N_f - 0.194 \approx 2.50, \quad (2.143)$$

$$\Delta_{\Phi\Phi\Phi} = 1.186N_f - 0.422 \approx 4.32. \quad (2.144)$$

Numerical quantum Monte Carlo studies of lattice QED<sub>3</sub> imply that  $\Delta_{\Phi\Phi} > 3$  is already irrelevant (Karthik and Narayanan, 2019, 2024). On the triangular lattice, the lowest-order symmetry-allowed operator constructed from many monopoles is

$$\lambda(\Phi_1\Phi_2\Phi_3 + \text{h.c.}). \quad (2.145)$$

The symmetry transformation of this composite operator can be checked by hand using Table 2.3. It is useful to briefly note that a prerequisite for this object being trivial under lattice symmetries is the absence of a phase under translation. This triple monopole has a momentum equal to zero  $\mathbf{X}_1 + \mathbf{X}_2 + \mathbf{X}_3 = 0$ . Double monopoles will always have momenta at the  $\mathbf{M}$  or  $\mathbf{K}$  points, and must thus be excluded from the continuum theory.

The reader might notice that there is an operator (constructed from monopoles) which does satisfy this condition:  $\Phi_a^\dagger\Phi_a$ . However, caution is advised in interpreting this as a monopole operator. The topological charge of this composite operator under  $U(1)_{\text{topo}}$  is zero  $q = 0$ . In fact in conformal field theory, we should think about the two monopoles fusing through the operator product expansion to form another operator. The operators in the charge-zero sector can be categorised by their  $SU(4)$  irreducible representation. The monopole-antimonopole lives in several of these:  $\mathbf{6} \otimes \mathbf{6} = \mathbf{1} + \mathbf{15} + \mathbf{20}$ , where  $\mathbf{15}$  is the adjoint and  $\mathbf{20}'$  the 20-dimensional traceless symmetric irrep (He *et al.*, 2022; Zhang *et al.*, 2025). The charge-zero sector can be understood in terms of fermion operators. We list these operators, following Chester and Pufu (2016a,b):

- The trivial irrep  $\mathbf{1}$  contains the parity-even singlets  $(\bar{\psi}\psi)^2$  and  $f_{\mu\nu}^2$ . These have scaling dimension

$$\Delta_{\mathbf{1},0} = 4 + \frac{64(2 - \sqrt{7})}{3\pi^2 N_f} \approx 3.65. \quad (2.146)$$

This is constructed from the trace element of the monopole OPE  $\sum_a \Phi_a^\dagger\Phi_a$ .

- The antisymmetric combinations of  $\Phi_a^\dagger\Phi_b$  produce fermion bilinears in the adjoint representation,  $M_{ij}$ . A form of this OPE was written down by (Luo *et al.*, 2022). As already written in Eq. (2.95), this has the scaling dimension  $\Delta_M = 1.46$  in the large- $N_f$  approximation.
- The traceless symmetric irrep  $\mathbf{20}'$  contains four-fermion interactions, including  $SU(2)$ -symmetric terms  $(\bar{\psi}\vec{\sigma}\psi)^2$  (Xu, 2008; Xu and Sachdev, 2008; Jian *et al.*, 2018). These have scaling dimension

$$\Delta_{\mathbf{20}',0} = 4 - \frac{64}{\pi^2 N_f} \approx 2.38, \quad (2.147)$$

and are hence relevant in the large- $N_f$  approximation.

- Finally, there is another class of strongly-irrelevant four-fermion interactions in  $\mathbf{84}$ . These come from higher order  $\Phi^\dagger\Phi^\dagger\Phi\Phi$  operators, but we will ignore them here.

The four-fermion terms in  $\mathbf{1}$ ,  $\mathbf{20}'$ , and  $\mathbf{84}$  are symmetry-allowed in the lattice model, and must therefore be irrelevant if the spin liquid is to be stable. As discussed briefly in Section 2.2.2, the fact that the fermion interactions  $(\bar{\psi}\vec{\sigma}\psi)^2$  are relevant could lead to a potential

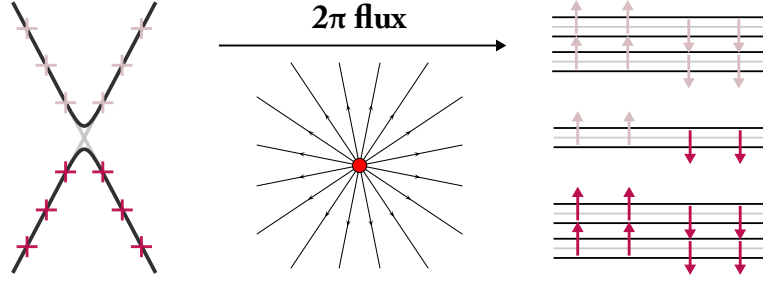


**Figure 2.11:** *Splitting of the fermion zero mode levels.* The fermion mass  $m_z$  splits the  $\uparrow\downarrow$  degeneracy, attaching two down-spin zero modes to every flux. This leads to in-plane magnetic order after monopole proliferation.

spontaneous symmetry breaking of the conformal fixed point. We repeat the point here that other recent approaches seem to point towards this operator being irrelevant, including the epsilon expansion (Pietro and Stamou, 2017) and numerical works (Karthik and Narayanan, 2016a,b). This highlights the need to go beyond the large- $N_f$  approximation for quantum magnets with  $N_f = 4$ .

As a final exercise, let us consider the effect of applying a perturbation by tuning an irrelevant four-fermion (Gross–Neveu) interaction  $(M_{ij})^2$ . Depending on which matrix elements are present, this will select some chiral mass term  $M_{ij}$  to condense. The gapped state will undergo Polyakov confinement and lead to a conventionally ordered state (Song *et al.*, 2019). To understand how this transition can occur, let us decouple the chiral spin interaction using an auxiliary field<sup>7</sup>

$$h^2(\bar{\psi}\vec{\sigma}\psi)^2 = (\bar{\psi}\vec{\sigma}\psi) \cdot \vec{\varphi} + \frac{1}{h^2}\vec{\varphi}^2. \quad (2.148)$$

Then as we take the mass of the boson to zero  $1/h^2 \rightarrow 0$ , the effective interaction  $h^2$  diverges and the boson condenses  $\langle\varphi\rangle \neq 0$ . As soon as there is a finite order mass for the fermions, the degeneracy of the fermion zero modes is broken (Song *et al.*, 2019; Dupuis *et al.*, 2019). For example, if the mass  $M_{30}$  is precipitated, the  $\uparrow\uparrow$  and  $\downarrow\downarrow$  states from Fig. 2.6 are split. The result is that the each monopole comes with the  $\downarrow\downarrow$  states filled. This is shown in Fig. 2.11, and described by the wavefunction  $(Z^-)^{\alpha\beta}c_{+,\alpha}^\dagger c_{-,\beta}^\dagger$ . This then selects an ordered state. Because the fermions are now gapped, the monopoles confine via the Polyakov mechanism. Eq. (2.133) then associates a finite monopole density  $\langle\mathcal{M}\rangle$  with in-plane magnetic order, given by

$$\langle S^- \rangle = \langle S^1 + iS^2 \rangle \neq 0. \quad (2.149)$$

The mapping to spin operators (2.135) then tells us that this is a 120-degree ordered phase. Note that condensing different masses  $M_{ij}$  leads to different competing orders (Song *et al.*, 2019; Dupuis *et al.*, 2022).

<sup>7</sup>This is called a Gross–Neveu–Yukawa coupling in this form, where the boson has a UV completion including a kinetic term (Janssen and He, 2017; Dupuis *et al.*, 2019).

### Summary

Taking a step back, let us review the theoretical understanding we have built. We have investigated two Ansätze which have Dirac cone dispersion, on the square and triangular lattices. In the continuum limit, both realise a 2+1 dimensional version of quantum electrodynamics. We described how the operators in the theory transform as neighbouring order parameters. The difference between the two lattices is in the transformation properties of the monopoles. On the frustrated triangular lattice, all monopoles transform like competing order parameters, but on the square lattice there is a trivial monopole that destroys the phase.

Taken all together, the U(1) Dirac spin liquid is intrinsically stable on the triangular lattice. This relies on the analysis of all operators in the spectrum, checking that there are no symmetry-allowed perturbations to the conformal fixed point. The work of (Song *et al.*, 2019, 2020) was critical for this, as well as others who described the CFT operators and exponents (Pufu, 2014; Dyer *et al.*, 2013; Chester and Pufu, 2016a). This tells us that in theory, such a state could exist (McGreevy, 2019). However, much work still needs to be done to understand *where*. It is impossible to know *a priori* what sort of model will realise the conformal fixed point, and it is possible that even irrelevant operators could destabilise it in a real spin model. We will investigate several such mechanisms in this Thesis.

#### 2.3.2 Phase diagram of the $J_1$ – $J_2$ model

Now we will discuss another reason to be interested in the U(1) Dirac quantum spin liquid. In addition to the theoretical understanding of its intrinsic stability, there is a growing amount of numerical evidence which points to this state appearing in the  $J_1$ – $J_2$  Heisenberg model on the triangular lattice.

As discussed in the Introduction, this model has a maximally frustrated point at  $J_2/J_1 = 1/8$ . Classically, this represents a highly degenerate point. Although it was considered possible that quantum fluctuations would stabilise an intermediate liquid phase, a gapless spin liquid was seen as unlikely. This comes from the belief that U(1) quantum spin liquids would be unstable in first-order mean-field theory (Wen, 2004). However, a decade ago Kaneko *et al.* (2014) provided the first surprising numerical evidence of a gapless spin-disordered state in this model. This kicked off a series of works which muddled the waters. A set of numerical studies which used the density-matrix renormalisation group (DMRG) method pointed to a gapped spin liquid (Zhu and White, 2015; Hu *et al.*, 2015), whereas a variational Monte Carlo study suggested that actually the gapless U(1) Dirac spin liquid was the ground state (Iqbal *et al.*, 2016). This variational work importantly claims that the  $\pi$ -flux Ansatz has the lowest variational energy among the possible QSL Ansätze characterised by Lu (2016). This state, which has no free variational parameters, turns out to be remarkably stable to symmetry breaking or lowering of the U(1) gauge structure to  $\mathbb{Z}_2$  (Iqbal *et al.*, 2016). Despite disagreement regarding the nature of the QSL, the phase diagrams agree well, see Fig. 2.12. All competing methods find a QSL within the region approximately  $0.07 \lesssim J_2/J_1 \lesssim 0.16$ . Furthermore, there was consensus that the QSL–stripe order transition is first order, and the QSL–120-degree order transition could be continuous.

The tension between the competing methods was resolved when Hu *et al.* (2019) showed that the apparent measured gap was definitively due to a finite-size effect. To summarise the

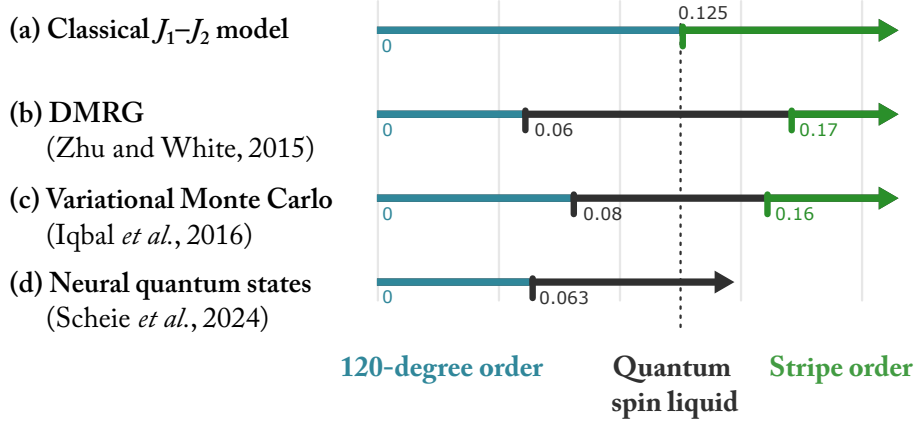


**Figure 2.12:** *Numerical phase diagram of the  $J_1$ - $J_2$  Heisenberg model on the triangular lattice.* We show the numerical values of the transitions as found by Zhu and White (2015); Iqbal *et al.* (2016); Scheie *et al.* (2024). (a) Classical phase diagram of the model; first-order transition from 120-degree to stripe magnetic order at  $J_2/J_1 = 1/8$ . Numerical results using (b) density matrix renormalisation group (DMRG), (c) variational Monte Carlo, and (d) neural quantum states. All methods find a continuous transition from liquid to 120-degree order; the transition to stripe order in (b,c) is first order. The final work (d) does not specify the stripe transition point.

problem, the DMRG calculations are performed on a highly anisotropic cylindrical geometry. Depending on the boundary conditions used, it is possible that the discretised Brillouin zone does not pass through the gapless points  $\mathbf{K}$  and  $\mathbf{M}$ . By properly twisting the boundary conditions to access these points, they were able to show that the DMRG simulation predicts a gapless state. In fact, they claim the state is also compatible with the U(1) Dirac Ansatz.

Each of these methods have different limitations. On the one hand, DMRG struggles with representing highly entangled states, and is typically restricted to anisotropic cylinder geometries on two-dimensional lattices. While new methods like projected-entangled pair states (PEPS) promises to solve some of these issues (Verstraete and Cirac, 2004), the computational cost still severely limits its application to frustrated magnets (Liu *et al.*, 2021). On the other hand, variational Monte Carlo has the fundamental problem that one risks being biased towards the state written in the Ansatz. The introduction of the the Jastrow factor can help describe competing ordering tendencies, but there is still a risk of bias (Iqbal *et al.*, 2016). Encouragingly, a new related method has arisen which serves to confirm the previous works: Deep neural quantum states. This method is based on the variational method to optimise the wavefunction. However, the storage of the wavefunction in a neural network permits the efficient handling of many more variational parameters, on the order of  $10^6$ , reducing the risk of bias. Returning to the  $J_1$ - $J_2$  model, two works have studied the spin liquid at the  $J_2/J_1 = 1/8$  point and concluded it has a gapless ground state (Roth *et al.*, 2023; Chen and Heyl, 2024).

Another fruitful line of numerical work has been investigating the *dynamics* of this quantum spin liquid on the triangular lattice (Ferrari and Becca, 2019; Drescher *et al.*, 2023;

Sherman *et al.*, 2023). Energy-resolved measurements of the quasiparticle spectrum provide more insight into the nature of the excitations (Hu *et al.*, 2019). These numerical works find low-energy features around both the  $M$  and  $K$  points, consistent with the predictions for the U(1) Dirac QSL state. It is not yet possible to exactly determine the nature of the low-lying excitations, with some degree of informed speculation being necessary for the interpretation of results.

Wietek *et al.* (2024) provide a more quantitative picture which seems to wholly support this perspective of quantum electrodynamics ‘as the organising principle’ of the triangular lattice  $J_1$ – $J_2$  model (Starykh, 2024). They perform exact diagonalisation on clusters with up to 48 sites, and directly compare the states in the spectrum to those predicted by QED<sub>3</sub>. This comparison begins by constructing the possible wavefunctions for fermion bilinear and monopole excitations in the QED<sub>3</sub> spectrum. Next, they calculate the overlap with all states in the very dense<sup>8</sup> numerical spectrum. The results show remarkable agreement. At the point  $J_2/J_1 = 1/8$ , the ground state has a 92% overlap with the QED<sub>3</sub> vacuum. That is despite the Hilbert space dimension being on the order  $2^{48} \approx 10^{14}$ . Furthermore, almost every low-lying state has a finite overlap with the trial excitation wavefunctions (without any variational parameters).<sup>9</sup> As expected from the field theory, there are two classes of monopoles: spin-triplet monopoles with momentum  $K$ , and spin-singlet monopoles with momentum  $X$ . The wavefunction overlaps in this sector reach 67%. Finally, Budaraju *et al.* (2025) study this same problem variationally on larger system sizes. They measure the same quantum numbers for monopoles, and project that they are gapless in the thermodynamic limit.

## 2.4 Open questions

This body of understanding serves as the starting point for our research. Before beginning, we will now briefly outline what is *not understood*. Firstly, it remains a challenge to make concrete predictions for experimental signatures of the U(1) Dirac spin liquid. Despite much numerical effort, it remains a challenge to interpret the results of simulations. It is even harder to make connection with experiment. To highlight a concrete example, we can ask a simple question: do numerics show algebraic correlations and an emergent SU(4) symmetry? We provide our first results in Fig. 2.13, a numerical calculation of the spin-spin and dimer-dimer correlation functions of the  $J_1$ – $J_2$  Heisenberg model on the triangular lattice at the maximally frustrated point. The field-theoretical predictions of Section 2.3.1 tell us that the monopoles should control the algebraic decay of both correlation functions. Furthermore, the emergent SU(4) symmetry fixes the exponents to be equal. We note that this is *not clearly* observed in the simulations. Although the dimer-dimer correlation functions are a clear power law, suggesting monopole exponent  $\Delta_\Phi = 1.20(3)$ , the spin-spin correlation function is dominated by another feature. It is possible that the algebraic correlations take over at longer distances. However, we point out that the difference between the monopole model, the shaded gray area, describes 90% of the total correlations. Explaining this result will be our initial focus in the next Chapter 3.

<sup>8</sup>On a cluster  $N = 48$ , they find on the order of 100 states below energy  $J_1$ . This is a sign of high frustration.

<sup>9</sup>Curiously the overlaps are even large in the ordered phases.

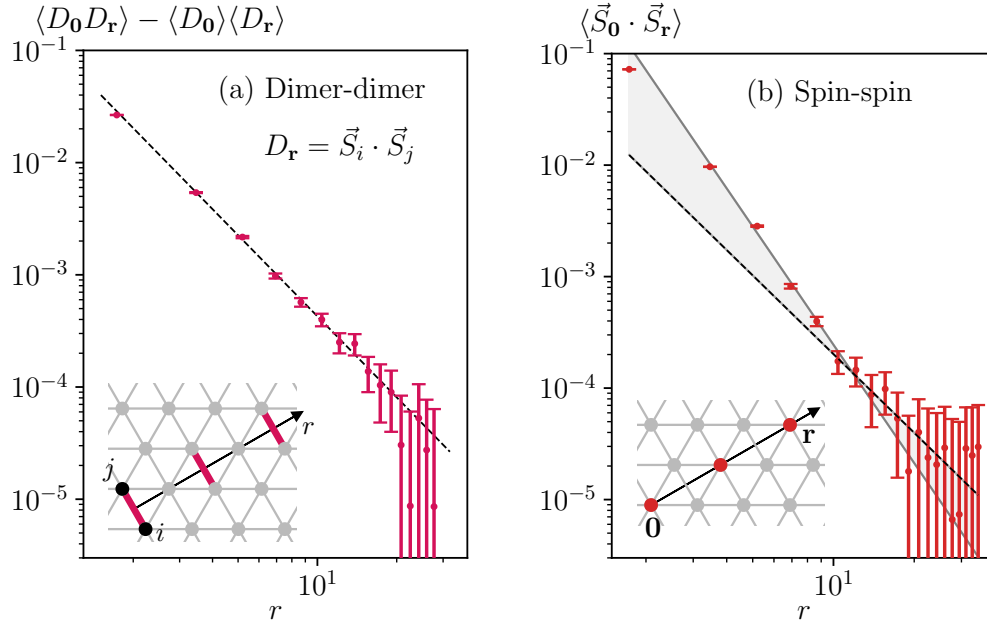


**Figure 2.13:** *Dimer-dimer and spin-spin correlation functions of the U(1) Dirac spin liquid.* Measured on a  $J_2 = J_1/8$  Heisenberg model on the triangular lattice using variational Monte Carlo; see Appendix C. Both correlation functions along the path which cancels any oscillating phase associated with the  $\mathbf{K}$  or  $\mathbf{X}$  momenta. (a) Dimer-dimer correlations (on the  $L = 42$  cluster) show a clear algebraic behaviour. Black dashed-line is a fitted power law  $r^{-2\Delta}$  with  $\Delta = 1.20(3)$ . (b) Spin-spin correlations (on the  $L = 60$  cluster) show a mixed behaviour; there is a dominant feature at low- $r$  and a possible sub-leading power-law tail. We fit successive intervals piecewise to power laws, with the two extremal gradients plotted. Black dashed-line is the minimal fitted power law  $r^{-2\Delta}$  with  $\Delta = 1.17(30)$ .

Expanding to consider spin liquids more generally, predictions for the quasiparticle spectrum and dynamical structure factor are only known in certain fine-tuned cases. We want to expand this to more general spin liquids, by using a toolbox that can be applied to any of the parton mean-field states, categorised by Wen (2002).

In addition, very little is understood about the stability of algebraic spin liquids beyond mean-field theory. To this end, we return to our points from Section 1.2.

- i. The wavefunction of the U(1) Dirac QSL is the  $\pi$ -flux mean-field Ansatz in the Abrikosov parton representation.
- ii. This is stable at first-order mean-field theory. Monopole proliferation is forbidden by the lattice symmetries (Song *et al.*, 2019, 2020).
- iii. Mean-field theory cannot predict the phase diagram of spin Hamiltonians. It widely overestimates the stability of QSL phases. In our case, the  $\pi$ -flux Ansatz is a valid

mean field for all values of  $J_2$ , which is in strong disagreement with the numerical results of Fig. 2.12.

- iv. Very little has been studied regarding the stability of the U(1) Dirac QSL to experimental perturbations. We are only aware of the studies which think about the influence of disorder on the conformal fixed point (Thomson and Sachdev, 2017; Dey, 2020).

Where should we look for gapless spin liquids, and how can we measure their signatures beyond mean-field theory? This will be the focus of the rest of the Thesis. We will see that dynamical signatures provide an especially valuable insight into the properties of this spin liquid.

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## Introduction

What are the signatures of critical quantum spin liquids in experiment? We have introduced the U(1) Dirac quantum spin liquid in Chapter 2, taking two different perspectives. On the one hand, we described it as a mean-field state that emerges from the  $\pi$ -flux Ansatz on the triangular lattice. This is a ‘high-energy’ picture, in the sense that it is a lattice-scale model valid up to high energies. On the other hand, we covered the more recent field-theoretic description of the ground state. Here, we showed that the model flows to a conformally-invariant ground state in the IR limit. This motivates a particularly compelling comparison to 1D spin chains, which have an equivalent description in terms of a conformal fixed point with relevant instantons that carry quantum numbers of competing orders. This continuum model has clear implications for the spectrum, but is strictly only applicable at low energies and long wavelengths. The relevant regime of validity is not known, i.e. below which energies it might appear. The conformal field theory should have measurable consequences for experimental and numerical works alike. We aim to make concrete predictions in this Chapter that support the measurement of this exotic type of quantum spin liquid.

How can these high- and low-energy pictures be united? This will be the starting point for the present Chapter. We solve this outstanding problem by noting a crucial aspect: fermion interactions are strong and controlled by lattice-scale physics. They may be irrelevant in the CFT perspective, but they are by no means irrelevant for the physics of the model. Rather, we will show that their consideration will allow us to extend mean-field theory in two ways. First, interactions lead to the formation of a new mode that dominates the spectral response at high frequency. Second, interactions control the stability of the mean-field Ansatz. Recall that the mean-field energy is agnostic to the next-nearest neighbour Heisenberg exchange  $J_2$ . However, we discussed in Chapter 1 that such an interaction is necessary to stabilise a liquid state. The resolution is that this interaction affects the dynamical stability of the state only beyond mean-field theory. We treat these two effects perturbatively using the random phase approximation. The results are in remarkable agreement with numerical studies of the  $J_1$ – $J_2$  Heisenberg model.

This Chapter is based on work in the preprint Willsher and Knolle (2025). It relies heavily on code written and techniques learned during a previous related project, Willsher, Jin, and Knolle (2023). Here, we studied the Hubbard model of interacting electrons on a triangular lattice. The structure of this Chapter is as follows. We first make two simple attempts at describing the dynamical response of the U(1) Dirac QSL state, and highlight their limitations. These are the conformal field theory and mean-field approaches. We identify fermion interactions as a key missing ingredient of the latter model, and then attempt to account for them at high energies using a diagrammatic technique. We first ignore the

gauge fluctuations necessary for a consistent low-energy description, but add them back after lattice-scale interactions have been taken into account. This approach allows us to describe the phase diagram of the  $J_1$ - $J_2$  model and predict the universality of critical points in our model. Finally, we discuss the generality of our approach by applying it to the chiral spin liquid. This is generated by a more complex three-spin interaction term, which we show is able to be approximately treated in our method.

### 3.1 Dynamical structure factor

To evaluate the dynamical structure factor, we first make use of the fluctuation-dissipation theorem (Auerbach, 1998). This relates the spectral function (which measures fluctuations) to the imaginary part of the dynamical spin susceptibility (which measures dissipative response). The theorem states

$$S(\mathbf{q}, \omega) = \text{Im } \chi(\mathbf{q}, \omega), \quad (3.1)$$

where the susceptibility is defined in terms of the retarded correlation function  $S_{ij}(t)$  using the Kubo formula. In imaginary time  $\tau = it$ , the susceptibility reads

$$\chi(\mathbf{q}, i\omega_n) = \frac{1}{N} \sum_{ij} e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \int d\tau e^{-i\omega_n \tau} S_{ij}(\tau), \quad (3.2)$$

where the time-ordered Green's function is

$$S_{ij}(\tau) = \langle T_\tau S_i^z(\tau) S_j^z(0) \rangle. \quad (3.3)$$

This form will be more amenable to computing correlation functions of CFT operators and fermions. After evaluating correlation functions in this basis, we may then analytically continue the frequencies back to real time  $i\omega \rightarrow \omega + i\eta$ .

#### 3.1.1 Monopoles in QED<sub>3</sub>: Low-energy response

We can calculate the contribution of monopoles to the dynamical susceptibility. We use the mapping Eq. (2.135) from spin operators to spin-triplet monopoles  $\mathcal{S} = \mathcal{S}_3$ . Substituting into the time-ordered correlation function, we get

$$\chi_S(\mathbf{q}, i\omega_n) = \frac{1}{N} \sum_{ij} e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \int d\tau e^{-i\omega_n \tau} \langle T_\tau S_i^z(\tau) S_j^z(0) \rangle, \quad (3.4)$$

$$= \frac{1}{N} \sum_{ij} e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \int d\tau e^{i\omega_n \tau} e^{-i\mathbf{K} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle \mathcal{S}^\dagger(\mathbf{r}_i, \tau) \mathcal{S}(\mathbf{r}_j, 0) \rangle. \quad (3.5)$$

Next we use translational invariance and perform the sum over  $j$  to yield

$$\chi_S(\mathbf{q}, i\omega_n) = \sum_i \int d\tau e^{-i(\mathbf{q} - \mathbf{K}) \cdot \mathbf{r}_i - i\omega_n \tau} \langle \mathcal{S}^\dagger(\mathbf{r}_i, \tau) \mathcal{S}(\mathbf{0}, 0) \rangle. \quad (3.6)$$

We can change variables to space-time coordinates  $x = (\tau, \mathbf{r}_i)$  in Euclidian space (imaginary time). We define the relative momentum  $q = (\omega_n, \mathbf{K} - \mathbf{q})$  and substitute the two-point function of the CFT operators

$$\chi_S(\mathbf{q}, i\omega_n) = \int d^3x e^{-iq \cdot x} \langle \mathcal{S}^\dagger(x) \mathcal{S}(0) \rangle, \quad (3.7)$$

$$= \int d^3x e^{-iq \cdot x} |x|^{-2\Delta_\Phi} = c |q|^{2\Delta_\Phi - 3}, \quad (3.8)$$

where  $c = \pi^{2\Delta_\Phi - 3/2} \Gamma(3/2 - \Delta_\Phi) / \Gamma(\Delta_\Phi)$  when  $0 < \Delta_\Phi < 3/2$ . This integral is simply the Fourier transform of a power law, which is therefore another power law. Writing the components explicitly,

$$\chi_S(\mathbf{q}, i\omega_n) = \frac{c}{(|\mathbf{K} - \mathbf{q}| + \omega_n^2)^{3/2 - \Delta_\Phi}}, \quad (3.9)$$

we can analytically continue back to real-frequency (when  $\omega > 0$ ) by taking  $i\omega_n \rightarrow \omega + i\eta$ . The spin susceptibility due to the monopoles is

$$\chi_S(\mathbf{q}, \omega + i\eta) = \frac{c}{(|\mathbf{K} - \mathbf{q}|^2 - \omega^2 - i\eta)^{3/2 - \Delta_\Phi}} = S^z \text{~~~~~} S^z. \quad (3.10)$$

In this Feynman diagram, we represent the monopole propagator as a wavy line. By taking the imaginary part, this produces the contribution of monopoles to the dynamical structure factor

$$S(\mathbf{q}, \omega) = \text{Im } \chi_\Phi(\mathbf{q}, \omega + i\eta) = \text{Im} \left[ \frac{c}{(|\mathbf{K} - \mathbf{q}|^2 - \omega^2 - i\eta)^{3/2 - \Delta_\Phi}} \right]. \quad (3.11)$$

This result resembles the spectral function across quantum critical transitions in one dimension where the quasiparticle picture breaks down (Hermele *et al.*, 2008). It is also equivalent to the result for the Luttinger liquid Eq. (2.34) when one replaces the exponents  $3/2 - \Delta_\Phi \rightarrow 1 - K_*$ .

This expression Eq. (3.11) for the susceptibility is the one that will be computed and worked with going forward. We briefly evaluate the imaginary part explicitly to show that there is a closed-form expression for the result. Firstly, write the magnitude of momentum transfer  $\delta q = |\mathbf{q} - \mathbf{K}|$  and note that (3.11) is purely real<sup>1</sup> if  $\delta q > |\omega|$ ; this will be responsible for the lightcone structure in  $S(\mathbf{q}, \omega)$ . We rewrite the susceptibility as a complex logarithm

$$(\delta q^2 - \omega^2 - i\eta)^{-(3/2 - \Delta_\Phi)} = e^{-(3/2 - \Delta_\Phi) \log(\delta q^2 - \omega^2 - i\eta)}, \quad (3.12)$$

which we can evaluate on the principle branch (we take the branch cut along the negative real axis)

$$\log(\delta q^2 - \omega^2 - i\eta) = \begin{cases} \log|\delta q^2 - \omega^2| & \delta q > |\omega|, \\ \log|\delta q^2 - \omega^2| - i\pi & \delta q < |\omega|. \end{cases} \quad (3.13)$$

<sup>1</sup>Up to the vanishing infinitesimal constant which we take to zero  $\eta \rightarrow 0^+$ .

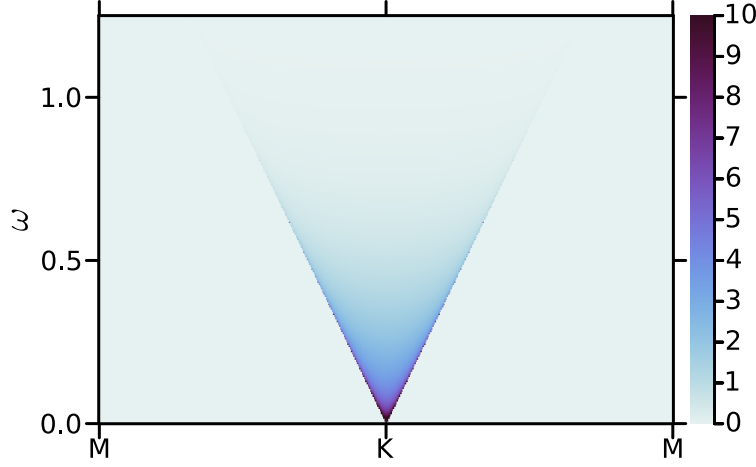


**Figure 3.1:** *Monopole contribution to the dynamical structure factor  $S(\mathbf{q}, \omega)$ .* The calculation is done within the low-energy conformal field theory. Energy  $\omega$  is in units of  $J_1$ .

Therefore we have

$$S(\mathbf{q}, \omega) = c \operatorname{Im} \exp\{-(3/2 - \Delta_\Phi) [\log|\delta q^2 - \omega^2| - i\pi \theta(\omega^2 - \delta q^2)]\} \quad (3.14)$$

$$= c \operatorname{Im} \left[ e^{i\pi(3/2 - \Delta_\Phi) \theta(\omega^2 - \delta q^2)} |\delta q^2 - \omega^2|^{-3/2 + \Delta_\Phi} \right]. \quad (3.15)$$

Finally, we get the structure factor by taking the imaginary part

$$S(\mathbf{q}, \omega) = \theta(\omega^2 - \delta q^2) \frac{c \sin[\pi(3/2 - \Delta_\Phi)]}{|\omega^2 - \delta q^2|^{3/2 - \Delta_\Phi}}. \quad (3.16)$$

This momentum-resolved structure factor is plotted in Fig. 3.1, where we have taken  $\Delta_\Phi = 1.25$ . At the  $\mathbf{K}$  point,  $\delta q = 0$ , the structure factor diverges as a power law

$$S(\mathbf{K}, \omega) \sim \omega^{2\Delta_\Phi - 3}. \quad (3.17)$$

The lightcone structure is enforced by the step function, and the divergence as  $\omega \rightarrow |\delta q|$  is  $\sim |\omega - \delta q|^{\Delta_\Phi - 3/2}$ .

This result is derived using the limit of large distances compared to the lattice spacing, where the continuum theory holds. It consequently describes the limiting behavior as  $\omega \rightarrow 0$ . At lattice-scale distances, the monopole (diverging) correlation function must be cut-off by a UV regulator. In the corresponding regime  $\omega \sim J_1$ , we therefore suppress the correlation function, such that its Fourier transform converges as  $r \rightarrow 0$ . We implement this simply using a Gaussian cutoff in our calculations of the monopole susceptibility where we take the lattice-scale to be  $\omega_l = 0.5 J_1$ .

### 3.1.2 Free fermions in mean-field theory: High-energy response

We now turn to a high-energy, lattice-scale calculation of the spin structure factor. We will first calculate the spinon contribution in the mean-field approximation. In contrast to

the monopoles, the spinons are not gauge-invariant objects. This means we must perform our calculation within a specific gauge. In particular, we must worry about the sublattice structure of the mean-field Ansatz. Moving Eq. (3.2) into momentum space, in the sublattice  $X = A, B$  basis, we define the matrix elements

$$[\chi(\mathbf{q}, i\omega)]^{XY} = \frac{1}{N} \int d\tau e^{-i\omega\tau} \langle T_\tau S_{X,\mathbf{q}}^z(\tau) S_{Y,-\mathbf{q}}^z(0) \rangle. \quad (3.18)$$

We can get the total susceptibility (3.2) by summing over sublattices including a relative phase. This gives the gauge-invariant result

$$\chi(\mathbf{q}, i\omega) = \sum_{X,Y=A,B} e^{-i\mathbf{q} \cdot (\mathbf{r}_X - \mathbf{r}_Y)} [\chi(\mathbf{q}, i\omega)]^{XY}, = \vec{R}_\mathbf{q}^\dagger \cdot [\chi(\mathbf{q}, i\omega)] \cdot \vec{R}_\mathbf{q}, \quad (3.19)$$

with the vector

$$\vec{R}_\mathbf{q} = \begin{pmatrix} 1 \\ e^{-i\mathbf{q} \cdot \delta_{AB}} \end{pmatrix} = \begin{pmatrix} 1 \\ e^{-ik_1/2} \end{pmatrix}, \quad (3.20)$$

where  $\delta_{AB}$  is the offset of the  $B$  site in the unit cell and  $k_j = \mathbf{q} \cdot \mathbf{q}_j$ , as defined in Eq. (2.121). Finally, the structure factor is the imaginary part  $S(\mathbf{q}, \omega) = \text{Im } \chi(\mathbf{q}, \omega)$ .

To proceed, represent the spin operator  $S^z$  in the Abrikosov fermion representation

$$S_{X,\mathbf{q}}^z = \frac{1}{2} \sum_{\mathbf{k}} f_{\alpha X,\mathbf{k}}^\dagger (\sigma^z)_{\alpha\beta} f_{\beta X,\mathbf{k}+\mathbf{q}}, \quad (3.21)$$

$$= \frac{1}{2} \sum_{\mathbf{k}} \Psi_\mathbf{k}^\dagger \cdot (\sigma_X^z) \cdot \Psi_{\mathbf{k}+\mathbf{q}}. \quad (3.22)$$

Here, we move into the combined index  $m = (\alpha, X)$ . The sublattice Pauli matrix  $\sigma_X^z$  only has non-zero elements when  $m, n$  are in sublattice  $X$ . In other words,  $\sigma_X^z = \sigma^z \otimes P_X$ , where  $P_A = \text{diag}(1, 0)$  and  $P_B = \text{diag}(0, 1)$  are the projectors onto the  $A, B$  sublattices.

The susceptibility matrix Eq. (3.18) can be written as the following four-fermion correlation function

$$\begin{aligned} [\chi(\mathbf{q}, \omega)]^{XY} &= \frac{1}{2} \sigma_X^z \text{---} \text{---} \text{---} \frac{1}{2} \sigma_Y^z \\ &= \frac{1}{4N} (\sigma^z)_{\alpha\beta} (\sigma^z)_{\gamma\delta} \int d\tau e^{-i\omega\tau} \sum_{\mathbf{k}} \langle T_\tau [f_{\alpha X,\mathbf{k}}^\dagger f_{\beta X,\mathbf{k}+\mathbf{q}}](\tau) [f_{\gamma Y,\mathbf{k}'}^\dagger f_{\delta Y,\mathbf{k}'-\mathbf{q}}](0) \rangle. \end{aligned} \quad (3.23)$$

This susceptibility matrix still has sublattice indices  $XY$ , since it is defined in momentum space in terms of gauge-dependent fermions. This object itself should however be gauge invariant since it represents a physical observable.

### Bare susceptibility

In the mean-field approximation, we can evaluate the four-fermion susceptibility by assuming non-interacting fermions. This neglects gauge fluctuations, as well as the Heisenberg

interactions which generated our mean-field Hamiltonian. In a diagrammatic language, the susceptibility gets a contribution from the free fermion bubble

$$[\chi^0(\mathbf{q}, \omega)]^{XY} = \frac{1}{2} \sigma_X^z \text{---}\text{---}\text{---} \frac{1}{2} \sigma_Y^z \quad (3.24)$$

The opposing fermion Green's functions carry momenta  $\mathbf{k}$  and  $\mathbf{k} + \mathbf{q}$ . Given that we are measuring longitudinal  $\sigma^z$  spin fluctuations, the fermions carry equal spin  $\uparrow, \downarrow$ . The calculation of this free four-fermion correlation function is shown in Appendix A. The result as a function of real frequency reads

$$[\chi^0(\mathbf{q}, \omega + i\eta)]^{XY} = -\frac{1}{4N} \sum_{\mathbf{k}, mn} \frac{(n_{\mathbf{k}}^m - n_{\mathbf{k}+\mathbf{q}}^n) \mathcal{V}_X^{mn} (\mathcal{V}_Y^{mn})^*}{\omega + \varepsilon_{\mathbf{k}}^m - \varepsilon_{\mathbf{k}+\mathbf{q}}^n + i\eta}. \quad (3.25)$$

The Fermi–Dirac occupation functions are  $n_{\mathbf{k}}^m = n_f(\varepsilon_{\mathbf{k}}^m)$  and the matrix elements are defined as

$$\mathcal{V}_X^{mn} = \vec{\alpha}_{\mathbf{k}}^\dagger \cdot (\sigma_X^z) \cdot \vec{\alpha}_{\mathbf{k}+\mathbf{q}} = (\alpha_{\mathbf{k}}^m)^*_{\alpha X} (\sigma^z)_{\alpha\beta} (\alpha_{\mathbf{k}+\mathbf{q}}^n)_{\beta X}, \quad (3.26)$$

in terms of the Hamiltonian (2.122) eigenvalues  $\alpha_{\mathbf{k}}^n$ . We calculate this complex susceptibility function Eq. (3.25) numerically<sup>2</sup>. We perform this calculation on a finite-size system with linear dimension  $L = 720$  [ $N_{\text{UC}} \cdot N = 2L^2 \sim \mathcal{O}(10^6)$  sites]. The infinitesimal is taken as  $i\eta = 0.8i/L$ , such that it scales with the level spacing of the fermion bands on a finite-size system. The imaginary part of this free susceptibility contributes to the dynamical structure factor can be written in the alternative analytic form

$$S(\mathbf{q}, \omega) = \frac{\pi}{4N} \sum_{\mathbf{k}, mn} (n_{\mathbf{k}}^m - n_{\mathbf{k}+\mathbf{q}}^n) \mathcal{M}^{mn} \delta(\omega + \varepsilon_{\mathbf{k}}^m - \varepsilon_{\mathbf{k}+\mathbf{q}}^n), \quad (3.27)$$

where  $\mathcal{M}^{mn} = \sum_{XY} (R_{\mathbf{q}}^X)^* R_{\mathbf{q}}^Y \mathcal{V}_X^{mn} (\mathcal{V}_Y^{mn})^*$ . Here, we used the Sokhotski–Plemelj formula (Auerbach, 1998)

$$\lim_{\eta \rightarrow 0} \left( \frac{1}{x + i\eta} \right) = \mathcal{P} \frac{1}{x} - \pi i \delta(x). \quad (3.28)$$

In a finite-size calculation, the delta functions should be broadened with width  $\eta \sim 1/L$ .

The contribution of the free fermion bubble  $\chi^0(\mathbf{q}, \omega)$  to the dynamical structure factor is plotted in Fig. 3.2. The gray dashed lines show the maximum and minimum energy difference  $\varepsilon_{\mathbf{k}}^m - \varepsilon_{\mathbf{k}+\mathbf{q}}^n$  of two spinon bands separated by momentum  $\mathbf{q}$ . From Eq. (3.27), we can see that the imaginary part of the susceptibility must be identically zero outside of these lines. The real part will generally be finite even outside of these limits. The form in  $S(\mathbf{q}, \omega)$  is determined by the density of states of fermions, as well as the spin-matrix elements  $\mathcal{M}^{mn}$  between transition states.

The continua are gapless at the  $\mathbf{M}$  and  $\Gamma$  points. These represent inter- and intra-Dirac cone transitions. This was also seen in the field theoretic-classification of low-energy excitations; see Fig. 2.10 and Table 2.3. It is important to note that the spectral weight is highest at high energies  $\omega \gtrsim J_1$ . It vanishes linearly  $S(\mathbf{M}, \omega) \sim \omega$  as  $\omega \rightarrow 0$  due to the vanishing

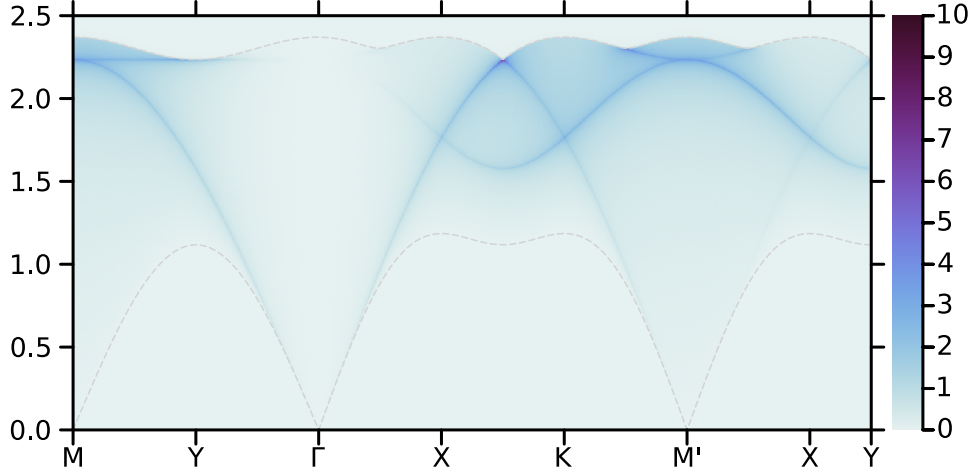


**Figure 3.2:** *Contribution to the dynamical structure factor given by the free fermion susceptibility.* Plotted is  $S(\mathbf{q}, \omega)$ , calculated from the imaginary part of  $[\chi^0(\mathbf{q}, \omega)]$ . We neglect all fermion-fermion interactions in this zeroth order mean-field approximation. Energy  $\omega$  is in units of  $J_1$ . Boundaries of the continuum are shown as dashed lines.

density of states in the low-energy Dirac cones. The spectral weight also vanishes as  $\mathbf{q} \rightarrow \Gamma$  because of vanishing matrix elements.

Note that we may also calculate generalised spin-spin susceptibilities by resolving the different spin components  $i, j = x, y, z$ , defined as time-ordered correlation functions of  $S_i^i(\tau)S_j^j(0)$ . The resulting susceptibility matrix can then be written as a  $6 \times 6$  matrix  $[\chi(\mathbf{q}, \omega)]_{XY}^{ij}$ . The physical response function is then found by tracing over the diagonal spin indices. This is often necessary when studying magnetically ordered states, such as stripe or 120-degree states on the triangular lattice (Willsher *et al.*, 2023). However this is not necessary here, since we consider a QSL Ansatz with SU(2) spin-rotation symmetry. This guarantees that the diagonal elements are equal, and the off-diagonal elements vanish  $[\chi(\mathbf{q}, \omega)]_{XY}^{ij} = \delta^{ij} [\chi(\mathbf{q}, \omega)]^{XY}$ . This was checked numerically, and will be important when considering interactions.

We have provided two models for the dynamical correlations of the U(1) Dirac spin liquid. Approaching the problem from two different perspectives gave vastly different results. The perspective inspired by QED<sub>3</sub> is only valid at asymptotically low energies (Hermele *et al.*, 2008). As stated before, this model cannot explain why the static correlations of spins and dimers are so different. The high-energy perspective however does not provide any insight. Fig. 3.2 shows no strong correlations at the  $K$  point which would correct the QED picture.

### 3.2 Interacting susceptibility

To move beyond the mean-field picture, we must include the effect of fermion-fermion interactions, which are naturally present in the Abrikosov representation of Heisenberg-type

<sup>2</sup>These calculations are not particularly expensive. All results shown in this Chapter were done on a local workstation.

Hamiltonians. In this Section, we will introduce the random phase approximation (RPA) and apply it to the U(1) Dirac QSL. This provides a new theoretical prediction for the spin structure factor, which we compare to previous numerical studies. Contrary to traditional understanding, we will find the spectrum of the liquid state is dominated by sharp features. Next, we are able to develop a deep understanding of the phase diagram of the model.

### 3.2.1 Random phase approximation

#### Fermion interactions

Here, we consider only the effect of interactions  $[J(\mathbf{q})]_{XY}$  on dynamical response functions (Zhou and Wen, 2003; Ghioldi *et al.*, 2018; Zhang and Li, 2020), given by the real-space nearest- and next-nearest-neighbour interaction  $J_{ij}$ . Transforming the Heisenberg interaction into the sublattice Fourier basis, we express it as

$$\sum_{\mathbf{q}} \delta_{ij} J_{\mathbf{q}}^{XY} S_{X,\mathbf{q}}^i S_{Y,-\mathbf{q}}^j = \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \delta_{ij} J_{\mathbf{q}}^{XY} \frac{1}{4} \sigma_{\alpha\beta}^i \sigma_{\gamma\delta}^j \times \left( f_{\alpha X, \mathbf{k}+\mathbf{q}}^\dagger f_{\beta X, \mathbf{k}} \right) \left( f_{\gamma Y, \mathbf{k}'-\mathbf{q}}^\dagger f_{\delta Y, \mathbf{k}'} \right). \quad (3.29)$$

The Fourier interaction strength in momentum space is defined as

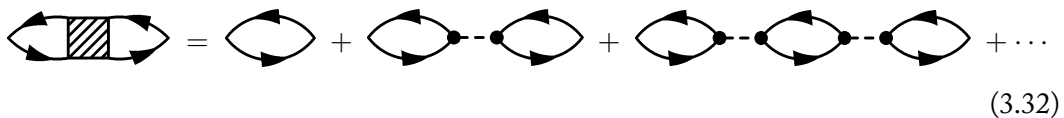
$$J_{\mathbf{q}}^{XY} = \sum_{\delta_{ij}: X \rightarrow Y} J_{ij} e^{i\mathbf{q} \cdot \delta_{ij}}, \quad (3.30)$$

where  $\delta_{ij} = \mathbf{r}_i - \mathbf{r}_j$  is the vector connecting all interacting sites where interactions  $J_{ij} \neq 0$  are non-zero. The matrix elements in the sublattice basis are explicitly given by

$$\begin{aligned} J_{\mathbf{q}}^{XX} &= J_{\mathbf{q}}^{YY} = 2J_1 \cos(k_2) + 2J_2 \cos(k_1 - k_2) \\ J_{\mathbf{q}}^{XY} &= J_1 \left[ 1 + e^{-ik_1} + e^{i(k_2 - k_1)} + e^{-ik_2} \right] \\ &\quad + J_2 \left[ e^{ik_2} + e^{i(2k_2 - k_1)} + e^{-i(k_1 + k_2)} + e^{-2ik_2} \right] \end{aligned} \quad (3.31)$$

and where  $J_{\mathbf{q}}^{XY} = (J_{\mathbf{q}}^{YX})^*$ . The momentum components within the reduced Brillouin zone are defined  $k_{1,2} = \mathbf{k} \cdot \mathbf{a}_{1,2}$  as defined by Eq. (2.121). Note that the elements  $J^{XY}$  differ from the Hamiltonian (2.123) in two ways. First, the signs do not alternate on different bonds in the unit cell. Second, the interaction matrix includes a contribution from  $J_2$  to the matrix elements. These are absent in the Hamiltonian  $M^{XY}$  because the self-consistent amplitude  $t$  is only non-zero on nearest-neighbour bonds. Importantly, this means that next-nearest neighbour interactions are non-zero and will modify the physics of the model beyond the self-consistent mean-field approximation!

Beyond the leading free fermion bubble, interactions produce a whole series of bubble diagrams of the following form



$$\text{Bubble with shaded region} = \text{Bubble} + \text{Bubble with dot} + \text{Bubble with dot} + \text{Bubble with dots} + \dots \quad (3.32)$$

These all contribute to the interacting fermion susceptibility. A perturbative calculation theory is performed in Appendix A, where the first terms in this series are

$$[\chi(\mathbf{q}, \omega)]^{XY} = [\chi^0(\mathbf{q}, \omega)]^{XY} - 2[\chi^0(\mathbf{q}, \omega)]^{XX'} J_q^{X'Y'} [\chi^0(\mathbf{q}, \omega)]^{Y'Y} + \dots \quad (3.33)$$

We therefore identify the interaction matrix

$$U_q^{XY} = \bullet - \bullet = -2J_q^{XY}, \quad (3.34)$$

where  $J_q^{XY}$  is the Fourier transform of the Heisenberg interaction  $J_{ij}$  in the sublattice basis.

### RPA susceptibility

We employ the RPA to treat the fermion interaction term (3.34), by summing up an infinite series of bubble diagrams (Schrieffer *et al.*, 1989; Chubukov and Frenkel, 1992). Note that similar self-consistent theories have successfully described the dynamical spin response and collective spin-wave modes in itinerant *ordered* magnets described by Hubbard-like models (Kampf, 1996; Peres and Araújo, 2002; Singh, 2005; Knolle *et al.*, 2010, 2011). This was only recently extended to the triangular lattice with next-nearest-neighbour hoppings by us (Willsher *et al.*, 2023). Large extended hoppings stabilise competing stripe orders, and at lower values cause magnetoroton-like minima in itinerant magnets such as PdCrO<sub>2</sub> (Le *et al.*, 2018).

Previous applications within parton mean field theory treated a phenomenological on-site Hubbard  $U$ . This approximately imposes the on-site single-filling constraint (Ho *et al.*, 2001; Ma *et al.*, 2018), or arises due to screened gauge fluctuations in a magnetised QSL with a Fermi surface (Balents and Strykh, 2020). We also added a phenomenological Hubbard repulsion, but realised that it is insufficient to describe the momentum-dependent spectrum. Instead, we focus only on the dominant interactions caused by the  $J_1$  and  $J_2$  terms present in the Hamiltonian (3.29). We will not attempt to impose the single-occupancy with fermion interactions. Instead, we return to this issue later by including temporal fluctuations of the gauge field.

To make progress towards calculating the interacting susceptibility, we can re-express the series (3.32) as a Dyson–Schwinger equation

$$\text{bubble with shaded box} = \text{bubble} + \text{bubble with shaded box} - \text{bubble} \quad (3.35)$$

or equivalently

$$[\chi(\mathbf{q}, \omega)]^{\mu\nu} = [\chi^0(\mathbf{q}, \omega)]^{\mu\nu} + [\chi(\mathbf{q}, \omega)]^{\mu\rho} U_q^{\rho\sigma} [\chi^0(\mathbf{q}, \omega)]^{\sigma\nu}. \quad (3.36)$$

Rearranging some terms, we find

$$[\chi(\mathbf{q}, \omega)]^{\mu\rho} \left( \delta^{\rho\nu} - U_q^{\rho\sigma} [\chi^0(\mathbf{q}, \omega)]^{\sigma\nu} \right) = [\chi^0(\mathbf{q}, \omega)]^{\mu\nu}, \quad (3.37)$$

which we solve to find the RPA susceptibility

$$\chi(\mathbf{q}, \omega) = \chi^0(\mathbf{q}, \omega) \cdot \text{inv} \left[ 1 - U_q \cdot \chi^0(\mathbf{q}, \omega) \right] \quad (3.38)$$

$$= \chi^0(\mathbf{q}, \omega) \cdot \text{inv} \left[ 1 + 2J_q \cdot \chi^0(\mathbf{q}, \omega) \right]. \quad (3.39)$$

Once again, we must calculate the scalar susceptibility by tracing over sublattices, according to Eq. (3.19). The elements of the interaction matrix  $U_q^{XY}$  are given in terms of  $J_{1,2}$ , and the energy scale of the bare susceptibility  $\hat{\chi}^0$  is normalised by the MFT QSL order  $t/J_1 = |\langle f_{i\alpha}^\dagger f_{j\alpha} \rangle| = 0.395$ . There are hence no free parameters in the model. The self-consistent nature means we can produce *quantitative* predictions for the dynamical response as a function of the microscopic exchange interactions  $J_2/J_1$ .

### 3.2.2 Results

#### Dynamical structure factor

The spinon contribution to the dynamical structure factor is shown in Fig. 3.3. Here, we show  $J_2/J_1 = 0.15, 0.09$  in the stable regime (upper two panels). The most striking effect of the spinon interactions is to create a sharp paramagnon mode coming down to low energy; this *spinon exciton*, a quasiparticle with quantum numbers of a magnon arising as a two-spinon bound state, displays a magnetoroton-like minimum around  $\mathbf{K}$ . The gap here  $m \approx 0.4J_1$  is at low energy relative to the magnetic exchange scale. In this regime, the low-energy mode is a signature of the proximate 120-degree order.

The bottom panel in Fig. 3.3 with  $J_2/J_1 = 0.0716$  shows that this spinon exciton gap approaches zero  $m \rightarrow 0$ . The condensation of this mode signals the onset of 120-degree order. In the ordered phase, the gapless mode at  $\mathbf{K}$  is the Goldstone mode of the spontaneously broken continuous spin-rotation symmetry.

We include a comparison to recent VMC results from Ferrari and Becca (2019) in Fig. 3.4, showing remarkable agreement. The spinon-exciton mode is sharp around  $\mathbf{K}$ , but broadens when entering the two-spinon continuum around  $\mathbf{M}$  and between  $\mathbf{K}$  and  $\mathbf{X}$ . It reemerges above the continuum around the  $\mathbf{\Gamma}$  point between  $\mathbf{Y}$  and  $\mathbf{X}$ , in strong agreement VMC results (Ferrari and Becca, 2019). Overall, the spinon exciton dominates the response; the only broad continuum at low energies is present at the  $\mathbf{M}$  points from inter-Dirac cone transitions. This has weaker spectral weight than a sharp mode around  $\mathbf{K}$ , but is enhanced compared to the free-fermion MFT case (c.f. Fig. 3.2). These observations are also in agreement with time-dependent DMRG calculations (Drescher *et al.*, 2023).

The differences between the two methods are minimal. The exact position of the modes differ at low energy, but this may be strongly affected by finite-size effects in the variational approach. Although both continua reach up to about  $\omega/J_1 = 2.25$ , the paramagnon mode extends to higher energies around  $\mathbf{\Gamma}$  in the numerical calculation. Also, there is more disperse spectral weight in the continuum of the VMC data, but this may be due to the stochastic nature of the sampling method used.

The nature of the low-lying mode around  $\mathbf{K}$  was an important outstanding question in the literature (Ferrari and Becca, 2019; Drescher *et al.*, 2023). It was unclear whether this is a monopole on a finite-size geometry, or if it's due to bound states of spinons. We show that an interacting fermion model alone is able to describe the numerical findings well.

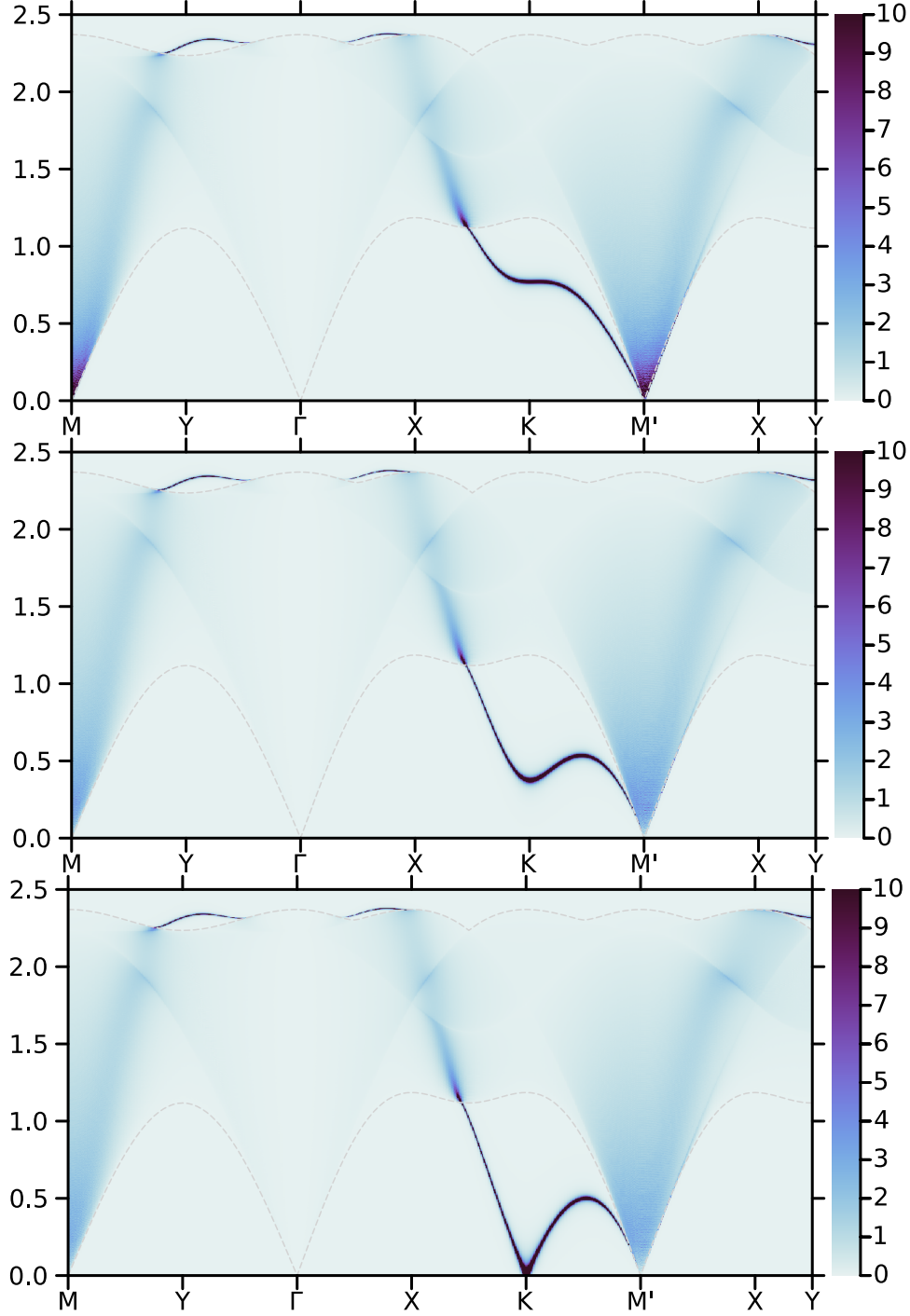


**Figure 3.3:** *Fermion contribution to the dynamical structure factor  $S(\mathbf{q}, \omega)$  in the random phase approximation.* We consider fluctuations of the  $\pi$ -flux Ansatz, with various interactions  $J_2/J_1$ . (Top)  $J_2/J_1 = 0.15$  in the U(1) Dirac QSL phase, close to the transition to stripe order. Here, the mode is low energy at  $M$ . (Middle)  $J_2/J_1 = 0.09$  in the stable Dirac spin liquid phase. (Bottom)  $J_{2,c}/J_1 = 0.0716$  at the transition to 120-degree order. All energies  $\omega$  in units of  $J_1$ .

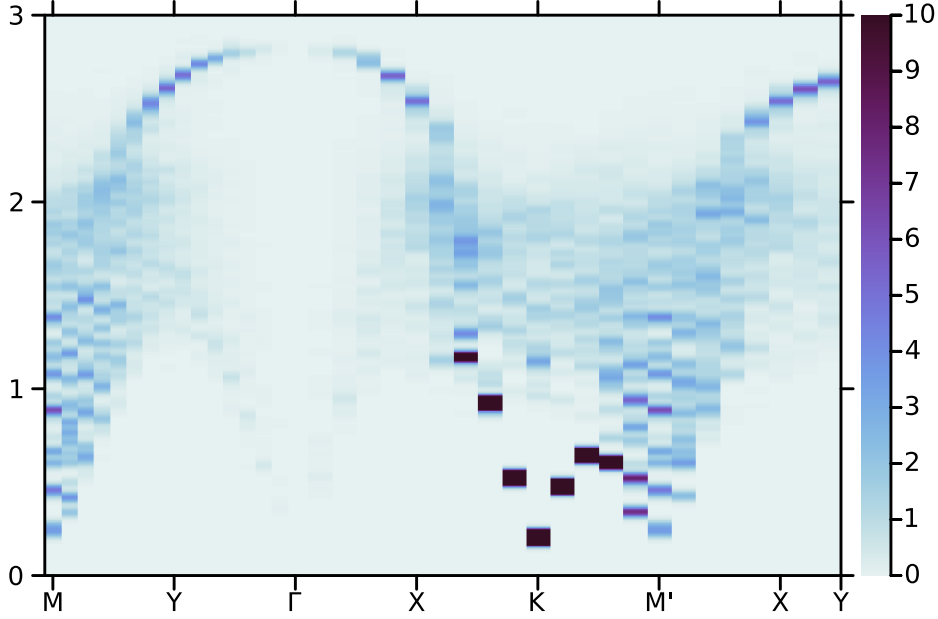


**Figure 3.4:** *Fermion contribution to the dynamical structure factor  $S(\mathbf{q}, \omega)$ .* Variational Monte Carlo study of the  $J_1$ – $J_2$  Heisenberg model on the triangular lattice; here  $J_2/J_1 = 0.09$ . Data taken from Ferrari and Becca (2019), reproduced with permission. All energies  $\omega$  in units of  $J_1$ .

### Spin-spin correlations

Let us revisit the problem of spin-spin correlation functions in real space. In terms of spin observables, it is

$$g_{ij} = \langle \vec{S}_i \cdot \vec{S}_j \rangle \quad (3.40)$$

evaluated at equal time. This is simply the dynamical spin-spin correlator  $S_{ij}(0)$  at equal time, defined in Eq. (3.3). This, in turn, is the Fourier transform of the spin-spin susceptibility Eq. (3.2). Together, we can write

$$g_{ij} = \text{Re} \sum_{\mathbf{q}} e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \int d\omega \chi(\mathbf{q}, \omega). \quad (3.41)$$

The real-space correlation function can be written as a Fourier transform over one momentum dimension of the susceptibility function, and a sum over the other momentum and frequency directions. We choose a specific path of the correlation function along next-nearest-neighbour bonds  $\mathbf{r}_i - \mathbf{r}_j = r(\mathbf{a}_1/2 + \mathbf{a}_2)$ , see Fig. 2.8. This probes the excitations around the  $\mathbf{K}$  point. The resulting real-space correlations are shown in Fig. 3.5(a) for a range of  $J_2/J_1$ . For large  $J_2$ , the response is approximately a power law with exponent 3.0(1). For critical  $J_2$ , such that the spinon exciton gap  $m$  goes to zero energy, the power law is 1.75(15). For intermediate interaction strengths, there is a dominant exponential-like behaviour at short distances.

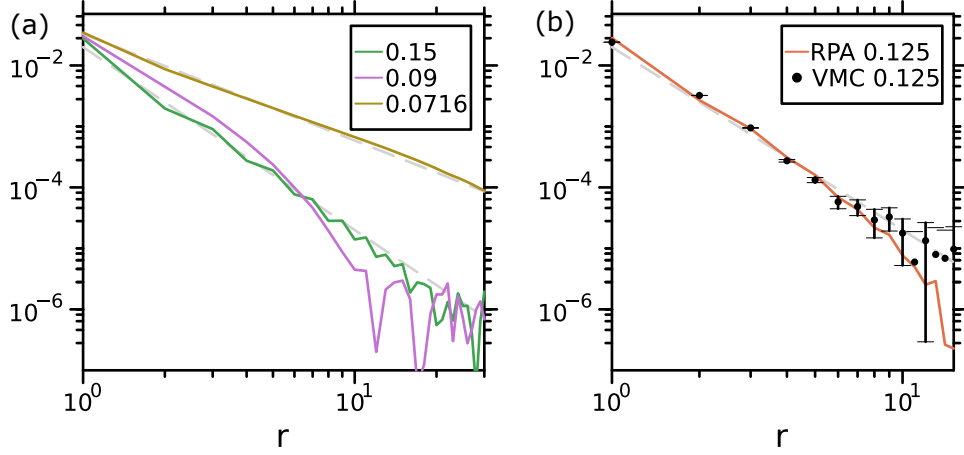


**Figure 3.5:** *Real-space correlation function*  $g(r)$  in the direction  $\mathbf{a}_2 + \mathbf{a}_1/2$ . (a) Comparison of the RPA method with VMC for  $J_2/J_1 = 0.125$ . (b) RPA method for various  $J_2/J_1 = 0.15$ , 0.09, and at the critical point 0.0716.

We plot a direct comparison between VMC calculations and our RPA method evaluated at  $J_2/J_1 = 0.125$  in Fig. 3.5(b) [data from Fig. 2.13(b)]. We are once again able to reproduce the numerical results very accurately. In fact, this result lets us put a bound on the contribution of monopoles to the static spin correlations. If monopoles with scaling dimension  $\Delta_\Phi \leq 1.25$  are present in spin correlation functions, they must have a prefactor that is of order  $\mathcal{O}(10^{-3})$ . Otherwise, they would dominate over the fermion contribution and our RPA result would clearly predict the wrong power law.

### 3.2.3 Spinon exciton

#### RPA pole condition

The results show a dominant pole in the low energy spectrum, with a gap controlled by the interaction strength  $J_2$ . We plot a direct comparison between the free fermion result and the RPA in Fig. 3.6 to highlight this difference. How does this collective mode arise in the RPA? In particular, how do interactions produce (dominant) spectral weight in a regime that had none in the non-interacting approximation, Fig. 3.2?

The spinon exciton emerges as a pole in the dynamical structure factor. It is sharp outside the two-spinon continuum. We can derive the dispersion of the spinon-exciton bound state  $m_{\text{RPA}}(\mathbf{q})$ , by seeing where Eq. (3.39) diverges. Labelling the RPA denominator as  $\mathcal{D}(\mathbf{q}, \omega) = 1 + 2J_{\mathbf{q}} \cdot \chi^0(\mathbf{q}, \omega)$ , we define the mass implicitly by setting its determinant to zero

$$0 = \det \mathcal{D}(\mathbf{q}, m_{\text{RPA}}(\mathbf{q})) = \det \left[ 1 + 2J_{\mathbf{q}} \cdot \chi^0(\mathbf{q}, m_{\text{RPA}}(\mathbf{q})) \right]. \quad (3.42)$$

This mass  $m_{\text{RPA}}(\mathbf{q})$  depends on the interaction  $J_2/J_1$  through the matrix  $J_{\mathbf{q}}$ . Outside of the two-spinon continuum, the bare susceptibility  $\chi^0(\mathbf{q}, \omega)$  is Hermitian, and so the Eq. (3.42) has a real solution for  $m_{\text{RPA}}(\mathbf{q})$ . Expanding around this pole, we may write  $\det \mathcal{D}(\mathbf{q}, \omega)^{-1} \sim$

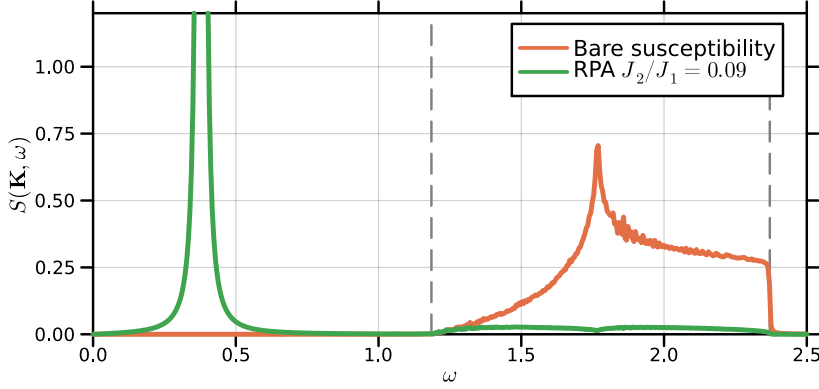


**Figure 3.6:** *Direct comparison between the spin structure factor in the mean-field and RPA approximations.* In the interacting case, the parameters are  $J_2/J_1 = 0.09$ . Dashed lines show the bandwidth of the continuum.

$(m_{\text{RPA}}(\mathbf{q})^2 - \omega^2)^{-1}$ . The leading behavior of the susceptibility is hence

$$\chi(\mathbf{q}, \omega + i\eta) = \frac{Z_{\text{RPA}}}{m_{\text{RPA}}(\mathbf{q})^2 - \omega^2 - i\eta} + (\text{continuum}), \quad (3.43)$$

or in diagrammatic form

$$\text{Diagram with a shaded box and arrows} = \text{Diagram with two parallel lines} + (\text{continuum}). \quad (3.44)$$

The spectral weight  $Z_{\text{RPA}}$  is a real function of the bare susceptibility matrix  $\chi^0(\mathbf{q}, \omega)$ , given by tracing over sublattices [via Eq. (3.19)]. Taking the imaginary component  $\chi''(\mathbf{q}, \omega)$ , we can evaluate the spin structure factor

$$S(\mathbf{q}, \omega) = \pi Z_{\text{RPA}} \delta(\omega^2 - m_{\text{RPA}}(\mathbf{q})^2), \quad (3.45)$$

which is indeed a pole at energy  $m_{\text{RPA}}(\mathbf{q})$ . Returning to the slice at  $\mathbf{K}$  in Fig. 3.6, we see that the pole dominates the response. Quantitatively, it carries 97.5% of the spectral weight at  $J_2/J_1 = 0.09$ .

### Stability & phase diagram

For the phase to be stable, the spinon exciton must be gapped for all momenta. Condensation of this bosonic mode, when any  $m_{\text{RPA}}(\mathbf{Q}, \omega) = 0$ , will signal a condensation to magnetic order with wavevector  $\mathbf{Q}$ .

Numerical solutions of the RPA pole condition Eq. (3.42) define the mode energy  $m_{\text{RPA}}(\mathbf{q})$ . This is shown as a function of  $J_2/J_1$  in Fig. 3.7(a). The precise optimisation performed is a minimisation of  $|\det \mathcal{D}(\mathbf{q}, \omega)|$  over  $\omega$ . Near the corners of the Brillouin zone  $\mathbf{K}$ , we find good convergence. The resulting masses shows a continuous closing to zero energy

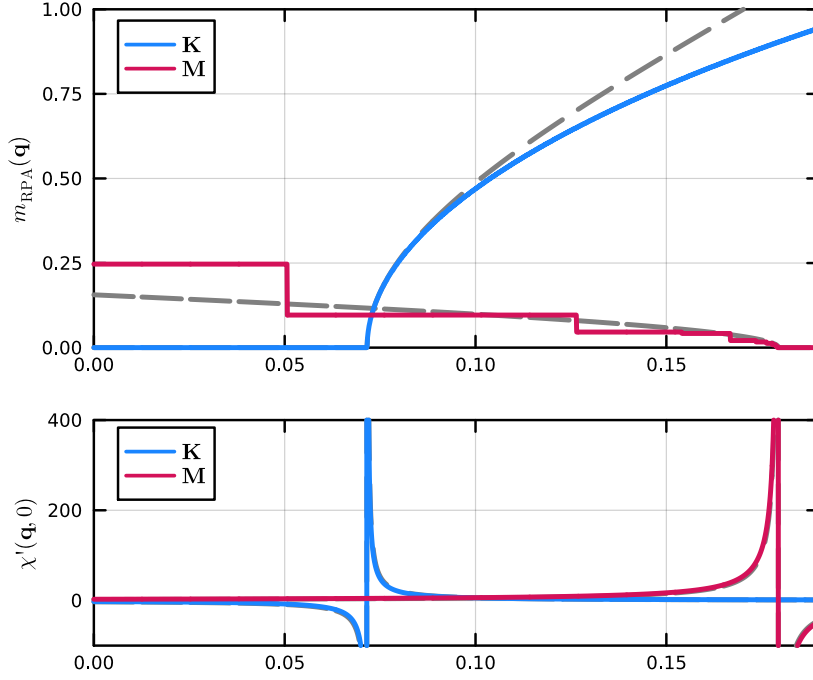


**Figure 3.7:** *Phase transitions to 120-degree and stripe order, caused by condensation of the spinon-exciton mode.* (Top panel) Energy of the RPA poles  $m_{\text{RPA}}(\mathbf{q})$  at the  $\mathbf{q} = \mathbf{K}, \mathbf{M}$  points. Dashed lines show the mode energy as calculated in the single-mode approximation  $\tilde{m}(\mathbf{q})$ , see Eq. (3.71). (Bottom panel) real part of the interacting susceptibility  $\chi'(\mathbf{q}, \omega) = \text{Re} \chi(\mathbf{q}, \omega)$  in the RPA at  $\omega = 0$ ; poles indicate the mode condensing.

$m_{\text{RPA}}(\mathbf{K}) \rightarrow 0$  as  $J_2/J_1$  is lowered towards the critical value 0.0716. However, we observe that the equivalent calculation for the centres of the zone edges  $\mathbf{M}$  is less numerically well-behaved. Within the continuum at finite frequencies, the free fermion susceptibility is complex, and so the pole at  $\mathbf{M}$  is broadened for  $\omega > 0$ . The zeros of  $|\det \mathcal{D}(\mathbf{q}, \omega)|$  then become minima, which makes the numerical optimisation less stable. However if we focus on  $\omega = 0$  we can better locate the transition point. Importantly, the imaginary part of the bare susceptibility vanishes  $\chi^0(\mathbf{M}, 0) = 0$  here. We can then define the critical point instead by modifying  $J_q$  until  $\det \mathcal{D}(\mathbf{M}, 0) = 0$ . From Eq. (3.43), we can read off that

$$\chi'(\mathbf{q}, 0) = \text{Re}[Z_{\text{RPA}}]/\text{Re}[m_{\text{RPA}}(\mathbf{q})^2] + \dots, \quad (3.46)$$

where we suppress terms higher order in  $\omega/J_1$ . We plot the real part of the RPA susceptibility as a function of  $J_2/J_1$  in Fig. 3.7(b). The poles represent the critical points:

$$J_{2,c}^{120}/J_1 = 0.0716, \quad J_{2,c}^{\text{stripe}}/J_1 = 0.1794. \quad (3.47)$$

Tuning  $J_2 \rightarrow J_{2,c}^{120}$  from above, we condense the spinon exciton at  $\mathbf{K}$ , leading to 120-degree order. Similarly, taking  $J_2 \rightarrow J_{2,c}^{\text{stripe}}$  from below, we condense the spinon exciton at  $\mathbf{M}$ , leading to stripe magnetic order.

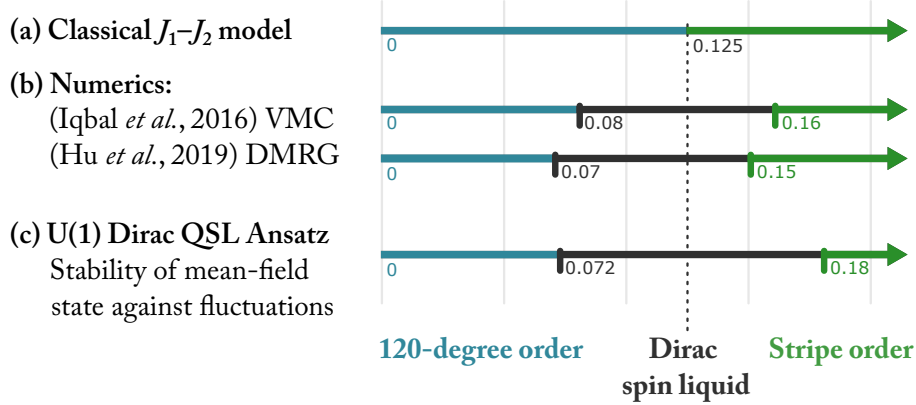


**Figure 3.8:** *Phase diagram of the  $J_1$ – $J_2$  Heisenberg model on the triangular lattice from the RPA.* We compare our results to other numerical methods in the literature. (a) Classical phase diagram of the model; first-order transition from 120-degree to stripe magnetic order at  $J_2/J_1 = 1/8$ . (b) Numerical phase diagram found using density-matrix renormalization group (DMRG) (Hu *et al.*, 2019) and variational Monte Carlo (VMC) (Iqbal *et al.*, 2016). (c) Phase diagram inferred from the stability of the U(1) Dirac QSL Ansatz beyond mean field theory. Stable regime is when the spinon-exciton mode is gapped, see Fig. 3.7. Critical values of  $J_2/J_1$  listed in Eq. (3.47).

Between these values, there is an extended regime where the Dirac QSL is stable against fluctuations of magnetic order. We plot the phase diagram in Fig. 3.8. Our analytic approach, which studies mean-field theory plus fluctuations in the RPA shows excellent agreement with various numerical approaches (Hu *et al.*, 2015; Iqbal *et al.*, 2016). We find particularly good agreement for the position of the 120-degree transition. A limitation of this approach seems to be that it overestimates the stability of the QSL with respect to stripe ordering. Furthermore, this analysis predicts a continuous transition, whereas numerics consistently point to a first order transition at lower  $J_2/J_1$  (see Section 2.3.2). Crucially, up to now we have ignored the effect of gauge fluctuations on the stability of the phases. We will later show that the gauge dynamics of the QSL affects the nature of the phase transitions. As such, we delay further discussion of the position, order and the universality classes of these transitions to Sec. 3.3.1.

### Continuum theory of the spinon exciton as a Hubbard–Stratonovich field

This spinon exciton behaves like a fluctuating competing magnetic order parameter. We have described how it must remain gapped for the QSL to be stable. In this section, we will show how this fluctuating boson can be derived from the original Hamiltonian. We also develop a Ginzburg–Landau theory for the phase transitions and examine an approximate single-mode model for the spectrum at low energies.

To begin, let us build on the field-theoretic description of zeroth-order mean-field theory

in Section 2.2.1. The spin Hamiltonian in the parton basis reads

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \frac{1}{4} \sum_{\langle ij \rangle} \left( f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta} \right) \cdot \left( f_{j\alpha'}^\dagger \vec{\sigma}_{\alpha'\beta'} f_{j\beta'} \right). \quad (3.48)$$

Previously, we decoupled this four-fermion interaction with a Hubbard–Stratonovich field  $\chi_{ij}$ . The (zeroth-order) mean-field theory came from taking the saddle point of  $\chi_{ij}$ . Given the insight that spin fluctuations are relevant to the stability of the mean field, let us now go one step further. We now perform a Hubbard–Stratonovich transformation to decouple the spin-spin interactions in terms of the bond-pairing  $\chi_{ij}$  and spin channel  $\vec{m}_i$  fields simultaneously

$$\begin{aligned} \mathcal{H}[f_i, a_i^0, \chi_{ij}, \vec{m}_i] = \sum_{ij} J_{ij} \left[ -\frac{1}{2} \left( \chi_{ij} f_{j\alpha}^\dagger f_{i\alpha} + \text{h.c.} - |\chi_{ij}|^2 \right) \right. \\ \left. + \left( f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta} \right) \cdot \vec{m}_j - \vec{m}_i \cdot \vec{m}_j \right] + \sum_i a_i^0 \left( f_{i\alpha}^\dagger f_{i\alpha} - 1 \right). \end{aligned} \quad (3.49)$$

A mean-field QSL Ansatz is consequently defined by the following *three* saddle point equations

$$n_i = \langle f_{i\alpha}^\dagger f_{i\alpha} \rangle = 1, \quad (3.50)$$

$$\chi_{ij} = \langle f_{i\alpha}^\dagger f_{j\alpha} \rangle, \quad (3.51)$$

$$\vec{m}_i = \frac{1}{2} \langle f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta} \rangle = 0. \quad (3.52)$$

These come from varying  $a_i^0$ ,  $\chi_{ij}$ , and  $\vec{m}_i$  respectively. The uniform zero-spin order  $\vec{m}_i = 0$  might appear trivial, but it is an independent constraint to the other two.<sup>3</sup>

We will now investigate the gap of the fluctuating magnetic order  $\vec{m}_i$ . In this Section, we will henceforth focus on the part of Eq. (3.52) containing only this Hubbard–Stratonovich field. Moving to momentum space in the sublattice basis, we find

$$\mathcal{H}[\vec{m}_q] = \sum_q J_q^{XY} \left( 2S_{-q,X}^i m_{q,Y}^i - m_{-q,X}^i m_{q,Y}^i \right) \quad (3.53)$$

Firstly, let us confirm that the amplitude fluctuations of spin order are gapped in the mean field. At this saddle point, we have  $\langle S_{q,X}^i \rangle = 0$  via Eq. (3.52). We may then change normalisation and work with Weiss exchange fields by defining  $\vec{h}_q = J_q \cdot \vec{m}_q^i$  (Bose and Paramakanti, 2025). The potential for this the Hubbard–Stratonovich field is

$$\mathcal{H}_{\text{MF}}[\vec{m}_q] = - \sum_q \vec{h}_{-q}^i \cdot [J_q]^{-1} \cdot \vec{h}_q^i. \quad (3.54)$$

<sup>3</sup>One can actually construct mean-field theories of fractionalised magnetically-ordered states within the Abrikosov fermion representation. In this context, there will be a saddle point where Eq. (3.52) is non-zero, and equal to some mean-field spin order.

Here we implicitly sum over the spin index  $i$ , and the multiplications are understood to be over the sublattice indices. We are interested in describing fluctuations of competing spin orderings. A spin momentum-eigenstate is  $S_q^i \sim \varphi_q \hat{n}_q^i$  in terms of a real amplitude  $\varphi_q$  and a complex ordering unit vector  $\hat{n}_q^i$ . Translating this into our sublattice basis, we can say that the phases of the vectors  $\hat{n}$  on  $A/B$  sublattices must be related by a constant. We therefore express the fluctuating order field as

$$\vec{h}_q^i = \varphi_q \vec{R}_q \hat{n}_q^i. \quad (3.55)$$

The vector  $\vec{R}_q$  is defined in Eq. (3.20) and serves the purpose of fixing the phase on the two sublattices. Taken together, the potential for the spin ordering amplitude simplifies to

$$\mathcal{H}_{\text{MF,free}}[\varphi_q] = - \sum_q \vec{R}_q^\dagger \cdot [J_q]^{-1} \cdot \vec{R}_q \varphi_q(\tau)^2 = \sum_q m_0^2(\mathbf{q}) \varphi_q^2, \quad (3.56)$$

where the mass is

$$m_0^2(\mathbf{q}) = -\vec{R}_q^\dagger \cdot [J_q]^{-1} \cdot \vec{R}_q = -1/j_q \quad (3.57)$$

where

$$j_q = \vec{R}_q^\dagger \cdot [J_q] \cdot \vec{R}_q / 4 = J_1 [\cos(k_2) + \cos(k_1/2 - k_2) + \cos(-k_1/2)] \\ + J_2 [\cos(k_1/2 + k_2) + \cos(k_1 - k_2) + \cos(2k_2 - k_1/2)]. \quad (3.58)$$

Focusing on the two relevant phase transitions, we can evaluate the mean-field gaps for the amplitude fluctuations  $\varphi_K$  and  $\varphi_M$ . Defining the interaction ratio  $r = J_2/J_1$  as our control parameter, we find

$$m_0^2(\mathbf{K})J_1 = \frac{2/3}{1-2r}, \quad m_0^2(\mathbf{M})J_1 = \frac{1}{1+r}. \quad (3.59)$$

The mean field gaps are indeed positive for  $-1 < r < 1/2$ .

### Landau–Ginzburg theory

Corrections to the effective potential (3.54) beyond the mean-field approximation is provided by the spinon-boson interaction written in Eq. (3.53). We evaluate the resulting effective action to leading order when integrating out the spinons in Appendix A (Weng *et al.*, 1991; Scholle *et al.*, 2024; Bose and Paramakanti, 2025). We find

$$\mathcal{H}_{\text{MF}}[\vec{m}_q] = - \sum_q \vec{h}_{-q}^i \cdot \left\{ [J_q]^{-1} + 2\chi^0(\mathbf{q}, \omega) \right\} \cdot \vec{h}_q^i. \quad (3.60)$$

We note that this matrix has determinant zero when the RPA pole condition (3.42) is fulfilled  $\omega = m_{\text{RPA}}(\mathbf{q})$ . Contracting with  $\vec{R}_q$ , the effective theory for amplitude fluctuations becomes

$$\mathcal{H}[\varphi_q] = \sum_q \left[ m_0^2(\mathbf{q}) - 2\chi^0(\mathbf{q}, \omega) \right] \varphi_q^2. \quad (3.61)$$

We can identify the self energy as  $-2\chi^0(\mathbf{q}, \omega)$ , proportional to the scalar susceptibility of the fermions. We will return soon to understanding the behaviour of these amplitude fluctuations at finite frequencies.

First, let us focus on the  $\omega = 0$  stability in order to understand the spinon exciton's condensation transition. This forms a Landau–Ginzburg theory of the spin order parameter. Here, Eq. (3.57) tells us that the stiffness of spin-amplitude fluctuations is positive in the mean field. Next, we define the limit of the self energy  $\Pi_q^0 = \chi^0(\mathbf{q}, 0)$ . This is purely real, and represents a shift of the stiffness due to RPA corrections. We can write the effective potential of the spin order parameter as

$$V(\varphi_{\mathbf{q}}) = \tilde{m}(\mathbf{q})\varphi_{\mathbf{q}}^2 = [m_0^2(\mathbf{q}) - 2\Pi_{\mathbf{q}}^0]\varphi_{\mathbf{q}}^2 + \dots \quad (3.62)$$

When this potential changes sign, there is a phase transition caused by the condensation of the parameter  $\varphi_{\mathbf{q}} > 0$ . This coincides with the RPA pole condition at  $\omega = 0$ . Focusing on the effective potential for the spin order parameters with wavevectors  $\mathbf{K}$  and  $\mathbf{M}$  at low energy, we derive a Landau–Ginzburg functional

$$V(\varphi_{\mathbf{K}}, \varphi_{\mathbf{M}}) = A^{120}(r - r_c^{120})\varphi_{\mathbf{K}}^2 + A^{\text{stripe}}(r_c^{\text{stripe}} - r)\varphi_{\mathbf{M}}^2, \quad (3.63)$$

for the transition. The critical ratios  $r = J_2/J_1$  are

$$r_c^{120} = \frac{1}{2} - \frac{2}{3\Pi_{\mathbf{K}}^0} = 0.071579 \quad (3.64)$$

$$r_c^{\text{stripe}} = \frac{2}{\Pi_{\mathbf{M}}^0} - 1 = 0.1800 \quad (3.65)$$

and the coefficients  $A$  are listed in the Appendix A.

### Single mode approximation

Returning to the  $\omega > 0$  problem, we will now calculate the mass gap of the spin fluctuations in the stable regime. From the Hamiltonian (3.61), the Green's function of this boson is

$$\begin{aligned} G_{\varphi}(\mathbf{q}, \omega) &= \text{=====} = \frac{1}{m_0^2(\mathbf{q}) - 2\chi^0(\mathbf{q}, \omega)} \\ &= \text{=====} + \text{===} \text{ (loop) } \text{===} + \dots \quad (3.66) \end{aligned}$$

This allows us to write a simplified form of the RPA pole condition

$$\frac{1}{2}m_0^2(\mathbf{q}) = \chi^0(\mathbf{q}, m_{\text{RPA}}(\mathbf{q})) = -\frac{1}{4N} \sum_{\mathbf{k}, mn} \frac{(n_{\mathbf{k}}^m - n_{\mathbf{k}+\mathbf{q}}^n) \mathcal{M}^{mn}}{m_{\text{RPA}}(\mathbf{q}) + \varepsilon_{\mathbf{k}}^m - \varepsilon_{\mathbf{k}+\mathbf{q}}^n}. \quad (3.67)$$

Solving this numerically for  $m_{\text{RPA}}(\mathbf{q})$ , we find the same mass of the RPA boson as shown in Fig. 3.7. This form for the pole condition allows us to develop a particularly simple ap-

proximate solution. Expanding the susceptibility to second order around  $\omega = 0$ , we find

$$\chi^0(\mathbf{q}, \omega) = \chi^0(\mathbf{q}, 0) + \omega^2 \left[ \frac{1}{2} \frac{\partial^2 \chi^0(\mathbf{q}, 0)}{\partial \omega^2} \right] + \dots \quad (3.68)$$

$$\equiv \Pi_{\mathbf{q}}^0 + \omega^2 (\Pi_{\mathbf{q}}^0)'' + \dots, \quad (3.69)$$

where we defined

$$(\Pi_{\mathbf{q}}^0)'' = -\frac{1}{4N} \sum_{\mathbf{k}, mn} \frac{(n_{\mathbf{k}}^m - n_{\mathbf{k}+\mathbf{q}}^n) \mathcal{M}^{mn}}{(\varepsilon_{\mathbf{k}}^m - \varepsilon_{\mathbf{k}+\mathbf{q}}^n)^3}. \quad (3.70)$$

Note that the linear contribution vanishes exactly. Solving Eq. (3.67) perturbatively  $\tilde{m}(\mathbf{q}) \approx m_{\text{RPA}}(\mathbf{q})$ , we get the approximate result

$$\tilde{m}^2(\mathbf{q}) = \frac{1}{2(\Pi_{\mathbf{q}}^0)''} \left[ m_0^2(\mathbf{q}) - 2\Pi_{\mathbf{q}}^0 + \dots \right]. \quad (3.71)$$

Now the Green's function of the amplitude-fluctuation field reads

$$G_{\varphi}(\mathbf{q}, \omega) = \frac{\tilde{Z}}{\tilde{m}^2(\mathbf{q}) - \omega^2} + \dots, \quad (3.72)$$

with  $\tilde{Z} = 1/[2(\Pi_{\mathbf{q}}^0)'']$ . This takes exactly the form that we argued for the spinon susceptibility in Eq. (3.43). Our approximate description of the spinon exciton's dispersion  $\tilde{m}(\mathbf{q})$  is expected to exactly agree with the RPA pole dispersion as  $m_{\text{RPA}}(\mathbf{q}) \rightarrow 0$ .

We show the energy of the modes  $\tilde{m}(\mathbf{q})$  at  $\mathbf{q} = \mathbf{K}, \mathbf{M}$  as a function of  $J_2/J_1$  in Fig. 3.7 as gray dashed lines. The approximation captures the critical properties of both transitions well. We also plot the momentum-resolved predictions for the quasiparticle mass in Fig. 3.9 for various  $J_2/J_1$ . This shows a dispersive mode which well captures the behaviour of the RPA pole. The results of this single-mode approximation differ from the RPA numerical solution at finite frequency, which is pronounced in this region for  $J_2/J_1 > 0.125$ . The approximation works particularly well around the  $\mathbf{K}$ , while it is slightly higher than the dispersive mode as it approaches the continuum. Interactions between the bound state and the continuum act to push the mode downwards relative to the single mode approximation, avoiding decay of the quasiparticle in this region (Verresen *et al.*, 2019).

### 3.3 Gauge fluctuations

What is the effect of gauge field fluctuations on these predictions for the phase diagram and resulting dynamical spin correlation functions? Up to now, we have included fermion interactions on top of the zeroth-order mean-field theory. In this Section, we will reintroduce the gauge field as a dynamical object. This is necessary, since the gauge field fluctuations are responsible for imposing the physical single-occupancy constraint on the fermions. Finally, we saw in Section 2.3.1 that the relevant low-energy gauge excitations are monopoles. In the spin sector, these have momentum  $\mathbf{K}$ . We will investigate here how these quasiparticles interact with the spinon exciton. Before investigating the spectral properties, we will turn to understanding how gauge fluctuations affect the critical points.

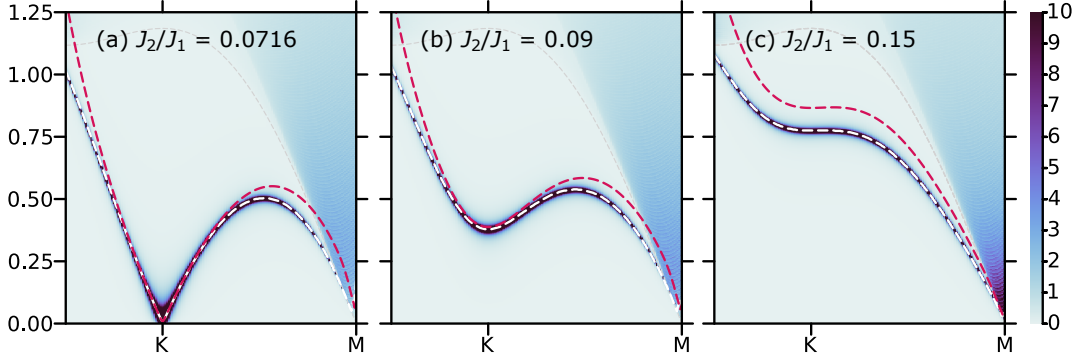


**Figure 3.9: Single-mode approximation for the spinon-exciton.** Spectral function  $S(\mathbf{q}, \omega)$  for three different values of  $J_2/J_1$ : (a) 0.15, (b) 0.09, and (c) 0.0716. White dotted lines show the zeros of the RPA denominator  $m_{\text{RPA}}(\mathbf{q})$ . Red dashed lines show the results of the single-mode approximation  $m_\varphi(\mathbf{q})$ , given by Eq. (3.71).

### 3.3.1 Critical points

#### Stripe transition

First, we will look at the low-energy theory of the boson closing at the  $M_j$  point. The Hubbard–Stratonovich field  $m_M^j$  transforms like the fermion bilinears in the low-energy description. Specifically,  $\vec{\varphi}^j = \vec{m}(M_j)$  transforms with phase  $e^{-iM_j \cdot \mathbf{a}}$  under translations by  $\mathbf{a}$ , is time-reversal odd, and permutes the index  $j$  under rotations and reflections. It transforms exactly as  $(b^j)^i = M_{ij} = \bar{\psi} \sigma^i \tau^j \psi$  in Table 2.2. In the continuum theory, the condensing boson couples to the SU(4) fermions via a mixed chiral Gross–Neveu coupling

$$\mathcal{L}_{\text{cGN}} = -h \sum_j \left[ (\bar{\psi} \vec{\sigma} \tau^j \psi) \cdot \vec{\varphi}^j + m^2 |\vec{\varphi}^j|^2 \right]. \quad (3.73)$$

The boson mass  $m^2 = \tilde{m}^2(M)$  is defined by Eq. (3.71) within the Landau–Ginzburg theory. The overall action is given by  $\mathcal{L}_{\text{QED}_3} + \mathcal{L}_{\text{cGN}}$ . The boson represents the fluctuating magnetic order at the  $M$  point, and naturally wants to precipitate stripe order when it condenses at  $m^2 = 0$ . When the spinon exciton condenses, it will also precipitate a mass for the fermions in some channel  $M_{ij}$ . This confines the gauge field by the Polyakov mechanism, which will in turn proliferate 120-degree or VBS order in the IR limit. The exact nature of the competing order depends on which of the chiral masses  $M_{ij}$  the interaction (3.73) selects.

We believe this picture will be modified when looking at the energetics of the competing magnetic orders around this transition point. Our calculations suggest this continuous transition would first occur when  $r_c^{\text{stripe}} = 0.18$ . We know that stripe order is energetically preferred to 120-degree order for all  $r > 0.125$ , even at the classical level. We suggest instead that this continuous transition at  $r = 0.18$  should be preempted by a *first-order* transition to stripe magnetic order. This perspective is compatible with the numerical works on this model which consistently see a first-order transition at lower  $J_2/J_1$ , see Section 2.3.2. Our method is not able to compare energies between liquid and ordered states, but we can provide

an upper bound to the regime of stability of a Dirac spin liquid in a lattice model. It is an open question how to understand the position of this first-order transition analytically.

### 120-degree transition

Next, we describe the effect of gauge fluctuations on the transition at low  $J_2/J_1$ . In contrast to the stripe transition, we believe this will realise a continuous transition in the presence of gauge fluctuations. We will show this is in a QED<sub>3</sub>-Gross-Neveu universality class by studying the low-energy continuum theory.

This transition occurs as the mass of the spinon-exciton mode goes to zero at the  $\mathbf{K}$  point. Here, the relevant symmetry-compatible operators are not fermion bilinears as in the typical Gross-Neveu-Yukawa models (Janssen and He, 2017; Song *et al.*, 2019; Dupuis *et al.*, 2019, 2022), but rather the relevant spin-triplet monopoles. The effective continuum theory reads

$$\mathcal{L}_{\Phi\text{GN}} = g \sum_{\alpha} \left( i S_{\alpha}^{\dagger} \varphi_{\alpha} + \text{h.c.} \right) + m^2 |\vec{\varphi}|^2, \quad (3.74)$$

where  $\vec{\varphi} = \vec{\varphi}_{\mathbf{K}}$  here, and  $m^2 = m_{\varphi}^2(\mathbf{K}) \sim (r - r_c^{120})$  from the Landau-Ginzburg theory. We call this a monopole-Gross-Neveu ( $\Phi\text{GN}$ ) coupling. The total theory is given by  $\mathcal{L}_{\text{QED}_3} + \mathcal{L}_{\Phi\text{GN}}$ . Integrating out the fluctuating bosons produces an interaction term

$$\mathcal{L}_{\text{QED}_3} + (g/m)^2 \left( S_1^{\dagger} S_1 + S_2^{\dagger} S_2 + S_3^{\dagger} S_3 \right). \quad (3.75)$$

What is the nature of the resulting critical point driven by  $m^2 \rightarrow 0$ ? As we introduced in Section 2.3.1, the OPE of two monopoles  $\Phi^{\dagger} \Phi$  produces charge-zero operators. The symmetric combination in (3.75) specifically leads to only four-fermion interactions appearing. The most dominant OPE channel from the above effective monopole interaction (3.75) is the four-fermion interaction in the irrep  $20'$  of SU(4)

$$\mathcal{O}_{\Phi\text{GN}} \sim (\bar{\psi}_i \vec{\sigma} \psi_i)^2. \quad (3.76)$$

This interaction is believed to be irrelevant, but will cause a phase transition as the spinon exciton condenses at  $m^2 = 0$ . The interaction (3.76) is a chiral Heisenberg Gross-Neveu interaction, like we wrote down in Eq. (2.148). We predict it will lead to the same fixed-point as the chiral Heisenberg Gross-Neveu-Yukawa model described by Dupuis *et al.* (2019) on the kagome lattice. We therefore suggest that the spin liquid-120-degree order transition at  $J_{2,c}/J_1 \approx 0.07$  on the triangular lattice is in this same universality class.

### Chiral Heisenberg Gross-Neveu-QED<sub>3</sub> fixed point

The chiral Heisenberg Gross-Neveu-QED<sub>3</sub> critical point describes the end point of a stable QED<sub>3</sub> CFT, driven through a phase transition by large fermion-fermion interactions (Dupuis *et al.*, 2019). It has a reduced  $\text{SO}(3) \times \text{SO}(3)$  symmetry group compared to the  $\text{SO}(6)$  of the original model, since these interactions only couple the spin components of the fermion masses. The degeneracy of the spin-triplet and spin-singlet monopoles is broken by the interactions, which tend to condense the spin-triplet order. In our model, the same is achieved via monopole-monopole terms (3.75) which only act in the spin-triplet subgroup.

This results in a hierarchy of different monopole scaling dimensions; the most relevant are the spin-triplet monopoles, with scaling dimensions

$$\Delta_S^{\text{GN}} = 0.195 N_f + \mathcal{O}(N_f^0) \quad (3.77)$$

in a large- $N_f$  expansion (Dupuis *et al.*, 2019). The spin-singlet monopoles have the dimension

$$\Delta_D^{\text{GN}} = \Delta_S^{\text{GN}} + 0.546 + \mathcal{O}(N_f^{-1}). \quad (3.78)$$

In our  $N_f = 4$  theory of the U(1) Dirac QSL, we find  $\Delta_S^{\text{GN}} \approx 0.78$  and  $\Delta_D^{\text{GN}} = 1.33$  (Dupuis *et al.*, 2019). Contrast this to the (degenerate) value  $\Delta_\Phi = 1.02$  in standard QED<sub>3</sub> (2.113).

Let us turn now to the physical consequences of these exponents for our model. The spin structure factor at the new critical point will take the same form as Eq. (3.9), but with a modified exponent

$$\chi_S(\mathbf{q}, \omega + i\eta) = \frac{c}{(|\mathbf{K} - \mathbf{q}|^2 - \omega^2 - i\eta)^{3/2 - \Delta_S^{\text{GN}}}} \quad (3.79)$$

due to the shifted spin-triplet monopole scaling dimension. The lower value of  $\Delta_\Phi$  represents a stronger divergence and hence a higher spectral weight in  $S(\mathbf{q}, \omega)$  at low energies. This is consistent with the spinon exciton coming down and transferring spectral weight towards zero.

Finally, we know the transition is driven by tuning  $m^2 = r_c^{120} - r$ . This coupling is the bosonic mass. Its scaling dimension was also calculated in the large- $N_f, N_b$  limit of the (noncompact) QED<sub>3</sub>-cHGN model in  $d = 4 - \epsilon$  dimensions (Dupuis *et al.*, 2019), giving  $\Delta_{\varphi^2} = 1 + 4.577\epsilon$  when  $N_f = 4$ . The Lagrangian for this coupling is  $m^2 \varphi^2$  and as such the coupling has scaling dimension  $3 - \Delta_{\varphi^2}$ . This means that in the critical regime, the correlation length will obey

$$\xi^{3 - \Delta_{\varphi^2}} \sim |r_c^{120} - r|^{-1}. \quad (3.80)$$

Hence, we can define the correlation length exponent

$$\xi \sim |r_c^{120} - r|^{-\nu} \quad (3.81)$$

with  $\nu^{-1} = 3 - \Delta_{\varphi^2}$ . Setting  $\epsilon = 1$ , we finally find that  $\nu = 1.644$  in our model.<sup>4</sup> Equivalent to Eq. (3.81), there is a mass that scales  $m \sim \xi^{-1} \sim |r_c^{120} - r|^\nu$ . In the Gaussian theory this was  $\nu = 1/2$ .

### 3.3.2 Dynamical structure factor

The Ansatz (3.79) is only possible because conformal symmetry is restored at the new critical point. We will now work to predict the spin structure factor away from the transition point. This becomes more difficult since both monopoles and spinons contribute to the structure factor.

<sup>4</sup>The value of  $\nu$  depends upon how the  $4 - \epsilon$  expansion is taken (Dupuis *et al.*, 2019).

The challenge will be to work out the effect of the quantum-critical continuum at the  $\mathbf{K}$  point on the response of the spinons. When adding these contributions, it is worth noting that although the fermion bilinears and monopoles both transform like spin operators, their normalization is different. In the case of spinons, the normalization is ‘fixed’ by the Abrikosov decomposition. The monopoles however are not defined as some local quasiparticle in this basis, and as such we can only write  $S_i^z \simeq \mathcal{S}(\mathbf{r}_i)$  as in Eq. (2.135) up to some arbitrary normalization (and a phase fixed by symmetry). We choose the following normalization for the two contributions to the spin operator

$$S_i^z = \frac{1}{2} f_i^\dagger \sigma^z f_i \quad (3.82)$$

$$S_i^z \simeq \alpha_\Phi \left( i e^{i\mathbf{K} \cdot \mathbf{r}_i} \mathcal{S}_3^\dagger(\mathbf{r}_i) + \text{h.c.} \right). \quad (3.83)$$

We initially describe the spin-spin correlation function as a sum of the fermion and gauge contributions, starting with a non-interacting fermion theory. In diagrammatic language, we write the mean-field susceptibility including gauge fluctuations as

$$\chi(\mathbf{q}, \omega) = \chi_f^0(\mathbf{q}, \omega) + \alpha_S^2 \chi_S(\mathbf{q}, \omega) = \text{fermion bubble} + \text{gauge wavy line}. \quad (3.84)$$

The monopole susceptibility Eq. (3.11), and hence also the relative magnitude of the terms in Eq. (3.84), is defined up to a constant  $\alpha_S^2$ . In Fig. 3.10(a) we plot this combined contribution with  $\alpha_S = 0.4$ .

### Gauge-matter coupling

In order to describe the effect of gauge fluctuations, we will now write down a fermion-monopole coupling and treat its effect perturbatively alongside the fermion-fermion interactions. In real space, this coupling is simply a coupling between the spin-order parameters of the fermions with wavevector  $\mathbf{K}$ , defined as

$$\langle S_i^\alpha \rangle = m_i^\alpha = e^{i\mathbf{K} \cdot \mathbf{r}_i} n_i^\alpha + \text{c.c.}, \quad (3.85)$$

and the monopole Eq. (2.135):

$$g_S \alpha_S [i \mathcal{S}_3^\dagger(\mathbf{r}_i) n_i^z + \text{h.c.}]. \quad (3.86)$$

In the fermionic parton representation, this leads to the vertex

$$\frac{1}{2} g_S \alpha_S \left( i \mathcal{S}_3^\dagger e^{i\mathbf{K} \cdot \mathbf{r}_X} \sum_{\mathbf{k}} f_{\mathbf{k}, X}^\dagger \sigma^z f_{X, \mathbf{k} + \mathbf{K}_\alpha} + \text{h.c.} \right) = \text{fermion vertex with wavy line}. \quad (3.87)$$

This result is written in the sublattice basis, where the phase  $R_X = e^{i\mathbf{K} \cdot \mathbf{r}_X}$  comes from the relative position of the site  $X$  in the unit cell.

In diagrams, we replace the free fermion bubble  $\chi_f^0(\mathbf{q}, \omega)$  in Eq. (3.84) by the interacting fermion susceptibility  $\chi_f(\mathbf{q}, \omega)$

$$\chi(\mathbf{q}, \omega) = \chi_f(\mathbf{q}, \omega) + \alpha_S^2 \chi_S(\mathbf{q}, \omega) = \text{interacting fermion bubble} + \text{gauge wavy line} \quad (3.88)$$

The diagrams which correct the bare susceptibility to leading order are as follows<sup>5</sup>

$$+ \dots \quad (3.89)$$

Beyond leading order, the series of diagrams will contain all combinations of Heisenberg interactions and monopole propagators. The Dyson equation is modified to include both intermediate states:

$$(3.90)$$

This can be formulated once again as a matrix equation (3.36), where the interaction now includes two terms: the Heisenberg four-fermion vertex, and an intermediate-monopole propagator

$$\hat{U}(\mathbf{q}, \omega)^{\mu\nu} = \delta^{ij} [-2J_{\mathbf{q}}^{XY} + (g_S^2 \alpha_S^2 / 4) (RR^\dagger)^{XY} \chi_S(\mathbf{q}, \omega)]. \quad (3.91)$$

The relative phases are  $(RR^\dagger)^{XY} = e^{i\mathbf{K} \cdot (\mathbf{r}_X - \mathbf{r}_Y)}$ . The Dyson equation for the fermion susceptibility in this language is exactly as before

$$[\chi_f(\mathbf{q}, \omega)]^{\mu\nu} = [\chi_f^0(\mathbf{q}, \omega)]^{\mu\nu} + [\chi_f(\mathbf{q}, \omega)]^{\mu\rho} [U(\mathbf{q}, \omega)]^{\rho\sigma} [\chi_f^0(\mathbf{q}, \omega)]^{\sigma\nu}; \quad (3.92)$$

resumming this series using the RPA produces the susceptibility in the presence of fermion-fermion and fermion-gauge interactions.

## Results

Here, we will numerically treat interactions between the fermions and spin-triplet monopoles by solving the Dyson equation (3.92). Taking  $J_2/J_1 = 0.09$  as a constant, we plot the RPA susceptibility for various values of the monopole-fermion coupling  $g$  in Fig. 3.10. In the decoupled limit (a), the mode remains sharp and unmoved. As interactions are turned on, the major effect is that the mode is broadened and shifted slightly. The spectral weight in the monopole continuum also appears to increase at low energies. Overall, we observe an interaction-dependent hybridisation between the mode and the critical continuum due to the monopoles. This is possible because the spinon exciton has identical quantum numbers to the spin-1 monopole  $\mathcal{S}^\alpha$ , see Table 2.3.

<sup>5</sup>Note that we ignore the correction of the fermion loop to the bare monopole propagator in (3.88). This would require a next-order self-consistent approach.

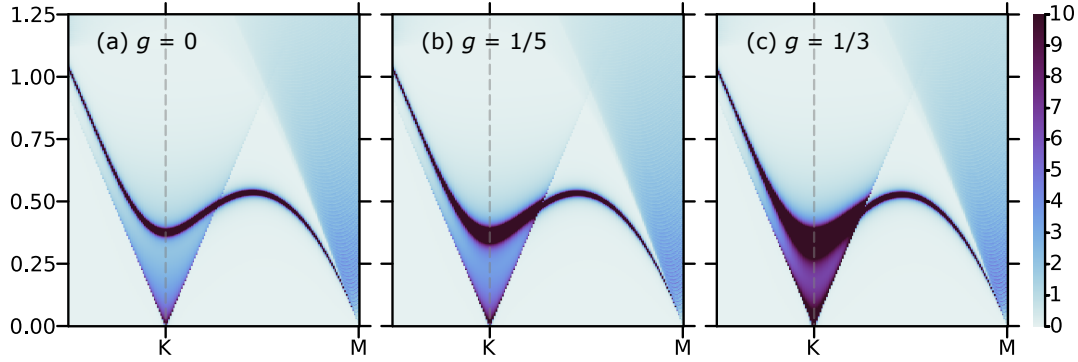


Figure 3.10: *Hybridisation of the spinon exciton with the monopole continuum through a modified RPA approach.* Coupling strengths (a)  $g = 0$  decoupled limit, (b)  $g = 1/5$  weak coupling and (c)  $g = 1/3$  strong coupling.

We expect effectively independent quasiparticles when the hybridisation correction to the RPA is negligible,  $g^2 \alpha_\Phi^2 \chi_\Phi(\mathbf{K}, m_{\text{RPA}}(\mathbf{K})) \ll 1$ . This can be simply achieved when the monopoles are weakly interacting  $g \ll 1$ , or they have a low spectral weight  $\alpha_\Phi \ll 1$ . Additionally, there is a complete separation of scales between the RPA mode and the low-energy monopole continuum when large  $J_2$  interactions push the spinon exciton to high energies. Away from this limit, the modes do not decouple. We have seen that the monopole broadens the spinon exciton through the RPA correction. Returning to Fig. 3.10(b) with  $g = 0.2$ , we plot a slice of the spin structure factor at  $\mathbf{q} = \mathbf{K}$  for various parameters  $J_2 \rightarrow J_{2,c}$  in Fig. 3.11. Focusing first on  $J_2/J_1 = 0.9$  and  $0.8$  where we can apply our perturbative RPA calculation. This shows that as the mass of the spinon-exciton mode approaches zero, the mode gets broader.

A simple understanding for this effect comes from including the monopole interactions into the effective theory of the dynamical spinon exciton. This is an approach discussed by Ghaemi and Senthil (2006) on the square lattice. In Appendix A we show the spinon exciton's Green's function is modified by an additional diagram, namely an intermediate monopole propagator

$$G_\varphi(\mathbf{q}, \omega) = \text{diagram 1} = \text{diagram 2} + \text{diagram 3} + \text{diagram 4} + \dots \quad (3.93)$$

The Green's function of the paramagnon hence reads

$$G_\varphi(\mathbf{q}, \omega) = \frac{1}{m_\varphi^2(\mathbf{q}) - g_S^2 \alpha_S^2 \chi_S(\mathbf{q}, \omega) - \omega^2}. \quad (3.94)$$

We can infer that the dispersive paramagnon mode  $m_{\varphi}^2(\mathbf{q})$  gets its energy renormalised by the gauge fluctuations, and it gets broadened. The real and imaginary parts are respectively responsible for these phenomena. The corrected energy and lifetime are given as follows,

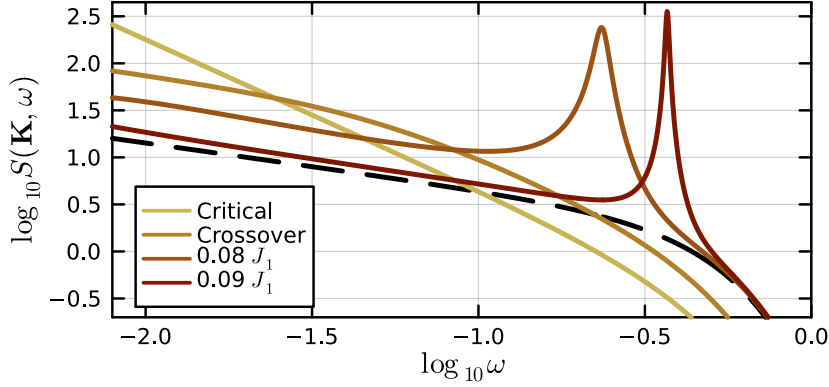


**Figure 3.11:** *Spectral function at the  $K$  point, showing hybridisation of the spinon exciton and monopoles.* This probes critical properties of the stable spin liquid phase and the transition to 120-degree magnetic order. The transition is tuned by the spinon exciton mass  $m$ . This is taken to be zero at the critical point  $m = 0$ ; the crossover relies on the Ansatz (3.97). The other two results are calculated within the modified RPA with monopole hybridisation. The coupling strength is  $g = 0.2$  and we tune  $J_2/J_1 = 0.09, 0.08$  towards the transition point. Black dashed line shows the (decoupled) monopole contribution.

where we evaluate the monopole susceptibility at the uncorrected mass:

$$\tilde{m}_\varphi^2(\mathbf{K}) = m_\varphi^2(\mathbf{K}) + g_S^2 \alpha_S^2 c \cos[\pi(3/2 - \Delta_\Phi)] |m_\varphi(\mathbf{K})|^{-(3-2\Delta_\Phi)}, \quad (3.95)$$

$$\Gamma_\varphi(\mathbf{K}) = g_S^2 \alpha_S^2 c \sin[\pi(3/2 - \Delta_\Phi)] |m_\varphi(\mathbf{K})|^{-(3-2\Delta_\Phi)}. \quad (3.96)$$

For  $1 < \Delta_\Phi < 3/2$ , the mode is drawn downwards and broadened.

### Critical regime

When the gap to the spinon exciton is small, the perturbative RPA approach will break down as the corrections diverge. Returning to Fig. 3.11, we now turn to the behaviour of the spectral function when the mode approaches the critical point. When  $J_2 = J_{2,c}$  we have a gapless boson  $m^2 = 0$  and we sit at the new QED<sub>3</sub>-cHGN fixed point. Here, we apply the Ansatz (3.79) to show  $S(\mathbf{K}, \omega) \sim \omega^{2\Delta_S^{\text{GN}}-3}$ . This shifted exponent is plotted as the critical line in Fig. 3.11. If, instead, we sit just away from the critical point, then we know that the gap scales as  $m \sim (r - r_c^{120})^{1.6}$  in the large- $N_f$  and  $4 - \epsilon$  approximations. Instead, here we can write a scaling Ansatz for the critical regime. To do this, first use that when  $\omega \ll m$ , the effective continuum theory is just QED<sub>3</sub>. The exponents in this regime should be dictated by  $\Delta_\Phi = 1.25$ . Alternatively, when  $\omega \gg m$ , the spectral function should scale with QED<sub>3</sub>-GN exponents, since at these energy scales it looks like the critical point  $m = 0$ . In the intermediate regime we can write down a scaling Ansatz

$$S(\mathbf{K}, \omega) = \omega^{2\Delta_\Phi-3} \mathcal{G}(\omega/m), \quad (3.97)$$

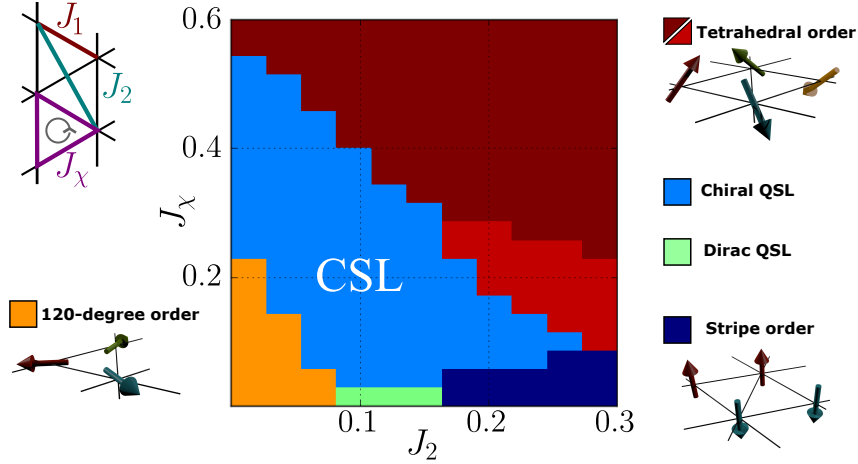


**Figure 3.12:** *Numerical phase diagram as calculated using exact diagonalisation.* Figure adapted from Wietek and Läuchli (2017). Phase diagram of the  $J_1$ - $J_2$ - $J_x$  triangular-lattice Heisenberg model. The authors find competing 120-degree, stripe, and tetrahedral magnetic orders, as well as both chiral and Dirac spin liquids.

where  $\mathcal{G}(x)$  is constrained by the two limiting cases discussed above. A basic example is plotted as the crossover line in Fig. 3.11, where we take  $\mathcal{G}(x) = (1 + x^2)^{\Delta_S^{\text{GN}} - \Delta_\Phi}$ . It recovers both limits as discussed, and has a crossover between power laws around  $m = 0.05$ . Imagining a numerical simulation or experiment where the interaction strength  $r$  could be tuned, this would allow a scaling collapse to be obtained and extract the relevant critical exponents. Combined with the scaling properties of  $m$ , we would expect a scaling collapse by plotting  $\omega^{3-2\Delta_\Phi} S(\mathbf{K}, \omega)$  against  $|r - r_c^{120}|^{\nu_{\text{GN}} \omega}$ .

We may also evaluate the real-space spin-spin correlations  $g_{ij}$  within these three regimes, given by Eq. (3.40). Away from the critical point, the long-distance behavior is dominated by a power-law tail, governed by the universal QED<sub>3</sub> monopole exponents  $g(r) \sim r^{-2\Delta_\Phi}$ . The finite-energy spinon exciton causes a non-universal correction at short distances, with a characteristic energy scale that goes as  $\xi \sim (r - r_c^{120})^{-1/2}$ . Numerical simulations suggest the monopole contribution is subleading to the fermionic one (cf. Fig. 3.5), but it must still dominate for large separations. Approaching the critical point, this correlation length will diverge, governed by new cHGN exponents  $\xi \sim (r - r_c^{120})^{-\nu_{\text{GN}}}$ . For lengths  $r \ll \xi$ , the correlations will be controlled by cHGN exponents  $g(r) \sim r^{-2\tilde{\Delta}_\Phi}$  such that at the critical point  $\xi \rightarrow \infty$  we have a picture of conformal correlations. Away from the transition, the correlations for lengths  $r \gg \xi$  will be given by QED<sub>3</sub> exponents. We equally expect a scaling collapse by plotting  $r^{2\Delta_\Phi} g(r)$  against  $|r - r_c^{120}|^{-\nu_{\text{GN}} \omega}$ .

### 3.4 Dynamical response of the chiral QSL

#### Chiral QSL on the triangular lattice

Next, we demonstrate the generality of the self-consistent approach by considering perturbing the U(1) Dirac QSL with a scalar spin chirality (SSC) term (Hu *et al.*, 2016)

$$\mathcal{H} = \mathcal{H}_{J_1 J_2} + J_\chi \sum_{ijk \in \triangle, \nabla} \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k), \quad (3.98)$$

where  $ijk$  is an ordered set of the three spins on each triangular plaquette. The SSC interaction  $J_\chi$  breaks time-reversal symmetry and opens up a gap for the fermion bands.

In the field-theory language of Section 2.3.1, this generates a finite mass  $M_{00} = \bar{\psi}\psi$  to the action. The result is gapped spinon bands, which acquire a non-zero topological Chern number. This is different to the cases we considered before, where adding a chiral mass term  $M_{ij}$  ( $i \neq j \neq 0$ ) led to monopole proliferation by the Polyakov mechanism (Song *et al.*, 2019). In this case, confinement and magnetic ordering are avoided. Integrating out the gapped fermion bands, we can see that a Chern–Simons term is generated

$$\bar{\psi} i \gamma^\mu (\partial_\mu - i a_\mu) \psi - m \bar{\psi} \psi \longrightarrow \frac{N_f/2}{4\pi} \epsilon^{\mu\nu\rho} a_\mu \partial_\nu a_\rho. \quad (3.99)$$

In our  $N_f = 4$  model, a finite mass  $m$  gives a mass to the gauge excitations and leads to the same effective theory as the  $\nu = 1/2$  Laughlin state (Kalmeyer and Laughlin, 1987; Wen *et al.*, 1989; Wen, 2004). Because the gauge excitations are gapped, the monopoles do not proliferate and we have a new, stable, liquid state: the chiral spin liquid. The spinons are the basic excitations in the chiral QSL, and we will treat them within the same framework as the U(1) Dirac model.

The triangular-lattice Heisenberg model has been studied by many numerical works, showing a rich array of unconventional phases upon adding spin-scalar chirality interactions (Wietek and Läuchli, 2017; Saadatmand and McCulloch, 2017; Gong *et al.*, 2017). As mentioned, the field-theoretic description points to the possibility of realising a chiral QSL upon breaking time reversal. Furthermore, recent works also suggests the presence of non-coplanar states at higher  $J_\chi$ . We show in Fig. 3.12 the phase diagram from Wietek and Läuchli (2017), showing rich competition between ordered and liquid phases. There is no obvious signal of non-coplanar ordered states within the competing orders of Song *et al.* (2019). We investigate here how it emerges from the spinon-exciton mode at intermediate  $J_\chi$ . Finally, we are able to directly study the dynamics of the chiral spin liquid phase.

To derive the properties of this chiral QSL, we will apply mean field theory. The SSC term induces six-fermion interactions. We can split the interaction to find (Maity *et al.*, 2025)

$$J_\chi \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k) = H_{ijk} + H_{jki} + H_{kij}, \quad (3.100)$$

where the explicit interaction in the parton basis is given by

$$H_{ijk} = \frac{iJ_\chi}{2} (S_i^+ S_j^- - S_i^- S_j^+) S_k^z \quad (3.101)$$

$$= \frac{iJ_\chi}{4} [f_{i\uparrow}^\dagger f_{k\uparrow} f_{k\uparrow}^\dagger f_{j\uparrow} f_{j\downarrow}^\dagger f_{i\downarrow} - f_{i\downarrow}^\dagger f_{j\downarrow} f_{j\downarrow}^\dagger f_{k\uparrow} f_{k\uparrow}^\dagger f_{i\uparrow} + (\uparrow \leftrightarrow \downarrow)]. \quad (3.102)$$

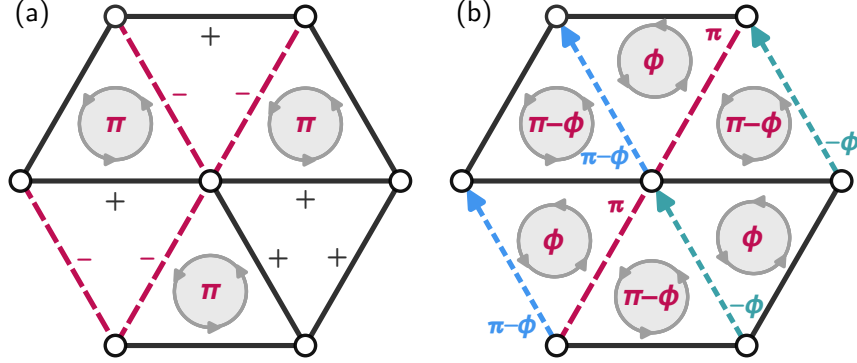


**Figure 3.13: Dirac and chiral spin liquid Ansätze.** (a) The  $\pi$ -flux Ansatz of the U(1) Dirac QSL, with  $[\pi, 0]$  flux through up- and down triangular plaquettes. (b) The general staggered  $[\pi - \phi, \phi]$ -flux Ansatz. Both states share the same unit cell and corresponding unit vectors, shown in Fig. 2.8. In this work, it is generated by a self-consistent mean-field treatment of a spin-scalar chirality interaction which breaks time-reversal symmetry.

As is familiar, we can now decouple the interacting Hamiltonian using parton mean-field theory. The Hamiltonian Eq. (3.98) takes the following form (Banerjee *et al.*, 2023)

$$\begin{aligned} \mathcal{H}_0 = & -\frac{1}{2} \sum_{ij} J_{ij} [(\chi_{ij} f_{j\alpha}^\dagger f_{i\alpha} + \text{h.c.}) - |\chi_{ij}|^2] \\ & + \frac{3i}{16} \sum_{ijk} J_\chi (\chi_{ik} \chi_{kj} f_{j\alpha}^\dagger f_{i\alpha} + \chi_{ik} \chi_{ji} f_{k\alpha}^\dagger f_{j\alpha} \\ & + \chi_{kj} \chi_{ji} f_{i\alpha}^\dagger f_{k\alpha} - \chi_{ik} \chi_{kj} \chi_{ji} - \text{h.c.}). \end{aligned} \quad (3.103)$$

In order to work with this mean-field Hamiltonian, we assume that the  $\chi_{ij}$  form a  $[\pi, 0]$ -flux Ansatz. The mean-field parameters  $\chi_{ij}$  in this context are all real, shown in Fig. 3.13(a). The mean-field hoppings that they induce in Eq. (3.103) will become complex. We write the Hamiltonian as

$$\mathcal{H}_0 = - \sum_{ij} (t_{ij} f_{j\alpha}^\dagger f_{i\alpha} + \text{h.c.}). \quad (3.104)$$

Focusing on a single triangle  $ijk$ , we can evaluate the  $ki$  hopping

$$t_{ki} = \frac{J_1 \chi}{2} \left[ 1 - i \left( \frac{3\chi J_\chi}{8J_1} \right) \right]. \quad (3.105)$$

The magnitude of the hopping increases with the added interaction, and there is an additional phase from the time-reversal symmetry-breaking contribution  $J_\chi$ . We find for the other two bonds that they are exactly the negative  $t_{ij} = t_{jk} = -t_{ki}$ . Therefore, a spinon hopping around this plaquette picks up a phase  $\phi$ , equal to three times the phase of Eq. (3.105). Likewise, on the upwards facing triangle, the result is  $-\phi$ . The parameters are

$$t = \frac{J_1 \chi}{2} \sqrt{1 + \left( \frac{3\chi J_\chi}{8J_1} \right)^2}, \quad \phi = -3 \arctan \left( \frac{3\chi J_\chi}{8J_1} \right). \quad (3.106)$$

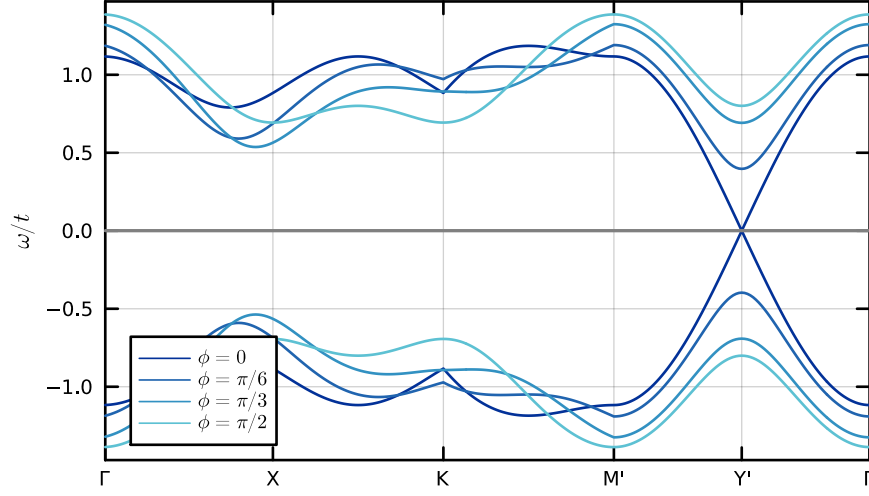


**Figure 3.14: Spinon bands of the chiral spin liquid.** Chiral phases are as follows: gapless Dirac spin liquid Ansatz  $\phi = 0$ ;  $\phi = \pi/6$ ;  $\phi = \pi/3$ ; and translationally invariant time-reversal odd Ansatz  $\phi = \pi/2$ .

This result shifts the mean-field state from  $[\pi, 0]$ -flux to  $[\pi - \phi, \phi]$ , with a modified normalisation of the Hamiltonian.

Performing a gauge transformation,<sup>6</sup> we find that the state can be parameterised as shown in Fig. 3.13. The Hamiltonian in the sublattice basis reads

$$H_{\alpha\beta}^{XY}(\mathbf{k}) = t \delta_{\alpha\beta} M_{\mathbf{k}}^{XY}, \quad (3.107)$$

where explicitly the phases are given by

$$\begin{aligned} M_{\mathbf{k}}^{AA} &= -M_{\mathbf{k}}^{BB} = 2 \cos(k_2) \\ M_{\mathbf{k}}^{AB} &= 1 + e^{-ik_1} + e^{i(\phi+k_2-k_1)} - e^{-i(\phi+k_2)}. \end{aligned} \quad (3.108)$$

The case  $\phi = 0$  recovers the U(1) Dirac spin liquid dispersion with gapless spinon bands. For finite  $\phi$  the bands have a gap, shown in Fig. 3.14. Note that this continuous evolution of the angle  $\phi$  is also seen in variational calculations (Hu *et al.*, 2016). Finally, we note that this state breaks time-reversal symmetry. To see this, note that the symmetry maps all triangle fluxes to their negative. For the Dirac state,  $\pi \rightarrow -\pi$  is equivalent up to a gauge transformation. But with the staggered phases,  $\pm\phi$  are not equivalent any more. Any Ansatz with  $\phi \neq 0$  has a finite gap. The case of  $\phi = \pi/2$  is the translationally invariant and time-reversal odd.

### Interacting susceptibility

Now let us evaluate the dynamical response of the chiral QSL phase of this model. We will evaluate the *interacting* susceptibility of the fermionic spinons. The interactions will

<sup>6</sup>See the work of Song *et al.* (2021) for another possible gauge choice.

come from both  $J_1$  and  $J_2$  Heisenberg interactions, as well as the scalar spin-susceptibility. The advantage of the self-consistent method defined above is that we may hope to produce quantitative predictions for the structure factor.

In this case, we are faced with treating a six-fermion interaction. In order to use the RPA, we have to make some further simplifications. The RPA sums over a series of bubble diagrams, where the interactions are four-fermion vertices. In the case of Heisenberg interactions, this was given by Eq. (3.29). Look again at the form of the SSC interaction in the parton basis, Eq. (3.102). We manipulate it into the form

$$J_\chi \sum_{ijj} \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k) = J_\chi \frac{1}{8} \epsilon_{ijk} \sigma_{\alpha\beta}^i \sigma_{\gamma\delta}^j \sigma_{\sigma\rho}^k \sum_{ijk} f_{i\alpha}^\dagger f_{i\beta} f_{j\gamma}^\dagger f_{j\delta} f_{k\sigma}^\dagger f_{k\rho}. \quad (3.109)$$

The RPA is based on a perturbative expansion of the interacting correlation function in terms of this interaction operator. The contribution of this interaction at first order would give an antisymmetric, off-diagonal (in spin indices  $ij$ ) contribution to  $\chi(\mathbf{q}, \omega)_{XY}^{ij}$ . However, this contribution is proportional to various expectation values of spin operators  $\langle f_{i\sigma}^\dagger \sigma_{\sigma\rho} f_{i\rho} \rangle$  and  $\langle f_{i\sigma}^\dagger \sigma_{\sigma\rho} f_{j\rho} \rangle$ . We expect these contributions to all vanish in the mean-field state. Therefore, the SSC interaction will only contribute at higher order.

We may now directly apply the RPA method to the chiral spin liquid in the regime<sup>7</sup> where  $J_\chi/J_1 \ll 1$ . Here, we also approximate Eq. (3.106) as  $t = J_1\chi/2$  and  $\phi = -9\chi J_\chi/8J_1$ . We use the form of the interactions exactly as described in Section 3.2. The spinon contribution to the dynamical structure factor is shown in Fig. 3.15. The chiral interactions  $J_\chi = 0.175$  induce a gap in the spinon continuum of the order  $J_\chi$ . Our mean-field analysis predicts a continuous transition from the U(1) Dirac to chiral QSL state upon addition of this time-reversal symmetry-breaking interaction.

We present results for the next-nearest neighbour interaction strength  $J_2/J_1 = 0.09$  and 0.18. In the pure Heisenberg model,  $\approx 0.18$  was the phase boundary of the U(1) Dirac QSL phase. Here, we see that the spinon exciton is gapped and we are still within the stable regime. The SSC interaction has hence *stabilised a spin liquid*. This has been observed by Wietek and Läuchli (2017) in an exact diagonalisation study of the same  $J_1$ - $J_2$ - $J_\chi$  model. Their results, shown above in Fig. 3.12, predict a chiral spin liquid extends over a wide range of  $J_2$  at small values of  $J_\chi$ . Note that a condition for this being realised in the phase diagram is that the chiral QSL must also have a ground state energy lower than the stripe phase. The aforementioned numerical results confirm that the SSC interaction stabilises the chiral QSL and quickly pushes the first-order transition to higher  $J_2$ .

For larger values of  $J_\chi/J_1$ , we predict that this sharp mode will be pushed downwards by the interactions that come in at order  $(J_\chi/J_1)^2$ . A scheme for how to evaluate the effect of these interactions within the RPA is as follows. The six-fermion SSC interactions have ‘legs’ on three sites around a triangular plaquette,  $ijk$ . There is a dominant correction to the four-fermion susceptibility that comes from two adjacent triangles which share two sites, one pointing up and one down. Here, we contract the operators on the shared sites  $j, j'$  and  $k, k'$ , leading to an effective next-nearest neighbour interaction  $i \leftrightarrow i'$ . At this order, there are contributions which do not vanish when  $j = j'$ , given by  $\langle f_{j\alpha}^\dagger f_{j\alpha} \rangle = 1$ . This leads

<sup>7</sup>Strictly speaking, we also require that  $(J_\chi/J_1)^2 \ll J_2/J_1$  in order to ignore SSC interactions.

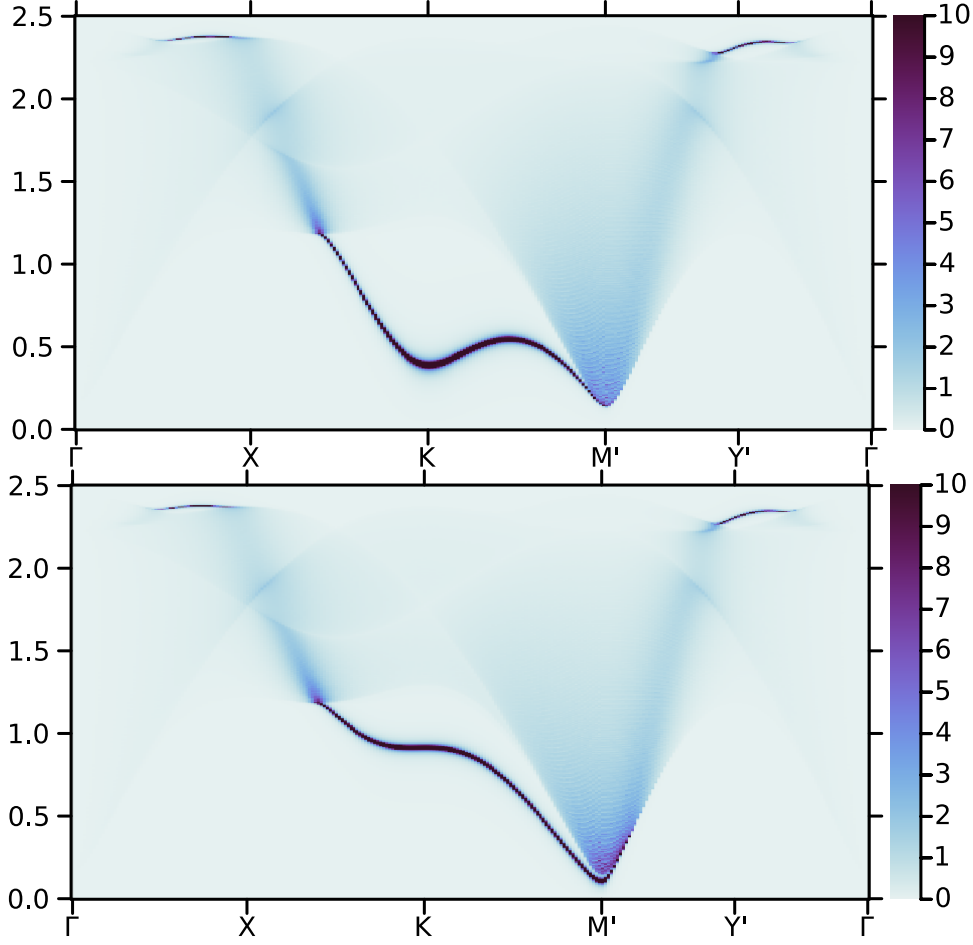


**Figure 3.15:** *Structure factor for the chiral QSL phase  $S(\mathbf{q}, \omega)$ .* We treat the spin-scalar chirality interaction in mean field theory, with magnitude  $J_\chi/J_1 = 0.18$  in both. We also take next-nearest neighbour exchange  $J_2/J_1 = 0.09$  (top figure) and  $0.18$  (bottom figure). All energies  $\omega$  in units of  $J_1$ .

to an effective next-nearest neighbour interaction that emulates an additional Heisenberg exchange  $J_2^{\text{SSC}}/J_1 \sim (J_\chi/J_1)^2$ . This acts to push the spinon exciton downwards at the  $M$  point. By calculating the order of energy scales, this transition is at about  $J_\chi/J_1 \approx 0.4$  for the mode plotted in Fig. 3.15 ( $J_2/J_1 = 0.18$ ).

The mode condensing will precipitate magnetic order with wavevector  $M$ . The SSC interaction naturally favours tetrahedral order, since it is non-zero when spins around a plaquette are non-coplanar. We therefore predict that the chiral QSL will transition continuously towards tetrahedral order (Wietek and Läuchli, 2017; Cookmeyer *et al.*, 2021). Because the gauge excitations of the spin liquid are gapped, they will not play a defining role in choosing the resulting ordered state (Hickey *et al.*, 2016). For lower  $J_2/J_1 \sim 0.09$ , the SSC interactions tend to destabilise the coplanar 120-degree order. In our interacting model, this is seen by the increasing effective next-nearest neighbour interaction, which acts to stabilise

the chiral spin liquid over 120-degree order. It would be a fruitful direction to explore the possibility of accounting for these effects quantitatively in future works.

### 3.5 Outlook

In this Chapter, we studied the dynamical response of the U(1) Dirac spin liquid on the triangular lattice. To do this, we used a self-consistent mean field theory of Heisenberg models in the parton basis. We find that interactions between spinons lead to sharp spinon-exciton bound states which dominate the spectral function over a large part of the finite-frequency response and interact with the broad spinon continuum. The results are in strong agreement with recent VMC (Ferrari and Becca, 2019) and tDMRG results (Drescher *et al.*, 2023; Sherman *et al.*, 2023).

From the condensation of the sharp modes we can deduce the stability of the QSL phases and predict the nature of neighbouring ordered phases. We therefore provide new concrete, analytical predictions for the stability of liquid states in these familiar Heisenberg Hamiltonians. The resulting phase diagram is in remarkable agreement with heavy-duty numerical methods. Overall, this points to a general applicability of our self-consistent method, which does not have any free parameters. If a parton MFT Ansatz is a good variational state, the RPA approach is a simple yet extremely powerful tool for describing the dynamical response and stability of the QSL phase.

This success is corroborated by a complementary study investigating the  $\mathbb{Z}_2$  Kitaev QSLs (Rao *et al.*, 2025). The Kitaev spin liquid is known to be the exact ground state of the model of bond-dependent Ising interactions (Kitaev, 2006). This ground state is a spin liquid of fractionalised, non-interacting Majorana fermions. Broad continua are observed in the dynamical properties of this model, which are interpreted as being a result of two-Majorana continua (Knolle *et al.*, 2014a,b). The  $\mathbb{Z}_2$  gauge fluxes play a key role in the resulting dynamics. However, realistic spin Hamiltonians introduce perturbations that break the exact solubility. This includes additional exchanges or magnetic fields needed to suppress ordering. Beyond this limit, dynamical properties are inaccessible using the free-Majorana approximation. The same RPA approach to treating interactions between fermionic partons was applied by Rao *et al.* (2025). Applied to the soluble limit, the interacting Majorana calculation is in surprising agreement with the previous work of Knolle *et al.* (2014a) which treats Majorana-gauge interactions. This implies that the fermion interactions somehow mimic the effect of a static flux degree of freedom. Beyond the soluble regime, this work also finds a dominant contribution to the dynamics coming from Majorana bound states.

It appears that sharp modes may be a general feature of realistic spin liquid models which are proximate to ordered states. As highlighted by Knolle and Moessner (2019), the definition of a spin liquid as being a *deconfined* phase of fractionalised spinons does not preclude finite-energy bound states in the spectrum. In our interpretation, the spinon bound states can be understood as fluctuating order parameters of neighbouring ordered states (Ghaemi and Senthil, 2006). We saw this explicitly through formulating the spinon exciton as a Hubbard–Stratonovich decoupling of the Heisenberg interaction. This has been experimentally observed in 1D chains (Coldea *et al.*, 2010) and we suspect it will play a key role in 2D experiments as well. We will discuss the implications of this observation for experimental

progress in the next Chapter.

On the theoretical side, let us note that many questions remain: First and foremost, it is unclear why the simple RPA works so well in describing the spin structure factor and stability of QSLs. In particular because the U(1) states are expected to have strong gauge fluctuations. The unreasonable effectiveness of the RPA in this context is yet another example of the successful application of a theory beyond its original development context (Wigner, 1990). We introduced a phenomenological understanding of the low-energy physics of the U(1) Dirac QSL by describing the monopoles and spinons as independent particles that are perturbatively coupled, but a deeper understanding of the physics remains a formidable open challenge.

Second, beyond extending the self-consistent approach to other models, we think a great insight could be gained by calculating other dynamical correlation functions, for example the dynamical dimer-dimer correlator (Läuchli *et al.*, 2008). Numerical results of the U(1) Dirac QSL show that static dimer-dimer correlations are dominated by monopoles and the role of spinon contributions at finite frequency is yet to be determined. We hope that it would also account for the QSL to valence bond solid (VBS) transition seen in the square-lattice  $J_1$ – $J_2$  model (Morita *et al.*, 2015). Furthermore, this response function would have predictive power for probes like resonant inelastic X-ray and Raman scattering (Koller *et al.*, 2025).

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## Introduction

The most basic criterium which defines a spin liquid state is the absence of magnetic order. This is the *negative* definition discussed in Chapter 1. In practice, this means there should be no magnetic Bragg peaks in elastic neutron scattering, and thermodynamic measurements must not show magnetic ordering transitions (Zhou *et al.*, 2017).

However, it is difficult to *positively* identify a quantum spin liquid by simply the absence of order. Inelastic neutron scattering may be able to provide signatures of the predicted dynamical, fractionalised quasiparticles. It directly probes the dynamical structure factor of frustrated spin systems (Lovesey, 1986), directly shining light on the excitation spectrum. Measuring the very emergent particles that make spin liquids theoretically interesting would be a true positive signature. In particular, much attention is often paid to the presence of continua in neutron scattering experiments as a signature of liquid behaviour. Spin fractionalisation naturally produces continua: there are a range of allowed momentum transfers when a spin-flip excitation produces two or more emergent particles. However, disorder and loss of translational symmetry have also been shown to cause responses that mimic a quantum spin liquid (Zhu *et al.*, 2017; Paddison *et al.*, 2017).

In this context, we need to be more careful to define reliable positive signatures which allow us to interpret neutron scattering data. Success has been found in 2D by measuring the temperature dependence of continuum responses in Kitaev-like materials (Nasu *et al.*, 2016). This directly probes the fermionic statistics of the Majorana continuum. Seeing such behaviour in a *bosonic spin model* is a truly surprising result, not easily explained by other conventional mechanisms. A related approach is familiar in the 1D context. The temperature dependence of the dynamical structure factor in Luttinger liquids should be governed by universal exponents. A scaling collapse of the dynamical structure factor can extract universal exponents from a continuum response (Lake *et al.*, 2005).

Beyond these universal aspects, it is also necessary to understand model-specific features. For example, the most simple explanation of sharp modes in the high-energy response of a spin liquid candidate material is sharp spin waves of a magnetically ordered state. Occam's razor then suggests we should choose this conventional description (Mazin, 2022). If we are to exclude this hypothesis in favour of an exotic model, we must prove its superiority. However, it is not always possible to make such concrete theoretical predictions which would provide sufficient weight to favour the interesting hypothesis. Our results in the previous Chapter 3 show that it is possible for the Hamiltonian-specific response to dominate in experiments. We will discuss a *quantitative* comparison to experimental works here.

This Chapter is based on our ongoing collaboration with the group of Scheie *et al.*, who investigated the dynamical response of a family of triangular-lattice magnetic insulators, the

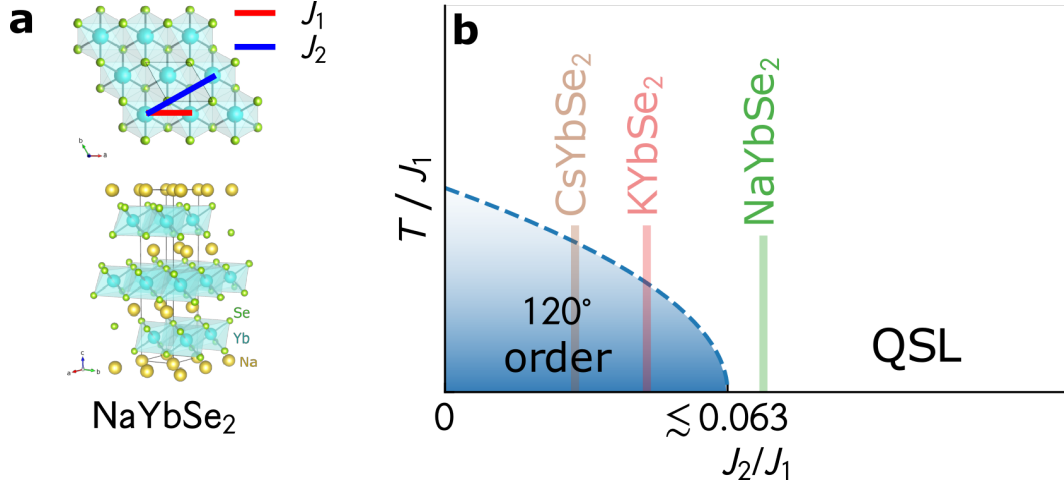


**Figure 4.1:** *Experimental search for a quantum spin liquid in the ytterbium delafossites.* (a) Crystal structure of the planar triangular lattice compounds  $\text{NaYbSe}_2$ . (b) Schematic phase diagram of the Heisenberg exchange parameters of  $\text{AYbSe}_2$  with  $A = \text{Cs}, \text{K}, \text{and Na}$ , as measured by (Xie *et al.*, 2023; Scheie *et al.*, 2024a).

ytterbium delafossites. The compounds in this family are well described by the  $J_1$ – $J_2$  model, and show signatures of fractionalisation in their neutron scattering spectra. The crystal structure and schematic phase diagram of the models is shown in Fig. 4.1. The three compounds are described by the series  $\text{AYbSe}_2$ , where the alkali earth metal  $A = \text{Cs}, \text{K}, \text{and Na}$ . The analysis of  $\text{NaYbSe}_2$  in this Chapter is to appear in Scheie *et al.* (2024b). We will also discuss several ongoing investigations into criticality in  $\text{KYbSe}_2$ , based on data published in Scheie *et al.* (2024c,a) and as part of an ongoing project. In these projects, we provide a theoretical analysis based on the  $\text{U}(1)$  Dirac spin liquid Ansatz. We critically compare our predictions for the dynamical structure factor with results from experiment in order to understand the nature of these correlated paramagnetic phases. We also include scaling data from  $\text{KYbSe}_2$ , and discuss the use of real-space correlations to positively confirm the nature of the critical regime and potential of a spin-liquid state.

## 4.1 Inelastic neutron scattering data

Inelastic neutron scattering data was collected using the Cold Neutron Chopper Spectrometer (CNCS) at Oak Ridge National Laboratory’s Spallation Neutron Source. For technical details, see Mason *et al.* (2006); Ehlers *et al.* (2011). The observed Hamiltonian parameters are extracted by applying an external field of 4 T and measuring the magnon modes in the  $1/3$  magnetisation plateau phase (Kamiya *et al.*, 2018). These modes are well described by non-linear spin wave theory, allowing parameter extraction from the  $J_1$ – $J_2$  model in an external field. The extracted parameters are shown in Table 4.1 and summarised in Fig. 4.1(b). It clearly shows that with the lessening atomic radius of the  $A$  ion, the relative strength of

|                     | $J_1/\text{meV}$ | $J_2/J_1$ | $T/\text{mK}$ | $J_1/k_B T$ |                  |
|---------------------|------------------|-----------|---------------|-------------|------------------|
| CsYbSe <sub>2</sub> | 0.395(8)         | 0.029(15) | 400           | 11          | 120-degree order |
| KYbSe <sub>2</sub>  | 0.456(13)        | 0.043(10) | 290           | 18          | 120-degree order |
| NaYbSe <sub>2</sub> | 0.551(13)        | 0.710(15) | 23            | 280         |                  |

Table 4.1: Model parameters of the ytterbium delafossites  $AYb\text{Se}_2$ . Data for  $A = \text{Cs}$  measured by Xie *et al.* (2023), and by Scheie *et al.* (2024a) for  $A = \text{K}, \text{Na}$ . The temperature  $T$  denotes the ordering temperature for two compounds, and the temperature of the susceptibility dip in NaYbSe<sub>2</sub>. In the former two cases, the parameter  $J_1/k_B T$  measures the frustration of magnetic order.

the next-nearest neighbour exchange  $J_2$  tends to increase. This, in turn, acts to suppress ordering by frustrating the 120-degree state and potentially stabilises a quantum spin liquid. We therefore study the inelastic scattering properties of these compounds in order to verify this possibility.

### Inelastic neutron scattering of KYbSe<sub>2</sub>

Let us first look at recent results for the compound KYbSe<sub>2</sub> in order to investigate the dynamical response and signatures of criticality. Scheie *et al.* (2024c) observe Bragg peaks emerging in the elastic scattering response of this material below  $T = 290$  mK. This is consistent with order at the  $\mathbf{K}$  point, signalling 120-degree order with purely in-plane correlations. The neutron spectrum at 300 mK, just above the transition temperature to 120-degree order, is shown in Fig. 4.2(a). It displays a diffuse continuum around the  $\mathbf{K}$  point with a sharp lower bound (Scheie *et al.*, 2024c).

There is a successful description of the 120-degree state in terms of Schwinger bosons (Arovas and Auerbach, 1988; Auerbach, 1998). This approach, which assumes fractionalised bosonic particles, can successfully capture the suppression of the magnetic moment in the ordered state. More recently, it has been extended to describe the dynamical response here too (Ghioldi *et al.*, 2018). However, here we will opt for a fermionic parton description for the critical regime. This is motivated by the fact that the 120-degree ordered state in the  $J_1$ – $J_2$  model is proximate to the U(1) Dirac spin liquid. In this phase, the relevant quasiparticles are fermionic spinons that are charged under an emergent U(1) gauge field. We highlight that it is still an Ansatz about the nature of the ground state, motivated by our understanding of the phase diagram of the  $J_1$ – $J_2$  model. We should compare the results to other predictions, such as  $\mathbb{Z}_2$  spin liquids or fractionalised ordered phases (Ghioldi *et al.*, 2018).

We present the structure factor of the U(1) Dirac QSL at the transition point  $J_2/J_1 = 0.0716$  in Fig. 4.2(b). This model displays only the spinon contribution to the structure factor, without the contribution of monopoles. Both the experimental data and our model of the critical point display similarities. Firstly, the sharp onset emanating from  $\mathbf{K}$  suggests the magnon mode in the ordered state continuously becomes the spinon exciton within the spin liquid. Both results also display a continuum above  $\mathbf{M}$ . In the critical spin liquid model, the continuum is gapless and due to the Dirac cones. However, the experimental data are more compatible with the continuum having a minimum of  $0.44 J_1 = 0.20$  meV. Such a

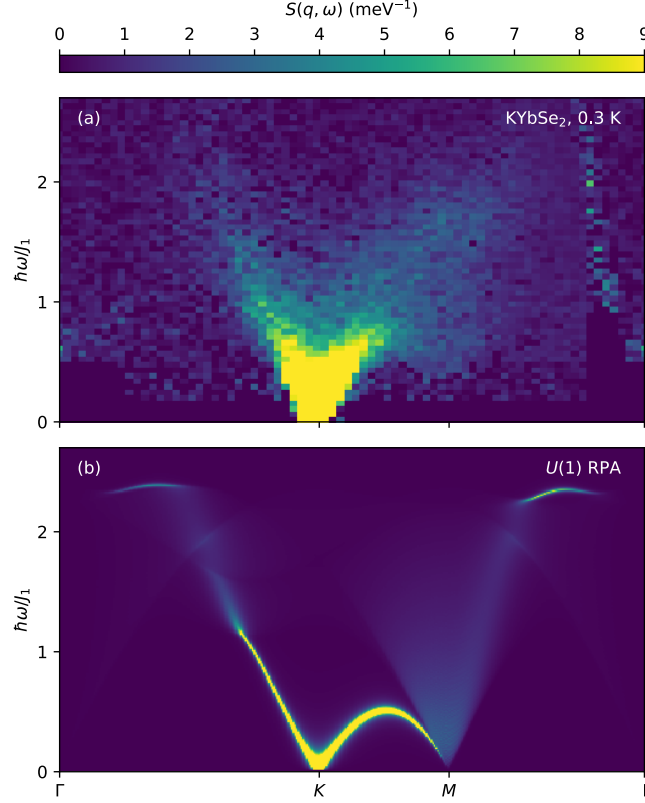


**Figure 4.2:** *Inelastic neutron scattering data in  $\text{KYbSe}_2$ , compared to the spectrum of the  $U(1)$  Dirac quantum spin liquid.* (a) Measured inelastic neutron scattering cross section at  $T = 0.3$  K. (b) Fermion contribution to the dynamical structure factor. Evaluated using the RPA method from Chapter 3.

gap in the two-spinon continuum can be induced by adding 120-degree magnetic order to the mean-field Ansatz (Zhang and Li, 2020). It would be a fruitful direction of research to perform this calculation in the fermionic parton basis (Ghioldi *et al.*, 2018). This would shed insight onto the other side of the 120-degree–Dirac QSL transition, as well allow a fully quantitative comparison with experimental data from  $\text{KYbSe}_2$ .

The value of  $J_2/J_1$  in this material is close to the critical point. It is estimated to be approximately 0.06 from numerical methods (see Fig. 2.12). As discussed, the neutron spectrum in zero field also shows signs of diffuse, fractionalised excitations. Scheie *et al.* (2024c) also present evidence for the proximity to a quantum critical point by measuring the quantum Fisher information, calculated from an energy integral at the momentum  $\mathbf{K}$ . This acts as a witness for multipartite entanglement (Hauke *et al.*, 2016). In the case of  $\text{KYbSe}_2$  at 0.3 K, the value of the QFI is 3.4(2), suggesting the presence of non-trivial entanglement. Importantly, this provides evidence to rule out glassiness or valence bond ground states, but does not definitively prove the presence of a quantum spin liquid.

We might then interpret the continuum of excitations as being within the quantum critical fan of a phase transition to a spin liquid. We can proceed to perform a scaling analy-

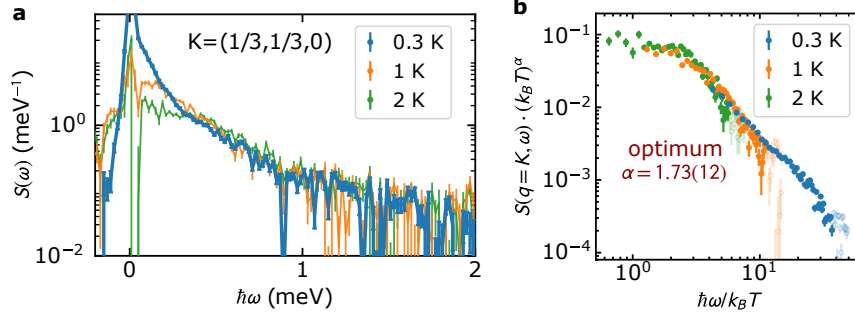


**Figure 4.3: Scaling collapse of the spectral function at the  $K$  point in  $KYbSe_2$ .** (a) Measured spectral function for three temperatures  $T = 2$  K, 1 K, and 300 mK. (b) Optimal data collapse, found by plotting  $S(\mathbf{K}, \omega)(k_B T)^\alpha$  against  $\omega/k_B T$ . The optimal collapse comes from  $\alpha = 1.73(12)$ . Data taken from (Scheie *et al.*, 2024c).

sis of the neutron scattering data to extract critical exponents. The temperature-dependent susceptibility was measured in Fig. 4.3(a) (Scheie *et al.*, 2024c). The divergent behaviour at low frequencies becomes sharper with lowering temperature, as is typical of quantum critical phases or points. Motivated by analogy to 1D, we show the scaling collapse in Fig. 4.3(b). To perform this, we plot  $T^\alpha S(\mathbf{K}, \omega)$  against  $\omega/T$ . The optimal extracted exponent is  $\alpha = 1.73(12)$ . We can compare this with the critical behaviour of the Dirac QSL at the transition to 120-degree order. Recall that this is described by a continuum theory of  $QED_3$  coupled to a condensing boson at  $\mathbf{K}$ . The resulting critical point is in the  $QED_3$ -Gross-Neveu universality class. The relevant critical exponent, as inferred from the large- $N_f$  results of Dupuis *et al.* (2019), is

$$\alpha = 3 - 2\Delta_{\Phi,1}^{GN} \approx 1.44, \quad (4.1)$$

with significant potential errors on the order  $1/N_f$ . These results appear compatible within errors, but we urge caution. Due to the large uncertainties due to both the large- $N_f$  approximation and difficulties fitting the experimental data, more progress is needed before the determining the universality class. One option would be to use numerical tools to provide a third independent measurement of the dynamical scaling. Alternatively, tuning the ratio  $J_2/J_1$  (for example with pressure) and performing an additional scaling in that parameter would probe another independent critical exponent  $\nu$  [see Eq. (3.81)].

### Inelastic neutron scattering of $NaYbSe_2$

The neutron spectra at 100 mK are shown in Fig. 4.4(a,b). We again observe a dispersive continuum of excitations at  $\mathbf{K}$  with a well-defined lower bound. This is reminiscent of the continua present in 1D spin chains (Mourigal *et al.*, 2013). No magnetic ordering is observed in Bragg peaks down to 100 mK  $= 0.016 J_1$ , and thermodynamic measurements of the specific heat capacity in the same range show no signs of a phase transition. Furthermore, the multipartite quantum Fisher information as extracted from the neutron scattering results of  $NaYbSe_2$  is lower than  $KYbSe_2$ , with a value of 2.3(5). This is compatible with the

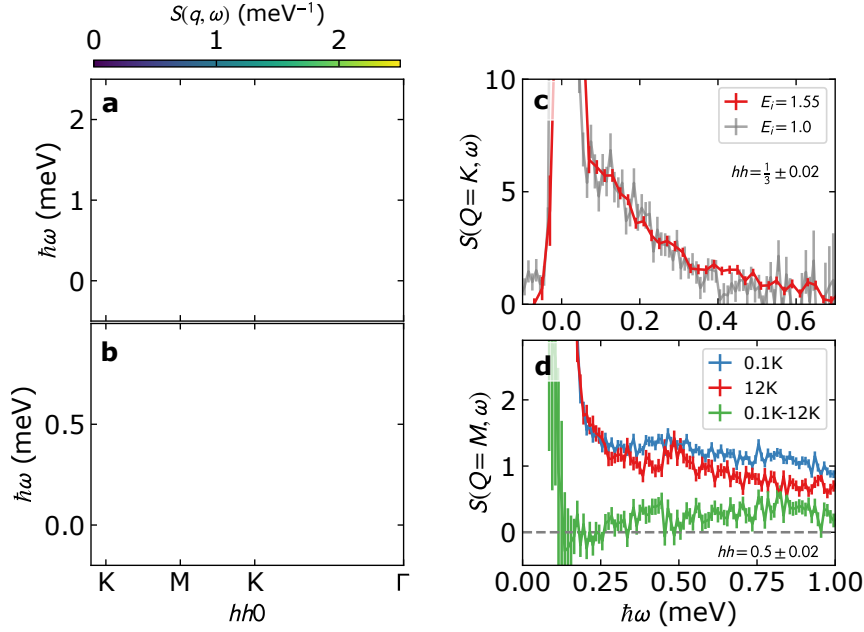


**Figure 4.4:** *Inelastic neutron scattering data in  $\text{NaYbSe}_2$ .* (a,b) Measured inelastic neutron scattering cross section at  $T = 100$  mK. (c) Slice at the  $\mathbf{K}$  point. (d) Slice at the  $\mathbf{M}$  point for various temperatures.

interpretation that the sodium compound is further from the quantum critical point than its potassium sibling.

Let us take a closer look at the inelastic neutron scattering data. Focusing on the  $\mathbf{K}$  point in Fig. 4.4(c), we see that no gap in the spectrum is resolved down to  $50 \mu\text{eV} = 0.09 J_1$ . This is the limit before the incoherent scattering on the elastic line obscures the scattering energy (for the incident energy of  $E_i = 1$  meV). Turning to the  $\mathbf{M}$  point, we observe a much lower spectral weight compared to  $\mathbf{K}$ . Fig. 4.4(d) shows the temperature-dependent background-subtracted scattering at this point, showing high uncertainties at low energies. It is therefore inconclusive whether the spectrum is gapped or gapless at this point. The model of the U(1) Dirac QSL predicts gapless excitations at both the  $\mathbf{K}$  and  $\mathbf{M}$  points. The excitations at  $\mathbf{K}$  will dominate the spectral weight. Fig. 4.5 shows a slice of the data here plotted on a log-log scale. Fitting the data to a power law, we see that the data at high energy transfers show some power-law behaviour. The best fit here is to  $\alpha = 1.74(6)$ . This is compatible with the result from  $\text{KYbSe}_2$ , although no data are available at different temperatures, which would allow a more rigorous scaling collapse. At lower energy transfers, around  $0.1 \text{ meV} = 0.18 J_1$ , there is a strong deviation from purely power-law behaviour. A full scaling collapse with temperature is needed to understand this effect, though we mention in passing that it is potentially compatible with the picture of a gapped spinon exciton within a monopole continuum [cf. Fig. 3.11 and the crossover Ansatz in Eq. (3.97)].

To see whether this spin-disordered behaviour holds down to lower temperatures, AC magnetic susceptibility measurements were additionally performed down to 20 mK. These show a low-field drop in susceptibility at  $23 \mu\text{eV} = 0.0036 J_1$ . This sets an upper bound on

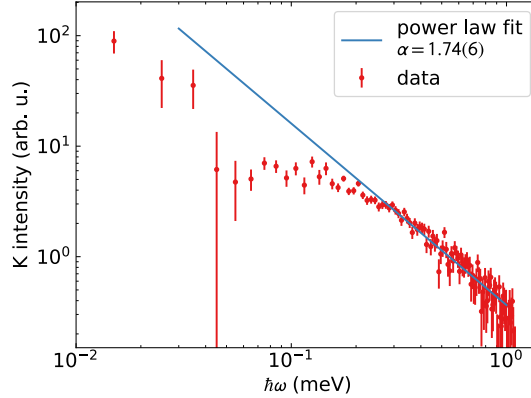


**Figure 4.5:** *Spectral function of NaYbSe<sub>2</sub> at K.* The background-subtracted data is shown. Structure factor at the **K** point. Some power-law behavior appears at high energy transfers, but it seems to deviate from this at low energy transfers. The fitted exponent strongly depends upon the region fitted, but the higher energy region follows  $\alpha = 1.74(6)$ .

the energy scale of magnetic impurities in the material, and is a sign of extremely good crystalline quality. There are three possible interpretations of this drop. First, in the absence of frequency-dependence, it signals a gap in the spectrum which is on the order  $10^{-3} J_1$ . Such a gap could be introduced in a spin liquid by introducing spinon pairing terms to the Hamiltonian, breaking the U(1) gauge symmetry down to  $\mathbb{Z}_2$ . However, such a small pairing gap would be extremely fine-tuned. We would expect dynamical properties to be continuously connected to the U(1) Dirac state since this  $\mathbb{Z}_2$  QSL is simply a Higgs descendent of the U(1) Dirac Ansatz. With such a small pairing it would be almost impossible to distinguish the two states spectroscopically. Second, we rule out the possibility of the downturn signalling magnetic order because the response is fully isotropic. Third, newer samples have shown signals of a frequency-dependent downturn. This would be a signature of a spin-freezing transition. It remains true that the temperature of this transition is exceptionally low. It would imply over an order of magnitude of temperatures where NaYbSe<sub>2</sub> shows liquid-like behaviour.

## 4.2 Outlook

In summary, we compared in this Chapter the experimental inelastic neutron scattering data from Scheie *et al.* (2024c,b) to our model of the U(1) Dirac quantum spin liquid. The spectra display a mixture of continua and sharp modes in both models, making concrete quantitative agreement between experiment and any one theoretical model ambiguous. Therefore, much work remains to be done. On the experimental side, we have discussed the need for more complete temperature scaling analysis. In addition, high-resolution, temperature-dependent data at the high-symmetry points would be incredibly helpful at distinguishing between competing models. Most decisively, the U(1) Dirac spin liquid should have a weak gapless continuum at low energies around the **M** point, where competing models are gapped.

On the theoretical side, we believe that simple extensions may improve the picture. For example, it is possible that refining the RPA calculation for the Dirac spin liquid Ansatz with spin-anisotropy will improve quantitative agreement. It would also be insightful to include spin ordering within the model, particularly in the case of  $\text{KYbSe}_2$ . On the more challenging end of the spectrum, we urgently need a better understanding of the effects of disorder in gapless quantum spin liquids. An ultra-low temperature spin-freezing transition in  $\text{NaYbSe}_2$  could potentially result from the interaction of sparse magnetic impurities through a long-range interaction mediated by the algebraic spin liquid.

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## Introduction

The Peierls instability describes the tendency of gapless states to spontaneously dimerise upon *infinitesimal* coupling to the lattice in one dimension (Peierls, 1996). This instability at weak electron-lattice coupling is unique to 1D. In spin chains, the same phenomenon leads to a weak-coupling instability of gapless algebraic spin-liquid ground states, often called the spin-Peierls instability (Bray *et al.*, 1975; Jacobs *et al.*, 1976). This mechanism is as general as the Peierls instability of electrons we introduced in Section 1.3. This is as there will generally be a non-zero spin-lattice coupling in any realistic system. To see this, recall that the origin of the Heisenberg exchange interaction is through the statistical interaction of neighbouring spinful orbitals. This naturally motivates us once again to write down the following form for its bond-length dependence

$$J_{ij} = J_0 e^{-g|r_i - r_j|}. \quad (5.1)$$

This spatial dependence of exchange is used implicitly when we construct toy models of nearest-neighbour Hamiltonians, and consider further exchanges as perturbations. However it also *necessarily* implies a bond-length dependence of the exchanges and therefore a non-zero spin-lattice coupling  $g$ .

In 1D, the effects are well-established. There are numerous examples of the spin-Peierls instability in the experimental literature. To name one, Hase *et al.* (1993) identify a drop in the magnetic susceptibility at  $T_{\text{SP}} = 14$  K in the spin-chain compound  $\text{CuGeO}_3$ . This is well below the energy scale of the magnetic exchange  $J = 88$  K, and they identify the ground state gap  $\Delta_{\text{gap}} = 24$  K. Importantly, the authors are able to show that this transition is driven by the magnetic spins transitioning to a dimer state, since the transition temperature is suppressed upon applying a magnetic field. Many experiments found compatible results in other Heisenberg chain compounds, see for example the earlier works (Bray *et al.*, 1975; Jacobs *et al.*, 1976; Huizinga *et al.*, 1979). The resulting spin state in this case is a gapped valence bond state on a dimerised lattice.

Although the presence of a weak-coupling instability has immediate and deep consequences for the fate of gapless QSL states, no such instability has been predicted in two dimensions. In this Chapter we investigate spin-Peierls-type instabilities in *higher-dimensional* frustrated quantum magnets. Previous works having focused on degenerate ground states in 2D (Becca and Mila, 2002; Ferrari *et al.*, 2021) or intrinsic nesting instabilities of spinon Fermi surfaces in 3D (Hermanns *et al.*, 2015; Krüger and Janssen, 2021). Other studies have also identified valence bond ordering upon a *finite* critical lattice coupling  $g_c > 0$  (Hou *et al.*, 2007; Ferrari *et al.*, 2021). Motivated by the paradigmatic algebraic spin chain instability in 1D, we study the crucial question concerning the stability of (otherwise intrinsically stable)

*gapless QSL ground states* to lattice distortions. In this Chapter, we will use this to show the lattice couples to relevant topological excitations in the Dirac spin liquid, which act like the instanton domain walls in 1D. We go on to present the first example of a spin-Peierls instability in two dimensions upon infinitesimal lattice coupling. This results in a spin-Peierls instability of the U(1) Dirac spin liquid, where we adopt the name of the one-dimensional instability of 1D spin chains. We therefore make steps towards understanding the stability of quantum spin liquid states in a realistic model. This extends the results of the previous Chapters, where we discussed the intrinsic stability of the U(1) Dirac spin liquid, and then studied the possibility of realising the phase in the  $J_1$ – $J_2$  model.

This Chapter contains the original work from two manuscripts: Seifert, Willsher, Drescher, Pollmann, and Knolle (2024), and Ferrari, Willsher, Seifert, Valenti, and Knolle (2024). Here, we predict the spin-lattice instability of the two-dimensional gapless Dirac QSL. We argue for this result using field theoretic arguments, and then go on to directly observe it in variational Monte Carlo simulations. This chapter focuses on the limit of *static distortions*, meaning classical deformations of the lattice. In this context, we find comprehensive evidence of an instability. We also investigate the effect of interlayer coupling on the stability of the spin liquid state. In the next Chapter 6 we will study quantum phonons.

## 5.1 Spin-Peierls instability in 1D

In this Section, we will introduce the spin-Peierls instability of 1D spin chains (Giamarchi, 2003). The Peierls instability, discussed in the Introduction, is an instability of a gapless electronic state to spontaneous lattice distortions. We have also seen in Chapter 2, how quantum magnets can be described in terms of emergent fermions through the Jordan–Wigner transformation. We will show here that these models of strongly *interacting*, emergent fermions are also unstable to the spin-Peierls instability.

For this, we rely on the field theoretical description of the XXZ model, described in Chapter 2. To summarise, we studied the spin Hamiltonian

$$\mathcal{H}_{\text{XXZ}} = \sum_i J \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right) = \sum_{i,\alpha} J^\alpha S_i^\alpha \cdot S_{i+1}^\alpha, \quad (5.2)$$

by using bosonisation to map it to the Sine–Gordon model

$$S_{\text{SG}} = \int dx d\tau \left[ \frac{1}{2\pi K} \left( (\partial_x \phi)^2 + (\partial_\tau \phi)^2 \right) + \mu \cos(4\phi) \right], \quad (5.3)$$

We will focus on the SU(2)-symmetric case  $\Delta = 1$  in the following, but let us first make a quick remark about the XY limit  $\Delta = 0$ . As we noted before, the Jordan–Wigner mapping in this case is to a system of free spinless fermions. That is Eq. (2.9) with interactions  $V = 0$ . In this limit, the theory is identical to our tight-binding model of polyacetylene. We have already shown that this exhibits a Peierls instability upon infinitesimal lattice coupling and has a finite ground state distortion (that is exponentially small in  $g$ ).

Now return to the isotropic, interacting, limit. From hereon we will consider Heisenberg interactions  $\mathcal{H}_J = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$  which is described by the field theory Eq. (5.3) with Luttinger parameter  $K = 1/2$ . In this Section, we consider the effect of dimerising the

|                                        |               | $Z_2^z$ | $T_x$ | $\mathcal{I}$ | $\mathcal{T}$ |
|----------------------------------------|---------------|---------|-------|---------------|---------------|
| $\eta_i \vec{S}_i \cdot \vec{S}_{i+1}$ | $\sin(2\phi)$ | +       | -     | -             | +             |
| $\eta_i(u_i - u_{i+1})$                | $\delta u$    | +       | -     | -             | +             |

Table 5.1: The symmetry properties of the field  $\phi$  under  $z$ -spin flip  $Z_2^z$ , as well as the external lattice symmetries: translation  $T_x$  and bond-inversion  $\mathcal{I}$  as is similarly obtained through bosonisation (Giamarchi, 2003). The order parameters are defined  $n_3 \sim \cos(2\phi)$  and  $v \sim \sin(2\phi)$ .

lattice. At lowest energies, only staggered lattice distortions are important, i.e. the ones with lattice momentum  $Q = \pi$  (Citro *et al.*, 2005). This means we take alternating sites from their equilibrium positions  $ia \rightarrow ia + u_i$  with an alternating displacement  $u_i$ , given as

$$u_i = (-1)^i \delta u \equiv \eta_i \delta u. \quad (5.4)$$

Distorting the lattice sites away from their equilibrium position will cost potential energy. We model this in the harmonic approximation

$$\mathcal{E}_{\text{lattice}} = \frac{\kappa}{2} u_i^2 = \frac{\kappa}{2} \delta u^2. \quad (5.5)$$

The other consequence of this distortion is that the exchange interactions will change strength. By Taylor expanding Eq. (5.1), we write

$$J_{i,i+1} = J - Jg(u_{i+1} - u_i) \quad (5.6)$$

$$= J - 2gJ \eta_i \delta u. \quad (5.7)$$

We include this bond-dependent term as an additional spin-spin interaction

$$\mathcal{H}(\delta u) = \mathcal{H}_J - 2g \delta u \sum_{i,\alpha} J \eta_i \vec{S}_i \cdot \vec{S}_{i+1}. \quad (5.8)$$

This is a direct coupling of the dimerisation parameter  $\delta u$  to spin bilinears.

Next, we can directly incorporate this interaction into the continuum field theory by using the bosonisation mapping

$$\eta_i \vec{S}_i \cdot \vec{S}_{i+1} = D_i \leftrightarrow \sin[2\phi(x_i)]. \quad (5.9)$$

The bosonised action therefore gets the following perturbation

$$S[\delta u] = S_{\text{SG}} + \tilde{g} \delta u \int dx d\tau \sin(2\phi), \quad (5.10)$$

where the field-theoretic coupling  $\tilde{g}$  can be written in terms of the lattice-coupling  $g$  (Orignac and Chitra, 2004; Citro *et al.*, 2005). We note that this is the same as the mapping (2.28) that we wrote down before between dimer order parameters and the soliton excitation  $\sin(2\phi)$ . In this case, we see that the lattice dimerisation couples linearly to dimer order. This order

parameter has scaling dimension  $\Delta = 1/2$  at the Heisenberg point and is therefore highly relevant. Note that translating by one lattice constant  $i \rightarrow i + 1$ , this order parameter transforms non-trivially:  $v_i \rightarrow -v_i$  and  $\sin(2\phi) \rightarrow -\sin(2\phi)$ . Before, we excluded these operators from the action on the grounds that they do not conserve the full symmetries of the system. The difference now is that we have explicitly broken translational symmetry by adding a staggered lattice distortion. The new coupling in Eq. (5.10) is symmetry-allowed, since the lattice distortion field also transforms identically  $\delta u \rightarrow -\delta u$ . The full transformation properties of both of these terms is shown in Eq. (5.1). The new continuum field theory therefore still obeys translational symmetry by construction. Critically, the staggered lattice distortion  $\delta u$  then allows a relevant soliton into the action. This will fundamentally change the nature of the ground state by destabilising the Luttinger liquid.

In the absence of spin-lattice couplings, the undistorted lattice (i.e.  $h \equiv 0$ ) minimises the system's elastic energy Eq. (5.5). We should therefore follow the same route as in the case of free fermions and ask what would make the lattice spontaneously distort. This will only occur if the energy gain due to a gap-opening in the spin sector out competes the energy cost associated with distorting the lattice.

The first task will be to calculate how the spin gap scales as a function of distortion. This follows from a straightforward RG argument, see e.g. (Giamarchi, 2003). The gap is opened by the coupling  $\lambda = \tilde{g}\delta u$  to the relevant operator  $\sin(2\phi)$ . This operator has scaling dimension  $K = 1/2$  in the Heisenberg case which we consider here. As we showed before in Eq. (2.26), adding a finite value of this coupling to the action  $\lambda_0 \sim 1$  creates a minimum for the field  $\phi_0 = \pi/4$ , where the excitations about this minimum have a finite gap  $\Delta_0$ . Under the RG flow, the coupling flows with exponent  $2 - K$ , meaning the gap will scale like

$$(\Delta/\Delta_0)^{2-K} \sim \lambda. \quad (5.11)$$

Therefore, we can define the correlation length exponent  $\nu^{-1} = 2 - K = 3/2$  and write the gap scaling

$$\Delta \sim \lambda^\nu \sim (\tilde{g}\delta u)^{2/3}. \quad (5.12)$$

The ground state energy density has dimensions energy per length. In the field-theory language, we say this has mass-dimension  $[\delta\epsilon] = 2$  in  $d = 1$ . In the free fermion case, we were able to evaluate this by integrating over a band; now we do not have such a clear quasiparticle picture. However, we can use dimensional analysis<sup>1</sup> to say that the energy density must scale like  $\delta\epsilon \sim \Delta^2$ . This gives us the following result for the ground state energy gain due to the distortion  $\delta u$ :

$$\delta\epsilon \sim (\tilde{g}\delta u)^{4/3}. \quad (5.13)$$

This is the Cross-Fisher exponent for the spin-Peierls energy gain (Cross and Fisher, 1979). Once again, the total energy of the system is then composed of a (harmonic) energy cost of the distortion, and this energy gain due to the opening of a gap in the Luttinger liquid. The total effective potential

$$\mathcal{E}(\delta u) = \frac{1}{N} (E_{\text{cost}} - \delta\epsilon) = (\kappa/g^2)(\tilde{g}\delta u)^2 - c(\tilde{g}\delta u)^{4/3}, \quad (5.14)$$

<sup>1</sup>This approach would miss the logarithmic correction seen for free fermions, but as we will see there are more dominant effects in the interacting Luttinger liquid.

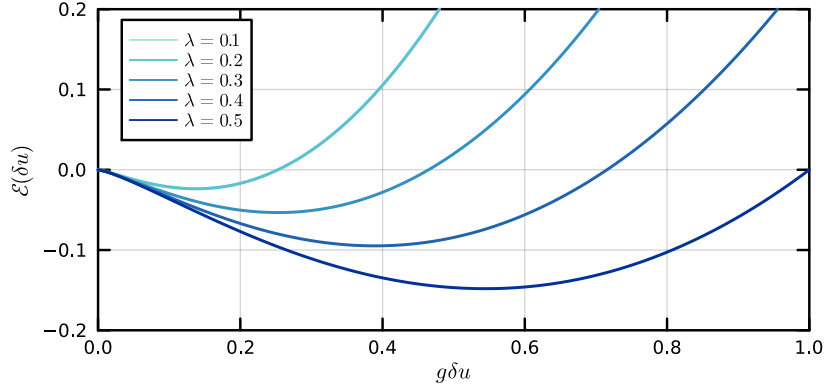


**Figure 5.1:** *Lattice instability of the Luttinger liquid.* The effective potential of the distortion field when coupled to a gapless spin system. We show various coupling parameters  $\lambda = g^2/(\kappa)$

for some constant  $c$ . This is plotted as a function of the coupling strength  $g^2/\kappa$  in Fig. 5.1. The non-analytic exponent of the energy gain  $4/3 < 2$  always out-competes the energy cost of distortion for small distortion  $\tilde{g}\delta u$ . Therefore, the ground state will have a spontaneously dimerised lattice  $\delta u_0 > 0$  and spins that form valence bond order. The gapped state breaks translational symmetry.

The Luttinger liquid is therefore unstable for any non-zero coupling  $g > 0$  (Giamarchi, 2003). Solving for the minimum of the potential Eq. (5.14) allows us to find the scaling of the equilibrium distortion and resulting gap:  $\Delta_0 \sim \delta u_0 \sim \tilde{g}^2$ . This algebraic behaviour is a *stronger instability* than the case of free fermions in Eq. (1.22). We note that interactions enhance the susceptibility of the gapless state to spontaneous dimerisation. In practice, we will argue that this is because the dimer correlations are enhanced by interactions.

## 5.2 Spin-Peierls instability of the U(1) Dirac QSL

### 5.2.1 Lattice distortion

We first consider static displacement fields by neglecting any intrinsic quantum dynamics of the lattice. This is often referred to as the *adiabatic limit* (Cross and Fisher, 1979; Orignac and Chitra, 2004) and it represents a classical approximation for the lattice. In this Section, we will describe the spin-Peierls instability of QED<sub>3</sub> on the triangular lattice, relying heavily on the field theory introduced in Section 2.3.1. In the spirit of generality, we first use this symmetry-based approach which is agnostic to specific microscopic models. That is as long as the following relevant spin rotation and lattice symmetries are preserved: translations  $T_1, T_2$ ,  $C_6$  rotations, parity  $\mathcal{P}$  and time reversal  $\mathcal{T}$ . We later study a microscopic model for spin-lattice couplings and test our findings using numerical methods, specific to the  $J_1$ – $J_2$  AFM Heisenberg model.

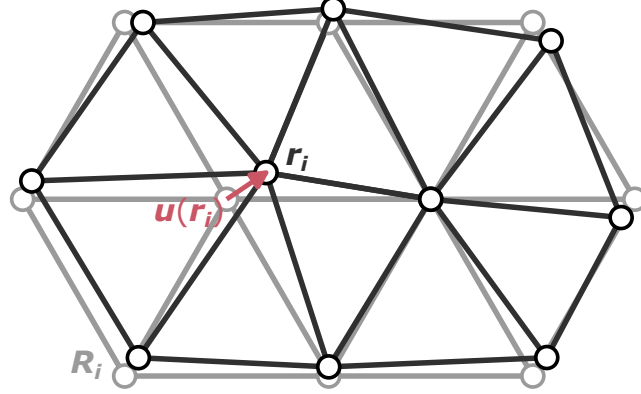


**Figure 5.2: Distorted triangular lattice.** The lattice sites are shifted by the displacement field  $\mathbf{u}(\mathbf{r}_i)$ . This will modify bond lengths and the exchange interactions.

### Lattice coupling

Our starting point on the triangular lattice is the observation that the valley-triplet (spin-singlet) monopoles  $\mathcal{D}_\alpha$  ( $\alpha = 1, 2, 3$ ) have lattice momenta  $\mathbf{X}_\alpha = -\mathbf{K}/2$ . These act as fluctuating order parameters for a competing VBS state. Although individual monopoles transform under lattice symmetry transformations, they can be combined with momentum-dependent prefactors to obtain a term which transforms trivially. Using Table 2.3, we write

$$\begin{aligned} H_{\text{pert}} &= \sum_i \sum_{\alpha=1,2,3} s_\alpha \left[ e^{i\mathbf{X}_\alpha \cdot \mathbf{R}_i} \mathcal{D}_\alpha(\mathbf{R}_i) + \text{h.c.} \right] \\ &= \sum_i \left[ e^{i\mathbf{X}_1 \cdot \mathbf{R}_i} \mathcal{D}_1(\mathbf{R}_i) + e^{i\mathbf{X}_2 \cdot \mathbf{R}_i} \mathcal{D}_2(\mathbf{R}_i) - e^{i\mathbf{X}_3 \cdot \mathbf{R}_i} \mathcal{D}_3(\mathbf{R}_i) + \text{h.c.} \right], \end{aligned} \quad (5.15)$$

where we use the sign factors  $s_\alpha = +1, +1, -1$  for convenience of notation. While Eq. (5.15) is symmetry-allowed, the oscillating prefactors average out on sufficiently long length scales, such that the perturbation is strongly irrelevant. This observation was key to showing that the U(1) Dirac QSL has a stable conformal ground state on the translationally-invariant triangular lattice.

We now consider the effect that a spontaneous breaking of the lattice symmetries has on this result. We will find that a specific commensurate lattice distortion will allow the monopoles to condense. Using Eq. (5.15) as a starting point, consider an in-plane deformation of the real-space lattice

$$\mathbf{R}_i \rightarrow \mathbf{r}_i = \mathbf{R}_i + \mathbf{u}(\mathbf{r}_i), \quad (5.16)$$

where  $\mathbf{u}(\mathbf{r}_i)$  is a displacement field, as shown in Fig. 5.2. Note that we work in the coordinates  $\mathbf{r}_i$  of the deformed system. We choose this implicit definition such that the fields  $\mathbf{u}(\mathbf{r}_i)$  and  $\mathcal{D}(\mathbf{r}_i)$  live at the same point in space, such that we can later take a consistent continuum limit. In these coordinates, the perturbation (5.15) becomes simply

$$H_{\text{pert}} = \sum_{i,\alpha} s_\alpha \left[ e^{i\mathbf{X}_\alpha \cdot (\mathbf{R}_i + \mathbf{u}(\mathbf{r}_i))} \mathcal{D}_\alpha(\mathbf{r}_i) + \text{h.c.} \right]. \quad (5.17)$$

Assuming that lattice distortions are small compared to the lattice constant  $a$ , expand Eq. (5.17) in the small parameter

$$|\mathbf{u}|/a \ll 1 \quad \text{or} \quad |\mathbf{X}_\alpha \cdot \mathbf{u}| \ll 1. \quad (5.18)$$

This gives

$$\sum_{i,\alpha} s_\alpha \left[ e^{i\mathbf{X}_\alpha \cdot \mathbf{R}_i} \mathcal{D}_\alpha(\mathbf{r}_i) + \text{h.c.} \right] + \sum_{i,\alpha} s_\alpha \left[ i\mathbf{X}_\alpha \cdot \mathbf{u}(\mathbf{R}_i) e^{i\mathbf{X}_\alpha \cdot \mathbf{R}_i} \mathcal{D}_\alpha(\mathbf{r}_i) + \text{h.c.} \right] + \dots \quad (5.19)$$

The first term here is simply equal to Eq. (5.15). We previously argued it is irrelevant due to the oscillating phases, and can hence be ignored. It is this second term which will contribute to the low-energy physics. Although it also has an oscillating phase, this can be cancelled by the conjugate factor in the Fourier modes of  $\mathbf{u}(\mathbf{R}_i)$ . Let us Fourier transform the lattice distortions in terms of crystal momentum  $\mathbf{Q}$ . The real distortion field in the Fourier basis is

$$\mathbf{u}(\mathbf{R}_i) = \sum_{\mathbf{Q}} \left( \mathbf{u}_{\mathbf{Q}} e^{i\mathbf{Q} \cdot \mathbf{R}_i} + \mathbf{u}_{\mathbf{Q}}^* e^{-i\mathbf{Q} \cdot \mathbf{R}_i} \right). \quad (5.20)$$

Substituting into (5.19), we see that the phase vanishes when  $\mathbf{X}_\alpha + \mathbf{Q} = 0$ ! Therefore, there will be a uniform contribution from the distortion mode commensurate with the monopole  $\mathcal{D}_\alpha$ . We call this relevant mode  $\mathbf{u}_{-\mathbf{Q}} = \mathbf{u}_{\mathbf{Q}}^*$ , which comes without an oscillating prefactor. The resulting relevant perturbation can be expressed in continuum form as

$$\mathcal{H} = \int d^2\mathbf{r} \sum_{\alpha} s_\alpha \left[ (i\mathbf{X}_\alpha \cdot \mathbf{u}_{\mathbf{X}_\alpha}^*) \mathcal{D}_\alpha(\mathbf{r}) + \text{h.c.} \right]. \quad (5.21)$$

This couples the monopoles to the *longitudinal* Fourier component

$$u_{l,\mathbf{X}_\alpha} = \hat{\mathbf{X}}_\alpha \cdot \mathbf{u}_{\mathbf{X}_\alpha} \quad (5.22)$$

where  $\hat{\mathbf{X}}_\alpha = \mathbf{X}_\alpha/|\mathbf{X}_\alpha|$ . In the field-theoretic language, we can formulate a perturbation to the QED<sub>3</sub> fixed point generated by the action

$$S_{\mathcal{D}}[u_\alpha] = g_{\mathcal{D}} \int d^3x \sum_{\alpha} u_\alpha^* \mathcal{D}_\alpha(x) + \text{h.c.}, \quad (5.23)$$

where the lattice distortion field is defined as

$$u_\alpha^* = i s_\alpha \sqrt{2} u_{l,\mathbf{X}_\alpha}^* = i s_\alpha \frac{\sqrt{2}}{N} \int d^2\mathbf{r} \hat{\mathbf{X}}_\alpha \cdot \mathbf{u}(\mathbf{r}) e^{i\mathbf{X}_\alpha \cdot \mathbf{r}}. \quad (5.24)$$

The lattice-monopole coupling constant  $g_{\mathcal{D}}$  has scaling dimension

$$[g_{\mathcal{D}}] = 3 - \Delta_\Phi \quad (5.25)$$

and is therefore strongly relevant. Table 5.23 shows the transformation of these distortion modes under all lattice symmetries alongside the monopoles. We highlight here that they transform identically.

| $T_j$                         |                                                                          | $R$                                   | $C_6$                                         | $\mathcal{T}$                         |
|-------------------------------|--------------------------------------------------------------------------|---------------------------------------|-----------------------------------------------|---------------------------------------|
| $s_\alpha \mathcal{D}_\alpha$ | $s_\alpha e^{-i\mathbf{X}_\alpha \cdot \mathbf{a}_j} \mathcal{D}_\alpha$ | $s_{\alpha-1} \mathcal{D}_{\alpha-1}$ | $s_{\alpha+1} \mathcal{D}_{\alpha+1}^\dagger$ | $s_\alpha \mathcal{D}_\alpha^\dagger$ |
| $s_\alpha u_\alpha$           | $s_\alpha e^{-i\mathbf{X}_\alpha \cdot \mathbf{a}_j} u_\alpha$           | $s_{\alpha-1} u_{\alpha-1}$           | $s_{\alpha+1} u_{\alpha+1}^*$                 | $s_\alpha u_\alpha^*$                 |

Table 5.2: Discrete symmetry transformations of monopole operators alongside the respective longitudinal lattice distortion modes. The sign factors are defined as  $s_\alpha = (+1, +1, -1)$ , and the distortion modes  $u_\alpha^* = i s_\alpha \mathbf{X}_\alpha \cdot \mathbf{u}_{\mathbf{X}_\alpha}^*$ . The coupling Eq. (5.23) is symmetry-allowed.

The monopole-lattice coupling is a strongly relevant operator in the QED<sub>3</sub> CFT and the coupling to the distortion field is symmetry-allowed. We emphasise that this does not *necessarily* imply an instability of the Dirac QSL, given the intrinsic elastic energy cost associated with a lattice distortion. In the decoupled system, the lattice distortion is zero. For an instability to occur, the system must *dynamically* generate such a distortion. The energy gain due to VBS ordering must outcompete the elastic energy cost, just as we saw in the 1D examples.

### Effective potential

The equilibrium lattice distortion will be determined by the competition between the potential energy cost of a lattice distortion, and the magnetic energy gain from opening a gap. As shown above, it is only the lattice distortion modes given by Eq. (5.24) which we expect to couple to the monopoles and which might lead to a spontaneous distortion.

A simple model for the lattice is given by independent harmonic site distortions

$$E_{\text{sites}} = \frac{\kappa}{2} \sum_i |\mathbf{u}_i|^2, \quad (5.26)$$

with stiffness  $\kappa$ . Fourier transforming with Eq. (5.20), the Fourier modes remain independent

$$E_{\text{sites}} = \kappa \sum_{\mathbf{Q}} |\mathbf{u}_{\mathbf{Q}}|^2 = \kappa \sum_{\mathbf{Q}, s=l,t} |\mathbf{u}_{s,\mathbf{Q}}|^2, \quad (5.27)$$

where we summed over transverse and longitudinal polarisations  $\mathbf{u}_{\mathbf{Q}} = \sum_{s=t,l} \epsilon_{\mathbf{Q},s} u_{s,\mathbf{Q}}$ . Assuming  $\mathbf{u}_{\mathbf{Q}} = 0$  unless  $\mathbf{Q} = \mathbf{X}_\alpha$ , and  $\mathbf{u}_{-\mathbf{X}_\alpha} = \mathbf{u}_{\mathbf{X}_\alpha}^*$ , we can write down an effective potential for these classical distortion parameters  $u_\alpha$ ,  $\alpha = 1, 2, 3$ ,

$$\mathcal{E}[\vec{u}]_{\text{lattice}} = \frac{\kappa}{2} |\vec{u}|^2, \quad (5.28)$$

as we did in 1D. We have switched to 3-vector notation  $\vec{u} = (u_1, u_2, u_3)$ . One can imagine several microscopic models which realise this potential for the longitudinal distortion modes at wavevector  $\mathbf{X}_\alpha$ . For simplicity we have taken an Einstein model of phonons, but the harmonic form will arise also from a model of acoustic phonons. The only constraints we assume are (i) the potential is harmonic with finite stiffness  $\kappa > 0$  for small distortions, and (ii) that it is the same for all three modes, since the undistorted lattice has a full  $C_6$  rotational symmetry.

Competing with this lattice-induced energy cost is the energy gain originating from the spin degrees of freedom in the presence of a distortion. In the continuum field theory, this will be caused by the distortion field introducing a relevant perturbation to the conformal fixed point with the coupling  $g_{\mathcal{D}}$ . We can define a free energy via the logarithm of the partition function of a CFT as

$$F_{\text{CFT}} = \beta^{-1} \log \int \mathcal{D}[\{\mathcal{O}_{\text{CFT}}\}] e^{-S[\{\mathcal{O}_{\text{CFT}}\}]}, \quad (5.29)$$

where  $S_{\text{CFT}}$  is the CFT fixed point action. We can consequently define the effective potential for the lattice distortion as the change in this quantity under a relevant perturbation  $S_{\mathcal{D}}$ :

$$\begin{aligned} \mathcal{E}[\vec{u}]_{\text{QED}_3} &= F[\vec{u}]_{\text{QED}_3} - F[\vec{0}]_{\text{QED}_3} = \beta^{-1} \log Z[\vec{u}]/Z_{\text{QED}_3} \\ &= \beta^{-1} \log \frac{1}{Z_{\text{QED}_3}} \int \mathcal{D}[\{\mathcal{O}_{\text{QED}_3}\}] e^{-S_{\text{QED}_3} - S_{\mathcal{D}}}. \end{aligned} \quad (5.30)$$

We will evaluate this potential in the next Section.

Bringing together these two terms, the effective potential of these particular longitudinal lattice distortion modes is hence given by

$$\mathcal{E}[\vec{u}] = \mathcal{E}[\vec{u}]_{\text{lattice}} + \mathcal{E}[\vec{u}]_{\text{QED}_3}. \quad (5.31)$$

The most simple case is the uncoupled limit  $g_{\mathcal{D}} = 0$ . The energy gain here must be equal to zero, and the potential is simply Eq. (5.28). The ground state is given by the U(1) Dirac QSL on an undistorted lattice  $\vec{u} = 0$ . At a large enough coupling  $g_{\mathcal{D}}$ , we expect there to be a transition to a symmetry-broken phase where the potential is minimised by a finite distortion  $\langle \vec{u} \rangle = \vec{u}_0 \neq 0$ . This signals that there will be a real-space lattice distortion with contributions from the modes  $\mathbf{Q} = \mathbf{X}_{\alpha}$ , and phases fixed by the three complex parameters  $(\vec{u}_0)_{\alpha}$ . Given that there is no coupling to other momenta at this stage, we assume that all other modes remain absent.

### 5.2.2 Lattice instability

The form of the potential  $\mathcal{E}[\vec{u}]_{\text{QED}_3}$  remains to be calculated. It will contain all of the physics of the phase transition. As a hint for how to approach it, it is worth taking a first attempt at using perturbation theory to calculate the energy gain of QED<sub>3</sub> under this lattice coupling. Recall the expression for the energy gain Eq. (5.30). In Appendix B, we discuss how to evaluate this potential using (conformal) perturbation theory. Here, we will discuss the basics of this method, and then apply the result. Imagine expanding the exponential in Eq. (5.30), justified by considering small monopole-lattice coupling  $g_{\mathcal{D}} \ll 1$ . The result can be expressed as a perturbative series of expectation values of the perturbation action at the unperturbed QED<sub>3</sub> fixed point. Up to quadratic order, this is

$$\begin{aligned} \mathcal{E}[\vec{u}]_{\text{QED}_3} &= F_{\text{QED}_3}[\vec{u}] - F_{\text{QED}_3} \\ &= \frac{1}{V} \left[ \langle S_{\mathcal{D}} \rangle_{\text{QED}_3} - \frac{1}{2} \left( \langle S_{\mathcal{D}}^2 \rangle_{\text{QED}_3} - \langle S_{\mathcal{D}} \rangle_{\text{QED}_3}^2 \right) + \cdots \right]. \end{aligned} \quad (5.32)$$

These expectation values of powers of  $S_{\mathcal{D}}$  can be evaluated using the conformal data of  $\text{QED}_3$ . Firstly, we can substitute the one-point function

$$\langle \mathcal{D}_\alpha \rangle = 0 \quad (5.33)$$

into (5.31). The potential then simplifies to

$$\mathcal{E}[\vec{u}]_{\text{QED}_3} = -g_{\mathcal{D}}^2 u_\alpha u_\beta^* \frac{1}{V} \int d^3x d^3y \langle \mathcal{D}_\alpha^\dagger(x) \mathcal{D}_\beta(y) \rangle + \dots \quad (5.34)$$

Next, substitute the two-point functions

$$\langle \mathcal{D}_\alpha(x)^\dagger \mathcal{D}_\beta(y) \rangle = \delta_{\alpha\beta} |x - y|^{-2\Delta_\Phi} \quad (5.35)$$

The energy gain due to this contribution is therefore

$$\mathcal{E}[\vec{u}]_{\text{QED}_3} = -g_{\mathcal{D}}^2 |\vec{u}|^2 \int d^3x |x|^{-2\Delta_\Phi} + \dots \quad (5.36)$$

If  $\Delta_\Phi < 3/2$ , the perturbative energy gain is IR divergent  $\mathcal{E}[\vec{u} \neq 0]_{\text{QED}_3} \rightarrow \infty$ . This result (5.36) implies an infinite energy gain which outcompetes the potential-energy cost of the distortion for all  $g > 0$ . In a more careful approach we must regulate the IR-divergent integrals and calculate the scaling of critical coupling strengths with system size. However at this level, we can already see that this divergence signals a breakdown of perturbation theory. This is a feature we can typically associate with an underlying instability of the state we are expanding around.

### Finite-temperature transition

Given this result that the U(1) Dirac QSL is unstable to lattice coupling at zero temperature, a few questions arise. How would the instability manifest as a phase transition in experiment, and what is the nature of the true ground state?

The result above is performed at zero temperature in the thermodynamic limit. Here, we relied on conformal symmetry to calculate correlation functions, and assumed an infinite spacetime volume  $V = \infty$ . We can make rigorous progress at describing the instability by moving away from this zero temperature assumption. Non-zero temperatures  $T > 0$  produce a finite (effective) length scale  $\beta = 1/T$ . This will act to regulate the spacetime integrals which are IR-divergent, due to the long-distance power-law tails of the correlation functions.

At finite temperatures  $\beta < \infty$ , we no longer have exact conformal invariance, but it is only recovered in the  $\beta \rightarrow \infty$  limit. Iliesiu *et al.* (2018) show that one can apply the conformal data to calculate correlation functions on finite-temperature systems, since OPEs converge for  $\sqrt{\tau^2 + |\mathbf{r}^2|} < \beta \rightarrow \infty$ . This lets us use the standard form of the 2-point function to do the integral over monopole correlation functions. We can now evaluate the integral from Eq. (5.36). In this regularization, we split the calculation into a spatial integral over  $\mathbb{R}^2$  and a regulated temporal integral

$$-\langle S_g^2 \rangle / 2V = -g_{\mathcal{D}}^2 |\vec{u}|^2 \int_0^\beta d\tau \int d^2\mathbf{r} \frac{1}{[\tau^2 + |\mathbf{r}|^2]^{\Delta_\Phi}} \quad (5.37)$$

The infinite spatial integral can be evaluated in polar coordinates with the substitution  $u = r^2 + \tau^2$ , giving

$$\begin{aligned} \int d^2\mathbf{r} \frac{1}{[\tau^2 + |\mathbf{r}|^2]^{\Delta_\Phi}} &= (2\pi) \int_0^\infty dr \frac{r}{[\tau^2 + r^2]^{\Delta_\Phi}} = \pi \int_{\tau^2}^\infty \frac{du}{u^{\Delta_\Phi}}, \\ &= \frac{\pi}{(\Delta_\Phi - 1)} |\tau|^{2-2\Delta_\Phi}, \end{aligned} \quad (5.38)$$

when  $\Delta_\Phi > 1$ . Substituting back into (5.37), we can perform the regulated imaginary-time integral to find

$$-\langle S_g^2 \rangle / 2V = \frac{g_D^2 |\vec{u}|^2 \pi}{(\Delta_\Phi - 1)} \int_0^\beta d\tau |\tau|^{2-2\Delta_\Phi} = -c_{\Delta_\Phi} g_D^2 |\vec{u}|^2 \beta^{3-2\Delta_\Phi}, \quad (5.39)$$

when  $\Delta_\Phi < 3/2$  and where at this final step we defined the constant

$$c_{\Delta_\Phi} = \frac{\pi}{(\Delta_\Phi - 1)(3 - 2\Delta_\Phi)}. \quad (5.40)$$

This coefficient is positive  $c_{\Delta_\Phi} > 0$  when the monopole scaling dimension satisfies  $1 < \Delta_\Phi < 3/2$ .

Combining with the harmonic lattice potential-energy cost Eq. (5.28), this result gives us an expression for the lowest-order effective potential for the distortion modes

$$\mathcal{E}[\vec{u}] = (\kappa/2 - c_{\Delta_\Phi} g_D^2 \beta^{3-2\Delta_\Phi}) |\vec{u}|^2 + \dots \quad (5.41)$$

Firstly, note that the symmetric phase is present for large temperatures  $T \rightarrow \infty$ ,  $\beta \rightarrow 0$ . Here, the potential is minimised by  $|\vec{u}| = 0$ . In the zero-temperature limit  $T = \beta^{-1} \rightarrow 0$ , the quadratic effective energy functional (5.41) inverts and diverges for any  $g_D \neq 0$ . This reproduces the result of Eq. (5.36) in the thermodynamic limit with conformal symmetry.

We can now apply this potential to understand the ordering phase transition. This perturbative result is well controlled for  $g^2 \beta^{3-2\Delta_\Phi} |\vec{u}|^2 \ll 1$ . This means we can describe the phase transition by the inversion of the quadratic potential at small  $|\vec{u}| \ll 1$  within perturbation theory. The critical temperature scale  $T_{\text{SP}} = 1/\beta_c$  for the ordering instability is called the spin-Peierls temperature. Solving (5.41) for where the quadratic potential inverts, we predict

$$T_{\text{SP}}^{3-2\Delta_\Phi} = 2c_{\Delta_\Phi} g_D^2 / \kappa = 2c_{\Delta_\Phi} \lambda_D. \quad (5.42)$$

Here, we introduced here the spin-lattice coupling  $\lambda_D = g_D^2 / \kappa$ . This is the first prediction in two dimensions of a spin-Peierls temperature that goes to zero as a power law of the spin-lattice coupling. This tells us that there is an ordered ground state for any non-zero spin-lattice coupling. The transition temperature is controlled by the conformal data.

### Symmetry of the ground state

What is the nature of the low-temperature phase  $T < T_{\text{SP}}$ ? To answer this, we have to go to next order of perturbation theory, as well as consider other perturbations to the conformal

fixed point. Both of these steps will let us learn more about the symmetries of the Ginzburg–Landau Hamiltonian Eq. (5.41) at higher order, and consequently the nature of the ground state manifold.

The higher order perturbation theory is performed in Appendix B. The resulting effective free energy as a function of distortion  $\vec{u}$ , up to fourth order of perturbation theory, is

$$\mathcal{E}[\vec{u}] = (\kappa/2 - c_{\Delta_\Phi} g_D^2 \beta^{3-2\Delta_\Phi}) |\vec{u}|^2 + \mathcal{C}_1(\beta) |\vec{u}|^4 + \mathcal{C}_2(\beta) |\vec{u} \cdot \vec{u}|^2 + \dots \quad (5.43)$$

We may write the functions as  $\mathcal{C}_{1,2}(\beta) = c_{1,2} g_D^4 \mathcal{C}(\beta)$ . Rewriting this expression in terms of the magnitude  $\delta u = |\vec{u}|$  and (complex) direction unit vector  $\hat{n} = \vec{u}/|\vec{u}|$  with normalisation  $|\hat{n}|^2 = \hat{n} \cdot \hat{n}^* = 1$ , we find that the quartic term becomes

$$= (\kappa/2 - c_{\Delta_\Phi} g_D^2 \beta^{3-2\Delta_\Phi}) \delta u^2 + g_D^4 \mathcal{C}(\beta) (c_1 + c_2 |\hat{n} \cdot \hat{n}|^2) \delta u^4 + \dots \quad (5.44)$$

Stability of this potential at fourth order in perturbation theory requires that  $c_2 > -c_1$  and  $c_1 > 0$ . We assume that both coefficients are positive  $c_{1,2} > 0$  in the perturbative expansion in Appendix B.

Given this, we infer that the ordered state with finite distortion  $\delta u > 0$  will try to *minimise* the magnitude of  $\hat{n} \cdot \hat{n}$ . The order parameter  $\hat{n}$  is a vector in  $\mathbb{C}^3$  now satisfies

$$\hat{n} \cdot \hat{n}^* = 1, \quad (5.45)$$

$$\hat{n} \cdot \hat{n} = 0. \quad (5.46)$$

Both of these relations are left invariant under  $O(3)$  rotations  $\hat{n} \rightarrow R\hat{n}$  where  $R^\top R = 1$ . This suggests a continuous manifold of ground states in the symmetry broken phase. We can parameterise the  $O(3)$  ground state manifold in  $\mathbb{C}^3$  in terms of a complex unit vector

$$\tilde{n} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{-2\pi i/3} \\ e^{+2\pi i/3} \end{pmatrix}, \quad (5.47)$$

which satisfies the conditions (5.45) and (5.46). The whole ground state manifold is generated by acting on it as  $\hat{n}(\theta, \phi) = R(\theta, \phi)\tilde{n}$  with general rotations  $R(\theta, \phi) \in SO(3)$ .

Each configuration  $\vec{u}$  represents a finite lattice distortion composed out of three momentum eigenstates. The phases of these three modes can be tuned within the  $SO(3)$  ground state manifold. If we consider this vector as a continuous order parameter field  $\vec{u}(\mathbf{r})$ , the continuous symmetry of the action Eq. (5.43) would imply an absence of a finite-temperature ordering transition. This is because the Mermin–Wagner theorem means that the  $SO(3)$  symmetry cannot be spontaneously broken in two spatial dimensions. Note that this is not a concern in previous 1D spin–Peierls models. In that case, the effective potential is Ising-like, and the ground state manifold is  $\pm \delta u$ . Since only a discrete  $\mathbb{Z}_2$  symmetry is spontaneously broken, long-range order will form and the lattice picks one dimerisation in the ground state.

However, in the 2D case, the  $SO(3)$  symmetry is of course not present in the parent spin Hamiltonian. The microscopic  $C_3$  valley symmetry is only enlarged to a  $SO(3)_{\text{valley}}$  symmetry in the low-energy QED<sub>3</sub> continuum theory. The VBS monopoles  $\mathcal{D}_\alpha$  transform as a vector under  $SO(3)_{\text{valley}}$ . We can understand the symmetry enlargement in the IR limit

as being because microscopically-allowed monopole terms  $S_{\Phi\Phi\Phi} = \lambda(\mathcal{D}_1\mathcal{D}_2\mathcal{D}_3 + \text{h.c.})$  are irrelevant. The bilinear coupling Eq. (5.23) is left invariant if the lattice coupling  $\vec{u}$  transforms under the same SO(3)-vector representation. In the effective theory for the distortion field Eq. (5.43), this symmetry becomes the enlarged SO(3) symmetry discussed above. However, in the presence of the relevant coupling  $g_{\mathcal{D}}$ , Eq. (5.23), we are driven away from the QED<sub>3</sub> CFT and towards an ordered state. Although the coupling  $\lambda$  is irrelevant at the QED<sub>3</sub> fixed point, it will be relevant about the new fixed point resulting from the spin-lattice coupling. This means the triple-monopole coupling is *dangerously irrelevant* (Chubukov *et al.*, 1994; Senthil *et al.*, 2004). It shows that although the coupling  $\lambda$  initially flows to zero, above a certain RG scale, it begins to grow again.<sup>2</sup>

Consequently, anharmonic terms must appear in the effective theory of the lattice distortions within the ordered state. These act to break the continuous symmetry back down to the discrete  $C_3$  of the lattice. We can write the resulting anharmonic potential

$$\mathcal{E}_{\text{anh}}[\vec{u}] = -\tilde{\lambda} \text{Re}(u_1 u_2 u_3) \quad (5.48)$$

which selects  $+\tilde{n}$  from the SO(3) ground state manifold for  $\tilde{\lambda} > 0$ , as defined in Eq. (5.47). Alternately,  $-\tilde{n}$  is selected as the ground state when  $\tilde{\lambda} < 0$ . A more explicit calculation in Appendix B derives this coupling in conformal perturbation theory in the presence of both perturbations  $S_{\mathcal{D}}$  and  $S_{\Phi\Phi\Phi}$ . We define the ground state configuration which minimises the energy Eq. (5.48) (when  $\tilde{\lambda} > 0$ ) as follows

$$\vec{u}_0 = +\delta u \tilde{n} = \frac{\delta u}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{-2\pi i/3} \\ e^{+2\pi i/3} \end{pmatrix}. \quad (5.49)$$

The remaining ground state symmetry is discrete, corresponding to permutations of the elements of Eq. (5.49) which represent the same physical state up to a phase  $e^{\pm 2\pi i/3}$ . This only acts to shift the unit cell and represents the same physical VBS ordering pattern. In the presence of this static distortion background, the monopole-lattice coupling Eq. (5.23) becomes

$$S[\delta u] = S_{\text{QED}_3} + g_{\mathcal{D}} \delta u \int d^3x \left[ \mathcal{V}^\dagger(x) + \text{h.c.} \right], \quad \mathcal{V}^\dagger = \sum_{\alpha} \tilde{n}_{\alpha} \mathcal{D}_{\alpha}^{\dagger} = \mathcal{D}_1^{\dagger} + e^{-2\pi i/3} \mathcal{D}_2^{\dagger} + e^{+2\pi i/3} \mathcal{D}_3^{\dagger}, \quad (5.50)$$

where  $\delta u$  is the strength of the distortion and we inserted the phases  $\tilde{n}_{\alpha}$ . The operator  $\mathcal{V}^\dagger$  proliferates 12-site VBS order (Song *et al.*, 2019).

Finally, we can calculate the resulting lattice distortion patterns and VBS order in real space. The real-space pattern is explicitly given by the inverse of the Fourier transform Eq. (5.24), in this case with  $\mathbf{u}_{\mathbf{Q}} = 0$  for all  $\mathbf{Q} \neq \pm \mathbf{X}_{\alpha}$ , given by

$$\mathbf{u}(\mathbf{r}_i) = \sum_{\alpha} \left[ \frac{i s_{\alpha}(u_0)_{\alpha}}{\sqrt{2}} e^{i \mathbf{X}_{\alpha} \cdot \mathbf{r}_i} \hat{\mathbf{X}}_{\alpha} + \text{c.c.} \right] = -\sqrt{2} \text{Im} \left[ \sum_{\alpha} s_{\alpha}(u_0)_{\alpha} e^{i \mathbf{X}_{\alpha} \cdot \mathbf{r}_i} \right] \hat{\mathbf{X}}_{\alpha}. \quad (5.51)$$

<sup>2</sup>A more detailed discussion of the meaning of dangerously irrelevant operators will come in Chapter 7.

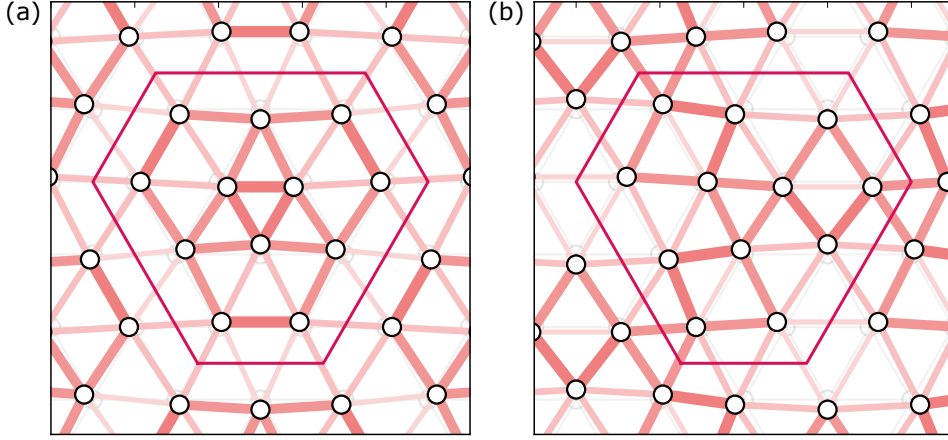


Figure 5.3: *The two possible spin-Peierls ground states which are instabilities of the  $U(1)$  Dirac QSL.* The patterns (a,b) are the ground state when the field theory coefficient  $\lambda$  is positive/negative. They are described by the phases  $\vec{v}_{\pm}$  in Eqns. (5.53) and (5.56).

Thus, we have a way of going from an effective potential (5.31) to a real-space distortion pattern. We start by finding its minimum  $\vec{u}_0$ , and then plugging this in the inverse Fourier transform (5.51). Substituting Eq. (5.49), we find

$$\mathbf{u}(\mathbf{r}_i) = -\delta u \sqrt{\frac{2}{3}} \operatorname{Im} \left[ \sum_{\alpha} s_{\alpha} \tilde{n}_{\alpha} e^{i\mathbf{X}_{\alpha} \cdot \mathbf{r}_i} \hat{\mathbf{X}}_{\alpha} \right] = -\delta u \sqrt{\frac{2}{3}} \sum_{\alpha} \sin(\mathbf{X}_{\alpha} \cdot \mathbf{r}_i + \vartheta_{\alpha}^{+}) \hat{\mathbf{X}}_{\alpha}, \quad (5.52)$$

where the phases are

$$\vartheta_{\alpha}^{+} = \arg(s_{\alpha} \tilde{n}_{\alpha}) = (0, -2\pi/3, -\pi/3)^{\top}. \quad (5.53)$$

The coupling Eq. (5.50) induces the following monopoles to condense:

$$\langle \mathcal{D}_{\alpha} \rangle \sim -\tilde{n}_{\alpha}, \quad (5.54)$$

fixing the VBS pattern. Using the leading-order mapping between VBS monopoles and nearest-neighbour dimer correlations [given by (2.136)], we can evaluate the nearest-neighbour spin-spin correlation function

$$\langle \vec{S}_{\mathbf{r}_i} \cdot \vec{S}_{\mathbf{r}_i + \delta_{\alpha}} \rangle \simeq \operatorname{Re} \left[ s_{\alpha} \langle \mathcal{D}_{\alpha} \rangle e^{i\mathbf{X}_{\alpha} \cdot \mathbf{r}_i} \right] \sim -\cos(\mathbf{X}_{\alpha} \cdot \mathbf{r}_i + \vartheta_{\alpha}^{+}) \quad (5.55)$$

where  $\vec{v}_{+}$  is defined via Eq. (5.53). The resulting spin-Peierls order for this configuration with  $\tilde{\lambda} > 0$  is shown in Fig. 5.3(a). Note that we take the positions  $\mathbf{r}_i$  in the middle of the bonds. If  $\tilde{\lambda} < 0$ , this distortion is the highest energy state in the  $SO(3)$  manifold. The ground state is instead  $-\tilde{n}$ , resulting in a different choice of phases

$$\vartheta_{\alpha}^{-} = (0, -2\pi/3, 2\pi/3)^{\top}. \quad (5.56)$$

This configuration is plotted in Fig. 5.3(b). The sign of the coefficient  $\tilde{\lambda}$ , and therefore the resulting ground state, cannot be fixed within this field theory approach but must rather be evaluated numerically. In both cases, the ground state spontaneously breaks symmetries by distorting the underlying lattice and inducing commensurate 12-site VBS order. This particular 12-site valence-bond ordered state is a strong sign of an underlying monopole instability (Moessner and Sondhi, 2001).

### 5.2.3 Strong-coupling limit

#### Scaling Ansatz

We have seen that perturbing the CFT fixed point with a monopole-lattice coupling leads to infrared divergences in the perturbative approach. We used a finite inverse temperature  $\beta < \infty$  to regulate these and evaluate a perturbative potential. Perturbation theory assumes a small parameter to justify the consideration of only leading terms. In our calculation above, the approximation holds when

$$g_{\mathcal{D}}^2 \beta^{3-2\Delta_{\Phi}} |\vec{u}|^2 \ll 1 \quad \leftrightarrow \quad g_{\mathcal{D}}^2 \delta u^2 \ll T^{3-2\Delta_{\Phi}}. \quad (5.57)$$

It is worth reiterating that we are able to predict the transition temperature when the quadratic potential inverts, since the perturbative expansion always holds for sufficiently small  $\delta u$ . If we are interested instead in understanding the zero-temperature limit, then we must take a different — non-perturbative — approach.

When  $T = 0$  (and in the thermodynamic limit  $L = \infty$ ), the monopole-lattice coupling constitutes the only energy scale in the otherwise conformally invariant theory. Therefore, we may use a scaling Ansatz which infers the CFT's response to the distortion from scaling and symmetry arguments. Instead of a  $\beta$ -dependent quadratic response, we expect the lattice deformation in the zero-temperature limit to lead to a critical power law energy gain. The critical exponents will be determined by scaling dimensions of operators at the fixed point. This approach will allow us to generalise the 1D energy response from Eq. (5.14) to the 2D model, as well as predicting ground-state properties like the induced gap size.

The continuum form of the spin-lattice coupling is written in Eq. (5.23). The distortion of the lattice introduces a symmetry-allowed, relevant perturbation to the CFT fixed point  $\mathcal{D}_{\alpha}$ , with scaling dimension  $\Delta_{\Phi}$ . The coupling strength is  $g_{\mathcal{D}} u_{\alpha}$ , with scaling dimension

$$[g_{\mathcal{D}} u_{\alpha}] = 3 - \Delta_{\Phi} \equiv \nu_{\Phi}^{-1}. \quad (5.58)$$

By conformal invariance, we may calculate the gap induced by the lattice distortion

$$\Delta_{\text{gap}} \sim |g_{\mathcal{D}} \vec{u}|^{\nu_{\Phi}}. \quad (5.59)$$

We can of course also evaluate the divergent behaviour of the correlation length  $\xi \sim 1/\Delta \sim |g_{\mathcal{D}} \vec{u}|^{-\nu_{\Phi}}$ .

From this power-counting within the QED<sub>3</sub> fixed point theory, we may further write down a strong-coupling Ansatz for the energy density gain from this relevant perturbation. The energy per area has dimension  $[\mathcal{H}] = 3$  and as such, the energy gain will scale with

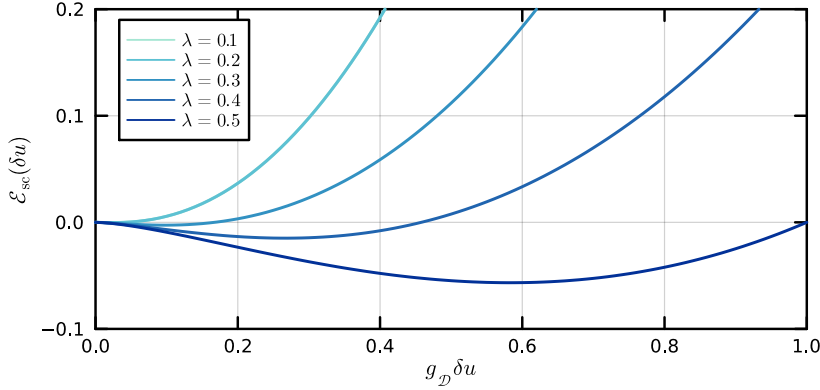


**Figure 5.4:** *Strong-coupling potential* for the lattice distortion field  $\mathcal{E}(\delta u)_{\text{sc}}$  as a function of coupling strength  $\lambda_{\mathcal{D}} = g_{\mathcal{D}}^2/\kappa$ .

the cube of the gap. The scaling form for the potential for the lattice distortion field at zero-temperature is

$$\mathcal{E}[\vec{u}]_{\text{sc}} = (\kappa/2)|\vec{u}|^2 - c_{\text{sc}}|g_{\mathcal{D}}\vec{u}|^{3\nu_{\Phi}}, \quad (5.60)$$

with  $3\nu_{\Phi} = 3/(3 - \Delta_{\Phi}) < 2$  when  $\Delta_{\Phi} < 3/2$ . We take  $c_{\text{sc}} > 0$  to be an undetermined positive scaling constant (Luo *et al.*, 2022). This non-analytic contribution to the ground-state energy must out compete the leading quadratic energy cost for the longitudinal displacements. We find it to be energetically preferable for the system to undergo a lattice distortion with amplitude  $u_0 \neq 0$  as long as  $\Delta_{\Phi} < 3/2$ . By defining the dimensionless coupling  $\lambda_{\mathcal{D}} = g_{\mathcal{D}}^2/\kappa$ , we can rewrite the potential simply as a function of  $g_{\mathcal{D}}\delta u$ :

$$\mathcal{E}[g_{\mathcal{D}}\delta u]_{\text{sc}} = (1/2\lambda_{\mathcal{D}})|g_{\mathcal{D}}\delta u|^2 - c_{\text{sc}}|g_{\mathcal{D}}\delta u|^{3\nu_{\Phi}}. \quad (5.61)$$

This is plotted in Fig. 5.4 for various couplings, and with  $c_{\text{sc}} = 1$ . It shows the minimum of the potential shifting to higher  $\delta u$  at higher coupling  $\lambda$ .

We stress that here, the form (5.60) possesses an accidental  $\text{SO}(3)_{\text{valley}}$  symmetry which is emergent at the CFT fixed point, which will be reduced to a discrete subgroup (compatible with the discrete UV symmetries of the model) by dangerously irrelevant operators or anharmonic terms, as discussed above.

Within this scaling Ansatz, we can further estimate the magnitude of the induced displacement field by minimising  $\mathcal{H}[\vec{u}]_{\text{sc}}$  and obtain

$$\delta u_0 = \left[ \frac{2/3}{\nu_{\Phi} c_{\text{sc}}} \left( \frac{\kappa}{g_{\mathcal{D}}^{3\nu_{\Phi}}} \right) \right]^{1/(3\nu_{\Phi}-2)}. \quad (5.62)$$

The corresponding equilibrium gap scales as

$$\Delta_{\text{gap}}[\delta u_0] \sim (g_{\mathcal{D}}^2/\kappa)^{1/(3-2\Delta_{\Phi})}, \quad (5.63)$$

in accordance with the spin-Peierls temperature Eq. (5.42). We predict that the ratio  $\Delta_{\text{gap}}/T_{\text{SP}}$  is system-independent and would be universal for all  $\text{U}(1)$  Dirac QSL materials which exhibit a spin-Peierls instability in the ground state.

### Spin-Peierls instabilities in general models

The above discussion is rather general in the sense that it only relies on the existence of a symmetry-allowed coupling between the distortion field and a relevant operator in the CFT. Given this, one may tentatively extend our results for the Dirac QSL to more general couplings between gapless deconfined phases of matter (described by a CFT) to lattice distortions in any dimension. The criterion for the spin-Peierls instability to occur is that there is a VBS-order parameter, expressed as an instanton of an underlying gauge theory, with scaling dimension

$$\Delta \leq d/2. \quad (5.64)$$

Note that this is stronger than relevance  $\Delta < d$ . Spin-Peierls instabilities are clearly highly dimensionally-dependent, but contrary to common knowledge they can exist beyond 1D!

Let us revisit the most basic example of a Peierls instability of free fermions. Inspecting the *free* Dirac fermion action in  $d$  dimensions, we identify the scaling dimension of the fermion bilinear term to be  $\Delta_M^{\text{free}} = [\bar{\psi}\psi] = d - 1$ . This corresponds to the fermion mass' scaling dimension. We derived our condition Eq. (5.64) in the context of monopoles, but it also applies to other operators in the spectrum which break lattice symmetries. Applied to the free Dirac fermion model, it implies we have a Peierls instability at weak coupling when  $d \leq 2$ , i.e. only in one spatial dimension. In the case of 2D Dirac fermions,  $\Delta_M^{\text{free}} = 2$  and we expect no instability (i.e. only a finite critical  $g_c$ ). Weak interactions will also be insufficient to cause an instability under this mechanism. Only *strong interactions* which cause a large anomalous dimension  $\Delta_M = 2 - \eta_M$  with  $\eta_M \geq 1/2$  will be sufficient.

In the case of 1D fermions, we have used bosonisation to show how interactions increase instability. The scaling dimension of the relevant dimerisation operator is  $\Delta = K$ . In the free fermion model (bosonised XY spins), we have  $K = 1$  which only just satisfies the inequality Eq. (5.64). For this model, it was logarithmic contributions which lead to a weak instability (Giamarchi, 2003). For the SU(2)-symmetric Heisenberg model, this is satisfied since  $K = 1/2$  is firmly within the unstable regime. By studying the U(1) Dirac QSL in  $d = 3$ , we have also provided an example of strong interactions exacerbating potential instabilities. The spin-Peierls instability of our model is the first such weak-coupling instability to be identified in this context.

## 5.3 Spin-Peierls instability of the $J_1$ - $J_2$ Heisenberg model

### 5.3.1 Numerical study

#### Spin-lattice Hamiltonian

In this Section, we numerically study the stability of the U(1) Dirac QSL ground state in the presence of lattice distortions. To do this, we use a variational numerical approach to study the  $J_1$ - $J_2$  model on a deformed triangular lattice. The starting point of our study is the  $S = 1/2$  Heisenberg model on the triangular lattice

$$\mathcal{H}_{J_1 J_2} = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j. \quad (5.65)$$

We take a next-nearest neighbour exchange  $J_2/J_1 = 1/8$  within the QSL phase. The interactions  $J_{1,2}$  are Heisenberg exchange interactions, which arise most simply from the overlap of localised electron orbitals. Such a process is naturally highly dependent upon the length of bonds. More explicitly, the coupling of distortions to the spins can be described by writing that the first-neighbour exchange interactions depend linearly on the relative site displacements as follows

$$\mathcal{H}[\mathbf{u}_i] = \mathcal{H}_{J_1 J_2} - g J_1 \sum_{\langle ij \rangle} \hat{\mathbf{r}}_{ij} \cdot (\mathbf{u}_i - \mathbf{u}_j) \vec{S}_i \cdot \vec{S}_j, \quad (5.66)$$

with  $g$  denoting the spin-lattice coupling constant and  $\mathbf{u}_i$  the local displacement operators. This expression can be seen as the leading expansion of the exponential form Eq. (5.1) for small displacements. Note that  $g$  is a lattice-scale constant with units inverse length that is non-trivially related to the field-theoretic coupling  $g_{\mathcal{D}}$ . We define the dimensionless spin-lattice coupling  $\lambda = J_1 g^2 / \kappa$ . The unit vectors  $\hat{\mathbf{r}}_{ij}$  are defined as  $\hat{\mathbf{r}}_{ij} = \frac{\mathbf{r}_i - \mathbf{r}_j}{\|\mathbf{r}_i - \mathbf{r}_j\|}$ , with  $\{\mathbf{r}_i\}$  indicating the site coordinates in the undistorted triangular lattice.

We choose to include a minus sign in Eq. (5.66) such that, for  $g > 0$ , stronger spin-spin correlations form on shorter bonds, as expected on physical grounds. In other words, the antiferromagnetic exchange interaction is enhanced when spins get closer. In the limit of *static distortions*, the displacements  $\mathbf{u}_i$  are classical variables which induce a static modulation of the exchange couplings. This allows us to modulate the site displacements in a specific distortion pattern and then compute the variational energy gain per site  $\delta\epsilon$  as a function of the strength of lattice distortions  $\delta u$ . Note that the next-nearest neighbour exchange  $J_2$  is also bond-length dependent. However we find it can be effectively neglected since it is already small compared to  $J_1$ .

### Variational Monte Carlo

We numerically simulate this model using variational Monte Carlo (VMC). In this method, the variational wavefunctions for spins are projected Abrikosov fermion states. These fermionic wavefunctions are ground states of an auxiliary Hamiltonian, which takes the form of the non-interacting  $\pi$ -flux Ansatz  $\mathcal{H}_0$  subjected to the one-fermion-per-site constraint (Wen, 2002). The *bonafide* Dirac QSL wave function is constructed by applying the Gutzwiller projector  $\mathcal{P}_G = \prod_i (n_{i,\uparrow} - n_{i,\downarrow})^2$  (with  $n_{i,\alpha} = f_{i\alpha}^\dagger f_{i\alpha}$ ) to the ground state of  $\mathcal{H}_0$ . Further details of the method are described in Appendix C.

On the triangular lattice we consider a 12-site distortion pattern that is commensurate with the monopole momenta  $\mathbf{X}_\alpha$  and with relative phases  $\vartheta_\alpha^+$ , given in Eq. (5.53). The pattern in real-space is given by Eq. (5.52) and plotted in Fig. (5.3). Within the 12-site unit cell, there are seven classes of symmetry-inequivalent first-neighbour bonds, according to their length after distortion, as depicted in Fig. 5.5(a). Therefore, we let the variational hopping parameters of  $\mathcal{H}_0$  take independent values on the symmetry-inequivalent bonds. More specifically, this optimisation is performed with the underlying sign structure kept fixed and equal to the one of the  $\pi$ -flux Ansatz. The absolute values of the inequivalent hoppings are independently optimised using the stochastic reconfiguration method (Sorella, 2005; Becca and Sorella, 2017). To verify the validity of our parametrization, we also performed a full

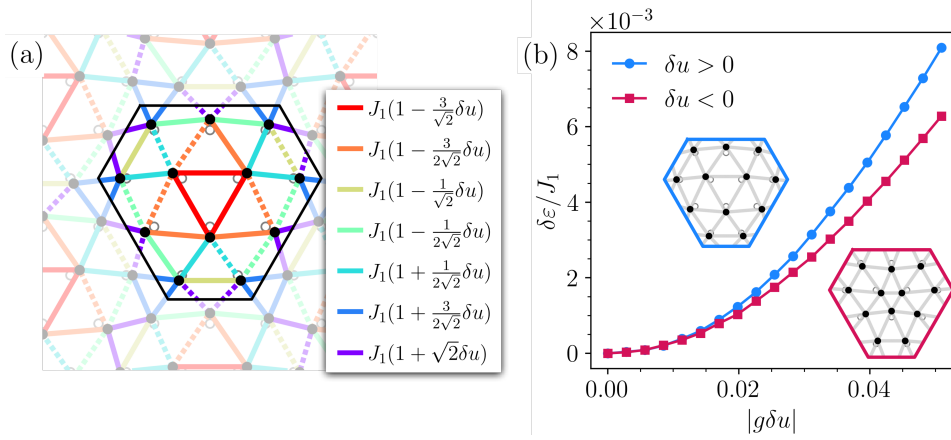


**Figure 5.5:** (a) 12-site lattice distortion on the triangular lattice. Lattice sites are displaced according to Eq. (5.52) (with  $\delta u > 0$ ). The resulting 12-site supercell is delimited by the solid black lines. Different colors represent symmetry-inequivalent first-neighbour bonds, grouped into distinct classes according to their bond length after distortion. For each class of bonds, the value of the exchange interaction in presence of a finite static distortion  $\delta u$  is reported. The variational parametrisation of  $\mathcal{H}_0$  follows the same symmetry of the distortions: hoppings with different absolute values are taken on the different classes of inequivalent bonds. The signs of the hoppings, instead, are kept equal to the ones of the Dirac QSL and are represented here by solid/dashed lines, which indicate positive/negative hoppings, respectively. (b) energy gain per site  $\delta\varepsilon$  as a function of the lattice distortions of Eq. (5.52), for different signs of  $\delta u$ . Results for the  $L = 12$  lattice. The respective site displacements are shown in the insets. The case  $\delta u > 0$  provides a larger energy gain beyond the weak-coupling regime of small distortions.

unbiased optimization of all the 36 hoppings within the 12-site supercell, which returned the same variational energy.

The spectrum of the optimal (auxiliary) fermionic Hamiltonian  $\mathcal{H}_0$  acquires a gap in the presence of finite distortions  $\delta u$ . From the field theoretical understanding, we expect this to drive monopole proliferation and VBS ordering. The energy gain per site is then calculated from the projected wavefunctions. It is defined as  $\delta\varepsilon = |E_{\text{var}}(\delta u) - E_{\text{var}}(0)|/N$ , with  $N = L^2$  being the number of sites on a  $L \times L$  cluster. Fig. 5.5(b) shows the energy gain  $\delta\varepsilon$  on a  $12 \times 12$  cluster as a function of distortion  $|g\delta u|$ . The result is a quadratic energy gain for small distortions. For larger  $g\delta u$ , there is a splitting between the energy gain from positive and negative signs of  $\delta u$ . Note that the amplitude of this response is larger than other distortion patterns with smaller unit cells. This shows that the pattern with positive  $\delta u$ , given in Eq. (5.52), is energetically preferred and will be selected. This can be explained by a positive value of the constant  $\tilde{\lambda} > 0$  in Eq. (5.48).

We perform the same numerical calculations on the 1D Heisenberg chain. Here, the lattice distortion is a dimerisation  $u_i = \delta u(-1)^i$  (Cross and Fisher, 1979). We normalise this distortion such that the energy cost (per site) of lattice displacements is  $(\kappa/2)\delta u^2$ . When  $\delta u$  is non-zero, the exchange interactions become  $J_1(1 \pm 2g\delta u)$  on even/odd bonds. We thus

compute the ground state energy of the spin model with alternating exchange interactions for different values of  $\delta u$ . Since the distortions lower the translational symmetry of the model and give rise to a doubled unit cell, we increase the variational freedom of our state accordingly. This means that we allow the hoppings and pairings of  $\mathcal{H}_0$  to take different values on even and odd bonds in the numerical optimization. This yields a gapped dimerised state at finite  $\delta u$ .

### 5.3.2 Weak-coupling regime

#### Finite-size systems

The quadratic response at small  $g \delta u$  motivates us to develop an alternative weak-coupling approach to the spin-lattice coupling on finite-size systems. We rely here on an alternative finite-system-size regularisation at zero temperature  $T = 0$ . The finite length  $L$  takes over the role of  $\beta$  in regulating the integrals. For a torus geometry with any finite length (smaller than the correlation length), the system's energy will be an analytic function in the spin-Peierls coupling  $g_{\mathcal{D}}$ . The change in energy  $\mathcal{E}[\vec{u}]_{\text{QED}_3}$  due to coupling to a distortion field can be obtained using the same perturbative expansion,

$$\mathcal{E}[\vec{u}]_{\text{QED}_3} = -\frac{1}{2V} \langle S_{\mathcal{D}}^2 \rangle_{\text{QED}_3} + \dots, \quad (5.67)$$

where  $\langle S_{\mathcal{D}}^2 \rangle_{\text{QED}_3}$  can be obtained in an analogous manner to (5.37), but now performing the space-time integral on the geometry  $\lim_{\beta \rightarrow \infty} S_{\beta}^1 \times S_L^2$ , such that

$$\mathcal{E}[\vec{u}]_{\text{QED}_3} = -\tilde{c}_{\Delta_{\Phi}} g_{\mathcal{D}}^2 |\vec{u}|^2 L^{3-2\Delta_{\Phi}}, \quad (5.68)$$

where the constant

$$\tilde{c}_{\Delta_{\Phi}} = \pi^{3/2} \frac{\Gamma(\Delta_{\Phi} - 1/2)}{(3 - 2\Delta_{\Phi})\Gamma(\Delta_{\Phi})} + \dots. \quad (5.69)$$

This explains the leading quadratic response shown in Fig. 5.5(b), but also predicts that the amplitude of this should be system-size dependent. Importantly, we notice that this result Eq. (5.68) is equivalent to Eq. (5.39) from the finite-temperature regularisation, up to a constant. This motivates us to identify the effective temperature due to the finite size of the system  $\tilde{T} = L^{-1}$ . A CFT at finite temperature is described by a finite-size ( $\beta = T^{-1}$ ) in the Euclidean time direction. In this construction, the effective temperature  $\tilde{T}$  is related to the true temperature  $T$  by a (geometry-dependent) constant factor.

We have not discussed the weak coupling case in 1D up to now. Orignac and Chitra (2004) performed a perturbative calculation to predict the spin-Peierls temperature  $T_{\text{SP}}/J_1 = 1.01\lambda = 1.01(g^2/\kappa)$ . Because of the bosonisation mapping, it is possible to predict the numerical coefficients in terms of the lattice constants  $g$ . There is a technicality that arises when calculating correlation functions of the Heisenberg chain. In the bosonised description of the SU(2)-symmetric model, the state flows to the point  $K = 1/2$  where the coupling  $\mu$  is marginal. The presence of this marginal operator acts to add logarithmic corrections to the power-law correlation functions. The effect of these logarithmic corrections on any finite system will be to effectively shift the Luttinger parameter  $1/2 \rightarrow K_* > 1/2$  (Orignac, 2004; Papenbrock *et al.*, 2003). This acts in turn to suppress  $T_{\text{SP}}$ .

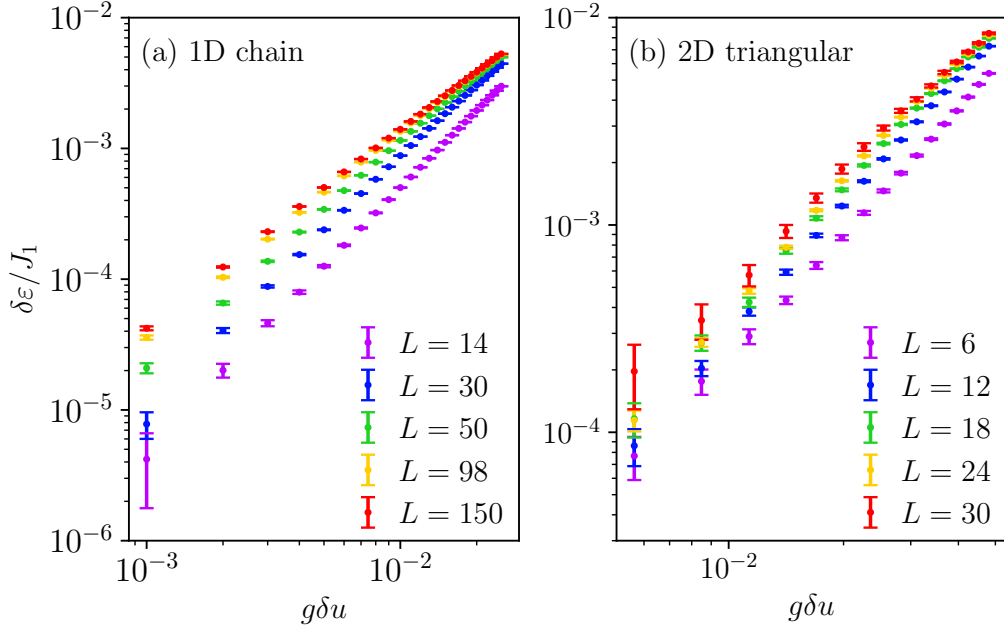


**Figure 5.6:** *The energy gain per site  $\delta\epsilon$ , as a function of static distortions, for various linear sizes  $L$ . Results shown in (a) 1D and (b) 2D, where  $N = L \times L$  sites.*

In 1D we can repeat the finite-temperature calculation from Orignac and Chitra (2004) on a zero-temperature system with periodic spatial boundary conditions. The resulting  $\mathbb{R} \times S^1$  geometry of the space-time manifold is identical to the finite-temperature  $L = \infty$  case. One may then use the same conformal mappings to evaluate correlation functions and consequently find that the effective critical temperature is equal to the true critical temperature of (Orignac and Chitra, 2004). That is, the inverse lattice size is exactly the effective temperature  $T = \tilde{T} = 1/L$  in 1D.

### Spin-Peierls temperature

We compute how the variational ground state energy of the  $J_1$ - $J_2$  model in Eq. (5.66) changes when the exchange couplings are modulated by lattice distortions. We extend this to a set of  $L \times L$  geometries compatible with the unit cell from  $L = 6$  to  $L = 30$ . The energy gain per site  $\delta\epsilon$  as a function of the distortion strength is shown in Fig. 5.6(b). The same calculation of the 1D Heisenberg chain's energetic response to dimerisation as a function of length  $L$  is shown in Fig. 5.6(a). Due to numerical limitations in 2D, we are only able to reliably measure the energy response in a regime at larger distortion  $g\delta u$ , and smaller linear system sizes.

For small distortions, we observe a quadratic gain in energy

$$\delta\epsilon = A(L)g^2\delta u^2, \quad (5.70)$$

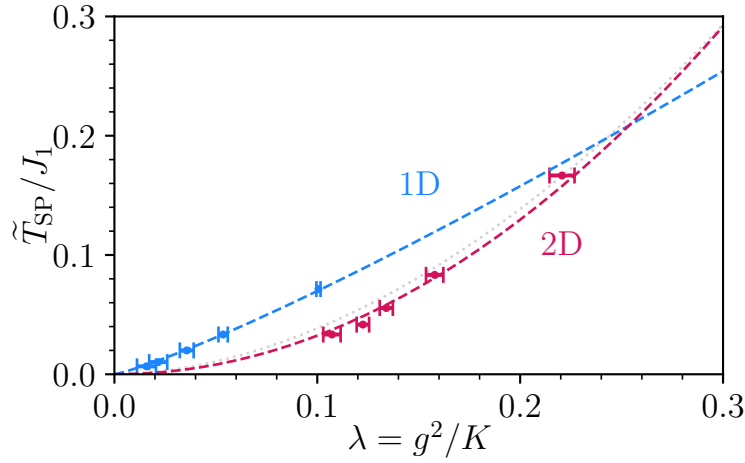


**Figure 5.7:** *Numerical results for the spin-Peierls temperature in 1D and 2D.* Calculated in the 1D Heisenberg chain and the 2D  $J_1$ - $J_2$  triangular-lattice Heisenberg model. Critical effective temperatures calculated from finite-size scaling  $\tilde{T}/J_1 = L^{-1}$  of the models under static lattice distortions. Results plotted as a function of (dimensionless) coupling strength  $\lambda$ . Blue and red dashed curves calculated from fits to the weak-coupling regime of the collapsed data, see Sec. 5.3.3. Grey dotted curve calculated from the independent dynamical calculations in Chapter 4.

where the amplitude  $A(L)$  is strongly dependent on system size. Both systems show quantitatively similar results, with comparable magnitudes of the response. For systems with  $L = 6$ , a 1% variation exchange induces an energy change on the order of  $10^{-3}J_1$ . This energy gain competes with the quadratic energy cost of static distortions to give the effective potential

$$\begin{aligned} \mathcal{E}(\delta u) &= (\kappa/2)(\delta u)^2 - \delta\varepsilon(\delta u) \\ &= [\kappa/(2g^2) - A(L)](g\delta u)^2. \end{aligned} \quad (5.71)$$

The lattice will spontaneously distort whenever the sign of this quadratic response changes to negative, i.e. when  $2A(L_c) = \kappa/g^2$ . This defines a critical system size  $L_c$  above which the lattice will spontaneously distort. As described above, we interpret this as a critical temperature  $\tilde{T}_{\text{SP}}/J_1 = L_c^{-1}$  for the spin-Peierls instability.

We estimate the spin-Peierls transition line by measuring the response  $A(\tilde{T})$  for various effective temperatures; then, the critical (dimensionless) spin-lattice coupling strength is  $\lambda_c(\tilde{T}) = J_1 g_c^2 / \kappa = J_1 / [2A(\tilde{T})]$ . For a given coupling strength, this equivalently defines an effective transition temperature  $\tilde{T}_{\text{SP}}$  which is plotted as points in Figure 5.6. The range of data to fit to a quadratic are chosen for each system individually. The error in the amplitudes  $A(L)$  is estimated by evaluating how far the first excluded data point lies from the fit curve. We then propagate this to an error in  $\lambda_c$  for a fixed  $L$ , plotted as error bars in Fig. 5.6. However, we see that only a subset of the data is well described by the weak-coupling prediction

of a quadratic response. The approach of predicting critical temperatures by excluding data and fitting the small quadratic regime is limited.

### 5.3.3 Scaling collapse

A more reliable approach to extracting the scaling of the spin-Peierls temperature will consist of performing a data collapse on the data before fitting. This collapse will provide an accurate description of the whole range of the response on different size systems. We highlight that our numerical results on larger systems show significant deviation from a simple quadratic (weak-coupling) response. The energy gain becomes significantly less  $L$ -dependent and is best described by a lower exponent  $(g\delta u)^\chi$ ,  $\chi < 2$ . We will now investigate this *strong-coupling* regime in the numerical data, and discuss the relationship to our strong-coupling predictions from field theory, given in Eq. (5.60).

In the thermodynamic limit, we predict that the static distortion will open a gap by inducing a relevant instanton to the low-energy model of the U(1) Dirac QSL. The respective field-theoretic coupling has scaling dimensions  $d - \Delta$ , where  $d = D + 1$  and we define  $\Delta = \Delta_*$ ,  $\Delta_\Phi$  in 1D and 2D, respectively. In our calculations, the system size also acts as a relevant operator with the coupling  $1/L$  (scaling dimension 1) which opens a finite-size gap (Cardy, 1996). To this end, we derive the following scaling Ansatz for the energy density gain  $\delta\varepsilon(\tilde{g}\delta u, 1/L)$ . This energy density (energy per spatial area) has scaling dimension  $[f] = d$ . Furthermore, we know the dimensions  $[L] = -1$ , and the coupling  $[g\delta u] = d - \Delta$  by power counting. We can hence constrain how the function  $f$  rescales under  $x \rightarrow bx$ , and find

$$\delta\varepsilon(g\delta u, 1/L) \rightarrow \delta\varepsilon(b^{-(d-\Delta)} g\delta u, 1/bL) = b^{-d} \delta\varepsilon(g\delta u, 1/L). \quad (5.72)$$

Choosing  $b = L^{-1}$  we recover

$$L^d \delta\varepsilon(g\delta u, 1/L) = \delta\varepsilon(L^{d-\Delta} g\delta u, 1) \equiv \tilde{\mathcal{F}}(L^{d-\Delta} g\delta u), \quad (5.73)$$

where  $\tilde{\mathcal{F}}(x)$  is a universal scaling function. This shows that plotting  $L^d \delta\varepsilon$  against  $L^{d-\Delta} g\delta u$  should produce a data collapse. The scaling Ansatz reads

$$\delta\varepsilon(g\delta u, 1/L)/J_1 = L^{-d} \tilde{\mathcal{F}}(L^{d-\Delta} g\delta u), \quad (5.74)$$

in terms of a universal scaling function  $\tilde{\mathcal{F}}(x)$ . In the weak-coupling (small distortions, small system) limit, i.e.  $x \rightarrow 0$ , the function must be quadratic  $\tilde{\mathcal{F}}(x) \sim x^2$ . Conversely, in the large-parameter limit  $x \rightarrow \infty$ , the function must follow  $\tilde{\mathcal{F}}(x) \sim x^{d/(d-\Delta)}$  and  $\delta\varepsilon$  becomes  $L$ -independent. This reproduces non-analytical scaling laws determined by the CFT fixed point theory.

We apply this analysis to the  $d = 2 + 1$  U(1) Dirac QSL in Fig. 5.8(b) and extract the exponent  $\Delta_\Phi = 1.25(2)$ . This agrees remarkably well with the fit of dimer-dimer correlations and is compatible with independent predictions of the QED<sub>3</sub> monopole scaling dimension (Karthik and Narayanan, 2019). We repeat the analysis for the  $d = 1 + 1$  Heisenberg chain data in Fig. 5.8(a). The extracted exponent is  $\Delta_* = 0.575$ , which is slightly above the Heisenberg Luttinger parameter  $K = 1/2$ . We attribute this shift due to the effect of logarithmic

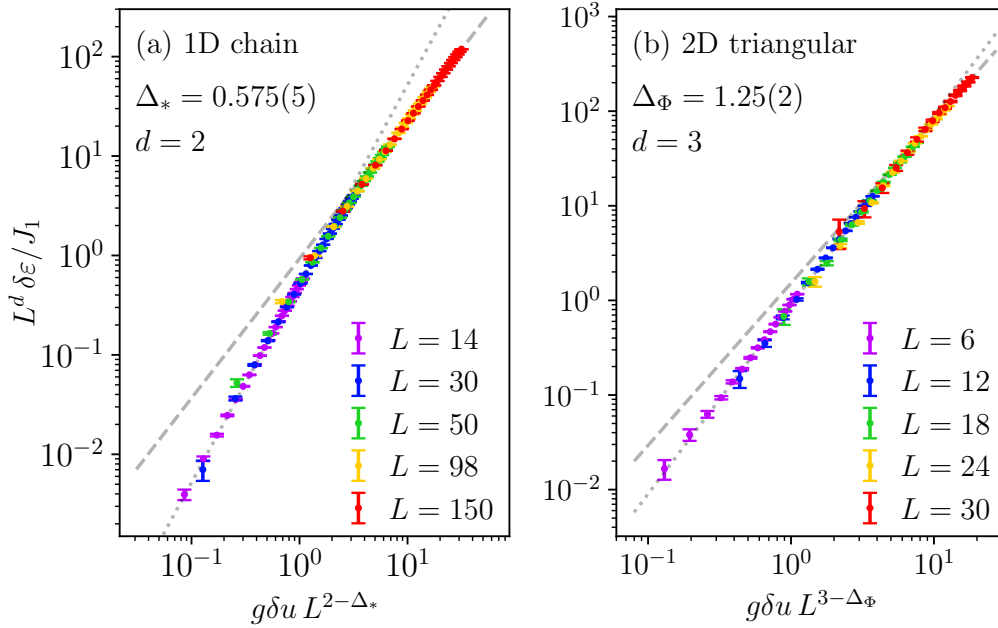


**Figure 5.8:** *Data collapse of the energy gain per site  $\delta\epsilon$  under static lattice distortion  $g\delta u$ .* Results for (a) the Heisenberg chain and (b) the triangular lattice  $J_1$ - $J_2$  model are shown. We plot  $L^d \delta\epsilon / J_1$  against  $g\delta u L^{d-\Delta}$  for dimension  $d = D + 1$  and optimise the scaling dimensions to get the best collapse, shown inset. Dotted and dashed lines represent asymptotic fitting functions for the regimes of weak and strong coupling, i.e. at small and large values of  $g\delta u$ .

corrections. Next, we can fit the collapsed data in the weak- and strong-coupling regimes to the appropriate power laws and extract the coefficients

$$\tilde{\mathcal{F}}(x \rightarrow 0) = A_0 x^2, \quad \tilde{\mathcal{F}}(x \rightarrow \infty) = A_\infty x^{d/(d-\Delta)}. \quad (5.75)$$

The resultant constants are shown in Table. 5.3. These limiting power laws are shown as dotted and dashed lines in Fig. 5.8.

The weak-coupling fit allows us to obtain the functional form of the critical temperature as a function of coupling strength by using the same procedure as for individual data points above. Explicitly, using Eq. (5.74) we may write  $A(L) = A_0 L^{d-2\Delta}$  and consequently

$$\tilde{T}_{\text{SP}}/J_1 = (2A_0 \lambda)^{1/(d-2\Delta)}. \quad (5.76)$$

We hence measure the following behaviour of the critical temperature as a function of coupling

$$\tilde{T}_{\text{SP}}^{2\text{D}}/J_1 = 3.24 \lambda^{2.0}, \quad \tilde{T}_{\text{SP}}^{1\text{D}}/J_1 = 1.05 \lambda^{1.18}, \quad (5.77)$$

as plotted with the dashed line in Fig. 5.7. Note that the 1D exponent is shifted from the bare scaling dimension 0.5 and the transition temperature is suppressed compared to the

|               | $\Delta$                | $A_0$ | $A_\infty$ |
|---------------|-------------------------|-------|------------|
| 1D chain      | $\Delta_* = 0.575(5)$   | 0.52  | 0.93       |
| 2D triangular | $\Delta_\Phi = 1.25(2)$ | 0.90  | 1.52       |

Table 5.3: Parameters fit to different regimes of VMC data.

approximate field theoretic prediction due to logarithmic corrections. Taken together, we find similar behaviour of static 1D and 2D spin-Peierls transitions at spin-lattice couplings comparable with 1D materials  $\eta \sim 0.3$  (Bray *et al.*, 1975; Jacobs *et al.*, 1976; Huizinga *et al.*, 1979). The temperature scale for such a spin-Peierls transition to VBS order in two dimensions could be of the same order as one dimension. Therefore, these results suggest that spin-Peierls instabilities of two dimensional quantum spin liquids could be equally experimentally significant as in one dimension.

In both models, the strong-coupling regimes are also well described by the proposed power-laws with fixed exponent  $\chi = d/(d - \Delta) < 2$ . In our 2D triangular lattice model, we write the effective potential for the distortion mode as

$$\mathcal{E}[\delta u]_{\text{sc}}^{2\text{D}} = (\kappa/2)\delta u^2 - A_\infty(g\delta u)^{1.714}. \quad (5.78)$$

This numerical analysis confirms that the spin energy gain will always outcompete the lattice stiffness in the thermodynamic limit, as in Eq. (5.60). The *static* lattice model has a distorted ground state with gapped spin excitations for any non-zero spin-lattice coupling. The magnitude of the strong-coupling response controls the size of the equilibrium lattice distortion and spin-gap, which may be potentially measured in experiments.

## 5.4 Interlayer coupling

Finally, we will use our intuition regarding the similarity between 1D spin chains and the U(1) Dirac QSL to investigate one final potential instability: interlayer coupling. This is also motivated by experiments. All realisations of a 2D triangular lattice QSL studied so far exist within bulk 3D lattices. In 1D, interchain couplings are widely responsible for the breakdown of QSL-like behaviour below an ordering temperature, set by some algebraic function of the interchain coupling strength (Lake *et al.*, 2005).

The multilayer Hamiltonian can be written as a sum over layers  $l$ :

$$\mathcal{H} = \sum_l \left[ \mathcal{H}_l + J_{\text{inter}} \sum_i \vec{S}_{i,l} \cdot \vec{S}_{i,l+1} \right]. \quad (5.79)$$

This is a direct Heisenberg exchange between sites  $i$  in neighbouring layers  $l$  and  $l + 1$ . In this setup, it is an unfrustrated antiferromagnetic coupling between equivalent sites. In direct analogy with 1D, we can treat this coupling in *interlayer mean-field theory* (Giamarchi, 2003; Luo *et al.*, 2022). This ignores fluctuations of the order parameters in adjacent layers, but couples  $\vec{S}_{i,l}$  to  $\langle \vec{S}_{i,l+1} \rangle$ . Each individual layer feels the average of the two adjacent mean-field spin order parameters. This acts as an effective magnetic field

$$\vec{h}_{i,l} = -J_{\text{inter}}[\langle \vec{S}_{i,l-1} \rangle + \langle \vec{S}_{i,l+1} \rangle] = 2J_{\text{inter}}\langle \vec{S}_{i,l} \rangle. \quad (5.80)$$

In the final step, we assumed that the magnetic order in the layers alternates. This assumes that the unfrustrated interlayer interaction leads to Néel order between the layers. We simulate a single-layer interlayer-mean-field Hamiltonian

$$\mathcal{H} = \sum_l \left[ \mathcal{H}_l + \sum_i \vec{S}_{i,l} \cdot \vec{h}_{i,l} \right]. \quad (5.81)$$

Together, Eqns. (5.80) and (5.81) define a self-consistent interlayer mean-field theory.

Beyond this point, we must specify the model and understand its correlations in order to work out the stability to interlayer coupling. In the context of the  $J_1$ – $J_2$  Heisenberg model, we should be particularly concerned about the stability of the liquid state to 120-degree ordering. In this case, the interlayer coupling acts through an effective 120-degree staggered external field. Let us first evaluate the response of monopoles to interlayer coupling. This was studied by Luo *et al.* (2022) in a bilayer model. It is also a natural candidate to cause an instability, since the monopoles are highly relevant gapless excitations. The interlayer mean-field couples to the spin-triplet monopoles  $\mathcal{S}_h = \alpha_S \int d^3x [i h_\alpha(x) \mathcal{S}_\alpha^\dagger(x) + \text{h.c.}]$ , where  $\alpha = 1, 2, 3$ . Given this perturbation, we can calculate the resulting one-point function of the monopole perturbatively in the field. With a finite-temperature regularisation, we derive

$$\langle \mathcal{S}_i^\alpha \rangle = \alpha_S \langle \mathcal{S}_\alpha(y) \rangle = -\alpha_S^2 \int d^3x \frac{h_\alpha}{|x-y|^{2\Delta_\Phi}} = -c\alpha_S^2 T^{2\Delta_\Phi-3} h_\alpha \equiv -B(T) h_\alpha, \quad (5.82)$$

where we have assumed here that  $h_\alpha$  is spatially-independent. Applying the self-consistent definition of the effective field (5.80), we can form a relation between these parameters and the critical (effective) temperature as

$$\langle \vec{S}_l \rangle = [2J_{\text{inter}} B(T)] \langle \vec{S}_l \rangle. \quad (5.83)$$

There are non-trivial solutions with  $\langle \vec{S}_l \rangle \neq 0$  only when  $2J_{\text{inter}} B(T) \geq 1$ . This defines the critical temperature

$$T_c = \left[ 2J_{\text{inter}} c \alpha_\Phi^2 \right]^{1/(3-2\Delta_\Phi)}. \quad (5.84)$$

This has the same scaling as the spin-Peierls temperature (5.42). Looking at this same problem alternatively, it implies an instability to 120-degree ordering upon infinitesimal interlayer coupling. This was a mean-field approach, but Luo *et al.* (2022) showed (in a bilayer limit) that the scaling of the resulting critical coupling is identical beyond this approximation.

Now we will attempt to apply these field-theoretical statements to the lattice model. This was successful in the case of the spin-Peierls instability. As we have seen in Section 2.4, the monopoles appear to contribute little spectral-weight to spin-spin correlation functions. The dynamical response appears to be better described by a model of a gapped spinon bound state mode. In this case, deep in the QSL phase of the  $J_1$ – $J_2$  model, the dominant excitations at  $\mathbf{K}$  are a gapped ‘paramagnon’ mode. We suggest that therefore, the response of the spin model to interlayer coupling will be dominantly that of a gapped paramagnet. Assuming no monopoles are present, we would find that as  $T \rightarrow 0$ , the susceptibility upon applying a staggered field remains finite. In the language above,  $B(T=0) = c_0$ , and so Eq. (5.83) tells us that there will be a non-zero critical interlayer coupling  $J_{\text{inter}}^c = 1/2c_0$ . At zero temperature, the ground state of the gapped paramagnet is stable for  $J_{\text{inter}} < J_{\text{inter}}^c$ .

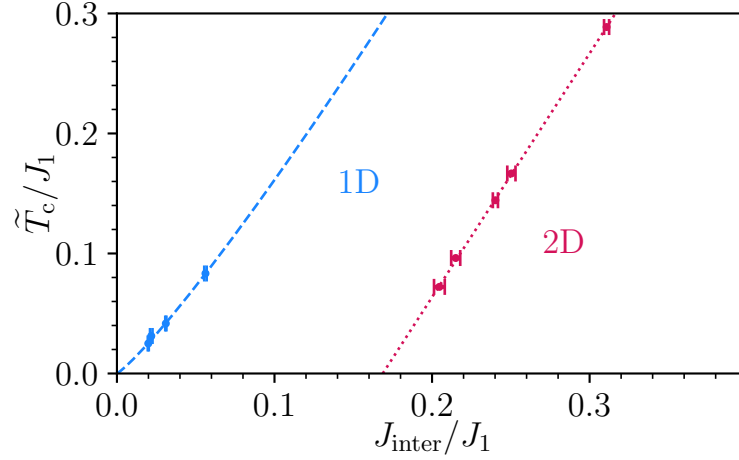


**Figure 5.9:** *Numerical results for the interlayer magnetic ordering temperature in 1D and 2D.* Calculated in the 1D Heisenberg chain and the 2D  $J_1$ - $J_2$  triangular-lattice Heisenberg model. Critical effective temperatures calculated from finite-size scaling  $\tilde{T}/J_1 = L^{-1}$  of the models under static lattice distortions. Results plotted as a function of interlayer coupling strength  $J_{\text{inter}}/J_1$ .

We can proceed again with a numerical treatment in order to see which of these scenarios describes the  $J_1$ - $J_2$  model. We simulate the  $J_1$ - $J_2$  Heisenberg model with a 120-degree staggered in-plane magnetic field using the variational Monte Carlo method (numerical details in Appendix C).

Similar to the spin-Peierls case, we can use the system size as an effective proxy for inverse temperature. In this case we measure the magnitude of induced 120-degree or Néel ordering upon varying the applied staggered field. Fitting the linear regime to extract the amplitude  $B(\tilde{T})$ , we can calculate the  $J_{\text{inter}}^c$  in the same way as for the spin-Peierls case. The results are plotted in Fig. 5.9. The 1D results are best described by a power law (5.84), where we extract the instanton exponent  $\Delta_* = 0.56(5)$ . The 2D results seem incompatible with such a model. The best fit to the data is a straight line, which intercepts the  $\tilde{T} = 0$  axis at  $J_{\text{inter}}^c = 0.169(1)$ . Although the numerical results on stability are wholly compatible with the response of a gapped paramagnet, it is possible that the monopole effects only emerge on much larger length scales. Consequently, we cannot rule a weak-coupling 120-ordering transition with a relative strength on the order  $\mathcal{O}(10^{-2})J_1$ . This is compatible with our analysis of real-space spin-spin correlation functions which were dominated by the spinon-exciton feature. If the stability of the phase is dominated by this lattice-scale mode, we propose that perturbations like hydrostatic pressure could be used to drive this instability. Tuning  $J_2$ , and hence the energy scale of the spinon exciton, could cause an interlayer-driven 120 ordering transition by lowering  $J_{\text{inter}}^c$ .

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## Introduction

In a quantum model of a lattice, the excitations are dynamical quasiparticles called phonons. The previously discussed picture of static distortions, while valid in some limits, could potentially overestimate the tendency to form ordered states. If we are interested in understanding a realistic model of a spin-lattice model, we must include the effect of dynamical quantum phonons. Such dynamics introduces an additional finite energy scale to the system. As such, there is the possibility that the U(1) Dirac QSL may remain stable even at zero temperature if this energy scale is large enough. One can imagine this by considering the effects of letting a distorted lattice oscillate. If this frequency is high enough, it is possible that the spin degrees of freedom see an average of the lattice positions, and the energy gain from dimerising the lattice is washed out.

Even more optimistically for the search for quantum spin liquids, we will discuss the potential of using phonons as a signature of fractionalised behaviour. In a system which remains liquid and avoids ordering, the presence of strong dimer-dimer correlations can still dramatically renormalise the dispersion of the lattice degrees of freedom. This ‘Kohn anomaly’ could in turn be measured in experiment.

This Chapter contains the original work from two manuscripts: Seifert, Willsher, Drescher, Pollmann, and Knolle (2024), and Ferrari, Willsher, Seifert, Valenti, and Knolle (2024a). This builds on the results of the previous Chapter 5 by extending both the field theoretical model and the lattice-scale simulations with a more realistic dynamical model of phonons. We first provide field-theoretic results, then discuss the implications for the phonon’s spectral response and the numerical phase diagram of the  $J_1$ – $J_2$  model in the presence of spin-phonon coupling.

## 6.1 Finite-coupling phase transition

### 6.1.1 Dynamical phonons

Next, we go beyond the assumption of adiabatic distortions by promoting the corresponding relevant components of the distortion field to be dynamical degrees of freedom  $u_a \rightarrow u_a(\tau, \mathbf{r})$ . While we explicitly treat in this section a model of non-dispersive (optical) phonons, we note that this is also an appropriate model for generic phonon bands away from the  $\Gamma$ -point, as we are explicitly interested in small momenta (compared to the inverse lattice spacing) around the finite lattice momentum of the singlet monopoles  $\mathbf{X}_a$ .

We add dynamics for the long-wavelength fluctuations of the  $\mathbf{X}_a$ -displacement modes via a kinetic energy term,  $S_{\text{kin}} = \rho \sum_a |\partial_\tau u_a(\tau, \mathbf{r})|^2$ , where  $\rho$  corresponds to a microscopic

phonon mass density. The physical phonon modes have energy

$$\omega_0^2 \equiv \kappa/\rho \quad (6.1)$$

at the momentum  $\mathbf{X}_a$ . We approximate this as an optical phonon with constant energy (Giamarchi, 2003; Citro *et al.*, 2005), governed by the action

$$S_{\text{ph}}[\vec{u}(\tau, \mathbf{r})] = \int d\tau \int d^2\mathbf{r} \left[ \rho |\partial_\tau \vec{u}(\tau, \mathbf{r})|^2 + \kappa |\vec{u}(\tau, \mathbf{r})|^2 \right], \quad (6.2)$$

$$= \rho \int d^3x u_a^*(x) [\partial_\tau^2 + \omega_0^2] u_a(x). \quad (6.3)$$

The Green's function of the free boson as a function of imaginary frequencies is  $G_{0,u}^{-1}(\omega) = \omega^2 + \omega_0^2$ . For now, this is fully independent of  $\mathbf{q}$  in this approximation. We can then analytically continue to real frequencies by replacing  $i\omega \rightarrow \omega + i\eta$  and then take the limit  $\eta \rightarrow 0$ . We find the (non-interacting) Green's function as a function of real frequency is

$$G_{0,u}(\mathbf{q}, \omega) = \frac{1}{\omega^2 - \omega_0^2}. \quad (6.4)$$

The poles  $\omega = \omega_0$  represent the physical phonon modes with momentum  $\mathbf{X}_a$ . In a realistic model where the phonon bands are dispersive, the stiffness  $\kappa$  and therefore  $\omega_0$  would be  $\mathbf{q}$ -dependent. In the previous Chapter 5, we studied the classical limit of non-dynamical phonons. This can be achieved by taking  $\rho \rightarrow \infty$  with constant  $\kappa$ , and so  $\omega_0 \rightarrow 0$ . We will refer to this as the adiabatic limit below. However, now we will deal with the dynamical case with finite  $\omega_0 > 0$ .

The interacting system has the action

$$S[u_a(x)] = S_{\text{ph}}[u_a(x)] + S_{\text{QED}_3} + S_{\mathcal{D}}[u_a(x)], \quad (6.5)$$

where  $S_{\text{QED}_3}$  is the fixed-point action for QED<sub>3</sub> and  $S_{\mathcal{D}}[u_a(x)]$  is the coupling between spin-singlet monopoles  $\mathcal{D}(x)$  and the lattice. This is given through Eq. (5.21),

$$S_{\mathcal{D}}[u_a(x)] = \int d^3x \left[ u_a(x) \mathcal{D}_a^\dagger(x) + \text{h.c.} \right], \quad (6.6)$$

where we now interpret  $u_a(\tau, \mathbf{r})$  as a dynamical phonon and not a static classical distortion.

Now we have defined the model, we are in a position to investigate how the phonon-monopole coupling affects its spectral properties and stability. To do this, let us start by integrating out the fluctuations of QED<sub>3</sub> perturbatively (Lee *et al.*, 2019). This approach is conceptually similar to our treatment of the coupling between monopoles and the spinon exciton in Section 3.3.2. Working at second order in perturbation theory, we find a correction to the imaginary-time Green's function of the phonon mode  $u_a$ :

$$G_u(\mathbf{q}, \omega)^{-1} = \omega^2 + \omega_0^2 - (g^2/\rho) \langle \mathcal{D}_a^\dagger \mathcal{D}_a \rangle_{\text{QED}_3}(\omega). \quad (6.7)$$

This appears like a self-energy of the phonon due to the intermediate monopole susceptibility. Diagrammatically, we write

$$G_u(\mathbf{q}, \omega) = \text{=====} = \text{=====} + \text{====}\text{~~~~~}\text{=====} + \dots \quad (6.8)$$

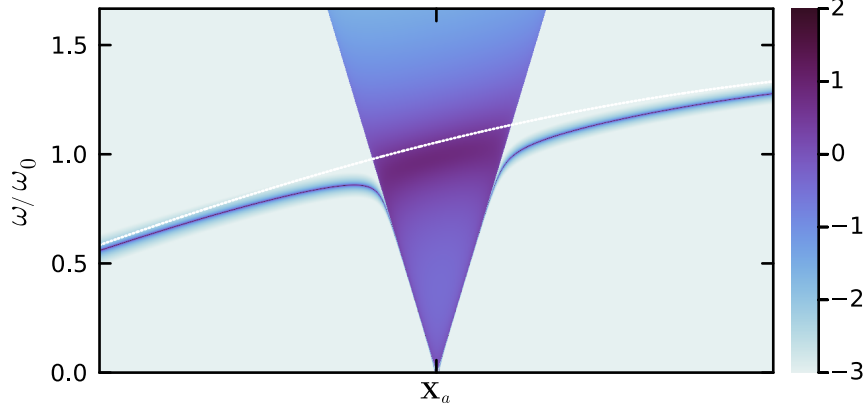


**Figure 6.1: Quantum critical continuum in the phonon selfenergy.** Phonon spectral function  $\log S_u(\mathbf{q}, \omega)$  plotted along the momentum slice between  $\Gamma$  and  $\mathbf{K}_a$ . Spin-phonon coupling is set to  $g = 0.3$ . The phonon spectral function is approximated by extending the interacting phonon propagator  $G_a(\omega) = G(\omega, \mathbf{X}_a)$  to momenta  $\mathbf{X}_a + \mathbf{q}$  given a microscopic model for the bare phonon dispersion  $\omega_0(\mathbf{q})$  (white dashed line).

Continuing to real frequencies, the interacting propagator is

$$G_u(\mathbf{q}, \omega) = \frac{1}{\omega_0(\mathbf{q})^2 - g^2 \rho^{-1} \chi_{\mathcal{D}}(\mathbf{q}, \omega) - \omega^2} \quad (6.9)$$

where we take the bare phonon dispersion  $\omega_0(\mathbf{k})^2 = \kappa_{\mathbf{k}}^2 / (\rho |\mathbf{k}|^2)$ , which is valid close to  $\mathbf{X}_a$  where it remains gapped. The phonon quasiparticle dispersion  $\omega_a$  becomes renormalised and is determined by solutions to the implicit equation

$$\omega^2 = \omega_0^2 - g^2 \rho^{-1} \chi'_{\mathcal{D}}(\omega, \mathbf{q}), \quad (6.10)$$

where  $\chi'$  is the real part of the VBS susceptibility

$$\chi'_{\mathcal{D}}(\omega, \mathbf{q}) \equiv \text{Re} \langle \mathcal{D}_a^\dagger \mathcal{D}_a \rangle_{\text{QED}_3}(\omega, \mathbf{X}_a + \mathbf{q}) = c \cos[\pi(3/2 - \Delta_\Phi)] \frac{1}{|\omega^2 - \mathbf{q}^2|^{\Delta_\Phi}}. \quad (6.11)$$

The power-law divergence as  $\omega \rightarrow 0$  implies a breakdown of the quasiparticle picture of the phonon. Instead, around the momenta  $\mathbf{X}_a$ , the phonon spectral function will display a quantum-critical continuum, a signature of deconfinement in the spin sector of the system (Lee *et al.*, 2019). To show this explicitly, we define the phonon spectral function. It is given in terms of the imaginary part of the phonon Green's function as  $S_u(\mathbf{q}, \omega) = 2 \text{Im} G_u(\mathbf{q}, \omega + i\eta)$ . In the non-interacting case, it only shows a quasiparticle pole at  $\omega = \omega_0(\mathbf{q})$ . Fig. 6.1 shows the second-order perturbative result, calculated from Eq. (6.9) at zero temperature  $T = 0$ .

We discussed the spectral signatures of the U(1) Dirac QSL in Chapter 3, and compared our predictions to inelastic neutron scattering data in the materials KYbSe<sub>2</sub> and NaYbSe<sub>2</sub> in Chapter 4. Both experimental results and the competing theoretical models all have low-energy modes around the  $\mathbf{K}$  point, which makes it particularly hard to distinguish the nature of the ground state. We suggest that progress may be made by instead looking at the

$\mathbf{X}$  points, at half of the wavevector. In other models, there are no low-energy signatures expected here. The spin-singlet monopoles of the U(1) Dirac QSL is unique for producing a critical continuum through the hybridisation with phonons.

What happens as we take the limit  $\omega_0 \rightarrow 0$ ? The results from the static model suggest there should be a spin-Peierls instability upon infinitesimal coupling. If the second term on the right-hand side of (6.10) is much smaller than first term, one can iteratively substitute (the square-root of) the left-hand side for  $\omega$  on the right-hand side, generating an order-by-order expansion. To leading order, we thus obtain

$$\omega^2 \approx \omega_0^2 - g^2 \rho^{-1} \chi'_D(\omega_0) + \dots \quad (6.12)$$

Using  $\chi'_a(\omega) \sim \omega^{-(3-2\Delta_\Phi)}$ , one obtains that the phonon dispersion is renormalised down to zero energy  $\omega = 0$  when  $\omega_0^2 \sim g^2 \rho^{-1} \omega_0^{-(3-2\Delta_\Phi)}$ . Therefore, the perturbative treatment of (6.10) breaks down above the critical coupling strength

$$\lambda_c = g_c^2 / \kappa \sim \omega_0^{3-2\Delta_\Phi} \quad \text{when } T = 0. \quad (6.13)$$

This defines the critical spin-Peierls coupling  $\lambda_c > 0$  at finite phonon frequency and zero temperature. This scaling law tells us that there may be a regime for small coupling  $g < g_c$  where the spin liquid is the stable ground state. The critical coupling depends analytically on the phonon frequency (6.13). We will discuss this further in the rest of this section.

### 6.1.2 Kohn anomaly

What is the behaviour of the phonon spectrum for finite temperatures  $T \gg \omega_0$ ? We will show that there is a temperature-dependent renormalisation of the phonon dispersion, and no breakdown of the quasiparticle picture. To describe this in the above framework, we have to understand how the monopole susceptibility behaves at finite temperature. For finite temperatures, the monopole susceptibility (6.11) is cut off. Scaling arguments tell us that the susceptibility for  $\omega \ll T$  is  $\omega$ -independent and scales as (Witczak-Krempa, 2015a)

$$\chi'_D(\omega, T) \sim T^{-(3-2\Delta_\Phi)}. \quad (6.14)$$

From (6.10) it follows that the phonon frequency is shifted downwards by a temperature-dependent constant

$$\omega^2 = \omega_0^2 - g^2 \rho^{-1} T^{-(3-2\Delta_\Phi)}. \quad (6.15)$$

We conclude that there exists a ‘Kohn anomaly’ in the phonon dispersion (Kohn, 1959; Luther and Peschel, 1974). This anomaly in the phonon branch manifests as a discontinuity in the derivative at zero temperature. At and close to the wavevector  $\mathbf{X}_a$ , there will be a characteristic softening of the otherwise gapped phonon with energy  $\omega_0$  depending analytically on temperature as  $T^{2\Delta_\Phi-3}$ .

In our model, the Kohn anomaly is more extreme than simply a kink in the quasiparticle dispersion as seen in other 2D materials (Zhao *et al.*, 2020). We see that the mode goes to zero energy and hybridises with the monopole continuum as  $T \rightarrow 0$ . This behaviour, and the resulting spin-Peierls instability, have only been predicted before in one-dimensional systems. Importantly, this theoretical prediction in two dimensions provides an experimentally

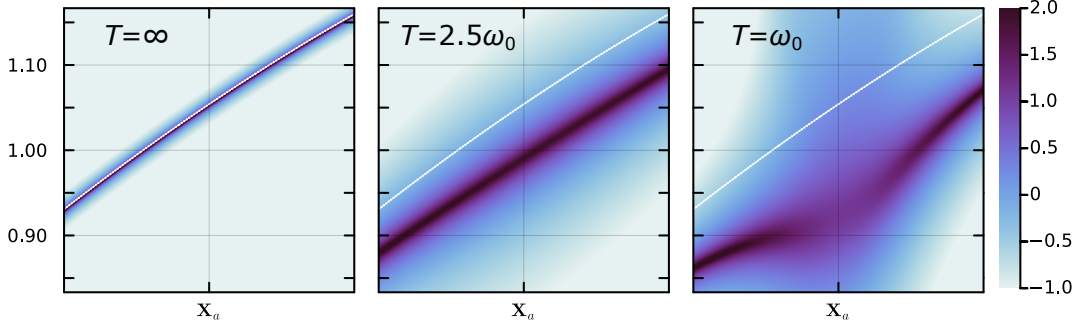


**Figure 6.2:** *Kohn anomaly of the phonon dispersion due to critical monopole fluctuations.* Phonon spectral function  $\log S_u(\mathbf{q}, \omega)$  for various temperatures along the momentum slice between  $\Gamma$  and  $\mathbf{K}_a$ . Spin-phonon coupling is set to  $g = 0.3$ .

accessible signature of a proximate U(1) Dirac QSL through the monopole-phonon couplings. Detailed measurement of low-energy phonon modes might provide new signatures in the search for fractionalised 2D quantum spin liquids. Moreover, a careful study of the divergent nature of the phonon continuum or the temperature dependence of the phonon anomaly, would allow measurement of the monopole scaling dimension. This would provide a quantitative measurement of critical exponents which may be compared to analytical and numerical studies of the QED<sub>3</sub> CFT.

In Figure 6.2, we plot the phonon spectral function in the large- $T$  regime which shows a temperature-dependent softening of the phonon mode towards zero at the spin-Peierls temperature. This is accompanied by the emergence of a sharp divergent continuum of excitations which blurs with the mode at low energies. We perform this calculation by making a simple scaling Ansatz for the monopole susceptibility function

$$\chi_{\mathcal{D}}(\omega, \mathbf{k}) = T^{2\Delta_{\Phi}-3} \Phi(\omega/T, |\mathbf{q} - \mathbf{X}_a|/T). \quad (6.16)$$

The universal scaling function  $\Phi(x, y)$  is unknown, but we may constrain it in the high-temperature limit (Sachdev and Ye, 1992; Sachdev, 2011; Witczak-Krempa, 2015b). For illustrative purposes, we assume a heuristic form similar to the expansion obtained by Sachdev and Ye (1992)

$$\Phi(x, y) = \frac{1}{(C + x^2 - y^2 + \dots)^{3/2-\Delta_{\Phi}}}, \quad (6.17)$$

where we choose  $C = 1 - 0.3i$ . This reproduces the high-temperature limit of Eq. (6.14). The exact form of this universal scaling function must be extracted from numerical or experimental studies.

We can now investigate the limit  $T \rightarrow 0$  with  $\omega_0$  constant. In this regime, the above scaling form (6.14) for  $\chi_{\Phi}$  becomes exact, since  $T \ll \omega_0$ . We can find an explicit solution to Eq. (6.14) for the mode condensation, given again by  $\omega = 0$ . This is solved when  $\omega_0^2 \sim g^2 \rho^{-1} T^{-(3-2\Delta_{\Phi})}$ , which precisely recovers the critical scaling of the static model

$$\lambda_c = g_c^2 / \kappa \sim T^{3-2\Delta_{\Phi}} \quad \text{when } \omega_0 = 0. \quad (6.18)$$

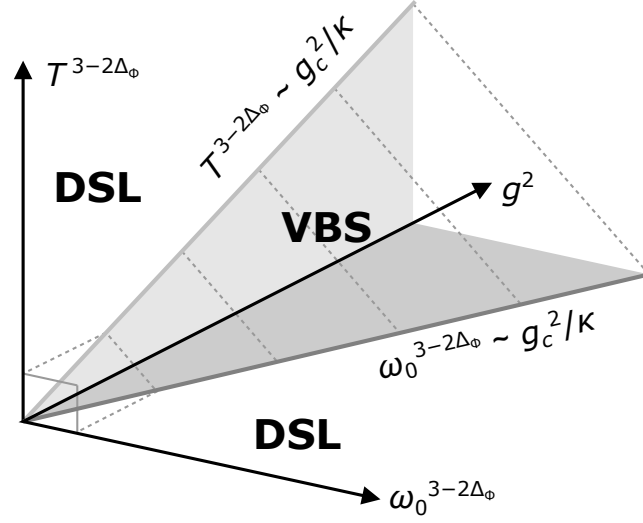


**Figure 6.3:** *Scaling phase diagram of the U(1) Dirac QSL with dynamical phonons.* Transition between the U(1) Dirac QSL, and 12-site VBS order. Phase diagram as a function of coupling  $g$ , temperature  $T$  and frequency  $\omega_0$ . The shaded regions indicate the unstable parameter regimes, based on the finite-temperature calculation in the classical ( $\omega_0 \rightarrow 0$ ) limit and the zero-temperature result for dynamical phonons ( $\omega_0 > 0$ ).

Reinterpreting this equation to predict the critical temperature as a function of coupling strength  $g_\Phi$ , this defines the spin-Peierls temperature  $T_{\text{SP}}$ , as in Eq. (5.42). Taking these two results Eqns. (6.13) and (6.18), we produce the phase diagram, shown in Fig. 6.3. The coupling-dependence of the two limits,  $T \rightarrow 0$  and  $\omega_0 \rightarrow 0$ , is seen to correspond. The phonon frequency  $\omega_0$  sets an effective temperature scale  $T \sim \omega_0$  which determines a correlation length for critical fluctuations in the Dirac QSL. We highlight this on the figure with the dashed lines, even though the exact phase boundary is not fixed by this scaling analysis.

### 6.1.3 Adiabatic and antiadiabatic limits

We can now take another perspective on the same problem: Instead of perturbatively integrating out the fluctuations of  $\text{QED}_3$ , we will integrate out the fluctuating phonon. This will let us analyse the stability within the framework of the  $\text{QED}_3$  CFT, introduced in Chapter 2. We take the Fourier transform of the phonon Green's function (6.2). In real-space (and imaginary time), we get

$$\langle u_a(x) u_b^*(y) \rangle = \delta_{a,b} G(x-y) = \delta_{a,b} \delta^{(2)}(\mathbf{r}_x - \mathbf{r}_y) \frac{1}{2\omega_0} e^{-\omega_0 |\tau_x - \tau_y|}. \quad (6.19)$$

As long as the phonons remain gapped  $\omega_0 > 0$ , these degrees of freedom can be integrated out exactly. The phonon then mediates a retarded interaction between  $\text{QED}_3$  monopoles,

$$S_{\mathcal{DD}} = -\frac{g^2}{\rho} \int d^3x d^3y \mathcal{D}_\alpha^\dagger(x) G(x-y) \mathcal{D}_\alpha(y). \quad (6.20)$$

We have used the fact that the phonon Green's function is diagonal in the valley index  $\alpha$  to simplify this expression. The total action is given by  $S = S_{\text{QED}_3} + S_{\mathcal{DD}}$ . We can understand the effect of this interaction in two limits:  $\omega_0 \rightarrow 0$  and  $\omega_0 \rightarrow \infty$ . We will call these the *adiabatic* and *antiadiabatic* limits respectfully.

In the adiabatic limit  $\omega_0 = 0$ , the monopole-monopole interaction in (6.20) becomes temporally non-local. The modes become correlated at large separations, which leads to the spin-Peierls instability at infinitesimal couplings (as per our treatment in Chapter 5). To make the statement more concrete, substitute (6.19) into  $S_{\mathcal{DD}}$  to get the following limiting adiabatic behaviour

$$S_{\mathcal{DD}}^{\omega_0 \rightarrow 0} \sim -\frac{g^2}{\rho\omega_0} \int d^2\mathbf{r} \, d\tau_x \int_0^{1/\omega_0} d\tau_y \, \mathcal{D}_\alpha^\dagger(\tau_x, \mathbf{r}) \mathcal{D}_\alpha(\tau_y, \mathbf{r}). \quad (6.21)$$

This shows that as  $\omega_0 \rightarrow 0$ , the effective monopole-monopole coupling becomes non-local in time. We can deal with this effect most simply by employing a mean-field theory of this monopole-monopole interaction. We decouple the interaction as follows:

$$\mathcal{D}_\alpha^\dagger(\tau_x) \mathcal{D}_\alpha(\tau_y) = \langle \mathcal{D}_\alpha^\dagger \rangle \mathcal{D}_\alpha(\tau_y) + \mathcal{D}_\alpha^\dagger(\tau_x) \langle \mathcal{D}_\alpha \rangle - |\langle \mathcal{D}_\alpha \rangle|^2. \quad (6.22)$$

The time-independent parameter  $\langle \mathcal{D}_\alpha^\dagger \rangle$  appears as an effective displacement field

$$S_{\mathcal{DD}}^{\omega_0 \rightarrow 0} \sim -\frac{g^2}{\rho\omega_0^2} \int d^3x \left[ \langle \mathcal{D}_\alpha^\dagger \rangle \mathcal{D}_\alpha(x) + \text{h.c.} \right]. \quad (6.23)$$

Taking  $\omega_0^2 \rightarrow 0$  with  $\kappa = \rho\omega_0^2$  fixed, we see this contribution remains finite.

There are solutions of Eq. (6.23) with condensed monopoles for any finite  $\lambda = g^2/\kappa > 0$ . By the same arguments as in Chapter 5, the ordered states with finite  $\langle \mathcal{D}_\alpha^\dagger \rangle \neq 0$  will lower the energy, representing an instability of the spin liquid. Because this instability happens exactly at zero coupling, we see it is the manifestation of the spin-Peierls instability from before (just now in a model with no explicit field representing the lattice, which we have integrated out). In both perspectives, we neglect the dynamics of the lattice. Here, we do this by assuming a constant monopole-monopole interaction (Luo *et al.*, 2022), ignoring all retardation effects of the interaction which are due to the finite value of  $\omega_0$ . In the previous study this was by explicitly only considering static distortion fields  $u(\mathbf{x})$ . To show how these approaches produce the same result, we can use Eq. (6.21) as the starting point for a brief finite-size analysis. Calculating the expectation value of this term, we find an IR-divergent expression. Regulating this with a finite size  $L$  we see<sup>1</sup>

$$\langle S_{\mathcal{DD}}^{\omega_0 \rightarrow 0} \rangle \sim -\frac{g^2}{\kappa} \int d^2\mathbf{r} \, d\tau \, \langle \mathcal{D}_\alpha^\dagger(\tau, \mathbf{r}) \mathcal{D}_\alpha(0, \mathbf{r}) \rangle \sim -\frac{g^2}{\kappa} L^{3-2\Delta_\Phi}. \quad (6.24)$$

By requiring that this correction to the action converges to an order-1 constant, we recover the static result for the scaling of the critical coupling

$$\lambda_c = g_c^2/\kappa \sim L^{2\Delta_\Phi-3}. \quad (6.25)$$

<sup>1</sup>Here we use an SO(3) symmetric regulator for convenience.

In the opposite, antiadiabatic, limit  $\omega_0 \rightarrow \infty$  (with  $\kappa = \rho\omega_0^2$  constant), the Green's function (6.19) becomes purely local

$$G(x-y) = \frac{1}{2\omega_0^2} \delta^{(3)}(x-y). \quad (6.26)$$

Substituting into the above, we write the effective monopole-monopole interaction as follows

$$S_{\mathcal{D}\mathcal{D}}^{\omega_0 \rightarrow \infty} = -\frac{g^2}{2\kappa} \int d^3x \mathcal{D}_\alpha^\dagger(x) \mathcal{D}_\alpha(x). \quad (6.27)$$

This is identical to the spin-triplet monopole interaction of Eq. (3.75) which was produced by integrating out the gapped spinon exciton. The only difference is that this interaction (6.27) is in the spin-singlet channel. We suggest that the resulting four-fermion operators (produced by the OPE) are of the form  $(\bar{\psi}\tau^j\psi)^2$ . Once again, this interaction is *irrelevant*. As such, the Dirac spin liquid will be stable in the  $\omega_0 \rightarrow \infty$  limit against spin-lattice coupling. In fact, the transition only occurs at infinite coupling  $g_\Phi^2/\kappa \rightarrow \infty$  here.

How does the critical coupling scale with  $\omega_0$  in the antiadiabatic limit? The Green's function (6.19) has an exponential form, meaning interactions  $|\tau_x - \tau_y| \geq 1/\omega_0$  will be exponentially suppressed. When this effective cutoff scale is less than the UV cutoff  $a$  (we can think of this as the lattice spacing), the monopole interaction becomes local [as in Eq. (6.27)]. The result is an irrelevant interaction. However when the interaction length scale is larger than the lattice cutoff, the retarded monopole-monopole interaction is relevant. We can now perform a scaling analysis to predict the scaling of the critical coupling strength in this case. Starting with an interaction

$$S_{\mathcal{D}\mathcal{D}} = -\frac{g^2}{2\rho\omega_0} \int d^2\mathbf{r} d\tau \int_0^{1/\omega_0} d\tau' \mathcal{D}_\alpha^\dagger(\tau, \mathbf{r}) \mathcal{D}_\alpha(\tau + \tau', \mathbf{r}), \quad (6.28)$$

we rescale all coordinates  $x \rightarrow x/(a\omega_0)$  to get

$$S_{\mathcal{D}\mathcal{D}} = -\frac{g^2}{2\rho\omega_0^{5-2\Delta_\Phi}} a^{2\Delta-5} \int d^3x \mathcal{D}_\alpha^\dagger(x) \mathcal{D}_\alpha(x). \quad (6.29)$$

This form of the monopole interaction is irrelevant, and the spin liquid is stable as long as we do not take the coupling to be infinite. Requiring that the coupling does not diverge defines the critical coupling strength

$$\lambda_c = g_c^2/\rho\omega_0^2 = \omega_0^{3-2\Delta_\Phi}. \quad (6.30)$$

This agrees with the form we derived using the self-consistent perturbative solution to the phonon Green's function, Eq. (6.13). We include a third, perturbative calculation of the critical phonon frequency in Appendix B.

## 6.2 Numerical phase diagram

### Method

In this Section, we calculate the phase diagram of the spin-Peierls transition as a function of phonon frequency  $\omega$  and assess how the static instability is dampened or resolved. For

this purpose, we turn again to the numerical variational Monte Carlo method to study the  $J_1$ - $J_2$  Heisenberg model on the triangular lattice. Here, we use a model in which lattice distortions are treated quantum mechanically. The combined Hamiltonian is

$$\mathcal{H} = \mathcal{H}[\mathbf{u}_i] + \sum_i \left( \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} m \omega_0^2 \mathbf{u}_i^2 \right), \quad (6.31)$$

where  $\mathbf{u}_i$  and  $\mathbf{p}_i$  are displacement and momentum operators of uncoupled harmonic oscillators, i.e. Einstein phonons. The spins and phonon degrees of freedom live on a triangular lattice. They are coupled through  $\mathcal{H}[\mathbf{u}_i]$ , which is taken as the Heisenberg spin Hamiltonian on a distorted lattice, Eq. (5.66), with  $J_2/J_1 = 1/8$ .

We pursue a full quantum treatment of the Hamiltonian (6.31), by means of a recently developed VMC approach. The variational Ansätze take the form  $|\Psi_{\text{sp}}\rangle = \mathcal{J}_{\text{sp}} |\Psi_{\text{p}}\rangle \otimes |\Psi_{\text{s}}\rangle$ , where  $|\Psi_{\text{s}}\rangle$  is a Gutzwiller-projected fermionic state,  $|\Psi_{\text{p}}\rangle$  is a phonon coherent state describing lattice distortions, and  $\mathcal{J}_{\text{sp}}$  is a spin-phonon Jastrow factor (Ferrari *et al.*, 2020, 2021, 2024b). In contrast to the case of static distortions, we do not impose a specific phonon mode, but we instead perform unbiased optimisations of the variational state to find the lowest energy distortion. Further details about the VMC method are provided in Appendix C.

When the spin-phonon interaction is turned on, we allow the variational state to (potentially) gain energy by creating lattice distortions. Concretely, we perform an unbiased search of the possible instabilities towards lattice distortions, by considering different supercells which can accommodate different patterns of sites displacements (Ferrari *et al.*, 2024b). We consider different shapes and sizes, up to a maximum of 24 sites. This approach enables an unbiased exploration of various potential Peierls orders. These supercells determine the periodicity of the wavefunctions  $|\Psi_{\text{p}}\rangle$  and  $|\Psi_{\text{s}}\rangle$ , and we optimise all variational parameters independently on each site.

## Results

The first important observation of our analysis is that for small values of the spin-phonon coupling  $g$ , the system remains in the DSL phase and no distortions are observed. Thus, the spin liquid state proves to be stable to the Peierls mechanism when the quantum nature of lattice distortions is accounted for. On the other hand, for spin-phonon interactions larger than a certain critical value  $g_c$ , we observe a phase transition towards the 12-site VBS order associated with the  $\mathbf{X}_\alpha$  phonon mode.

Similarly to what has been previously discussed in the static limit, also here the signs of the hopping parameters defining the optimal  $|\Psi_{\text{s}}\rangle$  state maintain the structure of the  $\pi$ -flux Ansatz. Their absolute values break the translational symmetry of the triangular lattice and introduce a gap. We estimate the critical point  $g_c$ , as a function of the phonon frequency  $\omega$ , by comparing the variational energy of the VBS state to the one of a DSL spin-phonon state in which only the Jastrow factors are optimised, while the distortion parameters are set to zero for all sites and the  $\mathcal{H}_0$  Hamiltonian is that of the pristine DSL Ansatz. The critical couplings  $g_c$  as a function of  $\omega_0$  are shown for varying system sizes  $L$  in Fig. 6.4(a). The coupling strength  $g$  is understood in units of  $\sqrt{J_1 m}$ . Firstly, note that as we take the adiabatic limit  $\omega \rightarrow 0$  the critical coupling approaches zero linearly (with an  $L$ -dependent

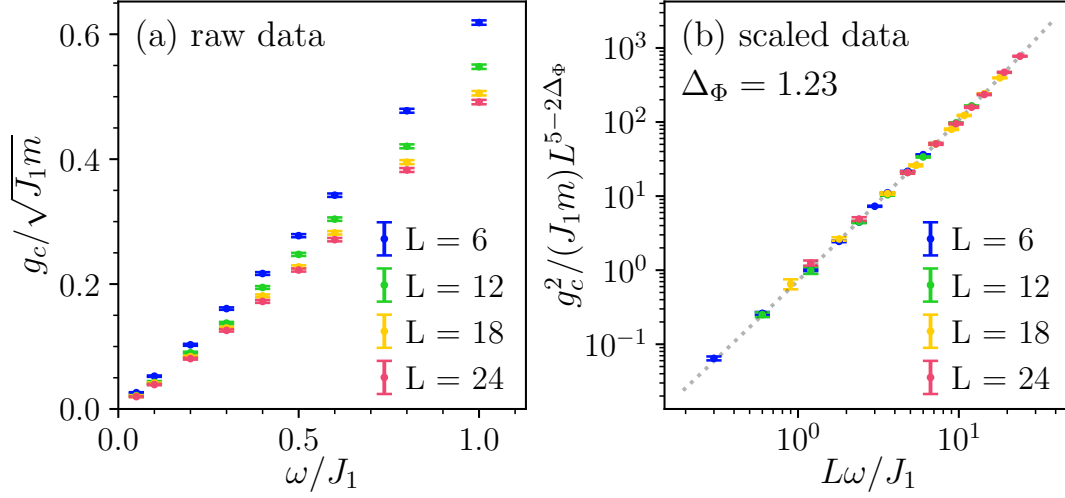


**Figure 6.4:** *Critical coupling strength  $g_c$  of the  $U(1)$  Dirac spin liquid with dynamical phonons.* (a) Measured critical coupling strength  $g_c^2/m$  as a function of phonon frequency  $\omega$  and linear system size  $L$ . (b) Data collapse, produced by plotting  $g_c^2/(J_1 m) L^{5-2\Delta_\Phi}$  against  $L\omega/J_1$ .

coefficient), in agreement with our static results that find an instability here. That is, the static critical coupling is zero  $g_c(\omega = 0) = 0$ . We observe a deviation from the linear trend for larger  $\omega$ . In order to capture the system-size dependence in this strong-coupling regime, we employ another scaling Ansatz.

In the field theoretic description of the model, dynamical phonons can be integrated-out exactly to leave an effective retarded interaction between monopoles, Eq. (6.20). This has an effective coupling constant  $\eta = g_\Phi^2/(J_1 m)$  with the field-theoretic scaling dimension  $d + 2 - 2\Delta_\Phi$ . To make progress in interpreting our numerical results, we make a scaling Ansatz for the *critical* lattice-scale coupling strength  $g_c^2/m$  at which the transition occurs. This is a function only of the phonon frequency and the finite size

$$\eta_c(\omega_0, 1/L) = [g_c^2/m](\omega_0, 1/L). \quad (6.32)$$

We constrain under rescaling  $x \rightarrow bx$ , finding

$$\eta_c(\omega, 1/L) \rightarrow \eta_c(b^{-1}\omega_0, 1/bL) = b^{-(5-2\Delta_\Phi)} \eta_c(\omega_0, 1/L). \quad (6.33)$$

Choosing  $b = L^{-1}$  we recover

$$L^{5-2\Delta_\Phi} \eta_c(\omega_0, 1/L) = \eta_c(\omega_0 L, 1) \equiv \tilde{\mathcal{G}}(\omega_0 L), \quad (6.34)$$

where  $\tilde{\mathcal{G}}(x)$  is a universal scaling function. A scaling collapse is achieved by plotting  $\eta_c L^{d+2-2\Delta_\Phi}$  against  $L\omega/J_1$ . Our Ansatz for the critical coupling  $\eta_c$  as a function of  $\omega/J_1$  and  $1/L$  in  $d = 2 + 1$  reads

$$\eta_c(\omega/J_1, 1/L) = g_c^2/(J_1 m) = L^{2\Delta_\Phi-5} \tilde{\mathcal{G}}(L\omega_0/J_1), \quad (6.35)$$

We can now constrain the form of this scaling function using the two limiting calculations performed in the last Section, namely Eqs. (6.30) and (6.25). In the large-parameter regime  $x \rightarrow \infty$ , we have  $\tilde{\mathcal{G}}(x) = a_\infty x^{5-2\Delta_\Phi}$  and so the  $L$ -dependence cancels out  $\eta_c = a_\infty \omega_0^{5-2\Delta_\Phi}$ . Using the relation that  $\lambda = g^2/K = \eta/\omega_0^2$ , we find that this implies

$$\lambda_c = a_\infty \omega_0^{3-2\Delta_\Phi} \quad \text{when } L \rightarrow \infty. \quad (6.36)$$

In the small-parameter limit  $x \rightarrow 0$ , the scaling form goes as  $\tilde{\mathcal{G}}(x) = a_0 x^2$  and so  $\eta_c = a_0 L^{2\Delta_\Phi-3} \omega_0^2$ . Once again using  $\lambda = \eta/\omega_0^2$ , we may write

$$\lambda_c = a_0 \tilde{T}^{3-2\Delta_\Phi} \quad \text{when } \omega_0 \rightarrow 0, \quad (6.37)$$

which defines the critical coupling strength as a function of  $\tilde{T} = 1/L$ .

In the 2D case considered here, we find the best collapse for  $\Delta_\Phi = 1.23(3)$ , as shown in Fig. 6.4(b). While no closed analytical expression for the full scaling form is available, we find that the whole range of the collapsed data is well described by the heuristic fit

$$\tilde{\mathcal{G}}(x)_{\text{fit}} = a_0 x^2 + a_\infty x^{5-2\Delta_\Phi} \quad (6.38)$$

with parameters  $a_0 = 0.58(2)$ ,  $a_\infty = 0.138(5)$  when  $\Delta_\Phi = 1.23(3)$ . This reproduces the expected asymptotic regimes and interpolates between them, implicitly defining an effective temperature as a function of  $\omega_0$  for a given coupling strength  $\eta$ . This fit is shown as a dotted line in Fig. 6.4. Here, the continuous line is implicitly defined through

$$\lambda = g_c^2/(m\omega^2) = \tilde{\mathcal{G}}(\omega/\tilde{T})_{\text{fit}}/\omega^2 = a_0 \tilde{T}_c^{3-2\Delta_\Phi} + a_\infty \omega^{3-2\Delta_\Phi}, \quad (6.39)$$

for various  $\lambda$ . The phase boundary  $\tilde{T}_c(\omega)$  for  $0 < \omega < \omega_c$  is plotted in Fig. 6.5 using this fit function for a given  $\lambda = 0.3$ . Taking the limit  $\omega_0 \rightarrow 0$  recovers the static model. Recasting Eq. (6.37) as a critical temperature for a given constant, we derive the spin-Peierls temperature  $\tilde{T}_{\text{SP}}/J_1 \approx 2.72 \lambda^{1.85}$ . This calculation is fully independent of the static results shown in Fig. 5.7, but the results are compatible up to uncertainties. In the large-parameter regime  $\tilde{T} \rightarrow 0$ , we similarly extract the critical frequency  $\omega_c/J_1 \approx 39 \lambda^{1.85}$ . Below this point, the  $\tilde{T} = 0$  ground state is spin-Peierls ordered. In Fig. 6.5 these critical points  $\tilde{T}_{\text{SP}}$  and  $\omega_c$  are plotted for  $\lambda = 0.3$ .

## 6.3 Discussion

Within the stable Dirac spin liquid, a monopole-phonon coupling is responsible for a Kohn anomaly visible in the phonon spectrum, which may provide insights into the critical correlations of a Dirac QSL, similar to elastic signatures of quantum critical points (Weickert *et al.*, 2010). We further suggest that the singular response of the Dirac QSL to *externally* induced lattice displacements, in particular via strain, may provide a fruitful avenue for experimental characterisation. We hope that a better understanding of the stability of QSLs with respect to coupling to phonons or structural disorder will help for the eventual discovery of these enigmatic quantum liquids in real materials.

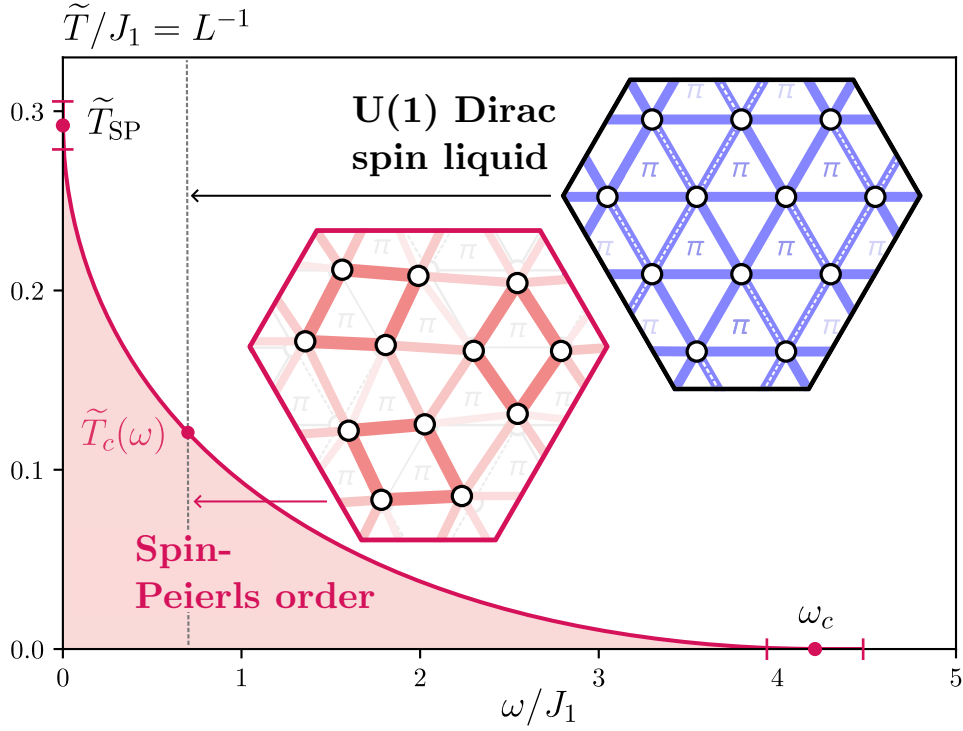


**Figure 6.5:** *Phase diagram of the frustrated triangular lattice Heisenberg model coupled to dynamical phonons* with energy  $\omega$ , for fixed spin-lattice coupling  $\lambda = 0.3$ . Below  $\omega_c$ , we measure a finite-temperature phase transition  $\tilde{T}_c(\omega)$  from the U(1) Dirac spin liquid to spin-Peierls order (i.e., simultaneous valence bond solid order and lattice distortion). We use a variational method, where the spin wave function in the liquid regime is the fermionic state with alternating 0 and  $\pi$  fluxes. The strengths of the  $\langle S_i^z S_j^z \rangle$  correlations of nearest-neighbours are shown in the insets through the thickness/shading of the bonds. Finite-temperature responses are inferred from the finite-size behaviour of the system. We find that a conformal scaling Ansatz well describes the scaling of critical temperature, using which we measure the scaling dimension of monopoles  $\Delta_\Phi = 1.23(2)$ .

By studying this model coupled to phonons in the full quantum regime, we confirm that the spin-Peierls instability is relevant in 2D. We show numerically that the transition temperatures are suppressed in the regime of large phonon frequencies. Since all recent triangular lattice Heisenberg candidate materials rely on rare-earth magnetism, the relevant exchange energy scales are typically lower than for the materials considered in 1D spin-chains. As an example,  $J_1$  in NaYbSe<sub>2</sub> is on the order of 6 K, an order of magnitude lower than CuGeO<sub>3</sub> with  $J = 88$  K (Hase *et al.*, 1993). The phonon scales in this system are correspondingly much larger relative to  $J_1$ , on the order of  $\omega_0/J_1 \approx 10$ . This has potentially significant implications for the stability. We show that in this highly non-adiabatic (high energy) phonon regime, the gapless U(1) Dirac state will be stable up to large (dimensionless) spin-phonon couplings on the order of  $\lambda = 0.5$ – $1$ . If the spin-lattice coupling were large enough to cause an instability, then the transition temperature would be anomalously low. For  $\lambda$  just greater than the critical temperature, the transition temperature is suppressed  $T_c \ll T_{\text{SP}} \sim \lambda_c^{1.85}$ . This tells us that the critical temperature towards an ordered VBS state would be suppressed down to very low temperatures. Turning again briefly to the experimental results of Section 4.1, we highlight the ultra-low temperature feature seen in the spin susceptibility of NaYbSe<sub>2</sub>. If this is the signature of a gap opening, then it would be potentially compatible with the picture of an ultra-low temperature spin-Peierls instability.

It remains important to search for signs of lattice symmetry breaking in candidate materials. If a low-temperature spin-Peierls ordering transition is measured, the ground-state symmetry and critical properties would serve as a distinctive signature of an underlying U(1) DSL state. This would manifest as symmetry breaking to a gapped state with a 12-site unit cell. If such a signal is seen in experiment, then it would be a sign of proximate Dirac spin liquid behaviour. Even if unstable in the ground state, these materials would allow us to probe universal properties of QED<sub>3</sub> through their spectral properties at finite temperature.

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# Spin-Peierls instability of deconfined quantum criticality

7

## Introduction

Deconfined quantum criticality (DQC) was originally proposed (Senthil *et al.*, 2004a,b; Senthil, 2023) as a continuous transition on the square lattice between two ordered states: an antiferromagnetic Néel state and a valence bond solid (VBS). Such a non-fine-tuned continuous transition between two phases that break independent distinct symmetries is forbidden in the Landau paradigm. Instead, this model shows a generally second order transition on the square lattice, as is shown in Fig. 7.1. The scenario of DQC relies on the fractionalisation of constituent degrees of freedom into spinon excitations interacting with emergent gauge fields which are deconfined *at the critical point*. We will see that we can view it as an unstable spin liquid, which acts to precipitate competing orders. In this way, it is closely related to the Dirac spin liquid that has been the focus of this Thesis so far.

While initially studied in the context of quantum magnets, several other systems have been proposed to possibly exhibit DQC (Christos *et al.*, 2020; Khalaf *et al.*, 2021; Liu *et al.*, 2022; Wang *et al.*, 2021; Liu *et al.*, 2019; Christos *et al.*, 2024). More generally, deconfined quantum critical points (DQCPs) are understood as a powerful tool to organise competing

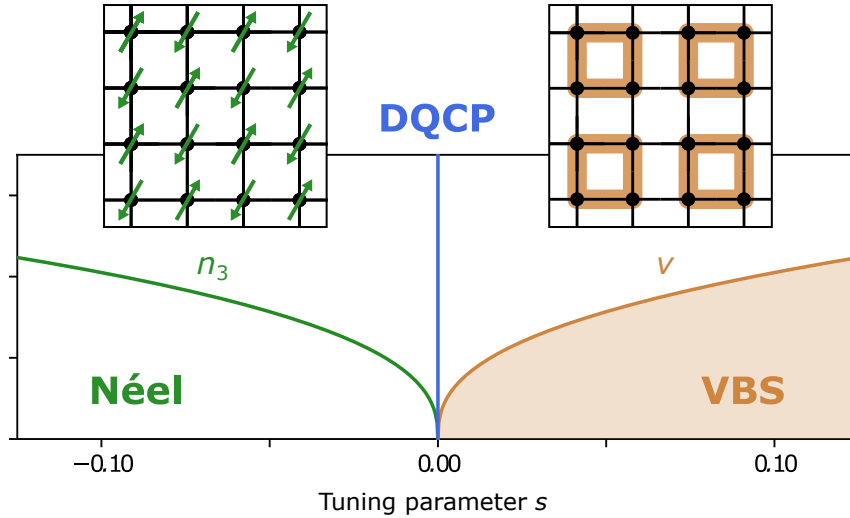


**Figure 7.1:** *Deconfined quantum critical transition on the square lattice.* Second order transition between non-compatible Néel and VBS orders, as predicted by Senthil *et al.* (2004a,b).

phases and their transitions (Nikolaenko *et al.*, 2023; Zhang and Sachdev, 2020). While significant progress has been made in identifying low-energy field theories that may describe deconfined quantum critical points and their dualities (Wang *et al.*, 2017), evidence for its realisation in a microscopic system is still sought for. Firstly on the numerical side: Several salient features of DQC have been observed in simulations of microscopic models or appropriate lattice-regularised field theories, but recent works cast doubt on a scenario of a truly continuous transition and instead point towards weakly first-order behaviour, the origin of which currently being under debate (Nahum *et al.*, 2015a; Poland *et al.*, 2019; Ma and Wang, 2020; Nahum, 2020; D’Emidio *et al.*, 2023; Takahashi *et al.*, 2024). For the purpose of this investigation, we will nevertheless focus on a scenario of a continuous DQCP, expecting that our results continue to hold upon considering *weakly* first order transitions. On the experimental side, systems exhibiting (possibly) continuous Néel–VBS transitions are scarce, with the exception of the candidate material  $\text{SrCu}_2(\text{BO}_3)_2$  (Cui *et al.*, 2023; Guo *et al.*, 2025). Although this material shows signs of DQCP in a magnetic field, the behaviour has recently been shown to turn strongly first order when tuning the lattice under hydrostatic pressure.

When connecting idealised microscopic models with possible material realisations, experimental realities must be taken into account. Disorder, defects, doping (Kaul *et al.*, 2007) and spurious interlayer couplings in quasi-2D systems (Lee *et al.*, 2019) can have significant impact on the stability and phenomenology of possibly exotic states. We take this as a motivation to study the stability of the DQCP to spin-lattice coupling.

This Chapter contains the original work from the manuscript (Hofmeier, Willsher, Seifert, and Knolle, 2024). Here, we show that the coupling to *static* lattice distortion modes renders the deconfined phase transition to exhibit strongly first order behaviour. Moving beyond our analysis of quantum critical *phases* in Chapters 5 and 6, we study quantum critical points coupled to the lattice. We show that these can also be unstable under a mechanism that resembles the 1D spin-Peierls instability of the Luttinger liquid. This extends works which study the effect of elastic couplings on general quantum critical points (Zacharias *et al.*, 2015; Sarkar *et al.*, 2023). We further go beyond (classical) lattice distortions and consider quantum mechanical phonons with finite frequency  $\omega_0$ . In this case DQCPs may persist and we derive scaling laws for a parameter regime of stable deconfined criticality

## 7.1 Deconfined quantum critical points

In this Section, we will present a brief introduction to the mathematical description of DQC. This will encompass both the original 2D model, as well as the recent 1D proposal. In the context of this Thesis, it makes sense to start with the 1D model since it is closely related to the Luttinger liquid model we have studied already.

### 7.1.1 DQC in general

Before we begin defining the transition mathematically, let us describe in more detail the phenomenology of the DQCP. We define a DQCP by the following three features.

First, the transition is a *continuous, Landau-forbidden* transition. This means the two competing states break independent subgroups of the spin and lattice symmetries. In our examples, we will consider Néel order which breaks spin-rotation symmetry, while VBS

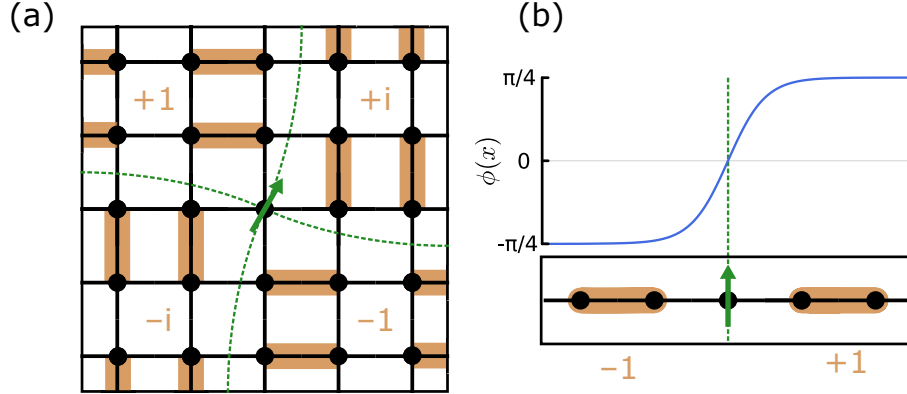


Figure 7.2: *Spin-1/2 moment localised in defects of VBS order.* (a) A  $\mathbb{Z}_4$  vortex of VBS order in 2D binds a spin-1/2 moment at its centre (Levin and Senthil, 2004). (b) A domain wall of VBS order in 1D binds a spin-1/2 moment (Sachdev, 2011; Mudry *et al.*, 2019).

order breaks lattice symmetries such as translation and rotation. Because the two phases break independent symmetries, the transition within Landau theory should generically be first order, or there must be an intermediate disordered phase. In the case of DQCP, we must tune *only one parameter* to reach this critical point.

Second, there is an *emergent symmetry* at the critical point. The critical point has no spin or VBS order, but the order parameters decay algebraically. This is a generic feature of a critical point. What makes the DQCP unique is that the critical exponents of the two competing ordered phases is the same. This represents the presence of an emergent symmetry between the two order parameters. Just like in quantum spin liquids, this symmetry can be seen as a result of an emergent deconfined gauge theory.

Third, the defects of one phase carry quantum numbers of the other phase. We say that the order parameters are *intertwined*. This means when the defects of one order proliferate, the result is a competing ordered phase, and not a simple disordered phase. A simple picture is presented in Fig. 7.2(a), following Levin and Senthil (2004). In the VBS phase, there are four types of columnar order on the square lattice. We define the VBS components

$$v_j^a = \langle \vec{S}_j \cdot \vec{S}_{j+\delta_a} \rangle, \quad (7.1)$$

and combine them into a complex order parameter  $v_j = v_j^x + iv_j^y$ . The states with  $v = e^{i\pi n/2}$  label the different columnar phases. A defect of the VBS order is a  $\mathbb{Z}_4$  vortex at the intersection of domain walls (shown in green). Levin and Senthil (2004) argued that the unpaired spin at the centre of the vortex is a free spin-1/2 moment. When the VBS order is destroyed by proliferating topological defects, then the resulting order is a Néel state. We show an analogous picture in the XXZ chain in Fig. 7.2(b) (Sachdev, 2011; Mudry *et al.*, 2019). Let us go back to our bosonised description of this model from Section 2.1. We draw a soliton of the field  $\phi(x)$  that maps between two VBS ordered phases  $\phi = \pm\pi/4$ . The domains have VBS order with signs  $\pm 1$  according to Eq. (2.28) and we see that the field passes through  $\phi = 0$  at the boundary between them. This has a magnetic moment

according to Eq. (2.27). We will return to this intertwining later when we write down concrete theories to describe the DQCP in 1D and 2D.

Before we attempt to describe the various deconfined transitions, let us first try to understand a more simple concept: How can we describe the Néel ordering transition, and how can VBS order arise in such a model? The 3-component Néel order parameter field is defined as

$$\mathbf{n}_j = \eta_j \langle \mathbf{S}_j \rangle, \quad (7.2)$$

where  $\eta_j = \pm 1$  alternates on neighbouring sites  $j$  of the lattice. To write down a continuum theory, we would typically then try to coarse-grain this field  $\mathbf{n}(\mathbf{r})$ . The effective low-energy theory for fluctuations of this ordering vector is the O(3) non-linear sigma model (NLSM) with an additional topological term (Haldane, 1988). In  $d = D + 1$  dimensions it reads

$$S_{\text{O}(3)} = \frac{1}{2e^2} \int_0^\beta d\tau \int d^D \mathbf{x} \left[ v^2 (\nabla \mathbf{n})^2 + (\partial_\tau \mathbf{n})^2 \right] + S_{\text{topo}}[\mathbf{n}]. \quad (7.3)$$

The field of the O(3) NLSM must also satisfy a non-linear constraint  $|\mathbf{n}(\mathbf{r})|^2 = 1$ . Note that we set the spin-wave velocity  $v = 1$  in the following. Here,  $S_{\text{topo}}[\mathbf{n}]$  is a topological term that follows from the Berry phase contribution of the spin path integral (Sachdev, 2011; Fradkin, 2013). Explicitly working on a lattice, the term  $S_{\text{topo}}[\mathbf{n}]$  is given by

$$S_{\text{topo}}[\mathbf{n}] = \frac{i}{2} \sum_j \eta_j \int d\tau \int_0^1 du [\mathbf{n}_j \cdot (\partial_u \mathbf{n}_j \times \partial_\tau \mathbf{n}_j)], \quad (7.4)$$

with  $\mathbf{n}(\tau)$  smoothly extended to  $\mathbf{n}(\tau, u)$  such that  $\mathbf{n}(\tau, u = 0) = (0, 0, 1)^T$  and  $\mathbf{n}(\tau, u = 1) = \mathbf{n}(\tau)$ .

What is the influence of the topological term? In this formulation it appears rather opaque. To get an intuition, we can try to ignore it and focus on the properties of the non-topological O(3) NLSM. Focusing on one dimension, the coupling in the theory  $e^2$  is marginally relevant. This would signal that the theory flows to the strongly coupled  $e^2 \rightarrow \infty$  fixed point. This corresponds to a gapped disordered paramagnet, which is in contradiction with our results for the Heisenberg chain from Chapter 2. To recap, in that case we found a gapless spin disordered phase which we called the Luttinger liquid. The topological term is necessary to capture the nature of this critical model.

Going beyond this and into 2D, Read and Sachdev (1989); Senthil *et al.* (2004a) show that the topological term is again of vital importance to understanding the nature of the strong-coupling disordered phase. First, it means the NLSM does not flow to a trivial disordered phase in the strong-coupling limit. Instead, a VBS phase is realised due to the proliferation of topological defects in  $\mathbf{n}$ . Second, the nature of the phases and transitions at finite  $e^2$  will be changed. While the possibility of a direct continuous phase transition between Néel and VBS order follows from the O(3) NLSM in 2D, the nature of the transition is difficult to access in this framework. This is because it is fundamentally an expansion about the Néel ordered phase. In the following, we will rely on alternative gauge-theory representations for these models. We present a complementary NLSM description in Appendix D.

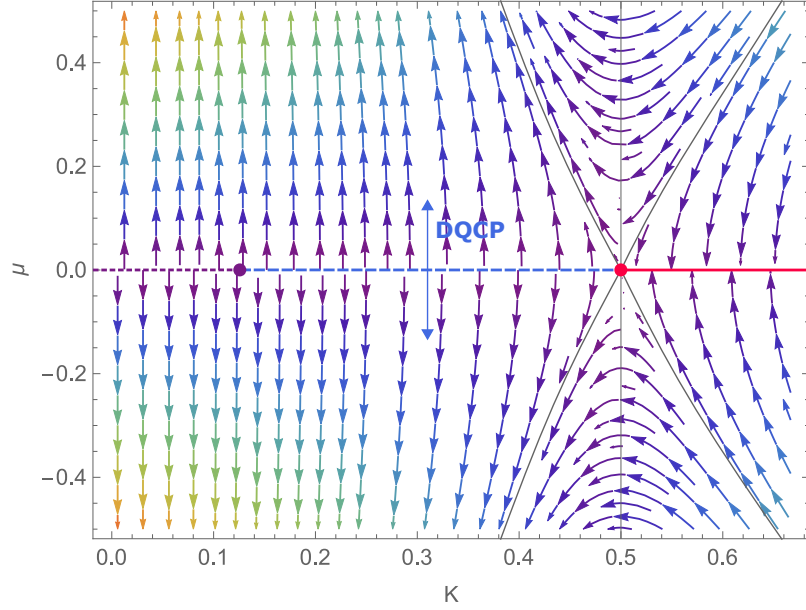


**Figure 7.3:** *RG flow of the Sine-Gordon model in the unstable regime.* The regime  $1/8 < K < 1/2$  displays a deconfined quantum critical point along the line  $\mu = 0$ , highlighted in blue here.

### 7.1.2 DQC in one dimension

Before describing in detail the original 2D model of DQCP, we will first study a simple 1D analogue. This will serve as a useful warm-up, since it is a model that we have encountered many times now. Let us take now the bosonised continuum theory for the XXZ model, (Giamarchi, 2003; Sachdev, 2011), Eq. (2.23), which we reproduce here:

$$S_{\text{SG}} = \int dx d\tau \left[ \frac{1}{2\pi K} \left( (\partial_x \phi)^2 + (\partial_\tau \phi)^2 \right) - \mu \cos(4\phi) \right]. \quad (7.5)$$

This is the Sine-Gordon model where  $K$  is the Luttinger parameter. For the isotropic model, we showed in Chapter 2 that there is a stable gapless, spin-disordered phase. This is the regime with Luttinger parameter  $K \geq 1/2$ , where the interactions  $\cos(4\phi)$  are irrelevant.

The DQCP in the XXZ model is found not in the stable regime, but is produced by adding a perturbation that makes the Luttinger liquid unstable. Assuming a sufficiently strong easy-axis anisotropy  $\Delta > 1$ , we move into the unstable region, where the Luttinger parameter is  $K < 1/2$  and the coupling  $\mu$  is relevant. Let us now rewrite the interaction directly in terms of the order parameters. Using the bosonisation mappings given by Eqns. (2.27) and (2.28), we find

$$-\mu \cos(4\phi) = \mu \left[ \sin^2(2\phi) - \cos^2(2\phi) \right] = \mu(v^2 - n_z^2), \quad (7.6)$$

such that Néel order is preferred when  $\mu > 0$ , and dimer order when  $\mu < 0$ . More precisely, we can say that the minima  $\phi_0$  of the potential with  $\mu > 0$  have finite Néel order

$$4\phi_0 = 0, 2\pi, \quad \implies \quad n_z = \cos(2\phi_0) \neq 0. \quad (7.7)$$

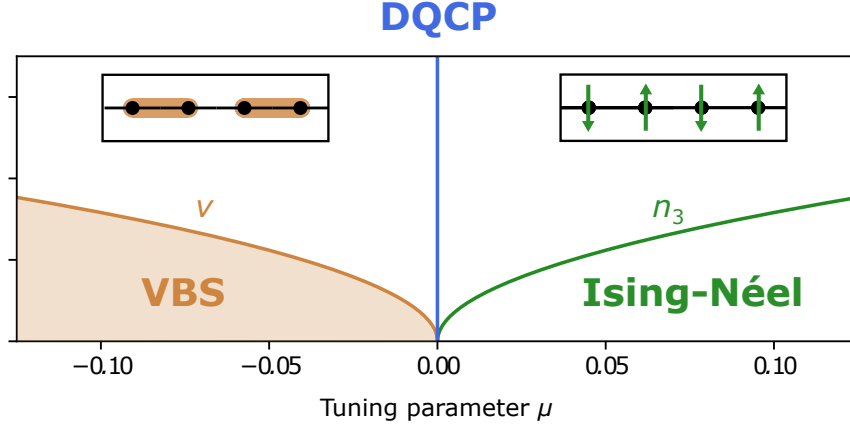


**Figure 7.4:** *Deconfined quantum critical transition in one dimension.* Continuous transition between competing Néel and VBS orders in the Heisenberg chain. Critical point is described by a Sine–Gordon field theory, here we take the Luttinger parameter  $K = 1/3$ .

Next, the minima  $\phi_0$  of the potential with  $\mu < 0$  have finite dimer order

$$4\phi_0 = \pm\pi, \quad \implies \quad v = \sin(2\phi_0) \neq 0. \quad (7.8)$$

The renormalisation group flow in this regime is plotted in Fig. 7.3 for both positive and negative  $\mu$ . We see that  $\mu$  is the only symmetry-allowed, relevant coupling when the Luttinger parameter is in the range  $1/8 < K < 1/2$ , and the resulting phase is dependent upon its sign.

This regime of interest will serve as an example of deconfined quantum criticality in one dimension. It satisfies all of the properties we discussed previously for the definition of a 2D DQCP. First, tuning the parameter  $\mu$  from negative to positive values will cause a direct phase transition between VBS and Néel order. The gap opens with exponent  $|\mu|^{\nu_\mu}$ , where  $\nu_\mu^{-1} = 2 - 4K$ . The order parameters onset with power-law behaviour  $n_3, v \sim |\mu|^\beta$  governed by the exponent  $\beta = \nu_\mu K$ . The continuous order-order transition is shown in Fig. 7.4. Second, at the critical point, the theory is given by the pure Sine–Gordon action. The  $U(1) \times U(1)$  symmetry of this model is not present in the original spin Hamiltonian, and can therefore be considered an emergent symmetry (Mudry *et al.*, 2019; Roberts *et al.*, 2019; Jiang and Motrunich, 2019). Finally, we note again that domain walls between VBS order  $\phi = \pm\pi/4$  host Néel order, as shown in Fig. 7.2. When domain walls of VBS order proliferate, they generate a Néel ordered state.

The presence of DQC in these spin chain models has recently been described in detail by a series of works (Jiang and Motrunich, 2019; Roberts *et al.*, 2019; Mudry *et al.*, 2019; Yang *et al.*, 2023; Lee *et al.*, 2023; Romen *et al.*, 2024). Let us now briefly study the problem numerically to confirm these field-theoretic predictions in an intuitive familiar setting. The above DQC regime corresponds to taking the XXZ Hamiltonian

$$\mathcal{H}_{\text{DQCP}} = \sum_i J_{ij} \left( S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z \right), \quad (7.9)$$

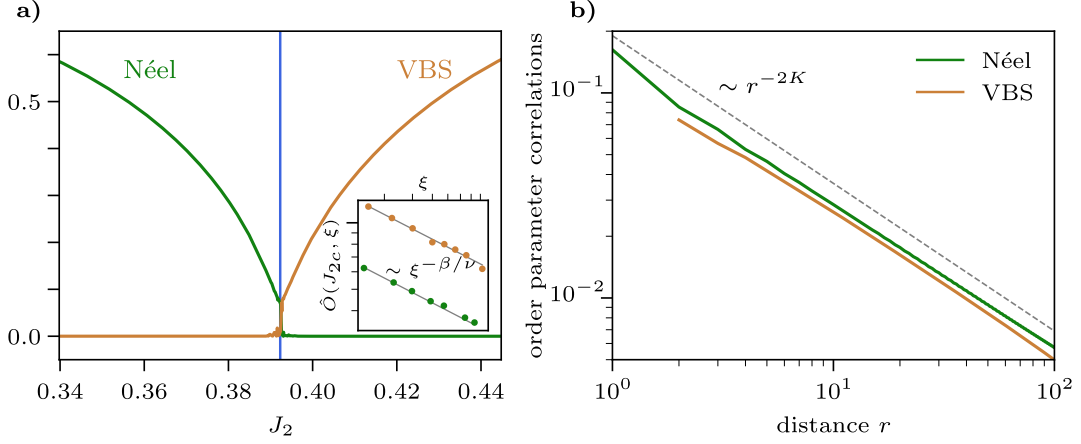


**Figure 7.5:** *Deconfined quantum critical point in the anisotropic  $J_1$ – $J_2$  chain.* (a) Continuous transition between competing Néel and VBS orders. The effects of cutting off the bond-dimension scale to zero with critical exponent  $\beta/\nu = K$  as the bond dimension  $\chi$  is increased. (b) Correlations of the order parameters, both described by exponent  $K = 0.370(5)$ .

with anisotropy  $\Delta = 4$  as well as exchange interactions  $J_{ij}$ . To access a DQCP, we must take both the nearest-neighbour exchange  $J_{i,i+1} = J_1$  and an additional next-nearest neighbour coupling and  $J_{i,i+2} = J_2$ . Because we have chosen a large spin anisotropy  $\Delta > 1$ , we are within the regime where the Luttinger liquid is unstable. By additionally tuning the ratio  $J_2/J_1$ , we can change the parameter  $\mu_0$  in the bosonised Hamiltonian. By adding the next-nearest-neighbour exchange  $J_2/J_1$ , we reduce the value of the relevant coupling  $\mu_0$ . Tuning this parameter through zero drives the DQCP.

We present numerical results of this model in Fig. 7.5. We use a 1D density matrix renormalisation group (DMRG) method to find the ground state of the spin Hamiltonian, and measure the resulting Néel and VBS order parameters. For  $J_2 = 0$ , we find Néel order, as predicted in Chapter 2 for the nearest-neighbour model. We see a phase transition about  $J_2/J_1 \approx 0.39$  to VBS order, shown in Fig. 7.5(a). There is a finite residual value of the order parameters at the transition point, but a scaling analysis shows that this is a numerical artefact. See Appendix C for more details. We show the correlations of the two order parameters at the critical point in Fig. 7.5, which show an algebraic decay with effective Luttinger parameter  $K_* = 0.370(5)$  (Jiang and Motrunich, 2019; Roberts *et al.*, 2019). The emergent symmetry of the order parameter correlations is a characteristic feature of the DQCP.

### 7.1.3 DQC in two dimensions

We can now return to the two-dimensional DQCP. Once again, we will argue that the topological Berry phase term affects the nature of the disordered state, as well as the critical properties of the Néel–VBS transition. Following the seminal work of Senthil *et al.* (2004a), we identify that the Néel order parameter in 2D has topological textures characterised by the

skyrmion number

$$Q = \frac{1}{4\pi} \int d^2\mathbf{r} \, \mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_y \mathbf{n}). \quad (7.10)$$

The Berry phase term in 2D (7.4) is exactly zero if this quantity is conserved. Only ‘hedgehog’ events, which add or remove integer numbers of skyrmion tetures, produce a Berry phase contribution (Haldane, 1988). Hedgehogs inserted on different sites contribute with a different phase factor, which can be accounted for by assigning them transformation properties under lattice symmetries (Haldane, 1988; Read and Sachdev, 1990a; Lee *et al.*, 2019). The result of this analysis is that the hedgehogs transform like VBS order parameters. This is another example of intertwining; we can think of the Néel melting transition as being due to a proliferation of skyrmions, which in turn may produce VBS order.

At this phenomenological level, it remains unclear whether this will actually be realised as a direct continuous transition. We can gain some insight by writing the sigma model in an alternative form. This observation about the transformation properties of the hedgehogs motivated a dual description of the transition (Senthil *et al.*, 2004a,c). Here, the Néel order parameter field is to be written as a composite object of spinons via the Hopf map

$$\mathbf{n} = z^\dagger \boldsymbol{\sigma} z. \quad (7.11)$$

This introduces a U(1) gauge degree of freedom into the new effective theory. Moreover, the constraint  $n^2 = 1$  becomes  $z_1^2 + z_2^2 = 1$ . From this mapping, it can be shown that the total flux of the U(1) gauge field is related to the skyrmion number of the Néel order parameter field (Auerbach, 1998). Monopoles are instantons which tunnel  $2\pi$  flux of the emergent gauge field, and can hence be identified with hedgehog events. Therefore, we write the NLSM as the following alternative form, in terms of the  $\text{CP}^1$  continuum model

$$\mathcal{L}_c = \sum_{\alpha=1}^2 |(\partial_\mu - ia_\mu)z_\alpha|^2 + s|z|^2 + u(|z|^2)^2 + \lambda_4 [\Phi^4 + (\Phi^\dagger)^4]. \quad (7.12)$$

This form is suggestive that we might be able to tune a phase transition by changing the sign of the bosonic mass  $s$ , as we will discuss shortly. We have additionally included possible anisotropies  $u$  which preserve SU(2) spin symmetry. The partons  $z$  transform as spinors under SO(3). The monopoles  $\Phi^\dagger$  transform like hedgehogs, and so they must pick up non-trivial phases under lattice symmetries (Haldane, 1988; Read and Sachdev, 1990a; Lee *et al.*, 2019). We can also identify its components with the VBS order parameter

$$v_1 \sim \text{Re } \Phi = \Phi_1 \quad \text{and} \quad v_2 \sim \text{Im } \Phi = \Phi_2. \quad (7.13)$$

The symmetry transformation properties are listed in Table 7.1. Note that this forbids single monopoles being added to the action. Instead, the most relevant instanton is  $(\Phi^\dagger)^4$ , with the coupling  $\lambda_4$ .

When the mass is negative  $s < 0$ , the bosons will condense and lead to magnetic order via Eq. (7.11). This is the Néel phase. When the mass is finite and positive  $s > 0$ , the U(1) gauge field will confine by proliferating monopoles. This is the VBS phase, since we identified monopoles with defects of the Néel order, which transform as dimer order (7.13).

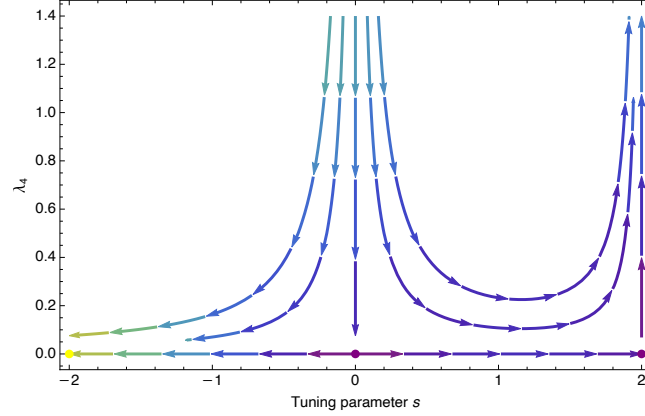


**Figure 7.6: *Dangerously irrelevant coupling.*** The quadruple monopole is irrelevant at the critical point, but is relevant in the VBS phase.

We will now briefly list the scaling dimensions of the operators at the critical point (Zhou *et al.*, 2024; Takahashi *et al.*, 2024)

$$\Delta_\Phi = 0.61, \quad \Delta_s = 2.27, \quad \Delta_4 = 3.723. \quad (7.14)$$

The mass is relevant  $\Delta_s < 3$  and transforms trivially under lattice symmetries. This means it can be tuned without breaking symmetries. Therefore tuning  $s$  from negative to positive moves from Néel to VBS order, with the critical point being gapless. At the transition  $s = 0$ , monopole events are forbidden by symmetries. Since the symmetry-allowed quadruple monopole is irrelevant, we have a deconfined phase of the U(1) gauge field. The theory is often called the non-compact  $\text{CP}^1$  (NC- $\text{CP}^1$ ) model at this point.

Even though symmetry-forbidden at the critical point, the  $\lambda_4$  coupling controls the behaviour of the VBS phase. As alluded to previously, this phase has the same  $\mathbb{Z}_4$  rotational symmetry as the lattice. This implies that the quadruple monopole is relevant in this order, despite being irrelevant at the transition. This is the picture of a dangerously irrelevant operator. A representative RG flow is shown in Fig. 7.6.

Let us review the properties of DQCP in our 2D model, as already sketched in the introduction. First, Fig. 7.2(a) shows us that a  $\mathbb{Z}_4$  vortex of VBS order must localise a spin-1/2 degree of freedom (Levin and Senthil, 2004). We have already relied on the observation that topological hedgehog defects of the Néel order parameter field transform as VBS order. Defects of the respective phases proliferate the competing orders. In the deconfined phase, the  $\mathbb{Z}_4$  lattice rotational symmetry is enhanced to U(1). Combining with the spin symmetry, the model's  $\text{SU}(2) \times \text{U}(1)$  symmetry may be further enhanced to  $\text{SO}(5)$  by tuning  $s$ . Equation (7.14) tells us the DQCP critical exponents for the correlation length  $\nu_s = 1/(3 - \Delta_s) = 1.38$  and order parameter onset  $\beta = \nu_s \Delta_\Phi$ , shown in Fig. 7.1. Surprisingly, the dimension  $\Delta_\Phi$  controls the correlations of both VBS and Néel order at the critical point. This is a signature of the enhanced emergent  $\text{SO}(5)$  symmetry (Nahum *et al.*, 2015b). This symmetry is not intuitively apparent in this gauge theory formulation (Senthil, 2023), but can be understood more clearly in a dual formulation. This is a ‘superspin’ NLSM,

formed by combining the order parameters of antiferromagnetic Néel  $(n_x, n_y, n_z)$  and VBS  $v^a = \eta^i \langle \vec{S} \cdot \vec{S}_a \rangle$  into the vector  $\tilde{n} = (\mathbf{n}, \mathbf{v})$ . The dynamics of this superspin order parameter is given by a non-linear sigma model supplemented by a topological Wess–Zumino–Witten (WZW) term, which intertwines the order parameters (Tanaka and Hu, 2005; Senthil and Fisher, 2006):

$$S_2^{\text{DQCP}}[\tilde{n}] = S_2^{\text{kin}}[\tilde{n}] + \int d^3x s(\mathbf{n}^2 - \mathbf{v}^2) + \Gamma_2^{\text{SO}(5)}[\tilde{n}]. \quad (7.15)$$

The 2D WZW term  $\Gamma_2^{\text{SO}(5)}$  reduces to the spin-1/2 Berry phase in the case of a single  $\mathbb{Z}_4$  vortex within the VBS phase (Levin and Senthil, 2004). The anisotropy  $s$  tunes between the two competing orders. The WZW term also serves to make this transition continuous. We discuss this mechanism in detail in Appendix D.

## 7.2 Spin-Peierls instability

There are two characteristic features of DQCPs that render the study of couplings to lattice distortion modes a particularly worthwhile endeavour. First, *emergent symmetries* are believed to be common at DQCPs, in this case an emergent  $\text{SO}(5)$  symmetry (Nahum *et al.*, 2015b). It is important to clarify the resilience of such emergent symmetries upon including lattice distortion modes which primarily couple to fluctuating VBS order parameters. Second, the DQCP has an equivalent description in terms of a *deconfined*  $U(1)$  gauge theory, the  $\text{CP}^1$  model as described above. In this language, VBS order is obtained after the proliferation of said monopoles, which may thus be identified with fluctuating VBS order parameters. Crucially, the conclusions of Senthil *et al.* (2004a) are based on the symmetry quantum numbers of the monopole operator and are thus lattice dependent (Block *et al.*, 2013); the key assumption being that the underlying microscopic Hamiltonian of the system respects the full symmetry of the square lattice. Lattice distortions, which might be generated by the system spontaneously (and are generally nonzero on the VBS side of the transition) explicitly break these symmetries, calling the underlying assumptions of deconfined criticality in question.

We approach these questions in a low-energy field-theoretical framework, which allows for general statements independent of putative microscopic realisations of DQCP. As an example of the generality, we present throughout this Section a parallel analysis of the proposed one-dimensional example of DQCP in antiferromagnetic spin chains with anisotropy (Jiang and Motrunich, 2019; Roberts *et al.*, 2019; Mudry *et al.*, 2019; Lee *et al.*, 2023). This makes especially clear the connection with the well-understood Peierls instability of the Luttinger liquid phase. In 2+1 dimensions, we primarily focus on the canonical example of the Néel–VBS deconfined phase transition, where we show that lattice distortion modes can couple to strongly relevant monopole operators and thereby strongly impact the nature of the phase transition.

### 7.2.1 Static model

#### In one dimension

Before we turn to the most prominent example of DQC, we focus on the 1D case (Jiang and Motrunich, 2019; Roberts *et al.*, 2019; Mudry *et al.*, 2019; Lee *et al.*, 2023). Here, we make use of low-energy field theory arguments, extending previous discussions in the context of one-dimensional Heisenberg chains without anisotropy. Writing  $u_n = (-1)^n \delta u$  and bosonising, we showed in Chapter 5 that the distortion field couples to the VBS order parameter in the Sine–Gordon action (7.5) via

$$H_{\text{sp}} \sim h \sin(2\phi), \quad (7.16)$$

where  $h = g \delta u$ . Recall that we derived this using a symmetry-based, top-down construction of the spin-lattice coupling. Equipped with the symmetry transformation behaviours of the field  $\phi$  in the Sine–Gordon model in Table 5.1, we deduce that the  $\sin 2\phi$  interaction, which is odd under translations  $T_x$  and inversion  $I$ , has a symmetry-allowed coupling to a staggered lattice distortion field  $h = g \delta u$ . A complementary approach finds the same result by explicitly bosonising the staggered coupling (Orignac and Chitra, 2004; Citro *et al.*, 2005).

Thus the field theory for the DQC upon coupling to lattice distortion modes becomes

$$S_u = S_{\text{SG}} + \int dx d\tau \lambda \sin(2\phi), \quad (7.17)$$

where we define the field theory coupling  $\lambda \sim h$ . This is exactly as we saw before in Eq. (5.10), but now we allow both spin anisotropy and next-nearest-neighbour coupling. The result is that the initial (lattice-scale) values of these parameters ( $K, \mu_0$ ) are fixed by  $\Delta$  and  $J_2$ . The new coupling  $\lambda$  is determined by the lattice distortion. With this in mind, we write the perturbative RG equations of this coupled model

$$\beta_K = -K^2(\lambda^2 + 4\mu^2), \quad (7.18)$$

$$\beta_\lambda = (2 - K)\lambda + \frac{2}{u}\lambda\mu K, \quad (7.19)$$

$$\beta_\mu = (2 - 4K)\mu + \frac{1}{2u}\lambda^2 K. \quad (7.20)$$

The leading terms of Eqns. (7.19) and (7.20) follow from the scaling dimensions of these operators, as we wrote in Eqns. (2.25) and (2.33). All other terms are calculated by Kadanoff (1980). Importantly, we see that no real-valued fixed points for the full three dimensional RG flow are found. This implies there is a breakdown of the DQCP.

We note that this is in contrast to previous works which predict a second-order Ising transition at finite  $\lambda$  (Kadanoff, 1980; Delfino and Mussardo, 1998). This apparent disparity stems from the fact that the analyses in Kadanoff (1980); Delfino and Mussardo (1998) did not account for the flow given by Eq. (7.18) of the Luttinger parameter  $K$ . Assuming  $K$  to be constant, we would indeed find two new fixed points for (7.19) and (7.20). However, these fixed points do not persist in the full three-dimensional RG flow. From Eqns. (7.18)–(7.20) we conclude that the RG flow for any finite  $\lambda \neq 0$  at the original DQCP line ( $1/8 <$

$K < 1/2, \mu = 0$ ) is non-zero, implying the absence of deconfined quantum criticality in the presence of a finite lattice distortion.

Once again, we note that in the absence of spin-lattice couplings, the undistorted lattice minimises the system's elastic energy. We must compare the energy gain of the spin system with the quadratic energy cost of the lattice distortion. Using Eq. (5.11) with general  $K$ , we write  $\nu^{-1} = 2 - K$  and write the gap scaling

$$\Delta \sim \lambda^\nu \sim (\tilde{g}\delta u)^{1/(2-K)}. \quad (7.21)$$

Within our approximation, the effective energy of the system is then composed of a (harmonic) energy cost of the distortion and an energy gain due to the opening of the gap,

$$\mathcal{E} = \frac{1}{N} (E_{\text{cost}} - E_{\text{gain}}) = (\kappa/g^2)(g\delta u)^2 - c(g\delta u)^{2/(2-K)}, \quad (7.22)$$

for some constant  $c$ . We have previously looked at the cases  $K = 1$  (XY model) and  $K = 1/2$  (Heisenberg model) and concluded there is an instability because the energy gain always outcompetes the potential energy cost. Of interest for DQC is the region  $1/8 < K < 1/2$ . We see that here too, the lattice is always unstable towards spontaneous distortion at the original DQCP.

The previous analysis implies an equilibrium VBS order, a lattice distortion  $h_0$ , and a corresponding gap  $(g^2/\kappa)^{1/(2-2K)}$  at the original DQCP  $\mu = 0$ . From this, it follows that deconfined criticality is spoiled, i.e. the Néel-VBS transition becomes a first order transition. It also tells us that the location of the critical point is shifted. Tuning  $\mu < 0$  in the pure DQCP model opens up an Néel gap which scales as  $\mu^{1/(2-4K)}$ . There will be a first-order transition when the energy gain due to this gap opening is equal to the aforementioned energy gain (driving the spin-Peierls gap at the original DQCP). There will be a corresponding discontinuous jump in the equilibrium lattice distortion. The first-order VBS to Néel order transition therefore occurs at the shifted value

$$\mu_{\text{static}} = -(g^2/\kappa)^{(2-4K)/(2-2K)}. \quad (7.23)$$

We exclude the possibility that the shifted transition remains deconfined, since no sort of second order Néel-VBS transition can exist in 1D on a lattice without translational symmetry. This effect can be elucidated by considering the 1D topological term Eq. (D.8) in the presence of a finite distortion it is no longer integer  $\delta u$ ,  $S_{\text{top}} = i\pi(1 + \delta u/J)Q_{x\tau}$ . This can be seen by using the Haldane expansion for the Heisenberg spin chain in the presence of an additional *staggered interaction* induced by a lattice distortion, see also (Affleck, 1986).

### Numerical results

Here, we return to the realisation of DQCP in the  $J_1$ - $J_2$  anisotropic Heisenberg chain. This is the spin Hamiltonian written in Eq. (7.9). We couple the spins to the lattice by way of a bond-length dependent exchange interaction. We write the bond-dependence in the linear approximation as

$$\mathcal{H}[\mathbf{u}_i] = \mathcal{H}_{\text{DQCP}} - 2g J_1 \sum_i \delta u (-1)^i \left[ S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right], \quad (7.24)$$

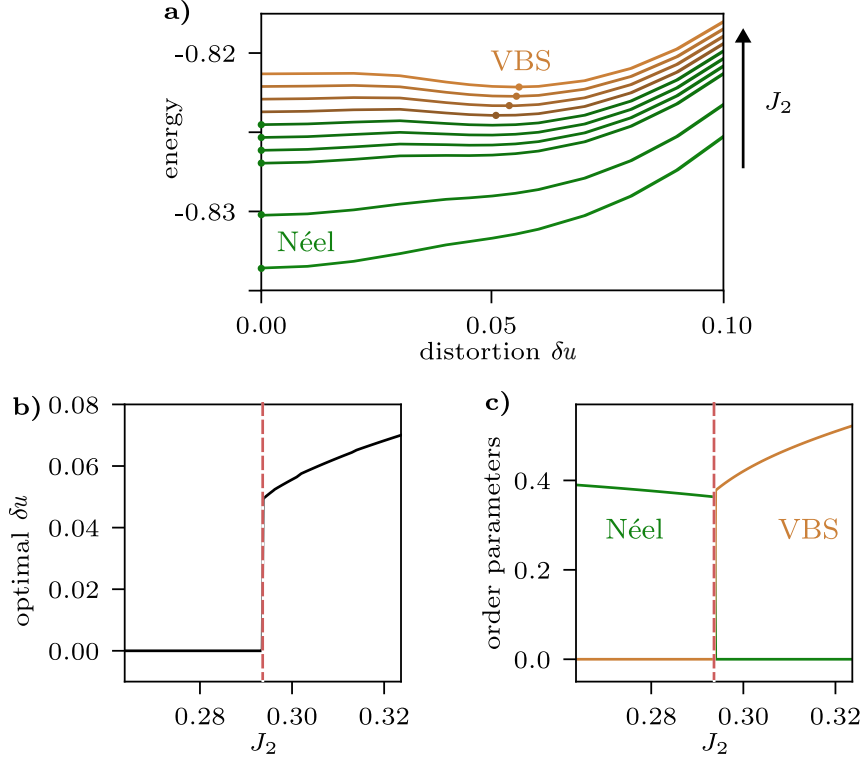


**Figure 7.7:** *First-order transition in the Heisenberg chain driven by spin-lattice coupling.* (a) The energy landscape  $\varepsilon(\delta u)$  as a function of varying  $J_2$  across the transition. The minimum jumps from  $\delta u = 0$  to a finite value at the first-order transition. The results show a strong discontinuity in (b) the equilibrium value of the spin-lattice coupling  $\delta u$  and (c) the order parameters. We take parameters  $g = 1$  and  $\kappa = 3.5$ ; all energies in units of  $J_1$ .

This is entirely equivalent to Eq. (5.66) which we previously used to study the isotropic Heisenberg chain (then using variational Monte Carlo).

In order to find evidence of the instability, we must measure the energy of the spin model as a function of lattice distortion and allow this to compete with a static potential-energy cost  $\kappa(\delta u)^2$ . This situation is more complex in the case of DQCP, since this calculation must be performed for a range of  $J_2$ . This is shown in Fig. 7.7(a) where we plot the energy as a function of distortion  $\varepsilon(\delta u)$  for various  $J_2$ . We take the coupling  $g = 1$  and the lattice stiffness  $\kappa = 3.5$ . In the Néel phase, we find the energy is minimised by the zero distortion state  $\delta u = 0$ . Upon increasing  $J_2$ , we lower the energy of higher-distortion states, leading to a double-well form of the effective potential in Fig. 7.7(a). At  $J_2/J_1 = 0.293$  there is a first-order transition to the distorted lattice state with a finite VBS order, shown in Fig. 7.7(b,c). Together, we conclude that the original DQPC has been destroyed. Instead, we see a strongly first order transition at a significantly reduced value of  $J_2$ . The lattice strongly favours VBS order, and destroys the emergent symmetry at the transition.

| Symmetry                     | $\mathbf{n}$         | $\Phi^\dagger$  | $u^*$  |
|------------------------------|----------------------|-----------------|--------|
| $\text{SU}(2)^{\text{spin}}$ | $R_{ab}\mathbf{n}_b$ | $\Phi^\dagger$  | $u^*$  |
| $T_x$                        | $-\mathbf{n}$        | $-\Phi$         | $-u$   |
| $T_y$                        | $-\mathbf{n}$        | $\Phi$          | $u$    |
| $R_{\pi/2}^{\text{site}}$    | $\mathbf{n}$         | $i\Phi^\dagger$ | $iu^*$ |
| $\sigma_x$                   | $\mathbf{n}$         | $\Phi$          | $u$    |
| $\mathcal{T}$                | $-\mathbf{n}$        | $\Phi$          | $u$    |

Table 7.1: Symmetry properties of the monopole operator  $\Phi^\dagger$  (Read and Sachdev, 1990b; Lee *et al.*, 2019) and the phonon mode  $u$  under the elementary lattice symmetries of the square lattice. The transformation of the lattice distortion field  $u = u_1 + iu_2$  is written for comparison. We include the action of spin rotation on the order parameters: the Néel order transforms under the representation  $R \in \text{SO}(3)$ , and the VBS order is a singlet, i.e., the monopole is left invariant (this latter fact is also true with possible anisotropy).

### In two dimensions

We observe that, just like in 1D, there exists an operator that is relevant at the DQCP but disallowed in the field theory due to its non-trivial behaviour under lattice symmetries. The role of  $\sin(2\phi)$  in 1D is taken over by the monopole operator  $\Phi^\dagger$ . Its transformation behaviour has been obtained by explicitly transforming the expression for the Berry phase in the presence of a single monopole (Read and Sachdev, 1989; Lee *et al.*, 2019). Table 7.1 summarises their symmetry properties. Again, we can now ask whether there exists a lattice distortion that transforms the same way such that the product of a monopole and a distortion would be symmetry allowed. To find this, we recall the definition of the VBS order parameters  $v^a(\mathbf{r}_i) = \eta_i \langle \vec{S}_{\mathbf{r}_i} \cdot \vec{S}_{\mathbf{r}_i + \hat{\delta}_a} \rangle$  where  $\hat{\delta}_{a=1,2} = \hat{x}, \hat{y}$  are the lattice unit vectors.

Defining a general distortion field  $\mathbf{u}(\mathbf{x})$  which shifts the lattice sites  $\mathbf{r}_i \rightarrow \mathbf{x} = \mathbf{r}_i + \mathbf{u}(\mathbf{x})$ , we expand in a Fourier basis  $\mathbf{u}(\mathbf{x}) = \sum_{\mathbf{Q}} \mathbf{u}_{\mathbf{Q}}^a e^{i\mathbf{Q} \cdot \mathbf{x}}$ , then we extract the two longitudinal components

$$u_a = \hat{\mathbf{Q}}_a \cdot \mathbf{u}_{\mathbf{Q}_a}, \quad \mathbf{Q}_a = (\pi, 0), (0, \pi). \quad (7.25)$$

Assuming that the distortion field at wavevectors  $\mathbf{Q}_1, \mathbf{Q}_2$  is purely longitudinal, we can thus write in real space

$$\mathbf{u}(\mathbf{x}) = \begin{pmatrix} u_x(\mathbf{x}) \\ u_y(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{i\pi x_1} u_1 + \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{i\pi x_2} u_2. \quad (7.26)$$

We may combine these two contributions into a complex field  $u^* = u_1 + iu_2$  as done for the VBS order parameters to form the monopole  $\Phi \sim v_1 + iv_2$ . We explicitly evaluate the transformation properties of this field  $u_a$  under transformations of the lattice  $\mathbf{r}_a \rightarrow g(\mathbf{r}_a) = M_{ab}\mathbf{r}_b + \delta_a$ . The components transform under the symmetry group of the lattice actively as  $u_a(\mathbf{x}) \rightarrow M_{ab}u_b(g^{-1}\mathbf{x})$ ; we summarise the results in 7.1, which shows that this field transforms identically to the VBS monopoles. We conclude that the monopole-lattice coupling

$$\mathcal{O}_{mp} \sim u \Phi^\dagger + \text{h.c.} \sim u_1 v_1 + u_2 v_2 \quad (7.27)$$

is therefore symmetry-allowed. This appears in the action through the coupling  $S_{mp} = -g \int d^3x \mathcal{O}_{mp}(x)$ . On the level of the NLSM, the lattice couples linearly to the VBS order parameters

$$S_2[\tilde{\mathbf{n}}, \mathbf{h}] = S_2^{\text{kin}}[\tilde{\mathbf{n}}] + \int d^Dx \left[ s(\mathbf{n}^2 - \mathbf{v}^2) - \mathbf{h} \cdot \tilde{\mathbf{n}} \right] + \Gamma_2^{\text{SO}(5)}[\tilde{\mathbf{n}}], \quad (7.28)$$

with  $\mathbf{h} \sim g(0, 0, 0, u_1, u_2)^T$ . This explicitly breaks the emergent  $\text{SO}(5)$  symmetry and will have the effect of pinning the VBS components of the topological NLSM field  $\tilde{\mathbf{n}}$  to the lattice distortion field  $\mathbf{h}$ . We expect this term to make the transition tuned by  $s$  first order whenever  $\mathbf{h}$  takes a non-zero value.

We are interested in understanding the gap induced by the perturbation  $\mathbf{h}$  when the NLSM of Eq. (7.28) is tuned to the strong-coupling fixed point. In analogy with the result in 1D, the gap scaling as a function of distortion is controlled by the conformal data at the fixed point

$$\Delta(\mathbf{h}) \sim |\mathbf{h}|^{\nu_\Phi} \quad (7.29)$$

with  $\nu_\Phi = 1/(3 - \Delta_\Phi) = 0.419$  being the correlation length exponent of the monopole operator (Takahashi *et al.*, 2024). We recall that the distortion  $\mathbf{h}$  in (7.28) is a (vector-valued) classical parameter that represents a static, non-local distortion of the lattice (we treat fluctuations of this field in the next section). Formally, the free energy of the coupled system may be written as  $\mathcal{F}(\mathbf{h}) = (\kappa/g^2)|\mathbf{h}| - \log \int \mathcal{D}\tilde{\mathbf{n}} e^{-S_2[\tilde{\mathbf{n}}, \mathbf{h}]}$ . The saddle-point behaviour of the lattice distortion field is determined by the respective scaling of the energy cost of a distortion and the induced energy gain. We tune  $s$  to the gapless DQCP with an emergent  $\text{SO}(5)$  symmetry and, in a result analogous to 1D [in Eq. (5.14)], we find the saddle point behaviour of the distortion field is governed by the effective potential

$$\mathcal{E}(\mathbf{h}) = (\kappa/g^2)|\mathbf{h}|^2 - c|\mathbf{h}|^{3\nu_\Phi}. \quad (7.30)$$

Hence, we conclude that a finite spontaneous equilibrium distortion  $\mathbf{h}_0 \neq 0$  is induced at the DQCP on the square lattice. The condition for a lattice instability in 2D reads  $3\nu_\Phi < 2$  or  $\Delta_\Phi < 3/2$ , as is believed to be satisfied for the DQCP.

The shifted transition must be rendered first order by this distortion, since the coupling  $-\mathbf{h} \cdot \tilde{\mathbf{n}}$  will always destroy the critical point. That is to say that on an explicitly distorted lattice, no DQCP can be present since both the strongly relevant single and double monopole  $\Phi^\dagger/(\Phi^\dagger)^2$  become symmetry-allowed (Nahum *et al.*, 2011) (this is stronger than the case of non-staggered rectangular-lattice distortions where translational symmetry is preserved (Block *et al.*, 2013; Wang *et al.*, 2017; Metlitski and Thorngren, 2018)). As for 1D, we also see that the transition is shifted away from the original DQCP and into the original Néel phase. The energies of the VBS and Néel phases cross when the  $s$ -induced gap to VBS excitations in the Néel phase becomes equal to the distortion-induced gap  $\Delta(\mathbf{h}_0)$  in the VBS phase. This produces a modified transition point

$$s_{\text{static}} = -[g^2/\kappa]^{(3-\Delta_s)/(3-2\Delta_\Phi)}. \quad (7.31)$$

From the energy density (7.30), it would naively follow that there are infinitely many degenerate distorted ground states. It should be noted, however, that we have neglected so

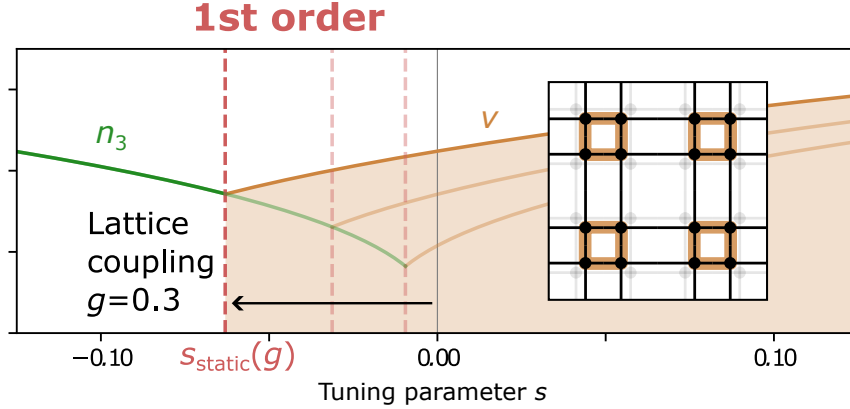


**Figure 7.8:** *Spin-phonon coupling shifts the transition and renders it first order.* The deconfined critical point becomes confined and gapped. Shown here is spin-phonon coupling  $g = 0.3$  (and lattice stiffness  $\kappa = 1$ ), with  $g = 0.2, -0.1$  in the background.

far higher order symmetry-allowed terms in the lattice potential. Taking these into account, the energy density up to fourth order reads

$$\mathcal{E}'(\mathbf{h}) = \mathcal{E}(\mathbf{h}) + c_1(h_1^4 + h_2^4) + c_2(h_1^2 h_2^2). \quad (7.32)$$

To ensure stability, we must require  $c_1 > 0$  and  $c_2 > -2c_1$ . The coefficient  $c_1$  reduces the unphysical  $U(1)$  symmetry to a more physical  $\mathbb{Z}_4$ -symmetry and  $c_2$  ultimately determines the type of distortion. For  $c_2 > 2c_1$ , the energy density is minimised for a distortion in columnar direction (with either  $h_{1,2} = 0$ ) and for  $c_2 < 2c_1$  the distortion is towards the plaquette centers (with  $h_1 = h_2 = h$ ). Accordingly, the system enters a columnar VBS (cVBS) or plaquette VBS (pVBS) phase, respectively. The value of  $c_2$  seems to be a microscopic property (determined by both the lattice dynamics and induced by spin interactions at the new strong-coupling fixed point) and we are not aware of any methods for accessing this from our top-down symmetry approach. To accurately specify the exact distortion, one must most likely resort to numerical methods. We summarise the different distortions in Figure 7.9.

### 7.2.2 Adding dynamics

Moving beyond the adiabatic approximation of the lattice, we will now develop a theory of dynamical optical phonons coupled to the DQCP. This will follow a similar approach to Chapter 6. This model has the advantage that it more accurately captures the physics of the lattice phonons which generally can be expected to have a finite energy  $\omega_0 > 0$  at non-zero (lattice) momenta.

#### Phonons in one dimension

From the static case, we know that the spins will couple to phonons with momentum  $\pi$  at the edge of the Brillouin zone. Hence, we now promote the Fourier component of the displacement field with lattice momentum  $\pi$  to be dynamical, which we henceforth for simplicity

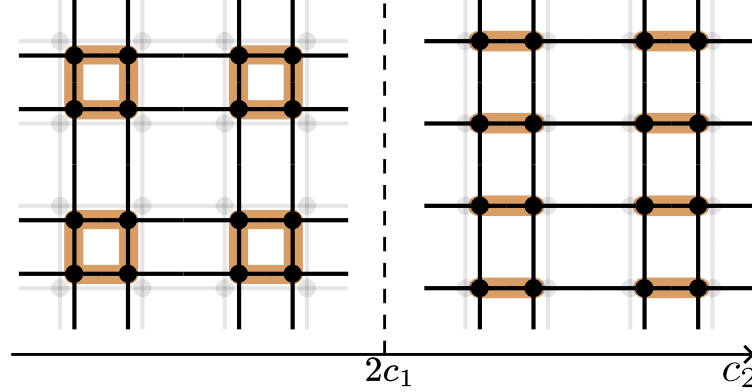


**Figure 7.9:** Possible lattice distortions of the square lattice, depending on the microscopic constant  $c_2$ . The ground state of the system has the corresponding VBS order, i.e. pVBS for  $c_2 < 2c_1$  and cVBS for  $c_2 > 2c_1$ .

denote  $u(x, \tau)$ . Then, the combined action of spins and phonons reads

$$S(\omega_0) = S_{\text{SG}} + \int dx d\tau \left\{ \frac{\rho}{2} [|\partial_\tau u|^2 + \omega_0^2 |u|^2] + 2u \sin(2\phi) \right\}, \quad (7.33)$$

with the phonon mass density  $\rho = m/a$  and frequency  $\omega_0 \sim \omega(\pi)$ . Integrating out the quadratic displacement field gives

$$S(\omega_0) = S_{\text{SG}} + g^2 \int dx d\tau d\tau' G_{\omega_0}(\tau - \tau') \times [\cos(2(\phi + \phi')) - \cos(2(\phi - \phi'))], \quad (7.34)$$

with the phonon propagator

$$G_{\omega_0}(\tau - \tau') = \frac{1}{2\rho\omega_0} e^{-\omega_0|\tau - \tau'|}. \quad (7.35)$$

For notational brevity, we drop the space-time dependence of  $\phi$  whenever it is clear and define  $\phi' = \phi(\mathbf{r}, \tau')$ . A similar action, without the  $\cos(4\phi)$  interaction in  $S_{\text{SG}}$ , has previously been derived by Citro *et al.* (2005) to describe the spin-Peierls transition of the SU(2)-symmetric Heisenberg model. Here, we analyse its meaning in the context of DQC where the  $\cos(4\phi)$  interaction is relevant. Let us begin by considering the two limits  $\omega_0 \rightarrow 0$  and  $\omega_0 \rightarrow \infty$ , called the adiabatic and antiadiabatic limits, respectively (Giamarchi, 2003). The former is simply the static case from above. There, we concluded that the deconfined quantum critical transition gets replaced by a first order transition.

Moving on to the antiadiabatic limit, we can use the representation of the delta-function (with appropriate normalization)

$$\frac{\omega_0}{2} e^{-\omega_0|\tau - \tau'|} \xrightarrow{\omega_0 \rightarrow \infty} \delta(\tau - \tau'), \quad (7.36)$$

to find that the dynamical phonons simply generate another  $\cos(4\phi)$  interaction and we have

$$S(\omega_0 \rightarrow \infty) = \int dx d\tau \left\{ \frac{1}{2\pi K} [(\partial_x \phi)^2 + (\partial_\tau \phi)^2] + \mu_{\text{new}} \cos(4\phi) \right\} \quad (7.37)$$

with a new coupling

$$\mu_{\text{new}} = \mu + \frac{g^2}{\rho \omega_0^2}. \quad (7.38)$$

This means that DQC persists and the critical line simply gets shifted from  $\mu = 0$  to

$$\mu_c = -\frac{g^2}{\rho \omega_0^2}. \quad (7.39)$$

Clearly, the model shows qualitatively different behaviour in the two opposite limits and so we can expect some critical frequency  $\omega_c$  where the transition changes between first-order to DQC. To find  $\omega_c$ , we assume  $\omega_0 \gg 1$  such that most of the weight of the propagator will still be concentrated around  $\tau = \tau'$ . We can then Taylor expand

$$\cos\{2[\phi(\tau) + \phi(\tau')]\} = \cos[4\phi(\tau)] + \text{irrel.} \quad (7.40)$$

up to terms irrelevant in the parameter range  $1/4 < K < 1/2$ . At  $K = 1/4$ , the next term in the Taylor expansion  $\partial_\tau \phi \sin(4\phi)$  would become relevant. Due the linearization of the fermionic dispersion in bosonisation and, as a consequence, the infinitely filled Fermi sea, fluctuations of  $\phi$  can in principle be infinite. Therefore, in order to Taylor expand the difference, we have to normal-order first. Making use of the identity (Knops and den Ouden, 1980; Nozières and Gallet, 1987)

$$\cos(\phi) = : \cos(\phi) : e^{-\frac{1}{2} \langle \phi^2 \rangle_0}, \quad (7.41)$$

where  $: \cos(\phi) :$  denotes the normal-ordered cosine and  $\langle \cdot \rangle_0$  denotes the vacuum expectation value with respect to the free part of (7.5), the expansion becomes

$$\cos\{2[\phi(\tau) - \phi(\tau')]\} = \left\{ 1 - 2(\tau - \tau')^2 [\partial_\tau \phi(\tau)]^2 \right\} e^{-2 \langle [\phi(\tau) - \phi(\tau')]^2 \rangle_0}. \quad (7.42)$$

Such correlation functions have been determined in full generality (Giamarchi, 2003). In our case, we find

$$\langle [\phi(\tau) - \phi(\tau')]^2 \rangle_0 = K \log |\tau - \tau'| \quad (7.43)$$

such that the expansion reads

$$\cos\{2[\phi(\tau) - \phi(\tau')]\} = \left\{ 1 - 2(\tau - \tau')^2 [\partial_\tau \phi(\tau)]^2 \right\} |\tau - \tau'|^{-2K}. \quad (7.44)$$

Inserting this back into our original action (7.34), performing the  $\tau'$  integration and rewriting the action back in Sine–Gordon form gives

$$S(\omega_0) = \int dx d\tau \left\{ \frac{1}{2\pi K_{\text{new}}} [\gamma (\partial_x \phi)^2 + \gamma^{-1} (\partial_\tau \phi)^2] + \mu_{\text{new}} \cos(4\phi) \right\}, \quad (7.45)$$

with new Luttinger parameter  $K_{\text{new}} = \gamma K$  and

$$\gamma = \left( \frac{2\pi K g^2 u^{-2K} \Gamma(3-2K)}{\rho \omega_0^{4-2K}} + 1 \right)^{-\frac{1}{2}}, \quad (7.46)$$

where  $\Gamma(x)$  is the Euler gamma function. Just like in the original Sine-Gordon model, this theory hosts a line of DQCPs for  $\mu_{\text{new}} = 0$  and  $\frac{1}{8} < K_{\text{new}} < \frac{1}{2}$ . The Taylor expansion itself holds for  $\frac{1}{4} < K < \frac{1}{2}$ , as explained above. Both conditions can be fulfilled simultaneously, at least for some values of  $K$ , if  $1/4 < \gamma < 2$ . The upper bound is trivially obeyed. For the lower bound, we find the condition

$$\rho \omega_0^{4-2K} > \frac{2\pi K \Gamma(3-2K)}{15} g^2 \quad (7.47)$$

which has to hold for DQC to persist even in the presence of phonons. Rewritten as a simple scaling relation, we find the critical scaling

$$\omega_c^{4-2K} \sim g_c^2 / \rho. \quad (7.48)$$

One can confirm this result agrees with Section 7.2.1 when we take the adiabatic limit  $\omega \rightarrow 0$  for a fixed  $\kappa$ , giving  $g_c^2 / \kappa \sim \omega_0^{2-2K} \rightarrow 0$ .

### Phonons in two dimensions

Just like in 1D, we integrate out the phonons, yielding a retarded monopole-monopole interaction on top of  $\mathcal{L}_c$  in (7.12), of the form

$$S_{\Phi\Phi} = -2g^2 \int d^d x d^d y \sum_{i=1}^2 \Phi_i(x) G(x-y) \Phi_i(y) \quad (7.49)$$

where we have written  $x = (\tau_x, \mathbf{x})$  and  $y = (\tau_y, \mathbf{y})$ . The phonon propagator is given by

$$G(x-y) = \frac{1}{2\rho\omega_0} e^{-\omega_0|\tau_x-\tau_y|} \delta(\mathbf{x}-\mathbf{y}). \quad (7.50)$$

Again, we consider first the adiabatic ( $\omega_0 \rightarrow 0$ ) and antiadiabatic ( $\omega_0 \rightarrow \infty$ ) limits separately. The adiabatic case has been studied above. In the antiadiabatic case, we can make use of the delta-function identity (7.36). Using the mapping between monopoles and the VBS order parameter in the NLSM, this coupling generates an additional anisotropy

$$\mathcal{L}_2^{\text{NLSM}}[\tilde{\mathbf{n}}] + s(\mathbf{n}^2 - \mathbf{v}^2) - \frac{2g^2}{\rho\omega_0^2} (v_1^2 + v_2^2), \quad (7.51)$$

At first, it might seem like this destroys the emergent symmetry at the critical point  $s = 0$ . But observe that we can rewrite

$$s(\mathbf{n}^2 - \mathbf{v}^2) + \frac{2g^2}{\rho\omega_0^2} (v_1^2 + v_2^2) = \left( s + \frac{g^2}{\rho\omega_0^2} \right) (\mathbf{n}^2 - \mathbf{v}^2) - \frac{g^2}{\rho\omega_0^2} (\mathbf{n}^2 + \mathbf{v}^2). \quad (7.52)$$

From  $(\mathbf{n}^2 + \mathbf{v}^2) = 1$ , we find that in the antiadiabatic limit, the transition is simply shifted by

$$s_c = 0 \xrightarrow{\omega_0 \gg 0} s_c = -\frac{g^2}{\rho\omega_0^2}, \quad (7.53)$$

as in the 1D case. Now, let us turn to the case between where the transition changes from first order to DQC. Observe first that we can rescale the theory by  $x_i = \frac{x'_i}{\omega_0}$  to move all dependence on  $\omega_0$  into the coupling. The interaction now reads

$$S_{\Phi\Phi} = \frac{g^2}{\rho_0\omega^{5-2\Delta_\Phi}} \int d^2\mathbf{x} d\tau'_x d\tau'_y \sum_{i=1}^2 \Phi_i(\tau'_x) e^{-|\tau'_x - \tau'_y|} \Phi_i(\tau'_y), \quad (7.54)$$

where from now on we suppress the space-dependence of the monopole. Now we can perform a formal expansion of the monopole

$$\Phi_i(\tau'_y) = \Phi_i(\tau'_x) + (\tau'_y - \tau'_x) \partial_{\tau'_x} \Phi_i(\tau'_x) + \frac{1}{2} (\tau'_y - \tau'_x)^2 \partial_{\tau'_x}^2 \Phi_i(\tau'_x) + \mathcal{O}((\tau'_x)^3). \quad (7.55)$$

and perform the  $\tau'_y$  integration to find

$$\sim \frac{2g^2}{\rho_0\omega^{5-2\Delta_\Phi}} \int d^2\mathbf{x}' \int d\tau'_x \sum_{i=1}^2 [\Phi_i^2 - (\partial_{\tau'_x} \Phi_i)^2]. \quad (7.56)$$

The first term simply generates an anisotropy, just like in the  $\omega_0 \rightarrow \infty$  limit. At first glance, the form of the anisotropy is different than in (7.53). However, we have to keep in mind that the coordinates in (7.56) have been rescaled. In order to add this to the anisotropy in the NLSM, we must revert back to the original coordinates resulting in the correct shift (7.53). The second term simply modifies the kinetic term in the NLSM description. We therefore believe that DQCP will break down when this perturbative treatment breaks down and higher orders in the Taylor expansion (7.55) have to be included; this is  $2g^2/(\rho\omega_0^{5-2\Delta_\Phi}) \sim 1$ . This suggests a critical scaling  $g_c^2 \sim \rho\omega_c^{5-2\Delta_\Phi}$ . This scaling argument can be performed in general dimension, revealing a critical

$$g_c^2 \sim \rho\omega_c^{3+d-2\Delta_\Phi} \quad \longleftrightarrow \quad g_c^2 \sim \kappa\omega_c^{1+d-2\Delta_\Phi}. \quad (7.57)$$

This is consistent with the results obtained in 1D (where  $\sin(2\phi)$  plays the role of  $\Phi$ ), and is also compatible with an alternative CFT-based stability analysis of the  $D = 2$  Dirac QSL.

We summarise our results for the stability of the DQCP in Figure 7.10 for a range of frequencies  $\omega$ . We simultaneously take the adiabatic  $\omega \rightarrow 0$  and antiadiabatic  $\omega \rightarrow \infty$  limits by keeping  $\kappa = \rho\omega_0^2$  constant. This choice to take  $\rho \rightarrow 0$  as  $\omega_0 \rightarrow \infty$  means that the shift of the transition (7.53) in the antiadiabatic limit remains finite.

### 7.3 Outlook

In this Chapter, we have outlined conditions regarding the stability of the DQCP under coupling to lattice degrees of freedom. The instability occurs for infinitesimal couplings when

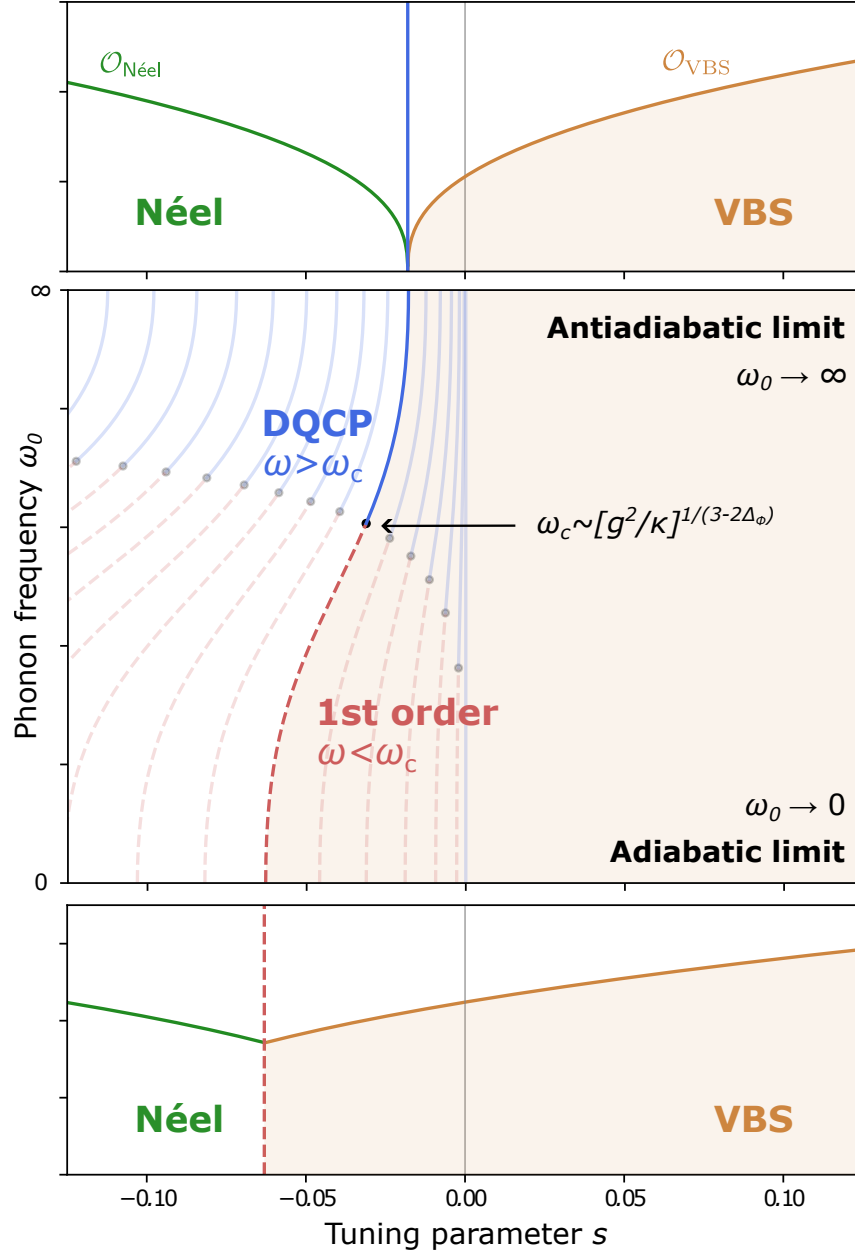


Figure 7.10: *Nature of the Néel–VBS phase transition on the square lattice as a function of phonon frequency  $\omega_0$ , with  $\kappa = \rho\omega_0^2$  constant. For  $\omega_0 \rightarrow \infty$  (the antiadiabatic limit, top panel), the critical  $s_c$  is shifted but the transition remains second order. This DQCP persists down to  $\omega_c$ , below which it becomes first order. For  $\omega_0 \rightarrow 0$  (the adiabatic limit, bottom panel), the transition occurs at  $s_{\text{static}}$ , given by Eq. (7.31). Shown here is  $g = 0.3$ ,  $\kappa = 1$ , with a range of  $g = 0.0$ – $1.0$  shown in the background.*

considering static distortions, while finite phonon frequencies protect the system up to some non-zero critical spin-lattice coupling. Hence, gapless systems that admit strongly relevant instantons which precipitate VBS order may be susceptible to a spin-Peierls distortion upon coupling to the lattice, in particular also in higher-dimensional systems (in addition to the familiar one-dimensional examples). For the DQCP to remain stable, the spin-lattice coupling must be smaller than some critical value that depends on the phonon frequency. The scaling relations obtained here are consistent with the ones obtained for the U(1) Dirac QSL. Though, of course, the exact microscopic instability is lattice- and even model-dependent.

While the existence of a true DQCP on the original square lattice model is still under debate (Nahum *et al.*, 2015a; Poland *et al.*, 2019; Ma and Wang, 2020; Nahum, 2020; D’Emidio *et al.*, 2023; Takahashi *et al.*, 2024), our results may be expected to hold also for a scenario of a weakly-first order regime and approximate criticality. More recently, it has been argued that QED<sub>3</sub> provides an effective theory for “unnecessary” quantum critical points and the surrounding critical regime (Zhang *et al.*, 2025), by starting with the observation that the U(1) Dirac QSL on the square lattice admits a G<sub>UV</sub>-singlet relevant monopole deformation  $\Phi_2$ . Tuning its coupling  $\lambda$  therefore can be understood as a DQCP-like control parameter. Crucially, in the scenario at hand, the nature of the resulting phase is argued to be independent of  $\lambda$ , and therefore  $\lambda = \lambda_c$  may be a critical point *within the same phase*. Adding spin-lattice couplings, the VBS monopole can be expected to couple to the distortion modes  $u_{1,2}$ , which are precisely those also discussed in Eq. (7.26). We expect that the system spontaneously generates a lattice distortion in the adiabatic limit. The impact on the unnecessary critical point depends on the surrounding phases: (i) In the case of the VBS–VBS critical point, it is plausible that the transition will be generically removed; instead of the VBS gap going to zero with a power law  $\beta = \nu_\Phi \Delta_\Phi$ , it will have a finite minimum on the order of  $\Delta_0 \sim (g^2/\kappa)^{1/(3-2\Delta_\Phi)}$ . (ii) For the Néel–Néel critical point, we hypothesise that the second order transition would split into two first order Néel–VBS transitions. There would be an island of VBS order within the Néel phase, induced by the interaction of the lattice with strongly relevant monopoles. This intermediate VBS order would exist for  $|\lambda| < [g^2/\kappa]^{(3-\Delta_\Phi)/(3-2\Delta_\Phi)}$ . In the antiadiabatic limit  $\rho \rightarrow \infty$ , we deduce that the unnecessary DQCP is preserved, which holds at finite- $\omega_0$  above a critical frequency  $\omega_c^2 \sim [g^2/\kappa]^{3-2\Delta_\Phi}$ .

We highlight that the  $\omega_0$ -dependent shift in the new transition point implies that a DQCP can be tuned *by varying phonon frequency*. This has recently been observed in a series of numerical studies (Götz *et al.*, 2024a,b). Quantum Monte Carlo simulations of lattice models for DQCP in 2D are notoriously hard due to the existence of a sign problem. Remarkably, it has recently been pointed out that a sign-problem free formulation of the Su–Schrieffer–Heeger–Hubbard model realises an effective unconstrained  $\mathbb{Z}_2$  gauge theory, with quantum Monte Carlo simulations providing evidence for a direct continuous Néel–VBS transition (Karakuzu *et al.*, 2018). Götz *et al.* (2024a) studied this model coupled to the lattice, and provide a first example of a DQCP tuned by phonon frequency. This is entirely compatible with our Fig. 7.10: For large  $\omega$  and taking a value of  $s$  close to the phase transition, we see that reducing  $\omega$  will drive the DQCP. By making  $s$  more negative, the value of  $\omega_0$  at the transition can be reduced. Our results imply that when  $\omega_0 < \omega_c$ , this transition must become first order. This behaviour has been confirmed in a follow-up study Götz *et al.* (2024b). We interpret the continuous phonon-driven transition as being a manifestation of

our spin-Peierls mechanism.

Going forward, it will be highly desirable to quantitatively extract the shift of the location of the DQCP as well as the regime of stable criticality as a function of spin-lattice coupling and phonon frequency. Given limited system sizes and the required double scaling, this is expected to be a more challenging task in 2D. In 1D, however, many numerical studies of quantum spin chains coupled to phonons exist, see, e.g. the works by Weber *et al.* (2020); Weber (2023); Uhrig (1998); Ferrari *et al.* (2020) and references therein. We expect it to be possible to extract the aforementioned features in 1D. The extracted critical exponents in higher dimension would provide interesting insight into the nature of the DQCP and the field theory’s operator content.

Turning towards experiments, a recent study observed “proximate-DQCP” behaviour between plaquette-solid and AFM phases in  $\text{SrCu}_2(\text{BO}_3)_2$  under tuning of the magnetic field (Cui *et al.*, 2023). The regime of quantum-critical scaling observed here was not reproduced in another work which instead tunes pressure to induce the transition (Guo *et al.*, 2025). Varying pressure is a standard technique to tune magnetic couplings, but inherently also changes the phonon energy scale. Due to the significant interplay of spin and lattice degrees of freedom in candidate DQCP materials, the strong first-order transition here does not necessarily exclude the potential of observing an underlying DQCP by tuning lattice-independent parameters. We emphasise, as has been previously suggested by Mila (2023), that clarifying the interplay of spin and lattice degrees of freedom in such system may be crucial for a more complete understanding. These results therefore constitute a step towards understanding the conditions for deconfined quantum criticality in realistic experiments (Lee *et al.*, 2019).

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## 8.1 Spin dynamics beyond mean-field theory

Quantum spin liquids are strongly interacting states. In Chapter 3, we introduced a method of calculating the dynamical spin structure factor for general spin liquid Ansätze. This used a self-consistent parton mean-field theory combined with the random phase approximation. This technique allows us to treat the interactions between the emergent spinons, going beyond pure mean-field approaches which have been applied previously. The results for the  $J_1$ – $J_2$  Heisenberg model on the triangular lattice are in superb agreement with numerical works. We also studied the chiral spin liquid using a perturbative treatment of the spin-scalar chirality interaction.

Our developments will find immediate application in several areas. It will be simple to include the effects of longer range hoppings  $J_3$  and spin anisotropy  $\Delta$  to this model. The predictions for dynamics in this context can be compared to other recent works (Bose and Paramakanti, 2025; Flores-Calderón *et al.*, 2025). Moreover, we are interested in describing fractionalised physics within ordered phases, and would like to understand if a self-consistent treatment is possible here too. Most significantly, we hope to extend our approach to other dynamical response functions. In this context, the immediate candidate is the dimer structure factor (Läuchli *et al.*, 2008). These can be probed using the same VMC and DMRG methods, and our analysis could once again provide very useful in interpreting the results. There is good reason to think that the dimer response function will not be dominated by spinon bound states in the same way as the spin structure factor. This result will also directly produce predictions for Raman and resonant inelastic X-ray scattering experiments. Because of the potential lack of low-lying bound states of spinons, we suggest that this dimer sector will be a more pure test of QED<sub>3</sub> physics. Experiments which probe it could be crucial in confirming this exotic phase in  $J_1$ – $J_2$  models.

The dynamical structure factor can be probed in experiment. We compared our results in Chapter 4 to recent inelastic neutron scattering data in the compounds KYbSe<sub>2</sub> and NaYbSe<sub>2</sub>. We find signatures of fractionalisation coexisting with sharp modes. While compatible with the picture of a spinon-exciton in a monopole continuum, we are cautious at this stage. Constraining the exact nature of the state will require pinning down the exact behaviour of the continua at  $\mathbf{M}$  and  $\mathbf{K}$ . There exist many possible competing explanations, and future work should focus on understanding which minimal model accurately describes the measured data.

Another line of investigation we are interested in pursuing in this context is in understanding dynamical *real-space correlations* of 2D frustrated magnets. Real-space correlations  $G(\mathbf{r}, t)$  can be defined simply through the Fourier transform of the dynamical spin susceptibility  $\chi(\mathbf{q}, \omega)$ . First proposed by Van Hove (1954), they have recently been used to interpret

fractionalised behaviour in 1D spin chains (Scheie *et al.*, 2022; Laurell *et al.*, 2022). The real-space correlations exhibit many interesting features in this case. Firstly, the imaginary part has a light-cone structure, typical of quantum-critical dynamics (Giamarchi, 2003). Furthermore, within this light-cone there are rich ‘wake dynamics’, which can be interpreted as being due to scattering dynamics of the spinons. These features make direct contact with the conformal field theory- and Bethe Ansatz-descriptions of spin chains. We believe the real power of this approach will lie in the future. Quantum simulators might exist in the next years which can calculate dynamics of spin models (Satzinger *et al.*, 2021; Bintz *et al.*, 2024). The dynamical spin correlations will be simulated directly in real space and time. Using quantum-matter realisations as a benchmark for this will require a combination of theoretical understanding of the underlying states, as well as knowing how effects like disorder and interactions manifest in this correlation function.

## 8.2 Roadblocks to emergence

Quantum spin liquids are enigmatic states that are defined by more than just the absence of spin-ordering. As states beyond Landau’s paradigm, they naturally break many intuitions about the properties of matter. In this Thesis, we have investigated some of the consequences and limitations of fractionalisation and emergent gauge fields. We did this by investigating the dynamics and stability of the Dirac spin liquid. We will soon summarise our contributions towards these two theoretical challenges in more detail, but let us first make some general comments about the fate of emergent gauge theories.

It remains truly surprising that such complexity can arise from a model of interacting spins. We saw that local gauge degrees of freedom naturally arise when we use the parton representation, which itself leads to novel types of monopole excitations. One theme that has been recurrent in this Thesis is the emergence of large continuous global symmetries. This behaviour represents an anti-GUT, an anti-grand unified theory, in the sense that the larger symmetry group occurs in the IR at low energy scales (Volovik, 2009; McGreevy, 2019). Specifically, we came across a  $U(1) \times U(1)$  symmetry in spin chains, an  $SU(4) \times U(1)_{\text{topo}}$  symmetry in the Dirac spin liquid, and an  $SO(5)$  symmetry in the DQCP. These are not present in the lattice scale model, but are an unexpected result of the emergent conformal theory. We discussed already in Section 2.4 that this emergent symmetry is not seen in simulations of the  $J_1$ – $J_2$  Heisenberg model, at least so far. We have given two mechanisms in this work which explain why. We found that this symmetry can be directly broken by coupling the spin-singlet and spin-triplet monopoles to different quasiparticles in the spectrum. In Chapter 3 this was the spinon exciton mode, and in Chapters 5–7 this was a phonon (in various incarnations). Spin-0 phonons only couple to one sector, and spin-1 spinon bound states only couple to another. The energy scales of these modes are fixed by Hamiltonian parameters, and hence also the upper bound on where we might see signs of anti-GUT emergence.

### Phase diagrams of spin models

The RPA approach also tells us something fundamental about the applicability of mean-field states to describe spin liquids. Typically, it is said that a mean-field Ansatz is defined by a

set of parameters, for U(1) symmetric states these are  $(\chi_{ij}, a_i^0)$ . Within the framework of mean-field theory, it is commonplace to consider the influence of gapless gauge fluctuations on stability. This is done at ‘first-order’ MFT by studying the stability of the emergent continuum gauge theory. However, it was thought that the amplitude fluctuations will remain gapped.

To this end, we were inspired to look at stability against competing spin orders by decades of studies of magnetic states in Hubbard models; see for example the works by Weng *et al.* (1991); Singh (2005); Scholle *et al.* (2024) among others. This includes our own work on the next-nearest-neighbour hopping ( $t-t'$ ) triangular lattice Hubbard model (Willsher *et al.*, 2023). There, we showed that it is possible to generate a phase diagram of competing stripe and 120-degree orders by mapping where the resulting collective modes are stable. This intuition has carried over to quantum spin liquids and our analysis of the spinon exciton. We must expand the definition of the mean-field parameters to include zero magnetic order  $\mathbf{n}_i = 0$ . Then, we must check that the fluctuations of this magnetic order around zero amplitude remain gapped. Their condensation signals a neighbouring ordered phase.

Given our observation that this method enjoys good quantitative success on the triangular lattice, we are urged to reproduce numerical works which include spin anisotropy (Gallegos *et al.*, 2025) or longer range  $J_3$  exchanges (Gong *et al.*, 2019). In these works, the authors find a variety of exotic phases including supersolid phases and chiral spin liquids (even without explicitly breaking time-reversal symmetry). Once again, describing fractionalisation within these ordered or competing spin liquids would provide a more comprehensive theoretical insight into these phase diagrams. We also suggest that a large number of other quantum magnets can be described in this way. This is because they often emerge around highly frustrated points which separate two competing orders. Another classic example here is the  $J_2/J_1 = 1/2$  square lattice Heisenberg model where numerical studies (Zhang *et al.*, 2003; Wang *et al.*, 2013; Ferrari *et al.*, 2020) point to a gapped spin liquid state. With our new self-consistent RPA approach for spin liquids, phase diagrams are no longer just in the purview of numerical simulation.

## Monopoles

Instantons pose an existential threat to gapless spin liquids. Critical phases with relevant, symmetry-forbidden operators have a tendency to spontaneously break the symmetries. We saw that this effect — while well understood in 1D as the Peierls and spin-Peierls instabilities — also occurs in 2D. The condition for this instability is as follows: (i) the system (in the absence of a distortion) is critical and (ii) the energy gain due to the gap opening stemming from the distortion coupling to the lattice-symmetry breaking operator  $\mathcal{O}$  scales with  $\frac{d}{d-\Delta_{\mathcal{O}}} < 2$ , where  $\Delta_{\mathcal{O}}$  is the scaling dimension of  $\mathcal{O}$  and  $d = D + 1$  is the space-time dimension. This is satisfied when  $\Delta_{\mathcal{O}} < d/2$ . Such a lattice symmetry breaking operator often exists in quantum magnets as a (fluctuating) VBS order parameter. Whenever such an operator is present, the state will have critical correlations of the VBS order parameter  $\chi_{\mathcal{D}}(\omega \rightarrow 0) \rightarrow \infty$  where the divergence is controlled by the exponent  $d - 2\Delta_{\mathcal{O}}$ . We identify these critical correlations as the origin of the strong Kohn anomaly and consequential instability of the lattice.

This leads us to ask whether there might be any other instances which are unstable in the same way. One such proposed model is the non-Lagrangian  $N = 7$  Stiefel liquid (Zou *et al.*, 2021). This is a non-Lagrangian phase which intertwines competing VBS and non-coplanar magnetic orders. The monopoles of this U(1) theory are potentially highly relevant (He *et al.*, 2022), and so we bring into question a spin-Peierls instability for this phase too. Our results may be generally understood as a natural obstacle to the intertwinement of VBS and anti-ferromagnetic orders. Any deconfined critical phases or points that lie between competing orders might be spoiled in magnetic realisations by the influence of the lattice.

### 8.3 Outlook

Many questions remain unanswered. Most pressing, we need better ways to distinguish competing spin-liquid and ordered states in materials. One route towards clarity is using perturbations to manipulate the ground state. Effects like magnetic field, hydrostatic pressure, and strain can change the magnetic state and sensitively probe the excitations of a quantum magnet (Balents and Starykh, 2020; Bachus *et al.*, 2020). By measuring the evolution of the spectrum and response functions in this way, we hope there might be less ambiguity fractionalised features. However this requires further theoretical advances.

It remains an open theoretical challenge to understand the monopoles we have discussed theoretically. Recent progress in forming their variational wavefunctions promises to shed light on them (Budaraju *et al.*, 2023, 2025). Studying the properties of these monopoles in the presence of perturbations might allow us to distinguish the universal from non-universal physics. These methods could allow for a richer understanding of these exotic excitations.

Quantitatively understanding the effects of disorder on spin liquids is another important theoretical challenge. Defects in the lattice locally break symmetries and can introduce interesting physics, for example binding local fermion modes (Willans *et al.*, 2010, 2011; Petrova *et al.*, 2014) which can then be measured using dynamical probes (Nambiar *et al.*, 2023; Kao *et al.*, 2024). Beyond this weak-disorder regime, it remains unknown what the fate of spin liquids are in amorphous materials, except for recent progress in Kitaev's exactly soluble model (Cassella *et al.*, 2023; Grushin and Repellin, 2023). Our understanding of spin liquids relies heavily on using lattice symmetries to classify states and guarantee stability. It would be an interesting discovery if there existed mean-field states which go beyond this paradigm.

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### Free fermion bubble

Defining each of the lines in Eq. (3.24) in terms of single-particle propagators

$$\mathcal{G}_{\alpha\beta}^{XY}(\mathbf{q}, \tau) = -\langle T_\tau f_{\alpha X, \mathbf{q}}(0) f_{\beta Y, \mathbf{q}}^\dagger(\tau) \rangle, \quad (\text{A.1})$$

and after imposing  $\mathbf{k}' = \mathbf{k} + \mathbf{q}$  the susceptibility reads

$$[\chi^0(\mathbf{q}, i\omega_n)]^{XY} = \frac{1}{4N} \int d\tau e^{-i\omega_n \tau} \sum_{\mathbf{k}} (\sigma^z)_{\alpha\beta} (\sigma^z)_{\gamma\delta} \mathcal{G}_{\delta\alpha}^{YX}(\mathbf{k}, \tau) \mathcal{G}_{\beta\gamma}^{XY}(\mathbf{k} + \mathbf{q}, -\tau) \quad (\text{A.2})$$

$$= \frac{1}{4N\beta} \sum_{\mathbf{k}, i\nu_n} \text{Tr}[\sigma_X^z \cdot \mathcal{G}(\mathbf{k} + \mathbf{q}) \cdot \sigma_Y^z \cdot \mathcal{G}(\mathbf{k})] \quad (\text{A.3})$$

We sum here over fermionic Matsubara frequencies  $\omega_n = (2n+1)\pi/\beta$ ; see Appendix D in (Auerbach, 1998). A summation over the free fermion Greens functions gives

$$[\chi^0(\mathbf{q}, i\omega_n)]^{XY} = -\frac{1}{4N} \sum_{\mathbf{k}, mn} \frac{(n_{\mathbf{k}}^m - n_{\mathbf{k}+\mathbf{q}}^n) \mathcal{V}_X^{mn} (\mathcal{V}_Y^{mn})^*}{i\omega_n + \varepsilon_{\mathbf{k}}^m - \varepsilon_{\mathbf{k}+\mathbf{q}}^n}. \quad (\text{A.4})$$

and analytic continuation back into real-frequencies gives the free susceptibility as written in Eq. 3.25. The matrix elements are defined in the main text.

### Interactions

Beyond the free-fermion approximation, the dynamical spin susceptibility will be corrected due to the Heisenberg interactions, written in Eq. (3.29). This contributes the following series of diagrams which we will resum with the random phase approximation (RPA)

$$\text{Diagram with shaded bubble} = \text{Diagram with empty bubble} + \text{Diagram with two bubbles} + \dots \quad (\text{A.5})$$

In the main text, we argue that these factorise into a geometric series with an interaction proportional to the Heisenberg interaction matrix in the sublattice basis. Here, we will fix the proportionality constant by perturbatively evaluating the first-order correction using Wick's theorem.

The Heisenberg interaction Eq. (3.31) in momentum space reads

$$\mathcal{H}_I = \sum_{X'Y', \mathbf{q}'} J_{\mathbf{q}}^{X'Y'} \mathcal{J}_{\alpha'\beta'\gamma'\delta'} \sum_{\mathbf{p}, \mathbf{p}'} f_{\alpha'X', \mathbf{p}-\mathbf{q}'}^\dagger f_{\beta'X', \mathbf{p}'} f_{\gamma'Y', \mathbf{p}'+\mathbf{q}'}^\dagger f_{\delta'Y', \mathbf{p}} \quad (\text{A.6})$$

where the spin matrix-elements are given by the tensor

$$\mathcal{J}_{\alpha'\beta'\gamma'\delta'} = \frac{1}{4}(\vec{\sigma})_{\alpha'\beta'} \cdot (\vec{\sigma})_{\gamma'\delta'} = \frac{1}{2} \left( \delta_{\alpha'\delta'} \delta_{\beta'\gamma'} - \frac{1}{2} \delta_{\alpha'\beta'} \delta_{\gamma'\delta'} \right). \quad (\text{A.7})$$

Correlation functions are given by

$$\langle T_\tau [f_{m,k}^\dagger f_{n,k+q}](\tau) [f_{r,k+q}^\dagger f_{s,k}](0) \rangle = \frac{\langle T_\tau [f_{m,k}^\dagger f_{n,k+q}](\tau) [f_{r,k+q}^\dagger f_{s,k}](0) S(\infty) \rangle}{\langle S(\infty) \rangle} \quad (\text{A.8})$$

where the S-matrix in imaginary time is

$$S(\infty) = T_\tau e^{-H_I}, \quad H_I = \int_{-\infty}^{\infty} d\tau \mathcal{H}_I. \quad (\text{A.9})$$

This is to be understood as a series expansion of  $S$  in powers of  $H_I$ . The denominator acts to cancel disconnected diagrams. The leading contribution  $S(\infty) = 1$  gives the bare susceptibility as written above. The next contribution comes from connected contractions of the following

$$\text{Diagram} \sim -\langle T_\tau [f_{m,k}^\dagger f_{n,k+q}](\tau) H_I [f_{r,k+q}^\dagger f_{s,k}](0) \rangle \quad (\text{A.10})$$

which is an eight-fermion correlator. The indices  $\alpha\beta\gamma\delta$  are to be contracted with external Pauli matrices, and the internal indices are to be contracted with the Pauli matrices Eq. (A.7). Now we will evaluate explicitly the correction to the susceptibility Eq. (3.23) due to this first-order correction in perturbation theory

$$\begin{aligned} &= \frac{1}{4N^2} (\sigma^z)_{\alpha\beta} (\sigma^z)_{\gamma\delta} \int d\tau e^{-i\omega_n \tau} \sum_{\mathbf{k}} \int d\tau' \\ &\quad \sum_{X'Y',q} J_q^{X'Y'} \mathcal{J}_{\alpha'\beta'\gamma'\delta'} \sum_{p,p'} \langle T_\tau [f_{\alpha X,k}^\dagger f_{\beta X,k+q}](\tau) \\ &\quad \times [f_{\alpha' X',p-q}^\dagger f_{\beta' X',p'} f_{\gamma' Y',p'+q}^\dagger f_{\delta' Y',p}](\tau') [f_{\gamma Y,k'}^\dagger f_{\delta Y,k'-q}](0) \rangle \quad (\text{A.11}) \end{aligned}$$

We keep only the connected diagrams which are non-zero; they come from the following contractions

$$\begin{aligned} &\langle f_{\beta' X',p'}(\tau') f_{\alpha X,k}^\dagger(\tau) \rangle \langle f_{\beta X,k+q}(\tau) f_{\alpha' X',p-q'}^\dagger(\tau') \rangle \\ &\quad \times \langle f_{\delta Y,k'-q}(0) f_{\gamma' Y',p'+q'}^\dagger(\tau') \rangle \langle f_{\delta' Y',p}(\tau') f_{\gamma Y,k'}^\dagger(0) \rangle \\ &\quad + \langle f_{\beta' X',p'}(\tau') f_{\gamma Y,k'}^\dagger(0) \rangle \langle f_{\beta X,k+q}(\tau) f_{\gamma' Y',p'+q'}^\dagger(\tau') \rangle \\ &\quad \times \langle f_{\delta Y,k'-q}(0) f_{\alpha' X',p-q'}^\dagger(\tau') \rangle \langle f_{\delta' Y',p}(\tau') f_{\alpha X,k}^\dagger(\tau) \rangle. \quad (\text{A.12}) \end{aligned}$$

The tedious calculation proceeds as follows: Express this in terms of Green's functions, substitute the interaction matrix elements (A.7), and simplify the resulting terms. At the end

we find

$$\begin{aligned}
&= -\frac{1}{N^2\beta^4} \int d\tau e^{-i\omega_n\tau} \sum_{\mathbf{k}\mathbf{k}'} \int d\tau' \sum_{X'Y',q} J_q^{X'Y'} \left\{ \right. \\
&\quad \text{Tr} \left[ \frac{1}{4} \sigma^z \mathcal{G}^{XX'}(\mathbf{k} + \mathbf{q}, \tau - \tau') \sigma^i \mathcal{G}^{X'X}(\mathbf{k}, \tau' - \tau) \right] \\
&\quad \times \text{Tr} \left[ \frac{1}{4} \sigma^i \mathcal{G}^{YY'}(\mathbf{k}', \tau') \sigma^z \mathcal{G}^{Y'Y}(\mathbf{k}, -\tau') \right] \\
&\quad + \text{Tr} \left[ \frac{1}{4} \sigma^z \mathcal{G}^{XX'}(\mathbf{k} + \mathbf{q}, \tau - \tau') \sigma^i \mathcal{G}^{X'X}(\mathbf{k}, \tau' - \tau) \right] \\
&\quad \left. \times \text{Tr} \left[ \frac{1}{4} \sigma^i \mathcal{G}^{YY'}(\mathbf{k}', \tau') \sigma^z \mathcal{G}^{Y'Y}(\mathbf{k}, -\tau') \right] \right\} \quad (\text{A.13})
\end{aligned}$$

Finally, perform the  $\tau$  integrals and then factorise the bare susceptibilities (A.3) to get the leading contribution (A.10) as a function of imaginary frequencies

$$\begin{aligned}
\text{Diagram} &= - \left\{ [\chi^0(\mathbf{q}, \omega)]^{XX'} J_q^{X'Y'} [\chi^0(\mathbf{q}, \omega)]^{Y'Y} + [\chi^0(\mathbf{q}, \omega)]^{XY'} J_{-q}^{X'Y'} [\chi^0(\mathbf{q}, \omega)]^{X'Y} \right\} \\
&= -2 [\chi^0(\mathbf{q}, \omega)]^{XX'} J_q^{X'Y'} [\chi^0(\mathbf{q}, \omega)]^{Y'Y}. \quad (\text{A.14})
\end{aligned}$$

where we used  $J_{-q}^{Y'X'} = (J_{-q}^{X'Y'})^* = J_q^{X'Y'}$ . We hence identify the interaction matrix

$$U_q^{XY} = \text{Diagram} = -2J_q^{XY}, \quad (\text{A.15})$$

where  $J_q^{XY}$  is the Fourier transform of the Heisenberg interaction  $J_{ij}$  in the sublattice basis. We use this form in the main text.

## Spinon exciton effective theory

### Bosonic perturbation theory

We will evaluate the effective potential for the spin-amplitude fluctuations  $\varphi_q$  in Fourier space. The interacting theory reads

$$- \sum_{ij} J_{ij}^{-1} \vec{m}_i \cdot \vec{m}_j + 2 \sum_i \vec{m}_i \cdot \vec{S}_i = \sum_q \left[ -J_q^{-1} |\varphi_q|^2 + (\varphi_q \hat{n}_q \cdot \vec{S}_{-q} + \text{c.c.}) \right] \quad (\text{A.16})$$

where  $\vec{m}_q = \varphi_q \hat{n}_q$ . The first term gives the bare mass of the bosonic propagator

$$J_q^{-1} |\varphi_q|^2 = \text{Diagram} \quad (\text{A.17})$$

where

$$\begin{aligned}
J_q &= J_1 [\cos(k_2) + \cos(k_1/2 - k_2) + \cos(-k_1/2)] \\
&\quad + J_2 [\cos(k_1/2 + k_2) + \cos(k_1 - k_2) + \cos(2k_2 - k_1/2)]. \quad (\text{A.18})
\end{aligned}$$

Following (Bose and Paramakanti, 2025), we find that integrating out the fermions creates a self-energy for this bosonic mode proportional to the free fermion bubble  $\Sigma_\varphi(\mathbf{q}, \omega) = -2\chi^0(\mathbf{q}, \omega)$ . The susceptibility is defined as the sum over the sublattice-resolved bare bubble (3.19)

$$\chi^0(\mathbf{q}, i\omega) = \frac{1}{4N} (R_{\mathbf{q},X}^\dagger R_{\mathbf{q},Y}) \sum_k \text{Tr}[\sigma_X^z \mathcal{G}(k) \sigma_Y^z \mathcal{G}(k+\mathbf{q})] = \text{bubble diagram} \quad (\text{A.19})$$

We can resum this one-loop contribution to form the self energy of the boson, which incorporates the sum of all 1PI-irreducible diagrams

$$\begin{aligned} G_\varphi(\mathbf{q}, \omega) &= \text{double line} = \text{dashed line} + \text{dashed line} \text{ bubble} \text{ dashed line} + \dots \\ &= \frac{1}{m_0^2 - 2\chi^0(\mathbf{q}, \omega) + \mathbf{q}^2 - \omega^2} = G_0(\mathbf{q}, \omega) - 2G_0(\mathbf{q}, \omega)\chi^0(\mathbf{q}, \omega)G_0(\mathbf{q}, \omega) + \dots \end{aligned} \quad (\text{A.20})$$

The form written in the main text includes the sublattice structure of the spin-order parameters.

### Landau–Ginzburg theory

The effective potential for the boson is Eq. (3.63)

$$V(\varphi_{\mathbf{q}}) = \tilde{m}(\mathbf{q})\varphi_{\mathbf{q}}^2 = \left[ \frac{-1}{j_1 + rj_2} - 2\Pi_{\mathbf{q}}^0 \right] \varphi_{\mathbf{q}}^2 + \dots, \quad (\text{A.21})$$

where here we have written  $j_{\mathbf{q}} = J_1(j_1 + rj_2)$ , via Eq. (3.57). Solving for the roots of this equation to identify the critical tuning parameter  $r_c$ , we find

$$r_c(\mathbf{q}) = \frac{1}{j_2} \left( \frac{2}{\Pi_{\mathbf{q}}^0} - j_1 \right). \quad (\text{A.22})$$

Finally, we expand the effective potential around the critical point to leading order to find

$$V(\varphi_{\mathbf{q}}) = j_2 \left( \frac{1}{2}\Pi_{\mathbf{q}}^0 \right)^2 [r - r_c(\mathbf{q})] + \dots. \quad (\text{A.23})$$

This is our Ginzburg–Landau theory for the spinon-exciton condensation transition.

Substituting in the momenta  $\mathbf{M}$  and  $\mathbf{K}$ , we find

$$\begin{aligned} \mathbf{K} : \quad & j_1 = -3/2, \quad j_2 = 3; \\ \mathbf{M} : \quad & j_1 = -1, \quad j_2 = -1. \end{aligned} \quad (\text{A.24})$$

This produces the mean-field masses Eq. (3.59). The zero-energy susceptibilities  $\Pi_{\mathbf{q}}$  are very inexpensive to numerically calculate, since it is just the evaluation of the sum Eq. (3.23) at one value of  $\mathbf{q}$  and  $\omega = 0$ .

$$\Pi_{\mathbf{K}}^0 = 1.556103, \quad \Pi_{\mathbf{M}}^0 = 1.6950. \quad (\text{A.25})$$

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These values were calculated on  $L = 3600$  systems within minutes on a laptop computer. The resulting critical points are written in the main text in Eqns. (3.64), (3.65). The coefficients in the linearised potential (3.63) are

$$A^{120} = 3(\Pi_K^0/2)^2 = 1.816, \quad A^{\text{stripe}} = (\Pi_M^0/2)^2 = 0.718. \quad (\text{A.26})$$

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## Landau theory of the spin-Peierls transition Appendix B

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### Conformal field theory

In this Appendix, we will first outline some technical details that were brushed over in the main text. These will be necessary to perform two perturbative calculations which support the results of Chapters 5 and 6. Firstly, we want to derive the potential Eq. (5.43). We will then provide a third calculation for the scaling of the critical frequency Eq. (6.13).

#### OPEs

The operator product expansion (OPE) states how operators approaching each other are expanded in the basis of primaries as

$$\lim_{x \rightarrow y} \mathcal{O}_i(x) \mathcal{O}_j(y) = \lim_{x \rightarrow y} \sum_k \frac{C_{ij}^k}{|x - y|^{\Delta_i + \Delta_j - \Delta_k}} \mathcal{O}_k(y), \quad (\text{B.1})$$

where the  $C_{ij}^k$  are the OPE coefficients. If the CFT is endowed with some global symmetry group  $\mathcal{G}$ , each term on the RHS of (B.1) will transform in some irreducible representation of  $\mathcal{G} \times \mathcal{G}$ . We stress that Eq. (B.1) corresponds to the asymptotic formulation of the OPE, but in general, OPEs can be shown to be convergent series if all primaries and their descendants are included. The full asymptotic form of the operators can be written in terms of the two real OPE coefficients  $C_{\Phi\Phi}^M$  and  $C_{M\Phi}^\Phi$  in the following way:

$$\Phi_a^\dagger(x) \Phi_b(y) \sim \frac{\delta_{ab}}{|x - y|^{2\Delta_\Phi}} + \frac{iC_{\Phi\Phi}^M}{|x - y|^{2\Delta_\Phi - \Delta_M}} \mathcal{F}_{\mu\nu}^{ab} M^{\mu\nu}(y) + \dots \quad (\text{B.2a})$$

$$\Phi_a(x) M^{\mu\nu}(y) \sim \frac{iC_{\Phi M}^\Phi}{|x - y|^{\Delta_M}} \bar{\mathcal{F}}_{ab}^{\mu\nu} \Phi_b(y) + \dots, \quad (\text{B.2b})$$

where the tensor  $\mathcal{F}_{\mu\nu}^{ab}$  maps elements of the adjoint-SU(4) representation to rank-2 antisymmetric representations of SO(6) and  $\bar{\mathcal{F}}_{ab}^{\mu\nu}$  its inverse. Implicit sums over  $(\mu, \nu)$  are taken to exclude the  $(0, 0)$  element. The nonzero components are

$$\begin{aligned} \mathcal{F}_{0i}^{ab} &= \epsilon^{abi} & \text{for } a, b \leq 3, \\ \mathcal{F}_{0i}^{ab} &= \epsilon^{a-3, b-3, i} & \text{for } a, b > 3, \\ \mathcal{F}_{ij}^{ab} &= \delta_j^a \delta_{i+3}^b - \delta_{i+3}^a \delta_j^b & \text{for } i, j = 1, 2, 3, \end{aligned} \quad (\text{B.3})$$

as defined in Ref. (Luo *et al.*, 2022). We can also write the components of its inverse  $\bar{\mathcal{F}}_{ab}^{\mu\nu} = \mathcal{F}_{\mu\nu}^{ab}/2$ .

### Conformal renormalisation group

We will briefly summarise the process of real-space renormalization group (RG) of general conformal theories, and show how the beta functions for the couplings are determined by the conformal data (Cardy, 1996).

The partition function of a conformal theory perturbed by a set of operators  $S_g = \sum_i a^{\Delta_i-3} \int d^3x g_i \mathcal{O}_i$  can be written

$$\mathcal{Z} = \int \mathcal{D}[\{\mathcal{O}_i\}] e^{-S_0 - S_g} = \mathcal{Z}_0 \left\langle 1 - S_g + \frac{1}{2} S_g^2 + \dots \right\rangle, \quad (\text{B.4})$$

where  $S_0$  is the action of the conformal fixed point. The theory is furthermore defined by a UV cutoff  $a$ , which acts as a minimum separation between any two operators. The long-distance IR is furthermore needed to regulate

The RG procedure proceeds in three steps: (1) raising the UV cutoff  $a \rightarrow (1 + dl)a$ ; (2) coarse-graining short-distance degrees of freedom, which in practice will mean integrating over operators which are closer than the new cutoff; (3) a scale transformation to restore distances. The effect of this RG step produces a different effective action  $e^{-S'_g}$ , which gets contributions at one-loop order from the trivial rescaling step (3) at linear order, as well as from integrating out  $\mathcal{O}_i(x)\mathcal{O}_j(y) \sim C_{ij}^k \mathcal{O}_k(x)$  at quadratic order, where  $x, y$  lie closer together than the new cutoff. This produces the flow equations at quadratic order

$$\frac{dg_k}{dl} = (3 - \Delta_k)g_k - 2\pi \sum_{ij} g_i g_j C_{ij}^k. \quad (\text{B.5})$$

We therefore find that RG-relevant operators will generally induce flow in operators in their OPE channels.

### Effective action including fermion mass couplings

We now write down a general set of couplings to the leading relevant operators in  $\text{QED}_3$ : the monopoles  $\Phi_a$  ( $a = 1 \dots 6$ ) and adjoint fermion masses  $M_{\mu\nu}$  [ $\mu, \nu = 0 \dots 3$ ,  $(\mu, \nu) \neq (0, 0)$ ]. The general form of this action is

$$S \sim \int d^3x \left[ \sum_{a=1}^6 (\varphi_a^* \Phi_a(x) + \text{h.c.}) + \sum_{\mu, \nu} m_{\mu\nu} M^{\mu\nu}(x) \right]. \quad (\text{B.6})$$

The monopoles transform under the UV symmetries as listed in Table 2.3, and the masses as listed in Table 2.2. In Chapter 5, we derived the symmetry-allowed monopole-lattice coupling  $S_D$  given by Eq. (5.23). Given the arguments above, we expect this to induce flow in the coupling

$$S_M = \int d^3x i m \epsilon^{abc} u_b^* u_c M_{0a}(x) \quad (\text{B.7})$$

We can check that this is a symmetry-allowed coupling using Table 2.2. When writing down a IR field theory and performing perturbation theory with it to higher orders, we should also

consider the effects of this term. We are now able to write the full symmetry-allowed action at lowest order in relevant operators as a sum of VBS monopole and mass terms:

$$S_I[u_a] = \int d^3x \left[ g (u_a^* \mathcal{D}_a(x) + \text{h.c.}) + im \epsilon^{abc} u_b^* u_c M_{0a}(x) \right]. \quad (\text{B.8})$$

Both terms are coupled to lattice distortions via Eq (5.24).

## Static model

The weak-coupling effective action is given as a function of the norm  $|\vec{u}|$  of the complex vector  $\vec{u} = (u_1, u_2, u_3)^T$ , implying invariance under global  $G \in \text{U}(3)$  transformations  $\hat{u} \mapsto G\hat{u}$ . However, this global continuous symmetry is accidental as it does not correspond to the physical symmetry group of microscopic lattice symmetries. We first note that the  $\text{U}(3)$  symmetry acts on the VBS monopoles, which transform as  $\text{SO}(3)_{\text{valley}}$ -vectors under the emergent symmetry group of the  $\text{QED}_3$  fixed-point action. To this end, we note that  $2\mathbf{X}_1 - 2\mathbf{X}_2 = 2\mathbf{X}_2 - 2\mathbf{X}_3 = 2\mathbf{X}_1 - 2\mathbf{X}_3 = 0$  up to reciprocal lattice vectors, and hence  $|\vec{u} \cdot \vec{u}|$  transforms trivially under the  $\text{SO}(6) \times \text{U}(1)_{\text{top}}$  symmetry group. This term will generically appear in a strong-coupling effective action obtained after ‘integrating out’ the DSL and breaks the  $\text{U}(3)$  redundancy down to  $\text{SO}(3)_{\text{valley}}$ .

We will now derive the subleading contribution to the perturbative free energy functional due to lattice-fermion mass couplings and recover exactly this term. Performing the same calculation as in the main text for lattice-monopole couplings, we enter the weak coupling regime  $g^2 \beta^{3-2\Delta_\Phi} |\vec{u}| \ll 1$  and perform a perturbative expansion of the free energy  $\langle S_M^2 \rangle / \beta V$ . Using the explicitly derived structure of the coupling, we find

$$\begin{aligned} \frac{\langle S_M^2 \rangle_{\text{QED}_3}}{\beta V} &= -m^2 \int d^3x \frac{\epsilon^{abc} \epsilon^{ade} u_b u_d^* u_c u_e^*}{|x|^{2\Delta_M}} \\ &= c_{\Delta_M} m^2 \beta^{3-2\Delta_M} \left( |\vec{u} \cdot \vec{u}|^2 - |\vec{u}|^4 \right). \end{aligned} \quad (\text{B.9})$$

This is IR-divergent if the exponent  $\Delta_M < 3/2$ . The monopole-monopole and monopole-mass terms produce additional divergent contributions, proportional to  $\mathcal{C}(\beta)(|\vec{u} \cdot \vec{u}|^2 - |\vec{u}|^4)$  (Luo *et al.*, 2022). At quadratic order there is a contribution from the  $M \times M$  OPE channel above, giving  $\mathcal{C}^{(2)}(\beta) = c_2 \beta^{3-2\Delta_M}$ . At higher order there are contributions from the following channels:  $\Phi^\dagger \times (M \times \Phi) \rightarrow \Phi^\dagger \times \Phi$  is asymptotically  $\mathcal{C}^{(3)}(\beta) = c_3 \beta^{6-2\Delta_\Phi - \Delta_M}$ ; and the channel  $(\Phi^\dagger \times \Phi) \times (\Phi^\dagger \times \Phi) \rightarrow M \times M$  contributes  $\mathcal{C}^{(4)}(\beta) = c_4 \beta^{9-4\Delta_\Phi}$ . We can constrain  $c_2 \sim m^2 > 0$  and  $c_4 \sim g^2 (C_{\Phi\Phi}^M)^2 > 0$  to be positive, but the sign of  $c_3$  cannot be fixed in this way. There will be multiple additional contributions at this order (e.g. from  $\langle S_D^2 \rangle^2 / \beta V$ ) which produce the potential  $|\vec{u}|^4$ , leaving the sign of this coefficient in the effective action indeterminate. However, we predict that the leading contributions to the  $|\vec{u} \cdot \vec{u}|^2$  term are positive.

The irrelevant three-monopole term

$$S_{\Phi\Phi\Phi} = \lambda \int d^3x [\Phi_1 \Phi_2 \Phi_3 + \text{h.c.}] \quad (\text{B.10})$$

is allowed by the microscopic (UV) symmetries. For example, this three-monopole term has zero lattice momentum since  $\mathbf{X}_1 + \mathbf{X}_2 + \mathbf{X}_3 = 0$ , but clearly breaks the emergent  $\text{SO}(6)$  symmetry at the  $\text{QED}_3$  fixed point.

Considering the coupling of the DSL to displacement fields, any finite  $\lambda \neq 0$  induces analogous corresponding anharmonic terms in the effective action,

$$\mathcal{E}_\lambda[\vec{u}] \sim \tilde{\lambda} [u_1 u_2 u_3 + \text{h.c.}] . \quad (\text{B.11})$$

Within perturbation theory about  $\text{QED}_3$ , one contribution to the effective action of this form arises from  $\langle S_{\mathcal{D}}^3 S_{\Phi\Phi\Phi} \rangle / (\beta V)$ . We stress that, since (B.11) is allowed by the microscopic symmetries of the system, it will also generically arise in any microscopic theory of lattice displacements upon going beyond the harmonic approximation, even in the absence of a coupling to the DSL (hence  $\tilde{\lambda}$  is not necessarily related to  $\lambda$  in  $S_{\Phi\Phi\Phi}$ ). We assume in the main text that this operator is dangerously irrelevant, such that instead of having a continuous  $\text{SO}(3)$  manifold of degenerate ground states, there are three degenerate ground states  $e^{2\pi i n/3} \vec{u}_0$ , with  $n = 0, 1, 2$ . The resultant lattice distortion preserves the  $C_3 = T_1 C_6^2$  lattice symmetry and has an additional reflection symmetry.

## Dynamical model

We now investigate the stability of the DSL in the presence of the interaction  $S_{\mathcal{D}\mathcal{D}}$  within perturbation theory. Considering a perturbative expansion of local observables, the expansion's breakdown is taken to signal an instability of the DSL. We employ the path-integral formalism, where the expectation value of some observable  $\mathcal{X}$  is written as

$$\langle \mathcal{X} \rangle = \mathcal{Z}^{-1} \int \mathcal{D}[\{\mathcal{O}_{\text{CFT}}\}] \mathcal{X} e^{-S} , \quad (\text{B.12})$$

where  $S$  is the system's interacting action and  $\mathcal{Z}$  its partition function without operator insertion, as above.

At the  $\text{QED}_3$  fixed point (i.e., zeroth order perturbation theory), all one-point functions vanish at zero temperature  $\beta \rightarrow \infty$  in the thermodynamic limit by conformal symmetry. We thus turn to the monopole two-point function at large distances  $|d| = |(\tau_d, \mathbf{r}_d)| \rightarrow \infty$ . Expanding the Boltzmann weight  $e^{-S_{\mathcal{D}\mathcal{D}}}$  in the path integral to first order, one finds the perturbative expansion

$$\langle \mathcal{D}_a^\dagger(d) \mathcal{D}_b(0) \rangle_{g^2} = \frac{\delta_{ab}}{|d|^{2\Delta_\Phi}} - \left( \langle \mathcal{D}_a^\dagger(d) \mathcal{D}_b(0) S_{\mathcal{D}\mathcal{D}} \rangle_{\text{QED}_3} - \frac{\delta_{ab}}{|d|^{2\Delta_\Phi}} \langle S_{\mathcal{D}\mathcal{D}} \rangle_{\text{QED}_3} \right) + \dots , \quad (\text{B.13})$$

where we have used the two-point functions evaluated at the CFT fixed point. The first term in the parenthesis is written explicitly as

$$\begin{aligned} \langle \mathcal{D}_a^\dagger(d) \mathcal{D}_b(0) S_{\mathcal{D}\mathcal{D}} \rangle_{\text{QED}_3} = & - \sum_c \frac{g^2 |\mathbf{X}_c|^2}{2\rho\omega_0} \int d^3x d^3y \\ & \times \left[ \delta^{(2)}(\mathbf{r}_x - \mathbf{r}_y) e^{-\omega_0 |\tau_x - \tau_y|} \langle \mathcal{D}_a^\dagger(d) \mathcal{D}_b(0) \mathcal{D}_c^\dagger(x) \mathcal{D}_c(y) \rangle_{\text{QED}_3} \right] . \end{aligned} \quad (\text{B.14})$$

Note that while 2- and 3-pt. functions of primaries are exactly determined by conformal symmetry, no closed forms are available for 4-pt. functions, making the evaluation of Eq. (B.13) challenging.

While Wick's theorem does not hold in interacting CFTs, we can successively apply operator product expansions (OPE) to decompose the 4-pt. function in (B.14). If the full (convergent) OPE is used, the choice of OPE channels is inconsequential. However, for analytical tractability, we will use the asymptotic forms of OPE [see also Eq. (B.1)]. A particular OPE channel then corresponds to a particular configuration of operator insertions which yield the most divergent contribution in the particular channel if they become 'close'.

Considering Eq. (B.14), we will focus on the leading monopole-antimonopole OPE channel (schematically  $\Phi^\dagger \times \Phi = \mathbb{1}$ ) corresponding to  $x \rightarrow 0$  and  $y \rightarrow d$ , with  $x$  and  $y$  sufficiently far apart, which means that we may assume  $0 < |x| \ll |y|$ . Explicitly, the first-order OPE in this channel then reads

$$\langle \Phi_a^\dagger(d) \Phi_b(0) \Phi_c^\dagger(x) \Phi_c(y) \rangle_{\text{QED}_3} \sim \delta_{ac} \delta_{bc} \frac{1}{|d-y|^{2\Delta_\Phi} |x|^{2\Delta_\Phi}}. \quad (\text{B.15})$$

We expect this channel to give the most dominant contribution: The other monopole-antimonopole channel corresponding to  $d \rightarrow 0$ ,  $x \rightarrow y$  is asymptotically equivalent to the disconnected contribution (second term in the parenthesis) in Eq. (B.14), and is thus expected to only weakly contribute to  $\langle \mathcal{D}_a^\dagger(d) \mathcal{D}_b(0) \rangle_{g^2}$ .

We use (B.15) in (B.14). As  $|d| \rightarrow \infty$ , we can take  $|d-y|^{-2\Delta_\Phi} \approx |d|^{-2\Delta_\Phi}$  and subsequently perform the  $\mathbf{r}_y$ -integration, yielding

$$\langle \mathcal{D}_a^\dagger(d) \mathcal{D}_b(0) S_{\mathcal{DD}} \rangle_{\text{QED}_3} \approx -\frac{\delta_{ab}}{|d|^{2\Delta_\Phi}} \frac{g^2}{2\rho\omega_0} \int d^3x \int d\tau_y \frac{e^{-\omega_0|\tau_x-\tau_y|}}{(|\mathbf{r}_x|^2 + \tau_x^2)^{\Delta_\Phi}}. \quad (\text{B.16})$$

We work on a cylindrical geometry  $S_\beta^1 \times \mathbb{R}^2 \xrightarrow{\beta \rightarrow \infty} \mathbb{R}^3$ . The spatial integration is performed in polar coordinates with  $0 < |\mathbf{r}_x| < L \rightarrow \infty$ ,

$$|d|^{2\Delta_\Phi} \langle \mathcal{D}_a^\dagger(d) \mathcal{D}_b(0) S_{\mathcal{DD}} \rangle_{\text{QED}_3} \approx -\delta_{ab} \frac{\pi g^2}{2(\Delta_\Phi - 1)\rho\omega_0} \int d\tau_x d\tau_y \frac{e^{-\omega_0|\tau_x-\tau_y|}}{|\tau_x|^{2\Delta_\Phi-2}}. \quad (\text{B.17})$$

Note that due to the  $\delta$ -distribution for the spatial components in (B.14), only configurations with  $\mathbf{r}_x = \mathbf{r}_y$  give a finite contribution. Thus, our previous assumption of  $|x| \ll |y|$  implies for the temporal coordinates  $|\tau_x| \ll |\tau_y|$ . With  $|\tau_x - \tau_y| \approx |\tau_y|$ , the remaining integrals are obtained as

$$\lim_{\beta \rightarrow \infty} \int_0^\beta d\tau_y \int_0^{|\tau_y|} d\tau_x \frac{e^{-\omega_0|\tau_y|}}{|\tau_x|^{2\Delta_\Phi-2}} \approx \frac{1}{3-2\Delta_\Phi} \frac{\Gamma(4-2\Delta_\Phi)}{\omega_0^{4-2\Delta_\Phi}}, \quad (\text{B.18})$$

which exists for  $\Delta_\Phi < 2$ , which is within the range of assumed scaling dimensions. Hence, one finds

$$|d|^{2\Delta_\Phi} \langle \mathcal{D}_a^\dagger(d) \mathcal{D}_b(0) S_{\mathcal{DD}} \rangle_{\text{QED}_3} \approx -\delta_{ab} \frac{c_{\Delta_\Phi} \Gamma(4-2\Delta_\Phi)}{4\rho\omega_0^2} \frac{g^2}{\omega_0^{3-2\Delta_\Phi}} \quad (\text{B.19})$$

Generically, perturbation theory breaks down when the  $(n + 1)$ -term in the expansion is no longer small compared to the  $n$ -th term. Here, we compare the first-order correction to the bare correlator,

$$\frac{\delta^{(1)} \langle \mathcal{D}_a^\dagger(d) \mathcal{D}_a(0) \rangle_{g^2}}{\langle \mathcal{D}_a^\dagger(d) \mathcal{D}_a(0) \rangle_{\text{QED}_3}} \approx \frac{1}{4} c_{\Delta_\Phi} \Gamma(4 - 2\Delta_\Phi) \frac{g^2}{\kappa \omega_0^{3-2\Delta_\Phi}}. \quad (\text{B.20})$$

Perturbation theory breaks down if this ratio is of order 1. This leads to a scaling relation for the critical coupling, given by

$$g_c^2 / \kappa \sim \omega_0^{3-2\Delta_\Phi}. \quad (\text{B.21})$$

In the thermodynamic limit at zero temperature, the finite phonon frequency  $\omega_0 \neq 0$  hence prevents a weak-coupling instability and rather determines a critical  $g_c$  as a function of  $\omega_0$ . The critical  $g_c$  matches precisely the result of the scaling analysis in the main text.

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## Variational methods

### Gutzwiller-projected states

The variational wave functions (for spins) are projected fermionic states of the form  $|\Psi_s\rangle = \mathcal{P}_G|\Phi_0\rangle$ , in which the Gutzwiller projector  $\mathcal{P}_G = \prod_i (n_{i,\uparrow} - n_{i,\downarrow})^2$  is applied to a wave functions of Abrikosov fermions  $|\Phi_0\rangle$  (Wen, 2002; Becca and Sorella, 2017). The latter is defined as the ground state of an auxiliary fermionic Hamiltonian  $\mathcal{H}_0$ , which in general contains real-valued hoppings  $t_{i,j}$  and singlet pairings  $\Delta_{i,j} = \Delta_{j,i}$  (variational parameters)

$$\mathcal{H}_0 = \sum_{i,j} \sum_{\alpha=\uparrow,\downarrow} t_{i,j} f_{i,\alpha}^\dagger f_{j,\alpha} + \sum_{i,j} \Delta_{i,j} f_{i,\downarrow} f_{j,\uparrow} + h.c. \quad (\text{C.1})$$

For the triangular-lattice  $J_1$ – $J_2$  model at  $J_2/J_1 = 1/8$  the optimal ground state is the U(1) DSL (Iqbal *et al.*, 2016). In this case  $\mathcal{H}_0$  contains only a nearest-neighbor hopping, with uniform absolute value and a bond-dependent sign, which creates a pattern of alternating 0 and  $\pi$  fluxes in the triangular plaquettes. The spectrum of  $\mathcal{H}_0$  is gapless with two Dirac points (for each spin component). We note that although the debate concerning the nature of the  $J_1$ – $J_2$  model’s QSL ground state and excitations is not fully settled, recent numerical results corroborate the DSL scenario (Hu *et al.*, 2019; Sherman *et al.*, 2023; Drescher *et al.*, 2023; Wietek *et al.*, 2024). For the 1D Heisenberg chain, the lowest variational energy is achieved by taking (translationally invariant) hopping and pairing at first-neighbor, plus an additional hopping at third-neighbors, within  $\mathcal{H}_0$  (Becca *et al.*, 2011; Ferrari *et al.*, 2018). The resulting fermionic band of  $\mathcal{H}_0$  is gapless at  $k = \pm \frac{\pi}{2}$ . The optimal values of the variational parameters can be obtained by a numerical minimization of the variational energy  $E_{\text{var}}$ . For this purpose, in all VMC calculations performed in this work, including the ones involving phonons, we use the stochastic reconfiguration method (Sorella, 2005; Becca and Sorella, 2017).

Where possible, we perform the Monte Carlo within the projected  $S_{\text{tot}}^z = 0$  subspace (Ferrari and Becca, 2019). In simulations regarding interlayer coupling in Sec. 5.4, we break SU(2) symmetry explicitly with the staggered in-plane magnetic, meaning a different sampling is used.

### Wave functions for spins and phonons

To pursue a full quantum analysis of the spin-phonon problem, we turn to study the dynamical spin-phonon Hamiltonian numerically. In addition to accounting for the potential energy cost of lattice distortions, this also includes the phonons kinetic energy, providing them with quantum dynamics. Specifically, the free phonon part of this Hamiltonian describes a set

of uncoupled harmonic oscillators, i.e. Einstein phonons. A full quantum treatment of the problem is achieved by the definition of a variational wave function for spins and phonons

$$|\Psi_{\text{sp}}\rangle = \mathcal{J}_{\text{sp}}|\Psi_{\text{p}}\rangle \otimes |\Psi_{\text{s}}\rangle. \quad (\text{C.2})$$

This ansatz is the product of a spin state,  $|\Psi_{\text{s}}\rangle$ , a phonon state,  $|\Psi_{\text{p}}\rangle$ , and a spin-phonon Jastrow factor  $\mathcal{J}_{\text{sp}}$  (Ferrari *et al.*, 2020, 2021, 2024). The spin wave function is a Gutzwiller-projected fermionic state supplemented by a (long-range) spin-spin Jastrow factor, namely  $|\Psi_{\text{s}}\rangle = J_{\text{s}}\mathcal{P}_G|\Phi_0\rangle$ , with  $J_{\text{s}} = \exp\left(\sum_{i,j} v_{i,j} S_i^z S_j^z\right)$ . The variational parameters of  $J_{\text{s}}$ ,  $v_{i,j} = v_{j,i}$ , depend only on the distance between sites in the undistorted lattice, i.e.  $\|\mathbf{r}_i - \mathbf{r}_j\|$ . As previously discussed, the fermionic state  $|\Phi_0\rangle$  is taken to be the ground state of a certain fermionic Hamiltonian  $\mathcal{H}_0$  [see Eq. (C.1)]. The phonon part of the variational Ansatz is a coherent state. Its amplitude on a generic element of the phonon Hilbert space (labelled by the local displacements) reads

$$\langle \{\mathbf{u}_j\} | \Psi_{\text{p}} \rangle = \prod_i \exp\left(-\frac{m\omega}{2} \|\mathbf{u}_i - \mathbf{z}_i\|^2\right), \quad (\text{C.3})$$

i.e. it is a product of Gaussians whose centers are controlled by the variational parameters  $\mathbf{z}_i \in \mathbb{R}^D$ . A nonzero  $\mathbf{z}_i$  upon optimization is associated with a finite displacement of site  $i$ . Finally, the variational state  $|\Psi_{\text{sp}}\rangle$  is completed by the Jastrow factor

$$\mathcal{J}_{\text{sp}} = \exp\left[\sum_{i,j} \mathbf{w}_{i,j} \cdot (\mathbf{u}_i - \mathbf{u}_j) S_i^z S_j^z\right], \quad (\text{C.4})$$

which connects spin and phonon degrees of freedoms. The variational parameters of  $\mathcal{J}_{\text{sp}}$  depend only on the distance  $\|\mathbf{r}_i - \mathbf{r}_j\|$ , but are antisymmetric under the swap of lattice sites, namely  $\mathbf{w}_{i,j} = -\mathbf{w}_{j,i}$ . Note that  $\mathbf{w}_{i,j} \in \mathbb{R}^2$  ( $\in \mathbb{R}$ ) for the 2D (1D) spin-phonon problem. Details on the implementation of the Monte Carlo procedure in the Hilbert space of spins and phonons are given in (Ferrari *et al.*, 2024).

## Density matrix renormalization group

The XXZ model (7.9) is simulated by sweeping over the parameter  $J_2$  for a number of bond dimensions. TeNPy is used to evaluate energies, order parameters, entanglement entropy, and correlation length (using the transfer matrix) (Hauschild and Pollmann, 2018; Hauschild *et al.*, 2024). The calculations are performed in the thermodynamic limit, with accuracy limited by the bond dimension. The results are shown in Fig. C.1. We observe a continuous evolution of the energy and a divergence in the correlation length that is cut off by finite bond dimension. The scaling with bond-dimension is included in Fig. 7.5(a).

In the model with lattice distortions, we see a strongly first order transition and so do not sweep over  $J_2$ , but run independent transitions (convergence is quicker in this case because the correlation lengths do not diverge). The spin energies are calculated using TeNPy and then the static energy cost of the lattice is added by hand. We find the minimum energy state and show order parameters at this point for each  $J_2$  in Figs. C.1(c,d) and 7.7(b,c).

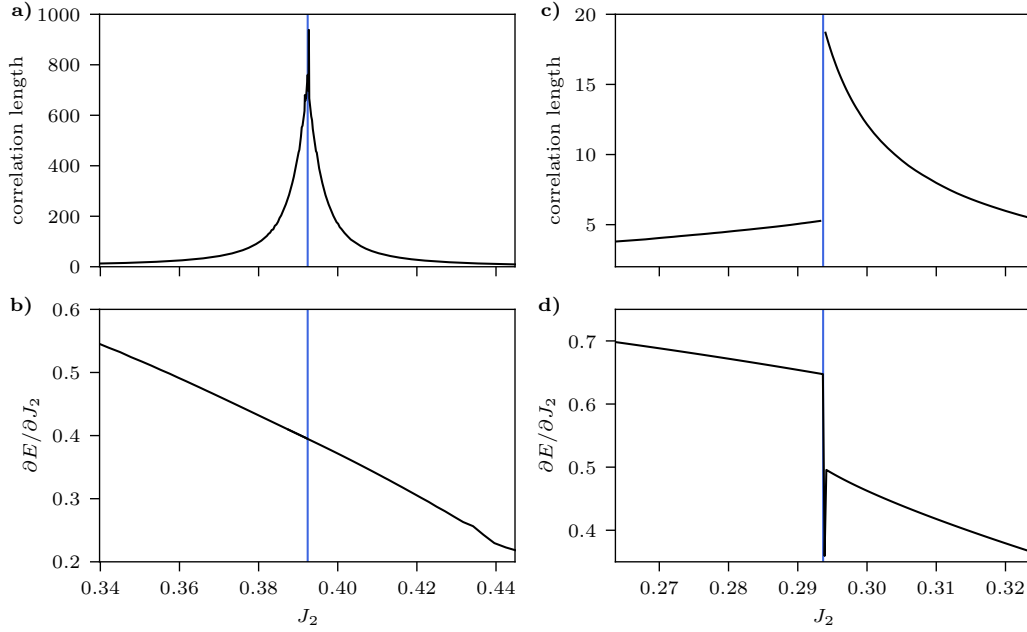


**Figure C.1:** *Evidence for a continuous transition becoming first order.* (a,b) Correlation length divergence and smooth energy derivative across the transition of the static model. (c,d) Finite correlation length and discontinuous energy over the first-order transition with spin-lattice coupling.

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### Non-linear sigma model description of DQCP

Let us now take another attempt at describing the transition and ordered phases within the NLSM framework. We are seeking a description which treats both competing orders on an equal footing. This differs from the approach of (Haldane, 1988) above, where we expanded about the ordered Néel state. To do this, unify the Néel vector  $\mathbf{n}$  and VBS order parameters  $v_j^a = \eta_j \langle \mathbf{S}_j \cdot \mathbf{S}_{j+\delta_a} \rangle$  into a  $N$ -component superspin vector

$$\tilde{\mathbf{n}} = (\mathbf{n}, \mathbf{v}). \quad (\text{D.1})$$

In the 1D example, the three Néel components and the scalar dimer order  $v$  are combined into an  $\text{SO}(4)$  vector. In the 2D model, the three Néel order parameters and two independent VBS order parameters  $v_{1,2}$  in the  $x$  and  $y$  directions are combined into an  $\text{SO}(5)$  vector. A simple model of the transition is given by

$$S_D^{\text{DQCP}}[\tilde{\mathbf{n}}] = \int d^{D+1}x \left[ \frac{1}{2e^2} (\nabla \tilde{\mathbf{n}})^2 + s(\mathbf{n}^2 - \mathbf{v}^2) \right]. \quad (\text{D.2})$$

The anisotropy  $s$  tunes between a VBS ( $v > 0$ ) and Néel-ordered state ( $v < 0$ ). However, the spontaneous symmetry-breaking transition at weak-coupling  $e^2 = 0$  tuned by this anisotropy is first order (Zou *et al.*, 2021). This is because in the ordered state  $e^2 = 0$ , the non-linear constraint  $\tilde{\mathbf{n}} = 1$  forces a jump in the order from the Néel components  $\tilde{n}_{1,2,3}$  to VBS  $\tilde{n}_4$ . The proposed continuous DQCP hence requires a non-trivial fixed point at finite  $e_*^2 > 0$ . It must represent a disordered, gapless critical point. This can be achieved by writing the following NLSM action for the superspin

$$S_1^{\text{SO}(D+3)}[\tilde{\mathbf{n}}] = \frac{1}{2e^2} \int d^{D+1}x (\nabla \tilde{\mathbf{n}})^2 + \Gamma_1^{\text{SO}(D+3)}. \quad (\text{D.3})$$

The topological WZW terms is explicitly

$$\Gamma_D^{\text{SO}(D+3)} = \frac{2\pi i}{\Omega_{D+3}} \epsilon_{j_1 \dots j_{D+3}} \int d^{D+1}x \int_0^1 du \tilde{n}_{j_1} \partial_{x_1} \tilde{n}_{j_2} \dots \partial_u \tilde{n}_{j_{D+3}} \quad (\text{D.4})$$

in  $D$  spatial dimensions. This term is responsible for intertwining the competing order parameters. It is responsible for endowing topological defects of one phase with the symmetry properties of the other phase (Wang *et al.*, 2017; Zou *et al.*, 2021). This Lagrangian form of the action should be extended to a non-trivial strong-coupling fixed point. Then, the DQCP is driven by the same anisotropy

$$S_D^{\text{DQCP}}[\tilde{\mathbf{n}}] = S_D^{\text{SO}(N)}[\tilde{\mathbf{n}}] + \int d^{D+1}x s(\mathbf{n}^2 - \mathbf{v}^2). \quad (\text{D.5})$$

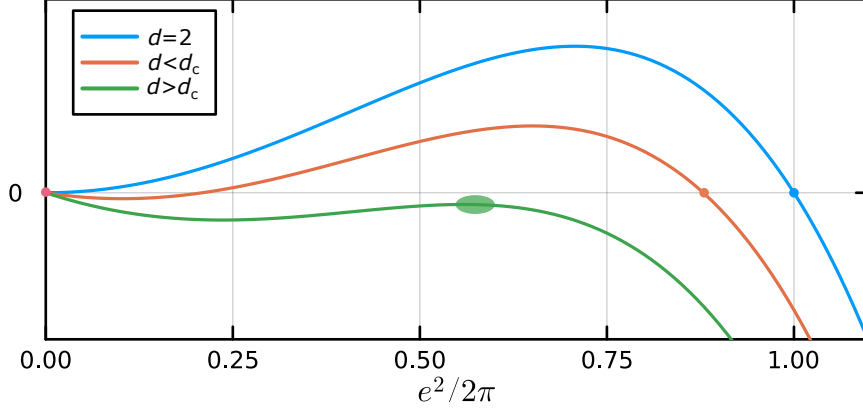


**Figure D.1:** *Beta function of the coupling strength in the NLSM with a WZW topological term.* Stable strong coupling fixed points are present for  $d < d_c$ , marked as points. For  $d$  just greater than  $d_c$ , there is a pseudocritical regime.

We will first discuss this model in  $D = 1$ , and then work towards recent results for the  $D = 2$  DQCP.

#### 1D DQCP: SO(4) NLSM with WZW term

Let us now write down a NLSM effective theory for the critical point and transition in 1D. We may unify the Néel vector  $\mathbf{n}$  and VBS order parameter  $v_j = \eta_j \langle \mathbf{S}_j \cdot \mathbf{S}_{j+1} \rangle$  into a four-component vector  $\tilde{\mathbf{n}} = (\mathbf{n}, v)$ . The field's dynamics is governed by an O(4) NLSM supplemented by a Wess–Zumino–Witten (WZW) term (Tanaka and Hu, 2005; Senthil and Fisher, 2006)

$$S_1^{\text{DQCP}}[\tilde{\mathbf{n}}] = \frac{1}{2e^2} \int d^2x (\nabla \tilde{\mathbf{n}})^2 + \Gamma_1^{\text{SO}(4)}. \quad (\text{D.6})$$

The non-Landau physics of a DQCP is contained in the topological WZW term  $\Gamma_1^{\text{SO}(4)}$ . This is responsible for creating a strong-coupling fixed point. Without this term, the transition would simply be a Landau-compatible first-order Néel–VBS transition. To see this, let us analyse the RG group flow for this model Eq. (D.6) (without any anisotropy, i.e. focusing on the DQCP itself). Witten (1984) showed that the leading perturbative beta function of the WZW model is given by

$$\frac{de^2}{d \log \ell} = \left( \frac{1}{2\pi} \right) e^4 \left[ 1 - \left( \frac{e^4}{4\pi} \right)^2 + \dots \right]. \quad (\text{D.7})$$

This is plotted in Fig. D.1. The first term comes from the renormalisation of the coupling strength of the kinetic term, and is strictly positive. We stated the same result for the O(3) NLSM without a topological term. This theory would flow to a trivial strong-coupling fixed point. However, in the presence of the WZW term, Eq. (D.7) has a non-trivial fixed point at strong coupling  $e_*^2 = 4\pi$  which preserves the SO(4) symmetries of the model.

In the AFM phase, the WZW action also recovers the O(3) NLSM's topological Berry phase term (Tanaka and Hu, 2005). This can be written explicitly

$$S_{\text{top}} = \frac{i}{4} \int dx d\tau \mathbf{n} \cdot (\partial_x \mathbf{n} \times \partial_\tau \mathbf{n}) = i\pi Q_{x\tau} \quad (\text{D.8})$$

in terms of the integer Pontryagin index  $Q_{x,\tau} \in \mathbb{Z}$ . The topological angle  $\pi$  guarantees that the transition at  $s = 0$  is gapless (Affleck and Haldane, 1987; Chubukov, 1991). The results of Lieb *et al.* (2004) tell us here that a gapped trivial phase is not allowed and this disordered critical point must be gapless.<sup>1</sup> Additionally, the WZW term is responsible for topological defects in the VBS phase carrying a  $S = 1/2$  degree of freedom, making them seeds for Néel order. Conversely, it also causes the topological defects in the Néel-ordered phase to transform non-trivially under lattice symmetries such that their condensation leads to VBS order. This so-called *intertwinement* of order parameters is a key underlying feature of the DQCP (Levin and Senthil, 2004; Metlitski and Thorngren, 2018).

In order to extend this critical point to a full model of DQCP, we must include two additional terms:

$$S_1^{\text{DQCP}}[\tilde{\mathbf{n}}] = S_1^{\text{DQCP}}[\tilde{\mathbf{n}}] + \int d^2x s(\mathbf{n}^2 - v^2) + S_{\text{aniso}}. \quad (\text{D.9})$$

Here,  $s$  is a tuning parameter for the transition between Néel ( $s < 0$ ) and VBS ( $s > 0$ ) orders. However, considering the SU(2) symmetric model (as implicitly assumed in the above formulation), the anisotropy  $\mathbf{n}^2 - v^2$  is an irrelevant perturbation. As such, we also include the anisotropy  $S_{\text{aniso}} = \alpha_{\text{aniso}} \int d^2x (n_3^2 + v^2)$  in order to stabilise the two ordered phases. In this anisotropic limit, we can parameterise the NLSM by a single angle  $2\phi$  like

$$\tilde{\mathbf{n}} = (0, 0, \cos(2\phi), \sin(2\phi)). \quad (\text{D.10})$$

First, note that the anisotropy then reads  $s \cos(4\phi)$ . Together with the kinetic term, the superspin NLSM action then reduces to the Sine-Gordon model with  $K = e^2/4\pi$ . Note to derive this, we used that the WZW term vanishes for these configurations.

## 2D DQCP: SO(5) NLSM

We now return to the 2+1-dim. case of putative DQCP on the square lattice. Here, the analogue of the NLSM with a WZW term takes the form (Tanaka and Hu, 2005; Senthil and Fisher, 2006)

$$S_2^{\text{DQCP}}[\tilde{\mathbf{n}}] = \frac{1}{2e^2} \int d^3x (\nabla \tilde{\mathbf{n}})^2 + \Gamma_1^{\text{SO}(5)}. \quad (\text{D.11})$$

where the three-component Néel order parameter  $\mathbf{n}$  and the two-component VBS order parameter  $v_j^a = \eta_j \langle \mathbf{S}_j \cdot \mathbf{S}_{j+\hat{r}_a} \rangle$  ( $a = x, y$ ) have been combined into 5-component vector  $\tilde{\mathbf{n}}$ . Extending this action to strong coupling, the proposed resulting conformal fixed point is believed to be dual to the CP<sup>1</sup> model (Wang *et al.*, 2017). The 2D WZW term  $\Gamma_2^{\text{SO}(5)}$  reduces to the spin-1/2 Berry phase in the case of a single  $\mathbb{Z}_4$  vortex within the VBS phase

<sup>1</sup>Alternatively there could be a crossover regime.

(Levin and Senthil, 2004). It once again serves the source of intertwinement in this theory (Tanaka and Hu, 2005; Senthil and Fisher, 2006).

However, it has been debated hotly in recent years whether a  $\text{SO}(5)$ -symmetric strong-coupling conformal fixed point exists in this theory (Senthil, 2023). As such, the existence of a continuous DQCP on the square lattice has been cast into doubt. Let us understand this from the perspective of the RG flow of the  $\text{SO}(5)$ -superspin NLSM with a topological WZW term, Eq. (D.11). Nahum (2020); Ma and Wang (2020) calculate the beta functions of the coupling strength to be

$$\frac{de^2}{d \log \ell} = -\epsilon e^2 + \left(\frac{1}{2\pi}\right) e^4 \left[ 1 - \left(\frac{e^4}{4\pi}\right)^2 + \dots \right]. \quad (\text{D.12})$$

Here, they analytically continue from an  $\text{SO}(4)$ -symmetric model in  $d = 2$ , Eq. D.7, to  $\text{SO}(4 + \epsilon)$  in  $d = 2 + \epsilon$ . The results are also plotted in Fig. D.1 for two values of  $\epsilon = 0.4, 0.8$ . For small  $\epsilon$ , it shows there is a stable strong coupling fixed point  $e_*^2$ . However, as  $\epsilon$  increases towards the physical value of 1, the stable and unstable fixed points at finite- $e^2$  annihilate. For all dimensions greater than this critical dimension, the DQCP disappears and the resulting transition is first order. However this picture also gives a clue as to why realisations of DQCP appear to have almost critical behaviour. If the true dimension is just greater than the critical dimension, the RG flow about the pseudocritical point will be very slow. This implies a very weakly first order transition, with an approximate emergent  $\text{SO}(5)$  (Wang *et al.*, 2017; Serna and Nahum, 2019).

The  $\text{U}(1)$  Dirac spin liquid is another critical phase with intertwined competing Néel and VBS orders. Recently this was highlighted by (Zou *et al.*, 2021), who unified such models into the class of ‘Stiefel liquids’. These Stiefel liquids generalise the intertwinement originally proposed in 1D spin chains and the DQCP. These phases are disordered critical states which may arise between competing VBS and (increasingly complex forms of) antiferromagnetic orders. They therefore generalise the DQCP, and have large emergent symmetry groups containing  $\text{SO}(N)$ . The NLSM and  $\text{U}(1)$  Dirac QSL are the  $N = 5$  and 6 instances of this (Senthil and Fisher, 2006; Jian *et al.*, 2018). The  $N = 7$  Stiefel liquids is also proposed to represent a potentially stable QSL state. It may exist at the boundary of competing VBS and non-coplanar orders on the triangular and kagome lattices. There is no proposed Lagrangian form of this action, as we have in the cases of the DQCP and  $\text{U}(1)$  Dirac QSL.

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