Deconfined Quantum Critical Points

A thesis submitted to the
Tata Institute of Fundamental Research, Mumbai
for the degree of
Master of Science, in Physics

by
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July, 2007

I dedicate this thesis to my parents.

Acknowledgements

First and foremost, I would like to acknowledge my advisor Kedar Damle for all his guidance and support. It is also a pleasure to acknowledge M. Barma, C. Dasgupta, A. Dhar, D. Dhar, G. Mandal, S. Minwalla, H. R. Krishnamurthy, S. Ramaswamy, T. Senthil, V. Shenoy and V. Tripathi for the physics I have learned from them. I thank the DTP office staff for being extremely helpful at all times. I thank Anindya for the computer guidance he has provided to me after I joined DTP. Among the students, I thank Argha, Loganayagam, Partha, Prasenjit and Shamik for many physics discussions. Finally, I would like to thank my parents for always being supportive to me.

Synopsis

The theory of continuous phase transitions is one of the foundations of statistical mechanics and condensed matter theory. A central concept in this theory is that of the ”order parameter”; its non-zero expectation value characterizes a broken symmetry of the Hamiltonian in an ordered phase and it goes to zero when the symmetry is restored in the disordered phase. According to the accepted paradigm due to Landau and Ginzburg, the physics near continuous phase transitions is dominated by the long distance fluctuations of the order parameter field(s) and can be described by a continuum field theory written in terms of the order parameter fields(s) and its gradients, where all terms consistent with the symmetries of the order parameter are allowed in general. The resulting field theory cannot be analyzed by a *simple* perturbation in general, as individual terms of the perturbation series diverge as the critical point is approached. However this difficulty is overcome by using general renormalization-group ideas, and this provides the sophisticated Landau-Ginzburg-Wilson (LGW) formalism for thinking about critical phenomena for a variety of different situations. For example, the LGW formalism gives us a method to calculate the critical exponents associated with a continuous phase transition, which are the numbers that characterize the power law divergences in various thermodynamic quantities on approaching the critical point.

In recent years, a different kind of phase transitions has generated a lot of interest, namely transitions that take place at zero temperature. In such transitions, a non-thermal control parameter like pressure, magnetic field or chemical composition is varied to access the transition point. In such cases, the order is destroyed or changed solely by quantum fluctuations which arise because of non-commuting (and hence, competing) terms in the Hamiltonian of the system. Such zero temperature phase transitions are called Quantum Phase Transitions. Theoretically, the LGW paradigm again provides the basic framework to understand these critical points. The critical modes are again presumed to be the long distance, long time fluctuations of the order parameter field, where the inverse temperature acts as the ”imaginary” time direction, and the d-dimensional quantum system can be mapped to some $d + 1$ dimensional classical system as $T \to 0$.

Are there quantum phase transitions which lie outside this well known LGW paradigm? In this thesis, we will review in detail the physics of the recently proposed ”deconfined critical point” [1]. Here the critical theory is most naturally expressed in terms of certain fractionalized degrees of freedom, instead of the order parameter fields. The order parameter fields characterizing the phases on either side of the critical point emerge as composites of the fractionalized fields. Moreover, in such cases, an emergent topological conservation law arises precisely at the quantum critical point. These type of critical points clearly violate the standard LGW paradigm. We set up the necessary background and review a particular example from $2d$ quantum magnetism with spin $S = 1/2$ on the square lattice to illustrate such critical points. There may be other examples of such deconfined critical points in strongly correlated electron systems, which might explain the experimental puzzles associated with such systems in the future.

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Chapter 1

Introduction

In this thesis, we would review the novel physics of ”deconfined critical points” which was recently proposed by Senthil *et. al* [1] as an example of a quantum phase transition (at $T = 0$) which violates the well established Landau-Ginzburg-Wilson paradigm to understand continuous phase transitions. In this chapter, we briefly explain the philosophy of the the LGW paradigm and how it explains the some of the remarkable properties associated with continuous phase transitions such as scaling and universality.

Phase transitions abound in nature and are familiar to us from a variety of everyday examples such as boiling of water and melting of ice. One can also think of more *complicated* examples such as the transition of a metal into the superconducting state and of a paramagnet into magnetically ordered state(s) upon lowering the temperature. These transitions occur by varying an external control parameter and normally, there is a qualitative change in the system properties on passing through the transition. In the examples given above, the transitions are temperature driven and are examples of finite temperature phase transitions. Here macroscopic order at low temperature (e.g., crystal structure of a solid) is destroyed at high enough temperature because of thermal fluctuations.

It is useful to categorize phase transitions into two types. The melting of ice into water is an example of a **first-order phase transition**. At the melting point of ice, the energy absorbed from the surrounding environment to melt the ice is called the latent heat which equals $T\triangle S$ where T is the temperature and $\triangle S$ is the change in entropy between ice and water at the melting point. The transition is first-order because the system's entropy, which is a first derivative of the Gibbs free energy, is discontinuous. A first-order transition also occurs at the boiling point of water. However, if water is at a sufficiently high temperature and pressure, there is no transition between a liquid and a gas. The limiting pressure and temperature above which there is no phase transition are called the critical pressure and critical temperature, respectively. At the critical pressure and temperature, there is a **continuous phase transition**, because the first derivatives of the Gibbs free energy are continuous (there is a divergence of the specific heat and the compressibility, which are second derivatives of the free energy). This point in the $p-T$ phase diagram is called the *critical point* and is at the end of

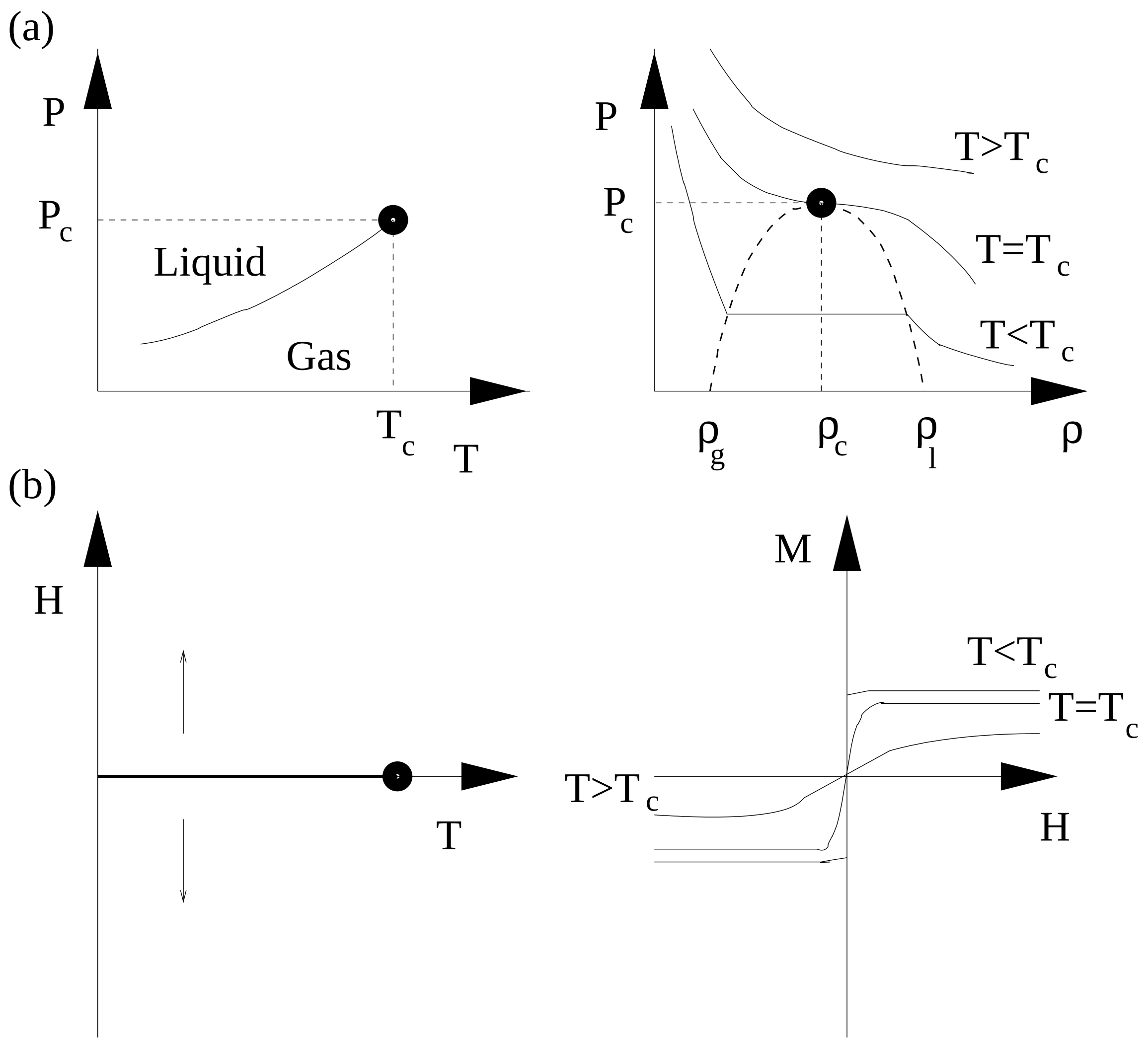

Figure 1.1: Phase diagrams of (a) the liquid-gas transition, and (b) the ferromagnetic transition for a uniaxial magnet. Notice the similarity between the two ($1/v = \rho \leftrightarrow M$, $P \leftrightarrow H$).

a curve of first-order transition points called the coexistence curve. Other examples of continuous phase transitions are the Curie point of ferromagnets, a similar transition for antiferromagnets and the transition between superconducting and normal metals.

A central concept in the theory of phase transitions is that of an ”**order parameter**” [2], which is essential to formulate a quantitative theory of the same. An order parameter is any quantity which is non-zero in the ordered phase where some symmetry of the microscopic interactions is broken, and is zero in the disordered phase where the symmetry is restored. Also, the value of the order parameter should reflect which of the symmetry-related states does a system choose when it spontaneously breaks a symmetry in the ordered state. To illustrate this concept, let us consider the example of uniaxial ferromagnets. In uniaxial magnets, the spins find it energetically favourable to only point along a certain axis (call it the z axis) because of crystal field effects. Thus, we can associate an Ising like variable $s_i = \pm 1$ at each site of the crystal, which indicates the state of the spin at that site. Note that the Hamiltonian is invariant under $s_i \to -s_i \; \forall \; i$, i.e., a global spin flip operation does not change the energy of a given microstate $\{s_i\}$. Here the average magnetization per site $\langle s \rangle = \langle 1/N \sum_i s_i \rangle$, where N is the number of sites in the system, acts as the correct order parameter. In the high temperature paramagnetic phase, the spins have an equal probability of pointing in both directions and therefore, $\langle s \rangle = 0$. However, in the low temperature ferromagnetic phase, the system chooses a direction (up or down with respect to the z axis) for the spins to order and therefore, $\langle s \rangle \neq 0$. Also, the order parameter $\langle s \rangle$ changes sign under global spin flip and hence differs in sign (but not in magnitude) for the two possible symmetry-related ordered states at a given T. The order parameter goes to zero smoothly when the system goes over from the ordered to the disordered state for continuous phase transitions. On the other hand, it jumps from a non-zero value to zero discontinuously at the critical point for a first-order phase transition.

We will focus primarily on continuous transitions from here. Continuous phase transitions are characterized by thermodynamic quantities such as the specific heat, the magnetic susceptibility and the isothermal compressibility, diverging at the critical point [3, 4]. The divergences typically follow a power law near the transition. The powers are called the **critical exponents**. Remarkably, transitions as different as the liquid-gas and uniaxial ferromagnetic transition can be described by the same set of critical exponents and are said to belong to the same **Universality class** [3, 4]. The phenomenon of Universality is the following: All phase transitions can be divided into a small number of *universality classes* depending upon the dimensionality of the system and the symmetries of the order parameter (long-ranged interactions bring additional complications). Within a universality class, all phase transitions have identical behaviour in the critical region, only the variables used to describe the critical region are different from case to case.

For example, the principal critical exponents for the uniaxial ferromagnetic transition are defined in the following manner [4]. It is useful to define two dimensionless measures of the deviation from the critical point: the reduced temperature $t = (T - T_c)/T_c$, and the reduced external magnetic field $h = H/k_B T_c$. Then the exponents are:

- α: The specific heat in zero field $C \sim A|t|^{-\alpha}$, apart from terms regular in t.
- β: The spontaneous magnetization $lim_{H \to 0+} M \propto (-t)^{\beta}$.
- γ: Zero field susceptibility $\chi = (\partial M/\partial H)|_{H=0} \propto |t|^{-\gamma}$.
- δ: At $T = T_c$, the magnetization varies with h according to $M \propto |h|^{1/\delta}$.
- ν: The spin-spin correlation length ξ diverges as $t \to 0$ (this is generally true for continuous phase transitions), with $h = 0$, according to $\xi \propto |t|^{-\nu}$.

- η: Exactly at the critical point, the spin-spin correlation function $G(r)$ does not decay exponentially, but rather according to $G(r) \propto 1/r^{d-2+\eta}$.

The critical exponents of the liquid-gas critical point can be defined by analogy with the uniaxial magnet case [4]:

- $C_V \propto |t|^{-\alpha}$ at $\rho = \rho_c$.

- $\rho_L - \rho_G \propto (-t)^\beta$ gives the shape of the coexistence curve near the critical point.

- isothermal compressibility $\chi_T \propto |t|^{-\gamma}$.

- $|p - p_c| \propto |\rho - \rho_c|^\delta$ gives the shape of the critical isotherm near the critical point.

The exponents ν and η are defined as for the ferromagnet, with $G(r)$ now being the density-density correlation function. The exponents of these two very different transitions are identical because of universality. Moreover, these critical exponents are normally not simple rational numbers (like 1/2, say) when measured in experiments. For example, the liquid-gas transition in sulphurhexafluoride [5] has been studied experimentally and it has been found that

$$|\rho_L - \rho_G| \propto |T - T_c|^{0.327 \pm 0.006} \tag{1.1}$$

The exponent has been measured in other fluids like He3 and the its value agrees within error bars. Similarly the exponent in uniaxial magnetic systems have been measured (e.g. in DyAlO3 [6]) and found to be identical to the liquid-gas transition exponents within error bars.

How does one explain universality and calculate quantities like critical exponents associated with continuous phase transitions? A key physical insight, largely due to Landau and Ginzburg [2], is that these universal critical singularities are associated with long-wavelength low-energy fluctuations of the order parameter field (call it $m(x)$ for concreteness). The idea is to construct an effective free energy (see Ref [2]) $\mathcal{L}$ which is local in terms of the order parameter field and its gradients, and is analytic. Thus $\mathcal{L}$ can be thought of as a Taylor expansion of a general function $f(m(x), \triangle m(x), \cdots)$. The only restriction on the expansion would be that each term in it is consistent with the symmetries of the order parameter field and that $\mathcal{L} \to \infty$ as $|m(x)| \to \infty$ so that the order parameter stays bounded. E.g., at zero magnetic field, the uniaxial magnet can be modeled by a scalar order parameter $m(x)$ and the effective free energy is invariant under $m(x) \to -m(x)$ because of the spin flip symmetry in the problem. The coefficients of the expansion can be thought to be phenomenological parameters which are non-universal functions of microscopic interactions and external parameters such as the temperature and magnetic field. Then we can write down the partition function $\mathcal{Z}$ as

$$\mathcal{Z} = \int \mathcal{D}m(x) \exp\left(-\beta \int d^d x \mathcal{L}(m(x), \triangle m(x), \cdot\cdot)\right) \tag{1.2}$$

Let us now motivate the Landau theory for the *simple* example of a uniaxial ferromagnet in zero magnetic field. Because the magnetic field is set to zero, only the temperature T is to be fine-tuned to T_c to achieve the critical point. Also, because of the $m(x) \to -m(x)$ symmetry,

$$\beta\mathcal{L} = \frac{1}{2}(\triangle m)^2 + a(t)m^2 + b(t)m^4 + \cdot\cdot \tag{1.3}$$

where $t = (T - T_c)/T_c$. Now how do we determine the functions $a(t), b(t)$ etc? Close to the critical point $t = 0$, we do not need to know the full functions $a(t), b(t)$ and can get away with their leading Taylor expansion terms. Also, we know that for $t > 0$, $\langle m \rangle = 0$ while for $t < 0$, $\langle m \rangle \neq 0$ and $\langle m \rangle$ falls continuously to zero as $t \to 0-$. We can expand the functions $a(t)$ and $b(t)$ as

$$a(t) = a_0 + a_1 t + \cdot\cdot$$

$$b(t) = b_0 + b_1 t + \cdot\cdot$$

If we want a single continuous phase transition at $t = 0$ and non-zero magnetization for $t < 0$, it is easy to see that $a_0 = 0$, $a_1 > 0$ and $b_0 > 0$. Thus we can take the effective free energy as

$$\mathcal{L} = \frac{1}{2}(\triangle m(x))^2 + a_1 t\, m(x)^2 + b_0 m(x)^4 \tag{1.4}$$

where a_1, b_0, T_c are all phenomenological constants in the theory. The Landau-Ginzburg way of looking at phase transitions brings universality to the forefront because the effective theory is only based on the symmetry properties of the order parameter field, and does not care about the microscopic origin of the order. In general, the functional integrals obtained cannot be solved analytically and approximations need to be made. Clearly, the simplest thing to do is to make a saddle-point approximation. This amounts to doing **Landau mean-field theory**, where we can ignore fluctuations of the order parameter field and take it to be a constant and minimize the resulting free energy. Thus, for the above example, we have

$$\mathcal{L}_{MF} = a_1 t\, m^2 + b_0 m^4 \tag{1.5}$$

where m is a constant now. Calculating the critical exponents in this formalism, we get $\alpha = 0, \beta = 1/2, \gamma = 1, \delta = 3, \nu = 1/2$ and $\eta = 0$, independent of the dimension d. However, these values are quite different from the experimentally obtained values of the critical exponents. The discrepancy between the mean-field results and experiments signal the failure of the mean field approximation. The problem arises because of the neglect of fluctuations of the order parameter field in the mean-field approximation. Because the correlation length diverges on approaching a continuous critical point, there are fluctuations of the order parameter field at all length scales, and these fluctuations get coupled due to interaction terms in the theory. One can check for the self-consistency of the Landau mean-field theory and see when the contribution due to fluctuations can be neglected. For the m^4 type theory above, it turns out that the fluctuations can be neglected only when $d > 4$, and thus the saddle-point type calculations are no longer reliable in $d = 3$.

The task of calculating the critical exponents correctly and capturing the non-analytic behaviour of various thermodynamic observables when approaching the critical point is achieved by combining **Renormalization Group** (RG) techniques to the Landau-Ginzburg effective theory (see Ref [3, 4]). Let us illustrate the basic idea of an RG through an example [4]. Consider the two-dimensional ferromagnetic Ising model on a square lattice. Instead of calculating the partition function at one go, let us integrate out the degrees of freedom in small steps or *coarse-grain*. Let us make the following transformation: we divide the square lattice into 3×3 blocks, each containing 9 spins. To each block, we assign a new variable $s' = \pm 1$, depending on whether the majority of spins in the block are up(+1) or down(-1). Notice that our blocking rule respects the up-down symmetry of the microscopic model because flipping the 9 spins of a block also changes the sign of the block spin s'. When this is done, we rescale the whole picture by a linear factor of 3, so that the blocks are the same size as the original squares. After a few iterations of this process a typical configuration with $T > T_c$ will evolve to complete randomness, while a configuration with $T < T_c$ will evolve to all spins up or all spins down. However, at $T = T_c$, the configuration obtained after the iterations is *statistically* the same as the first picture,i.e. it is an equally probable configuration at the critical point. This observation illustrates the scale invariance of the critical point ($\xi \to \infty$ as $T \to T_c$).

Let us formalize this blocking procedure. Suppose we have a set of spins $\{s\}$ and

$$\mathcal{Z} = \sum_{\{s\}} \exp(-H(\{s\})) \tag{1.6}$$

so that the probability distribution of a particular configuration $\{s\}$ is

$$P(\{s\}) = \frac{1}{\mathcal{Z}} \exp(-H(\{s\})) \tag{1.7}$$

where we have absorbed β in the definition of H. We set out to coarse-grain the system by defining general block spins. To do this, we introduce a conditional probability $P(\{s'\}|\{s\})$. This is the probability of finding the block spin configuration $\{s'\}$, given that the original spin configuration is $\{s\}$. For example, the 3×3 blocking introduced above would have

$$P(\{s'\}|\{s\}) = \prod_B \delta\left(s'_B - sgn \sum_{i \epsilon B} (s_i)\right) \tag{1.8}$$

Here s'_B labels the new block spin made out of the nine original spins. Because $P(\{s'\}|\{s\})$ is a probability, we must have

$$\sum_{\{s'\}} P(\{s'\}|\{s\}) = 1 \tag{1.9}$$

Using Eqn1.9, we can now write

$$\mathcal{Z} = \sum_{\{s\}} \sum_{\{s'\}} P(\{s'\}|\{s\}) \exp(-H(\{s\})) = \sum_{\{s'\}} \exp(-H'(\{s'\})) \tag{1.10}$$

where H' is the new Hamiltonian in terms of the block spin variables. Furthermore, because the new block spins are local functions of the old spins, this coarse-graining preserves all the long distance physics of the model. After blocking, it is convenient to shrink the system by a factor 1/3 in both directions so that each block spin occupies the same space as the old spin. Repeating this procedure, we thus get a sequence of Hamiltonians, all with the same long-distance physics.

$$H(\{s\}) \to H'(\{s'\}) \to H''(\{s''\}) \to \cdots \tag{1.11}$$

This is an example of a RG flow. Suppose there exists a Hamiltonian such that

$$H^* \to H^* \tag{1.12}$$

Such a Hamiltonian H^* is a **fixed point** of the renormalization group transformation and corresponds to a scale-invariant critical point. How do neighbouring hamiltonians behave under the RG ? Consider a hamiltonian H which lies near the fixed point H^*

$$H = H^* + \sum_i g_i O_i \tag{1.13}$$

where the O_i represent additional interactions. Under the RG flow, we will have

$$H \to H^* + \sum_i g_i' O_i \tag{1.14}$$

Near H^* the flow of g_i would be linear: $g_i \to g_i' = A_{ij} g_j + O(g^2)$. In general, A_{ij} is not symmetric, but let us assume that it is diagonalizable. Also, let us assume that O_i is chosen so that the matrix A_{ij} is diagonal with entries Λ_i. Then

$$g_i \to \Lambda_i g_i \to \Lambda_i^2 g_i \to \cdots \tag{1.15}$$

If $|\Lambda_i| < 1$ the coefficient of O_i decreases under the renormalization group flow and we say that such O_i are **irrelevant**. Conversely, if $|\Lambda_i| > 1$, the coefficient of O_i increases under the RG flow and we say that such O_i are **relevant** perturbations of H^*. When $|\Lambda_i| = 1$, we say that O_i is a **marginal** perturbation. Relevant operators take us away from criticality. For example, the magnetic field is a relevant perturbation for the Ising model critical point and any non-zero value of the field destroys criticality. The subspace spanned by the irrelevant directions is called the **basin of attraction** of the fixed point H^*, since the irrelevant couplings flow to zero under the RG. This provides an explanation of universality [3, 4] in that very many microscopic details of the system make up a huge space of irrelevant operators comprising the basin of attraction. Scaling arises [4] because the behaviour near the fixed point makes the singular part of the free energy a generalized homogeneous function of the form $F_s(\lambda^{a_h} h, \lambda^{a_t} t) = \lambda F_s(h, t)$, where h and t are the reduced magnetic field and reduced temperature defined earlier. Because thermodynamic observables can be obtained by suitable differentiation of the free energy, they also show scaling behaviour close to the critical point.

Although the idea of RG is relatively simple, calculating the flows explicitly can be quite difficult. Sophisticated approximation techniques [3] like the $\epsilon(= 4 - d)$-expansion and large N expansion can be used to solve the RG systematically but we will not discuss these here.

During recent years, a different class of phase transitions has generated a lot of interest, namely transitions which take place at zero temperature (see book by Sachdev [7]). A non-thermal control parameter such as pressure, magnetic field or chemical composition is varied to access the transition point. In these examples, the order is destroyed or changed solely by quantum fluctuations which come because of non-commuting (and hence competing) terms in the Hamiltonian of the system. These zero temperature phase transitions are called Quantum Phase Transitions (QPT).

At first glance, it might appear that the study of QPT is not of great interest because the transition only occurs at $T = 0$ which is impossible to access experimentally. However the presence of quantum critical points *can* affect finite temperature properties [7] as can be seen from the following argument [8]. Consider a quantum critical point separating two distinct ground states with very different quantum ordering and low-lying excitations. Close to the critical point, there is only a tiny difference between the energies of the two states, and only at very low temperatures is a particular one picked up as a ground state. At these temperatures, we can model the physics in terms of the low-lying excitations of *this* ground state, which are the "quasiparticles" associated with its ordering. At a somewhat different parameter value on the other side of the critical point, a different state will be picked up as the ground state and a quasiparticle picture would again apply at very low temperatures. However, the nature of the quasiparticles would in general be very different from the previous ones. At higher temperatures, it is impossible to ignore the competition between the two ground states and their respective quasiparticles, and complex behaviour which is not characteristic of either of the ground states can arise. In fact, it has been proposed that the anomalous properties of materials such as the cuprate superconductors is because of the proximity to quantum critical points separating two distinct phases.

How does one analyze quantum critical phenomena? Theoretically, the Landau-Ginzburg-Wilson (LGW) paradigm again provides the basic framework to understand these critical points. Critical modes associated with a QCP are again presumed to be the long-distance, long-time fluctuations of the order parameter field. In fact, a d-dimensional quantum system is equivalent (at least, formally) to some $d + 1$ dimensional classical system [7] as the temperature $T \to 0$. This statement may be understood by writing the partition function $\mathcal{Z}$

$$\mathcal{Z} = Tr(\exp(-\beta\hat{H}))$$

(where $\hat{H}$ is an operator now) as a path integral by splitting $\exp(-\beta\hat{H})$ as $[\exp(-(1/\hbar)\delta\tau\hat{H}]^N$ where $\delta\tau \to 0, N \to \infty$ such that $N\delta\tau = \beta\hbar$ in "imaginary time" $\beta\hbar$ (the operator $\exp(-\beta\hat{H})$ looks like the time-evolution operator of quantum mechanics $\exp(-i\hat{H}t)$ in imaginary time). Then the expression

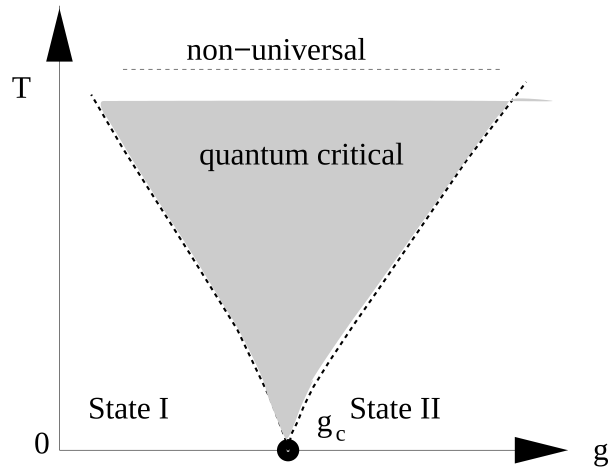

Figure 1.2: Schematic phase diagram in the vicinity of a QCP. The horizontal axis g represents the non-thermal control parameter tuning which drives the quantum phase transition,and the vertical axis is temperature T. In the region marked quantum critical, there is competition between the two ground states and their quasiparticles, which can lead to unconventional properties.

for the path integral looks like a classical partition function for a system with $d+1$ dimensions, expect that the dimension of the system in imaginary time is finite in extent and equals $\hbar\beta$. As $T \rightarrow 0$, the system size in this extra ”time” direction diverges, and we get a truly $d + 1$ dimensional effective classical theory.

Are there quantum phase transitions which lie outside the well-known LGW paradigm? Indeed there are cases where Landau order parameters do not capture the true order in a quantum phase. The well known phenomenon where this happens is the quantum Hall effect that occurs in a two-dimensional electron gas in high magnetic field. The electron does not survive as a quasiparticle in fractional quantum Hall states; and the order in such a state cannot be captured by a local Landau order parameter as the distinction between the states is not that of a symmetry but rather is *topological* in nature. There are continuous transitions between distinct quantum Hall state which cannot obviously be described by a conventional Landau-type treatment of the transition. But what about transitions between phases which can be characterized using Landau order parameters? Is it possible to violate the LGW paradigm in such cases? Recent work by Senthil *et. al* [1] show that such a breakdown is possible in certain phase transitions in two-dimensional quantum magnetism. For these critical points, the best starting point for the description of the critical theory is not in terms of the order parameter, but an emergent set of fractionalized degrees of freedom which are *natural* degrees of freedom only at the critical point.

In the next few chapters, we will set up the necessary background and then explain this remarkable possibility.

Chapter 2

Effective Theory of Quantum Antiferromagnets

Let us consider spin $S = 1/2$ moments on a $2D$ square lattice interacting with the following Hamiltonian:

$$H = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \tag{2.1}$$

where all couplings $J_{ij} > 0$ are antiferromagnetic in nature and respect lattice symmetries. Thus the interactions preserve both lattice symmetries and $SU(2)$ spin rotation symmetry. This model is the generalized antiferromagnetic Heisenberg model of spin half which emerges naturally as an effective Hamiltonian for Mott insulators (see Auerbach's book [9]).

What are the possible ground states of such a Hamiltonian? The simplest ground state we may think of is the so called Néel state (see Fig 2.1). Consider the nearest-neighbour Heisenberg antiferromagnet. Classically, the ground state is the state with $S_z = +1/2$ (z axis being arbitrary) on one sublattice and $S_z = -1/2$ on the other sublattice. However, the staggered magnetization, which acts as the order parameter for the Néel state, does not commute with the Hamiltonian and the simple-minded classical ground state is not the true ground state of the quantum problem. Does Néel order survive in the quantum ground state or is the ground state something else, without any long range Néel order? Clearly, quantum fluctuations increase as one decreases the value of spin S. It has been rigorously shown [10] that for the nearest-neighbour Heisenberg antiferromagnet on a d-dimensional hypercubic lattice, the ground state has Néel order for all S when $d \geq 3$ and for $S \geq 1$ when $d = 2$. The interesting case of $S = 1/2$ on the square lattice remains out of reach of these rigorous methods. However, numerical simulations [11] show that the ground state does have long range Néel order. The Néel state has been observed in a variety of insulators, which includes La_2CuO_4, the parent compound of the cuprate superconductors. The Néel state breaks spin rotation symmetry and the order parameter is a single vector $\vec{N}$ (the Néel vector), defined to describe a state of staggered magnetization,

$$\vec{S}_r = \epsilon_r \vec{N}_r \tag{2.2}$$

where ϵ_r equals +1 on one sublattice and −1 on the other sublattice. The Néel state has $\langle \vec{N}_r \rangle \neq 0$ and the low-energy excitations of the state are linearly dispersing spin waves. These spin waves are the gapless modes due to the broken spin rotation symmetry and have two independent polarizations (this follows very generally from the Goldstone Theorem).

What about possible ground states of this Hamiltonian which do not break spin rotation symmetry? From above, we know that the Hamiltonian must then consist of non-nearest neighbour interactions also. For example, we can think of the $J_1 - J_2$ model on the square lattice, where in addition to the nearest neighbour interaction J_1, one also has next nearest neighbour interaction J_2. The classical limit of this model has collinear Néel order for all J_2/J_1. For very small J_2, Néel order survives in the quantum ground state as well. However, numerical and series expansion studies [12] for $S = 1/2$ have shown that this model loses the order around $J_2/J_1 \approx 0.4$ and spin rotation symmetry is restored. The ground state breaks lattice symmetry instead.

More generally, such paramagnetic states can be broadly divided into two classes. Firstly there are states that can be described as "valence bond solid" (VBS) states. In a simple caricature of such a state, each spin forms a singlet with one of its neighbouring spins resulting in an ordered pattern of "valence bonds" (the singlets) (see Fig 2.1). For spin 1/2 systems on a square lattice, such states necessarily break lattice translational symmetry and the ground state is four-fold degenerate. The symmetry can be broken in two different ways, leading to what is called columnar order and plaquette order (Fig 2.1). In the plaquette state, singlets bonds resonate coherently between the two horizontal and vertical bonds of the elementary square plaquettes on the lattice (shown as dotted and undotted valence bonds in Fig 2.1). This type of ordering is called spin-Peierls ordering. A suitable order parameter for VBS order is the following :

$$\psi_{VBS} = \frac{1}{N} \sum_i \left((-1)^{x_i} \vec{S}_i \cdot \vec{S}_{i+\hat{x}} + i(-1)^{y_i} \vec{S}_i \cdot \vec{S}_{i+\hat{y}} \right) \tag{2.3}$$

The order parameter ψ_{VBS} is a complex number and ψ^4_{VBS} is real and positive for columnar order ($\psi_{VBS} = +1, +i, -1, -i$) and real and negative for plaquette order ($\psi_{VBS} = 1 + i, -1 + i, -1 - i, 1 - i$). In the S=1/2 VBS states there is an energy gap for spin-carrying S=1 quasiparticle excitations, which can be thought of as an adiabatic continuation of simply breaking a singlet valence bond into a triplet. Typically there is a coupling between the spin exchange energy and phonon displacements, which leads to lattice distortions whose pattern reflects the distribution of $\langle \vec{S}_i \cdot \vec{S}_j \rangle$.

A second class of more exotic paramagnetic states [13, 14, 15, 16, 17] is also possible in principle: in these states the valence bond configurations resonate amongst each other and form a "spin liquid". The resulting state has been argued to possess excitations with fractional spin 1/2 and interesting topological structure. However, we will not discuss these exotic states any further in this thesis.

In this chapter, our objective is to show that in the Néel phase or close to it, the long distance low energy fluctuations of the Néel order parameter are captured by the quantum O(3) non linear sigma model (NLσM) with the Euclidean action (here the lattice coordinate $r = (x, y)$ has been promoted to a continuum spatial coordinate and τ is imaginary time):

$$\begin{aligned} \mathcal{S}_n &= \mathcal{S}_0 + \mathcal{S}_B \\ \mathcal{S}_0 &= \frac{1}{2g}\int d\tau \int d^2r \left[\left(\frac{\partial \hat{n}}{\partial \tau}\right)^2 + c^2 \left(\nabla_r \hat{n}\right)^2\right] \\ \mathcal{S}_B &= iS\sum_r \epsilon_r \mathcal{A}_r \end{aligned} \tag{2.4}$$

We will then rewrite the quantum O(3) NLσM in another set of variables, the CP^1 representation, which would turn out to be very useful to describe the critical theory.

Here $\hat{n}_r \propto \epsilon_r \vec{S}_r$ is a unit three component vector that represents the Néel order parameter. The term $\mathcal{S}_B$ contains crucial quantum-mechanical Berry phase effects, and is sensitive to the precise quantized value, S of the microscopic spin on each lattice site: $\mathcal{A}_r$ is the (directed) area enclosed by the curve mapped out by the time evolution of $\hat{n}_r(\tau)$ on the unit sphere. These Berry phases play an unimportant role in the low energy properties of the Néel phase, but are crucial in correctly describing the quantum paramagnetic phase (VBS). In fact, the VBS state arises naturally in the large g limit if one carefully takes the Berry phases into account. Thus the NLσM field theory augmented by these Berry phase terms is, in principle, powerful enough to correctly describe both the Néel state and the VBS quantum paramagnet; and the quantum phase transition (QPT) between these two states. The Néel-VBS QPT for $S = 1/2$ spins on the square lattice has been argued to be an exotic phase transition outside the LGW paradigm in Ref [1].

2.1 Path Integral for Quantum Spins

Now we describe how to write the partition function of spins interacting via a generalized Heisenberg Hamiltonian (Eqn 2.1) in terms of a path integral. We shall consider the spin $S = 1/2$ case in detail here to show things very explicitly [18], the generalization to the case of an arbitrary spin is not difficult (a good reference for this is [7]).

2.1.1 Spin Coherent States

To write a path integral, clearly we cannot use the $S_z = |\uparrow, \downarrow\rangle$ basis. Instead, we go to an overcomplete basis $|\hat{N}\rangle$ where

$$\vec{S} \cdot \hat{N}|\hat{N}\rangle = \frac{1}{2}|\hat{N}\rangle \tag{2.5}$$

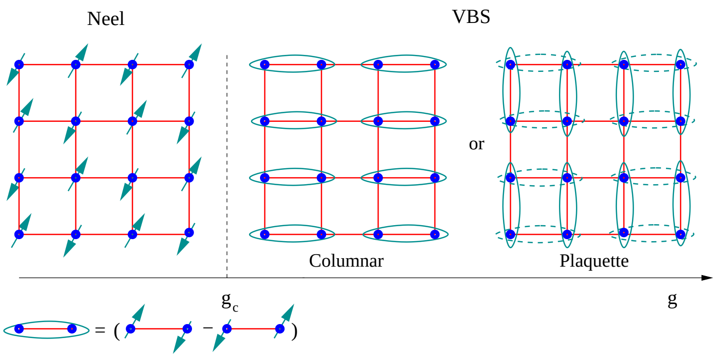

Figure 2.1: Ground states of the square lattice $S = 1/2$ quantum antiferromagnet. The coupling g controls the strength of quantum spin fluctuations about the magnetically ordered Néel state ($g = 0$ is the classical limit). There is broken spin rotation symmetry in the Néel state and broken lattice symmetry in the Valence Bond Solid (VBS) state. There can be two different orderings for the VBS state as shown in Figure, columnar ordering and plaquette ordering.

(more generally, the RHS is $S|\hat{N}\rangle$). $\hat{N}$ defines a direction on the unit sphere and the North Pole of the sphere may be identified with the state $|\uparrow\rangle$. One can easily figure out the state $|\hat{N}\rangle$ by rotating the "standard" state $|\uparrow\rangle$. The transformation is simply $|\hat{N}\rangle = \exp(-i\theta\hat{M}\cdot\vec{S})|\uparrow\rangle$, where the unit vector $\hat{M}$ is defined in Fig 2.2, where $\vec{S} = \vec{\sigma}/2$ (σ_x, σ_y and σ_z being the usual Pauli matrices). Writing it out explicitly, we have

$$|\hat{N}\rangle = \cos\frac{\theta}{2}|\uparrow\rangle + \sin\frac{\theta}{2}\exp(i\phi)|\downarrow\rangle \tag{2.6}$$

Clearly, this basis is overcomplete, which can be seen by computing $|\langle\hat{N}|\hat{N}'\rangle|^2 = (1+\hat{N}\cdot\hat{N}')/2$ (on the RHS, $\hat{N}$ denotes the unit vector $\hat{N}$). What is the resolution of identity in terms of these states? For spin $S = 1/2$,

$$\int\frac{d\hat{N}}{2\pi}|\hat{N}\rangle\langle\hat{N}| = \int\frac{d(\cos\theta)d\phi}{2\pi}|\hat{N}\rangle\langle\hat{N}| = \mathbb{I} \tag{2.7}$$

(More generally, the completeness relation is $(2S+1)\int\frac{d\hat{N}}{4\pi}|\hat{N}\rangle\langle\hat{N}| = \mathbb{I}$.) Another useful property to note is that

$$\langle\hat{N}|\vec{S}|\hat{N}\rangle = \frac{1}{2}\hat{N} \tag{2.8}$$

The RHS is $S\hat{N}$ in general. Now let us figure out how to write down the path integral representation for the partition function Z. First consider a single spin for notational convenience.

$$\begin{aligned} Z &= \sum_\alpha\langle\alpha|\exp(-\beta H)|\alpha\rangle \\ &= \int\mathcal{D}\hat{N}(0)\langle\hat{N}(0)|\exp(-\beta H)|\hat{N}(0)\rangle \end{aligned} \tag{2.9}$$

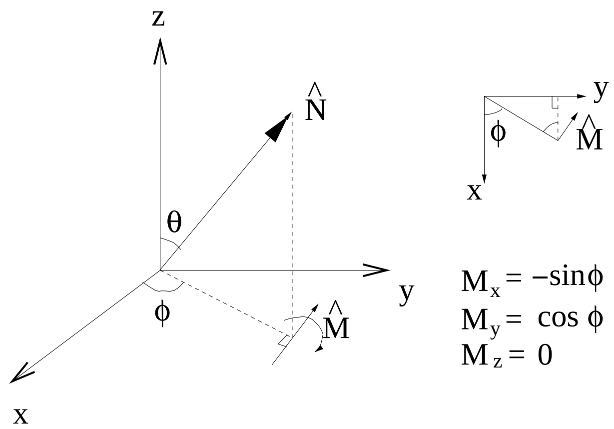

Figure 2.2: The rotation of the state $|\uparrow\rangle$ by an angle of θ about the axis $\hat{M}$ takes it to the state $|\hat{N}\rangle$. This can be used to determine the state $|\hat{N}\rangle$ easily.

We then perform the usual trick of breaking up the exponential $\exp(-\beta H)$ into a large number of exponentials of infinitesimal (imaginary) time evolution operators:

$$Z = \int \mathcal{D}\hat{N}(\tau_0)\mathcal{D}\hat{N}(\tau_1)\cdots\mathcal{D}\hat{N}(\tau_n)\prod_{i=0}^{n}\langle\hat{N}(\tau_i+\epsilon)|\exp(-\epsilon H)|\hat{N}(\tau_i)\rangle \tag{2.10}$$

where $|\hat{N}(\tau_0+n\epsilon)\rangle = |\hat{N}(\tau_0)\rangle$ (PBC) and $n\epsilon = \beta$. What is $\langle\hat{N}(\tau_i+\epsilon)|\exp(-\epsilon H)|\hat{N}(\tau_i)\rangle$ as $\epsilon \to 0$? It is easy to see that the answer is $\exp[-\epsilon(\langle\hat{N}|\frac{d\hat{N}}{d\tau}\rangle + H(S\hat{N}))]$. Then in the limit $\epsilon \to 0$, we may rewrite the partition function as

$$Z = \int \mathcal{D}\hat{N}(\tau)\exp\left(-\int_0^\beta d\tau(\langle\hat{N}|\frac{d\hat{N}}{d\tau}\rangle + H(S\hat{N}))\right); \quad |\hat{N}(0)\rangle = |\hat{N}(\beta)\rangle \tag{2.11}$$

Notice that $\int_0^\beta d\tau\langle\hat{N}|\frac{d\hat{N}}{d\tau}\rangle$ is a purely imaginary phase term. This term has an elegant geometric interpretation which we will work out in the next section.

2.1.2 Geometric Interpretation of the Phase Term

First, let us consider a single spin and define $\hat{M}(\tau)$ through the relation: $|\hat{N}(\tau)\rangle = \exp(-i\theta(\tau)\hat{M}(\tau)\cdot\vec{S})|\uparrow\rangle$. We further introduce the following notation, $|\hat{N}(u,\tau)\rangle = \exp(-iu\theta(\tau)\hat{M}(\tau)\cdot\vec{S})|\uparrow\rangle$ where $u \epsilon [0,1]$. Thus $|\hat{N}(0,\tau\rangle = |\uparrow\rangle$ and $|\hat{N}(1,\tau\rangle = |\hat{N}(\tau)\rangle$ and the vector $\hat{N}(u,\tau)$ moves from the north pole of the unit sphere to $\hat{N}(\tau)$ along the circle of constant ϕ as u is increased from 0 to 1. Then using the fact that $\hat{M}(\tau)\cdot\hat{N}(u,\tau) = 0$ and $\langle\hat{N}(u,\tau)|\vec{S}|\hat{N}(u,\tau)\rangle = S\hat{N}(u,\tau)$, we get the following relation:

$$\langle\hat{N}(\tau)|\frac{d\hat{N}(\tau)}{d\tau}\rangle = iS\int_0^1 du\theta(\tau)\hat{M}(\tau)\cdot\frac{d\hat{N}(u,\tau)}{d\tau} \tag{2.12}$$

We can further simplify the expression by using the relation $\hat{N}(u,\tau)\times\frac{\partial\hat{N}(u,\tau)}{\partial u} = \theta(\tau)\hat{M}(\tau)$. Putting this in the above formula, we get the following result for the phase term:

$$\int_0^\beta d\tau\langle\hat{N}(\tau)|\frac{d\hat{N}(\tau)}{d\tau}\rangle = iS\int_0^\beta d\tau\int_0^1 du\hat{N}(u,\tau)\cdot(\frac{\partial\hat{N}(u,\tau)}{\partial u}\times\frac{\partial\hat{N}(u,\tau)}{\partial\tau}) \tag{2.13}$$

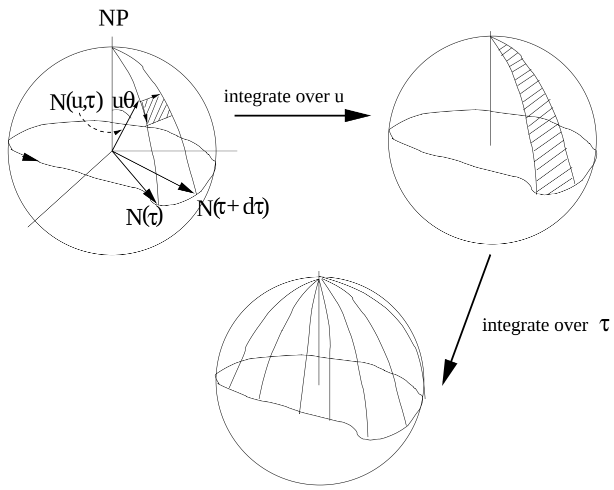

Figure 2.3: The geometric interpretation of the berry phase term as the directed area $\mathcal{A}$ swept by the "string" attached to the north pole and the instantaneous position of $\hat{N}(\tau)$. The phase term equals $iS\mathcal{A}$.

Eqn 2.13 has an elegant geometric interpretation [See Fig 2.3]. Because of the periodic boundary condition (PBC) on $\hat{N}(\tau)$, the vector $\hat{N}(\tau)$ traces a closed path on the surface of a unit sphere. Imagine attaching a "string" from the north pole of the sphere to the instantaneous position of $\hat{N}(\tau)$. Then the RHS of Eqn 2.13 is the (directed) area swept by this string on the unit sphere. If the path of $\hat{N}(\tau)$ is in the anticlockwise (clockwise) sense with respect to the north pole, the contribution is positive (negative). Note that the choice of the north pole on the unit sphere is arbitrary and the phase term is only defined modulo 4π. However, this is not a problem because of the quantization of the value of the spin S. The generalization to the case of a system of spins interacting via the generalized Heisenberg hamiltonian (Eqn 2.1) is immediate.

$$Z = \int \prod_i \mathcal{D}\hat{N}_i(\tau) \exp\left(-iS \sum_{i=1}^{N} \mathcal{A}_i - S^2 \int_0^\beta d\tau \sum_{i,j} J_{ij} \hat{N}_i \cdot \hat{N}_j \right) \tag{2.14}$$

with the boundary condition that $\hat{N}_i(0) = \hat{N}_i(\beta)$ for all i (i refers to the $2d$ lattice site).

2.1.3 Coarse Graining

The classical Heisenberg hamiltonian would have a staggered state as its ground state on the (bipartite) square lattice. Any pair of spins is either parallel or antiparallel, thus the ordering is collinear. Let us consider here quantum antiferromagnets whose classical ground state have collinear Néel order. Such an ordering can be expected to be present at least over short distances in the quantum case. Noncollinear ordering arises on nonbipartite lattices or even on bipartite lattices with certain types of further neighbour interactions. Such cases would not be considered here.

If the Néel order survives even for a few lattice spacings, we may think of doing a continuum theory in terms of new fields $\hat{n}$ and $\vec{L}$, where $\hat{n}$ and $\vec{L}$ refer to the staggered and uniform component of the magnetization. We write

$$\hat{N}_i(x_i,\tau) = \epsilon_i \hat{n}(x_i,\tau)\left(1-(\frac{a^d}{S})^2\vec{L}^2(x_i,\tau)\right)^{1/2} + \frac{a^d}{S}\vec{L}(x_i,\tau) \tag{2.15}$$

where $d(=2)$ id the dimension of the lattice and a is the lattice spacing. Because of the condition $\hat{N}_i\cdot\hat{N}_i = 1$, we get $\hat{n}_i\cdot\hat{n}_i = 1$ (that's why the notation $\hat{n}$) and $\hat{n}_i\cdot\vec{L}_i = 0$. Also, because of the implicit assumption of at least short range Néel order being present, we immediately have $\vec{L}^2 \ll S^2a^{-2d}$. Using Eqn 2.15, we can rewrite the Hamiltonian $H(S\hat{N}) = JS^2\sum_{ij}\hat{N}_i\cdot\hat{N}_j$ to the lowest order in $\vec{L}$ as $JS^2\sum_{ij}[(\hat{n}_i-\hat{n}_j)^2/2 + (a^{2d}/S^2)\vec{L}_i\cdot\vec{L}_j]$. Now, we go the continuum limit and get

$$Z = \int_{PBC}\mathcal{D}\hat{n}\mathcal{D}\vec{L}\delta(\hat{n}^2-1)\delta(\vec{L}\cdot\hat{n})\exp\left(-iS\sum_{i=1}^{N}\mathcal{A}_i - \int_0^\beta d\tau\int d^dx(\frac{\rho_s}{2}(\nabla_r\hat{n})^2 + S^2\frac{\vec{L}^2}{2\chi_\perp})\right) \tag{2.16}$$

where $\rho_s = JS^2/a^{d-2}$ and $\chi_\perp = S^2/(2dJa^d)$. Let us consider the Berry phase terms now. Insert the parameterization of the $\hat{N}$ field in terms of $\hat{n}$ and $\vec{L}$ and retain to first order in $\vec{L}$.

$$\begin{aligned}
S_B &= iS\sum_{i=1}^{N}\mathcal{A}_i \\
&= iS\sum_{i=1}^{N}\int_0^\beta d\tau\int_0^1 du\hat{N}_i(u,\tau)\cdot(\partial\hat{N}_i/\partial u\times\partial\hat{N}_i/\partial\tau) \\
&= iS\sum_i\epsilon_i\int_0^\beta d\tau\int_0^1 du[\hat{n}\cdot(\partial\hat{n}/\partial u\times\partial\hat{n}/\partial\tau)] \\
&+ i\int d^dx\int_0^\beta d\tau\int_0^1 du[\hat{n}\cdot(\partial\hat{n}/\partial u\times\partial\vec{L}/\partial\tau) + \hat{n}\cdot(\partial\vec{L}/\partial u\times\partial\hat{n}/\partial\tau) + \vec{L}\cdot(\partial\hat{n}/\partial u\times\partial\hat{n}/\partial\tau)]
\end{aligned} \tag{2.17}$$

Note that $\vec{L}$, $\partial\hat{n}/\partial\tau$ and $\partial\hat{n}/\partial u$ are all perpendicular to $\hat{n}$ and thus they lie in the same plane, and the last term in the above equation is zero. Moreover, we note that $\hat{n}\cdot(\partial\hat{n}/\partial u\times\partial\vec{L}/\partial\tau)+\hat{n}\cdot(\partial\vec{L}/\partial u\times\partial\hat{n}/\partial\tau)$ equals $\partial/\partial\tau[\hat{n}\cdot(\partial\hat{n}/\partial u\times\vec{L})]+\partial/\partial u[\hat{n}\cdot(\vec{L}\times\partial\hat{n}/\partial\tau)]$. Doing the "surface" integrals over τ and u in the two terms and noting that the first term vanishes because of the periodicity of $\hat{n}$ and $\vec{L}$ in τ and in the second term, the $u = 0$ term vanishes, we finally get

$$S_B = iS\sum_i\epsilon_i\int_0^\beta d\tau\int_0^1 du[\hat{n}\cdot(\partial\hat{n}/\partial u\times\partial\hat{n}/\partial\tau) - \int d^dx\int_0^\beta d\tau\vec{L}\cdot(\hat{n}\times\partial\hat{n}/\partial\tau) \tag{2.18}$$

Putting the above expression in Eqn 2.16 and integrating out the $\vec{L}$ field, we finally get the result (quantum O(3) NLσM) as shown in Equation 2.4.

2.1.4 Topological Nature of the Berry Phase Term

Let us first evaluate the Berry phase term $S_B = iS\sum_i \epsilon_i \mathcal{A}_i$ in $d = 1$. Let us examine the contribution of two neighbouring sites, i and $i+1$ to S_B. The weights ϵ_i will have opposite signs on the two sites, so the net contribution is the difference of these areas. We further assume that the order parameter field $\hat{n}$ only varies slightly between i and $i+1$. Then we can write

$$\mathcal{A}_{i+1} - \mathcal{A}_i \approx a\int_0^\beta d\tau\hat{n}(x_i)\cdot(\partial\hat{n}(x_i)/\partial x_i \times \partial\hat{n}(x_i)/\partial\tau) \tag{2.19}$$

The summation in S_B can be carried out over pairs of sites. All terms are of the same sign and the summation can thus be easily converted into an integral. We then get

$$\begin{aligned} S_B &= i(2\pi S)[\frac{1}{4\pi}\int dx\int_0^\beta d\tau\hat{n}\cdot(\partial\hat{n}/\partial x\times\partial\hat{n}/\partial\tau)] \\ &= i(2\pi S)Q \end{aligned} \tag{2.20}$$

The term Q is called the "Pontryagin index", is topological in nature and can only take integer values (see Polyakov's book [19]). In order for the NLσM action to be finite in the infinite volume limit, we have to consider the boundary condition:

$$\hat{n}(\vec{x}) \to \hat{n}_0; \quad |\vec{x}| \to \infty \tag{2.21}$$

where $\vec{x}$ is now a point in the (x,τ) plane. Therefore, since infinity can be viewed as one point, our $\vec{x}$-space is topologically a sphere. Each configuration $\hat{n}(\vec{x})$ defines a map of such a sphere in $\vec{x}$-space onto the sphere $\hat{n}^2 = 1$, which gives $S^2 \to S^2$. It is known that such maps can be classified by integers Q which define the number of times the second sphere is covered by the first one. The simplest example of the Q-map is described by the formulas [19]:

$$\tilde{\theta} = \theta; \quad \tilde{\phi} = Q\phi \pmod{2\pi} \tag{2.22}$$

where (θ,ϕ) and $(\tilde{\theta},\tilde{\phi})$ are the polar and azimuthal angles of the first and second sphere. $Q \neq 0$ configurations are called skyrmions. A $Q = 1$ configuration is shown in Fig 2.4. Thus the Berry phase in $d = 1$ is $S_B = i2\pi S\,Q$ where Q is the skyrmion number of the spin configuration.

What happens in higher dimensions e.g. $d = 2$? There, one has to calculate the Berry phase by summing over a given spin configuration in (x,y,τ) space. It is easy to see that the Berry phase vanishes for any *smooth* field configuration of $\hat{n}$ [20]. We calculate Q for each configuration of $\hat{n}$ in the $x-\tau$ plane and then sum up over all the $x-\tau$ planes [call that object $Q_{x,\tau}(y)$ where $y\epsilon\mathbb{Z}$ and refers to the y coordinate]. Now, by assumption, $\hat{n}$ is continuous, and hence $Q_{x,\tau}(y)$ is a continuous integer-valued function. Thus $Q_{x,\tau}(y)$ is a constant! Thus, $S_B = i(2\pi S)Q\sum_{n_y}(-1)^y$ which vanishes in the continuum limit. This argument holds for any spatial dimension greater than one.

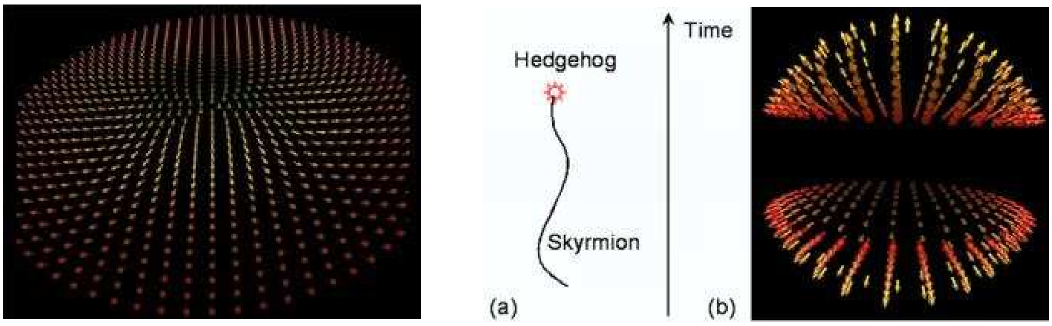

Figure 2.4: (a)Real-space representation of a skyrmion in the Néel field $\hat{n}$. Spins in the center are pointing down whereas spins on the boundaries point up. The charge of this skyrmion is $Q = 1$. Also shown in (b)The skyrmion number is suddenly changed at a hedgehog event in space time. The Real-space representation of a hedgehog event (the two spin configurations represent different time slices) is shown. A hedgehog corresponds to a singular configuration of $\hat{n}$ at one space-time point where the skyrmion number changes. All spins are pointing outwards of a hedgehog. Figures taken from F. Alet et al., Physica A 369 (2006) 122-142.

However, if one allows for singular configurations in the field $\hat{n}$, then the skyrmion number can change [20] and the Berry phase term might become important. For example, for $d = 2$, the $\hat{n}$ field *lives* in the (x, y, τ) space, and the natural topological defects in this situation are "hedgehogs" configurations. A hedgehog is a configuration of the $\hat{n}$ vectors, which is singular at one space-time point but smooth everywhere else (see Fig 2.4(b)). The skyrmion number Q changes when one crosses the singularity. What is the role of these topological defects? In the Néel phase, hedgehogs are very costly energetically and are therefore absent. Deep within a paramagnet, the spins fluctuate essentially independent of each other. In this case, the hedgehogs are indeed present. We will see in the next chapter that the proliferation of these hedgehogs not only destroy the Néel phase, but also break the lattice symmetry when they condense [20].

2.2 $\mathbf{CP}^1$ formulation of the theory

It would be helpful to rewrite the above NLσM field theory in the so-called CP^1 formulation (see review by Sachdev [21] or Auerbach [9]) to analyze the novel physics of the quantum critical point between the Néel and the VBS states, as it turns out to be the natural description of the critical point. The Néel order parameter $\hat{n}$ transforms as a vector and hence, is a spin 1 object. Suppose we decompose the $\hat{n}$ field into two complex fields $(z_\uparrow, z_\downarrow)$:

$$\hat{n} = z^*_\alpha \vec{\sigma}_{\alpha\beta} z_\beta, \quad (\alpha, \beta = \uparrow, \downarrow) \tag{2.23}$$

where $\vec{\sigma}$ are the usual Pauli matrices. The constraint $\hat{n} \cdot \hat{n} = 1$ translates to $|z_\uparrow|^2 + |z_\downarrow|^2 = 1$. z is nothing but a spinon (spin-1/2 object). Thus the physical Néel field has been written in terms of these spinons, which are fractionalized degrees of freedom. Remarkably, it turns out that these are the natural variables to describe the the critical point of the Néel-VBS transition for spin-1/2 moments on the square lattice. It will turn out that the theory is that of two *charged* complex fields $z_\uparrow, z_\downarrow$ interacting with a single $U(1)$ gauge field. It is easy to understand where the gauge field comes from. The physical field $\hat{n}$ has two independent components (remember the unit length constraint). However, the description is terms of z has three independent components instead (because of $|z_\uparrow|^2 + |z_\downarrow|^2 = 1$). This extra degree of freedom corresponds to the gauge freedom in the description. The local $U(1)$ gauge freedom is simply $z_\alpha \rightarrow z_\alpha \exp(i\phi)$ and $z^*_\alpha \rightarrow z^*_\alpha \exp(-i\phi)$ which leaves the physical Néel field $\hat{n}$ invariant. Also, because of the above transformation, the z field is charged with respect to the $U(1)$ gauge field (z and z^* are oppositely charged), while the Néel field $\hat{n}$ is neutral. Now let us explicitly do the steps see all this.

Firstly, by definition (Eqn 2.23), we have

$$\begin{aligned} n_x &= z^*_\uparrow z_\downarrow + z^*_\downarrow z_\uparrow \\ n_y &= i(z^*_\uparrow z_\downarrow - z^*_\downarrow z_\uparrow) \\ n_z &= z^*_\uparrow z_\uparrow - z^*_\downarrow z_\downarrow \end{aligned} \tag{2.24}$$

From this, we can easily verify that

$$\frac{1}{4}(\partial_\mu \hat{n}) \cdot (\partial_\mu \hat{n}) = (\partial_\mu z^*_\alpha)(\partial_\mu z^*_\alpha) + (z^*_\alpha \partial_\mu z_\alpha)(z^*_\beta \partial_\mu z_\beta) \tag{2.25}$$

The local $U(1)$ symmetry strongly reminds us of gauge theories. Suppose we invent a gauge potential A_μ (a real field) which has the following transformation:

$$\begin{aligned} z_\alpha &\rightarrow z_\alpha \exp(i\phi) \\ A_\mu &\rightarrow A_\mu + \partial_\mu \phi \end{aligned} \tag{2.26}$$

Then as is usual in gauge theories, we define the quantity $D_\mu = (\partial_\mu - iA_\mu)$. Then its transformation is simple.

$$\begin{aligned} D_\mu z_\alpha &= (\partial_\mu - iA_\mu) z_\alpha \rightarrow (D_\mu z_\alpha) \exp(i\phi) \\ (D_\mu z_\alpha)^* &= (\partial_\mu + iA_\mu) z^*_\alpha \rightarrow (D_\mu z_\alpha)^* \exp(-i\phi) \end{aligned} \tag{2.27}$$

which means that $(D_\mu z_\alpha)^*(D_\mu z_\alpha)$ is invariant under the gauge transformation. Then we write the gauge invariant quantity $1/4|\partial_\mu \hat{n}|^2$ as $(D_\mu z_\alpha)^*(D_\mu z_\alpha)$ and figure out the A_μ by comparison. This gives $A_\mu = -iz^*_\alpha \partial_\mu z_\alpha$, which is real and satisfies the transformation property of the gauge field stated earlier. Then, ignoring the Berry phase term, we may immediately write our earlier field theory as:

$$Z = \int \mathcal{D}^2 z \mathcal{D} A_\mu \mathcal{D}\lambda \exp\left(-\frac{1}{g} \int d\tau d^2 x [\sum_\mu |(\partial_\mu - iA_\mu) z|^2 - i\lambda(|z|^2 - 1)] \right) \tag{2.28}$$

The field A_μ can be promoted to an independent degree of freedom in the path integral above [9] because it appears only till quadratic order in the action and the Euler-Lagrange equation $\frac{\delta L}{\delta A_\mu} = 0$ gives back the correct definition of A_μ.

What about the Berry phase? It can be shown that [9]

$$\begin{aligned}\frac{1}{2}\hat{n}\cdot(\partial_\mu\hat{n}\times\partial_\nu\hat{n}) &= \partial_\mu(z^*_\alpha\partial_\nu z_\alpha)-\partial_\nu(z^*_\alpha\partial_\mu z_\alpha)\\ &= \partial_\mu A_\nu-\partial_\nu A_\mu\end{aligned} \qquad (2.29)$$

Now the skyrmion number Q at any instant of (imaginary) time is

$$2\pi Q=\int d^2x(\partial_x A_y-\partial_y A_x) \qquad (2.30)$$

The RHS is nothing but the flux of the gauge field at that instant of time. Now, we have already seen that Q changes due to hedgehog configurations of the Néel field. Also, taking the usual definition of $\vec{B}=\vec{\nabla}\times\vec{A}$, we see that the above implies that $\vec{\nabla}\cdot\vec{B}\neq 0$ at the cores of the hedgehogs. Thus monopoles of the gauge theory which change the flux by $\pm 2\pi$ are identified as the hedgehog configurations in the usual Néel field picture. The Berry phase term naturally forces us to consider configurations with monopoles (the total charge of the monopoles should be zero to respect periodicity) in our partition function and hence the gauge field A_μ is to be treated as a compact $U(1)$ gauge field, i.e., A_μ is an angle defined modulo 2π instead of being an ordinary number [There are no monopoles for non-compact A_μ, e.g. in the usual electrodynamics]. We will now do a careful analysis with the Berry phase term present and see what is the actual path integral for Z.

2.2.1 Analysis with the Berry Phase present

The main problem in calculating the Berry phase is that one has to keep track of the areas enclosed by the curves traced out by all the spins on the unit sphere (remember the Berry phase equals $iS\sum_r \epsilon_r\mathcal{A}_r$) . This seems complicated because the area is a global object defined by the whole curve, and cannot be obviously associated with a local portion of the curve. One convenient way to proceed is the following.

We discretize imaginary time, choose a fixed arbitrary point $\hat{n}_0$ on the unit sphere, and write the area of the closed loop as a sum of the areas of a large number of spherical triangles. Note that each triangle is associated with a local portion of the curve $\hat{n}(\tau)$. We now need an expression for $\mathcal{A}(\hat{n}_1,\hat{n}_2,\hat{n}_3)$, defined as half the area of the spherical triangle with vertices $\hat{n}_1,\hat{n}_2$ and $\hat{n}_3$ [think of $\hat{n}_1$ as $\hat{n}_j(\tau)$, $\hat{n}_2$ as $\hat{n}_j(\tau+d\tau)$ and $\hat{n}_3$ as $\hat{n}_0$ for concreteness, where $\hat{n}_0$ is identified with the north pole of the sphere]. The required expression is (see Sachdev and Park [22]):

$$\exp(i\mathcal{A})=\frac{1+\hat{n}_1\cdot\hat{n}_2+\hat{n}_2\cdot\hat{n}_3+\hat{n}_3\cdot\hat{n}_1+i\hat{n}_1\cdot(\hat{n}_2\times\hat{n}_3)}{[2(1+\hat{n}_1\cdot\hat{n}_2)(1+\hat{n}_2\cdot\hat{n}_3)(1+\hat{n}_3\cdot\hat{n}_1)]^{1/2}} \qquad (2.31)$$

The above formula looks very complicated. However, a far simpler expression [22] is obtained after transforming to the spinor variables. Let us define a variable $\mathcal{A}_{ij}$ associated with each pair of vertices

i, j.

$$\mathcal{A}_{ij} = \arg[z^*_{i\alpha} z_{j\alpha}] \tag{2.32}$$

[We are thinking of $2+1$ dimensions as a three dimensional lattice now.] Notice that $\mathcal{A}_{ij}$ is a compact field defined modulo 2π. Moreover, under the gauge transformation $z_\alpha \to z_\alpha \exp(i\phi)$, we have $\mathcal{A}_{ij} \to \mathcal{A}_{ij} - \phi_i + \phi_j$, thus $\mathcal{A}_{ij}$ behaves like a compact $U(1)$ gauge field (also note that $\mathcal{A}_{ji} = -\mathcal{A}_{ij}$). How is this compact field related to our earlier definition of the gauge field A_μ? A_μ is just the naive continuum limit of $\mathcal{A}_{ij}$. The classical result for the half-area of the spherical triangle can be written in the following simple form in terms of the present $U(1)$ gauge variables:

$$\mathcal{A}(\hat{n}_1, \hat{n}_2, \hat{n}_3) = \mathcal{A}_{12} + \mathcal{A}_{23} + \mathcal{A}_{31} \tag{2.33}$$

Note that the total area is invariant under the gauge transformation of $\mathcal{A}_{ij}$ and that the half-area is ambiguous modulo 2π (as it should be). We can finally write down a useful expression for $\mathcal{A}[\hat{n}(\tau)]$. We assume that imaginary time is discretized into times τ_j separated by intervals $\triangle\tau$. Also, we denote by $j + \tau$ the site at time $\tau_j + \triangle\tau$, and define $\mathcal{A}_{j,j+\tau} \equiv \mathcal{A}_{j\tau}$. Then

$$\mathcal{A}[\hat{n}(\tau)] = \sum_j \mathcal{A}_{j\tau} \tag{2.34}$$

Note that this expression is a gauge-invariant function of the $U(1)$ gauge field. We are now ready to write down the field theory with the Berry phase properly taken into account (see Sachdev's review [21]).

(i) Discretize space-time into a cubic lattice of points j.

(ii) On each space-time point j, we represent the quantum spin operator $\vec{S}_j$ by $\vec{S}_j = \epsilon_j S \hat{n}_j$ where ϵ_j is the staggering factor on the square lattice as before. In the quantum fluctuating Néel state, we can reasonably expect $\hat{n}_j$ to be a slowly varying function of j.

(iii) Associated with each $\hat{n}_j$, define a spinor $z_{j\alpha}$ using Eq 2.23.

(iv) With each link of the cubic lattice, we use Eq 2.32 to associate with it a $\mathcal{A}_{j\mu} \equiv \mathcal{A}_{j,j+\mu}$. Here $\mu = x, y, \tau$ extends over the 3 space-time directions.

Using this notation, the field theory (written on the lattice) becomes:

$$\tilde{\mathcal{Z}} = \prod_{j\alpha} \int dz_{j\alpha} \prod_j \delta(|z_{j\alpha}|^2 - 1) \exp\left(\frac{1}{g} \sum_{\langle ij \rangle} \hat{n}_i \cdot \hat{n}_j + i2S \sum_j \epsilon_j \mathcal{A}_{j\tau} \right) \tag{2.35}$$

The above expression can be made to look more like a conventional lattice gauge theory [21]by writing it in the following manner.

$$\mathcal{Z} = \prod_{j\mu} \int_0^{2\pi} \frac{dA_{j\mu}}{2\pi} \prod_{j\alpha} \int dz_{j\alpha} \prod_j \delta(|z_{j\alpha}|^2 - 1) \exp\left(\frac{1}{g} \sum_{j\mu} (z^*_{j\alpha} e^{-iA_{j\mu}} z_{j+\mu,\alpha} + c.c.) + i2S \sum_j \epsilon_j A_{j\tau} \right) \tag{2.36}$$

Note that we have introduced a new field $A_{j\mu}$, on each link of the cubic lattice, which is integrated over. Like $\mathcal{A}_{j\mu}$, this is also a compact $U(1)$ gauge field because all terms in the action above are invariant under an analogous gauge transformation of $A_{j\mu}$. The very close relationship between $\tilde{\mathcal{Z}}$ and $\mathcal{Z}$ may be seen by explicitly integrating over the $A_{j\mu}$ in the previous expression and using the relation

$$z^*_{i\alpha} z_{j\alpha} = \left(\frac{1 + \hat{n}_i \cdot \hat{n}_j}{2} \right)^{1/2} e^{i\mathcal{A}_{ij}} \tag{2.37}$$

The integrals over $A_{j\mu}$ can be done exactly because the integrand factorizes into terms on each link that depend only on a single $A_{j\mu}$. The Berry phase term obtained after the integrations is exactly the same as in $\tilde{\mathcal{Z}}$. Also, the integrand contains a real action that is solely a sum over functions of $\hat{n}_i \cdot \hat{n}_j$ on nearest neighbour links: in $\tilde{\mathcal{Z}}$ this function is simply $\hat{n}_i \cdot \hat{n}_j / g$, but the corresponding function obtained from $\mathcal{Z}$ is more complicated (it involves the logarithm of a Bessel function), and has distinct forms on spacial and temporal links. However, these details should not affect the universal properties and we will work with the form $\mathcal{Z}$ for convenience. We note two crucial ingredients in the present theory which would be crucial in what follows: firstly the $U(1)$ gauge field is compact and secondly, our model contains a Berry phase term which can be interpreted as a $J_\mu A_\mu$ term associated with a current $J_{j\mu} = 2S\,\epsilon_j \delta_{\mu\tau}$ of static charges $\pm 2S$ on each site.

The properties of $\mathcal{Z}$ are quite evident for small g [21]. Here one can ignore the Berry phase term and the ground state should have Néel order, with the low-lying excitations being linearly dispersing spin waves. How does one see it in this gauge theory picture? The Neel phase corresponds to the "**Higgs Phase**" of the gauge theory as given in Eqn 2.35.

The matter field z_α acquires a finite expectation value which automatically gives a mass to the gauge photon. However, crucially there are two complex fields $(z_\uparrow, z_\downarrow)$ in the problem and only one gets a finite mass by "higgsing" the $U(1)$ gauge field A_μ. The other complex field is still gapless and produces a doublet of spin-waves in the Néel field picture. Let us illustrate this by saying that the Néel vector picks up the z axis for ordering for notational simplicity. This corresponds to saying that $\langle z_\uparrow \rangle = 1$ and $\langle z_\downarrow \rangle = 0$ [note that $z_\uparrow$ and $z_\downarrow$ cannot be simultaneously be equal to one because of the constraint $|z_\uparrow|^2 + |z_\downarrow|^2 = 1$] . Then the $z_\uparrow$ field higgses the gauge field and itself gets gapped. However, the $z_\downarrow$ field is still massless and generates two linearly dispersing modes. These are nothing but the deformations of the n_x and the n_y fields because these are linear in $z_\downarrow$ (see Eqn 2.24). We will briefly describe the Higgs mechanism below.

When a continuous symmetry is spontaneously broken, there are gapless excitations called Goldstone modes connecting the possible vacua to each other. However, the situation is different in the presence of gauge fields. The Goldstone modes and the gauge fields conspire to create massive excitations, destroying both the massless photon mode of the gauge field and the massless Goldstone mode in the process [23]. This effect is what leads to the Meissner effect in a superconductor where an external magnetic field can penetrate the superconductor only upto a certain characteristic length known as the London penetration depth.

For clarity, consider a charged field ϕ coupled to an abelian gauge field A_μ, where the action is given by

$$\mathcal{S} = (\partial_\mu + iA_\mu)\phi^*(\partial_\mu - iA_\mu)\phi + r\phi^*\phi + u(\phi^*\phi)^2 + \frac{r^2}{4u} \tag{2.38}$$

where the minimum of $V(\phi) = r\phi^*\phi + u(\phi^*\phi)^2 + \frac{r^2}{4u}$ where $r < 0, u > 0$ occurs for a non-zero value of $\phi^*\phi$ $(-r/2u)$, and the action is invariant under the local transformation

$$\phi \to \exp(-i\theta)\phi$$

$$A_\mu \to A_\mu + \partial_\mu\theta$$

First, consider the case without the gauge fields. Also, let us make the choice that the field ϕ orders in the real direction. Thus, we have $\phi = \phi_1 + i\phi_2$ where $\phi_1 = \sqrt{-r/2u} + \phi_1^{'}(x)$ and $\langle\phi_1^{'}\rangle = \langle\phi_2\rangle = 0$. Putting this in the Lagrangian, we see that there is no (ϕ_2^2) term, showing that ϕ_2 is the Goldstone mode associated with the $U(1)$ symmetry breaking (however, the $\phi_1^{'}$ excitations are massive).

Now, we put in the gauge fields and do the same exercise. Then to quadratic order, we get the following result

$$\mathcal{S} = (\partial_\mu\phi_1^{'})(\partial_\mu\phi_1^{'}) + \frac{|r|B_\mu^2}{2u} + 2|r|(\phi_1^{'})^2 + \text{higher order} \tag{2.39}$$

where $B_\mu = A_\mu - \sqrt{2u/|r|}\partial_\mu\phi_2$. The net result is that the gauge field has acquired a mass while ϕ_2 has disappeared from $\mathcal{S}$. We started with a system describing a charged scalar field (two states) and a massless gauge field with two polarization states. After spontaneous symmetry breaking of the matter field, we are left with a massive vector field B_μ with three polarizations and one real scalar field, which leaves the correct number of degrees of freedom.

The situation is much more complicated for large g where one gets a paramagnetic phase due to strong quantum fluctuations. Here the Berry phase term in the action plays a crucial role and cannot be ignored. We will study the paramagnetic phase in the next chapter and see how to deal with the Berry phase.

Chapter 3

Quantum Paramagnetic Phase

What about the paramagnetic state of the generalized antiferromagnetic Heisenberg Hamiltonian, where spin rotation symmetry is restored. If we ignore the Berry phase terms in the field theory developed in the previous chapter, we would get an *ordinary* paramagnet with a non-degenerate disordered ground state with a finite energy gap to other states. However, a theorem recently proven by Hastings [24] for generalized Heisenberg models with periodic boundary conditions shows that the above mentioned plain paramagnet does not exist in $2D$ at $T = 0$. Barring exotic spin liquid states mentioned before, the ground state would then have to be degenerate, with a gap to the excited states; and would then break some other symmetry in the thermodynamic limit. In this chapter, we carefully take the Berry phase terms in account and show how a quantum paramagnet with the correct symmetry breaking arises in the large g limit.

3.1 Mapping to a Height Model

For large g, we can perform the analog of a "high-temperature" expansion [21] of $\mathcal{Z}$ (Eqn 2.35). We expand the integrand in powers of $1/g$ and perform the integral over $z_{j\alpha}$ term-by-term. The result is then an effective theory for the compact $U(1)$ gauge field $A_{j\mu}$ alone. An explicit expression for the effective action of this theory can be obtained in powers of $1/g$: this has the structure that higher powers of $1/g$ yield terms dependent upon gauge-invariant $U(1)$ fluxes on loops of all sizes residing on the links of the cubic lattice. For large g, it is sufficient to retain only the simplest such term on elementary square plaquettes, yielding the following partition function:

$$\tilde{\mathcal{Z}}_A = \prod_{j\mu} \int_0^{2\pi} \frac{dA_{j\mu}}{2\pi} \exp\left(\frac{1}{e^2} \sum_{\square} \cos(\epsilon_{\mu\nu\lambda} \triangle_\nu A_{j\lambda}) + i2S \sum_j \epsilon_j A_{j\tau} \right) \tag{3.1}$$

where e monotonically increases with g, in fact $e^2 \sim g^4$ ($\epsilon_{\mu\nu\lambda}$ is the totally antisymmetric tensor in three space-time dimensions). Here the cosine term represents the conventional Maxwell action for a compact $U(1)$ gauge theory: it is the simplest local term consistent with the gauge symmetry of $A_{j\mu}$ and which is periodic under $A_{j\mu} \to A_{j\mu} + 2\pi$. We would now perform a series of transformations

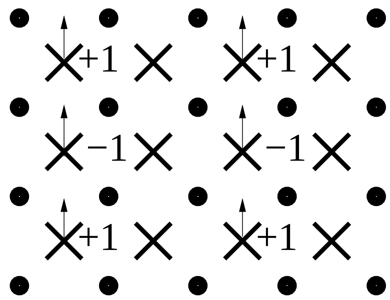

Figure 3.1: The non-zero values of $a^0_{j\mu}$ shown in the figure. The circles are the sites of the direct lattice, while the crosses are the sites of the dual lattice. The $a_{j\mu}$ are all zero for $\mu = \tau, x$ while the only non-zero values of a^0_{jy} are shown above. Note that the flux satisfies Eqn 3.3.

(see Vojta and Sachdev [25]) on Eqn 3.1 to bring it to a much more convenient form from which the properties of the paramagnet will be deduced. First the cosine term in Eqn 3.1 is replaced by a Villain sum over periodic Gaussians:

$$\mathcal{Z}_A = \sum_{a_{j\mu}} \prod_{j\mu} \int_0^{2\pi} \frac{dA_{j\mu}}{2\pi} \exp\left(-\frac{e^2}{2} \sum_{j,\mu} a^2_{j\mu} + i \sum_{\Box} \epsilon_{\mu\nu\lambda} a_{j\mu} \triangle_\nu A_{j\lambda} + i2S \sum_j \epsilon_j A_{j\tau} \right) \tag{3.2}$$

where $a_{j\mu}$ is an integer-valued vector field on the links on the dual cubic lattice (let us identify each dual lattice point with the direct lattice site closest to it on its top-right corner). Now, let us choose a 'background' $a_{j\mu} = a^0_{j\mu}$ flux which satisfies the following relation:

$$\epsilon_{\mu\nu\lambda} \triangle_\nu a^0_{j\lambda} = \epsilon_j \delta_{\mu\tau} \tag{3.3}$$

Any integer valued solution of Eqn 3.3 is an acceptable choice for $a^0_{j\mu}$, and a particularly convenient choice [21, 25] is shown in Fig 3.1. Then we can write Eqn 3.2 in a more symmetric form as

$$\mathcal{Z}_A = \sum_{a_{j\mu}} \prod_{j\mu} \int_0^{2\pi} \frac{dA_{j\mu}}{2\pi} \exp\left(-\frac{e^2}{2} \sum_{j,\mu} a^2_{j\mu} + i \sum_{\Box} \epsilon_{\mu\nu\lambda} a_{j\mu} \triangle_\nu A_{j\lambda} + i2S \sum_j \epsilon_{\mu\nu\lambda} a^0_{j\mu} \triangle_\nu A_{j\lambda} \right) \tag{3.4}$$

Define another integer-valued vector field $\tilde{a}_{j\mu}$ which satisfies $\tilde{a}_{j\mu} = a_{j\mu} + 2S\, a^0_{j\mu}$. Then, Eqn 3.4 can be rewritten as

$$\mathcal{Z}_A = \sum_{\tilde{a}_{j\mu}} \prod_{j\mu} \int_0^{2\pi} \frac{dA_{j\mu}}{2\pi} \exp\left(-\frac{e^2}{2} \sum_{j,\mu} (\tilde{a}_{j\mu} - 2S\, a^0_{j\mu})^2 + i \sum_{\Box} \epsilon_{\mu\nu\lambda} \tilde{a}_{j\mu} \triangle_\nu A_{j\lambda} \right) \tag{3.5}$$

Now the integration over $A_{j\mu}$ can be trivially performed, and it yields the constraint $\epsilon_{\mu\nu\lambda} \triangle_\nu \tilde{a}_{j\lambda} = 0$. We solve this constraint by writing $\tilde{a}_{j\lambda}$ as the gradient of an integer-valued 'height' field h_j which lives on the sites of the dual lattice:

$$\mathcal{Z}_h = \sum_{h_j} \exp\left(-\frac{e^2}{2} \sum_{j,\mu} (\triangle_\mu h_j - 2S\, a^0_{j\mu})^2 \right) \tag{3.6}$$

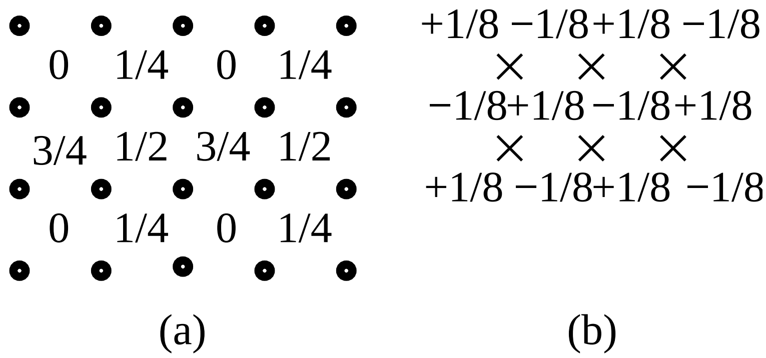

Figure 3.2: The new fields $\mathcal{Y}_j$ and $\mathcal{Z}_{j\mu}$ introduced in Eqn 3.7. Only the $\mu = \tau$ components of $\mathcal{Z}_{j\mu}$ are non-zero ($\mathcal{Z}_{j\mu} = \delta_{\mu\tau}\epsilon_i/8$) and are shown in (b). The field $\mathcal{Y}_j$ takes four different values on the four sublattices of the dual lattice as shown in (a).

The above expression can be cast into a more illuminating form by splitting $a^0_{j\mu}$ into a curl-free and a divergence-free part and writing it in terms of new fixed fields, $\mathcal{Y}_j$ and $\mathcal{Z}_{j\mu}$ as follows:

$$a^0_{j\mu} = \triangle_\mu \mathcal{Y}_j + \epsilon_{\mu\nu\lambda}\triangle_\nu \mathcal{Z}_{j\lambda} \tag{3.7}$$

The values of the new fields are shown in Fig 3.2. Putting in the decomposition of Eqn 3.7 into Eqn 3.6, we get

$$\mathcal{Z}_h = \sum_{H_j} \exp\left(-\frac{e^2}{2}\sum_{j,\mu}(\triangle_\mu H_j)^2\right) \tag{3.8}$$

where

$$H_j = h_j - 2S\,\mathcal{Y}_j \tag{3.9}$$

is the new height variable. Notice that $\mathcal{Z}_{j\lambda}$ has dropped out of the final expression. We have been able to reduce the problem with the Berry phase term into a height model where the action is purely real. From the above equation, we can easily get the following field theory:

$$\mathcal{Z}_c = \sum_{Q_{j\mu}} \prod_{j,\mu} \int_{-\pi}^{\pi} \frac{dA_{j\mu}}{2\pi} \exp\left(-\frac{1}{2e^2}\sum_j (\epsilon_{\mu\nu\lambda}\triangle_\nu A_{j\lambda} - 2\pi Q_{j\mu})^2 + i4\pi S \sum_j \mathcal{Y}_j \triangle_\mu Q_{j\mu}\right) \tag{3.10}$$

To get Eqn 3.10 from Eqn 3.8, simply introduce an integer field $M_{j\mu} = \triangle_\mu h_j$ and introduce an additional field $A_{j\mu}$ to enforce the constraint $\epsilon_{\mu\nu\lambda}\triangle_\nu M_{j\lambda} = 0$. Then we use Poisson Summation formula ($\sum_{n=-\infty}^{+\infty} g(n) = \sum_{m=-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\phi g(\phi) e^{2\pi i m\phi}$) to replace the integer field $M_{j\mu}$ by a real field $\phi_{j\mu}$. Then the variables $\phi_{j\mu}$ can be integrated out to finally give Eqn 3.10.

The partition function written in the form of Equation 3.10 gives us a remarkable piece of physics. $\triangle_\mu Q_{j\mu}$ is the magnetic monopole number at the dual lattice site j, which is equivalent to a hedgehog core being located there as we saw earlier. But notice that the monopoles (or, hedgehogs) carry a Berry phase of $e^{i4\pi S \mathcal{Y}_j}$, where $\mathcal{Y}_j$ takes four different values on the four sublattices of the dual square lattice. Thus, in a phase where the hedgehogs get condensed, lattice symmetry can be broken because of the Berry phase attached to them.

Now we analyze the height model given in Eqn 3.8 to get the nature of the paramagnetic ground state. Firstly, d-dimensional height models of the form considered here can be mapped to a d-dimensional lattice Coulomb Gas problem [22]. We elevate the height variable h_j (in Eqn 3.8) to a continuous field by using the Poisson Summation formula, to get

$$\mathcal{Z}_h = \sum_{m_j} \int_{-\infty}^{\infty} \prod_j dH_j \exp\left(-\frac{e^2}{2} \sum_{j,\mu} (\triangle_\mu H_j)^2 - 2\pi i \sum_j m_j (H_j + 2S \mathcal{Y}_i) \right) \tag{3.11}$$

Now the gaussian integrals over H_j can be easily performed to give the following result.

$$\mathcal{Z}_h = \sum_{m_j} \exp\left(-\frac{2\pi^2}{e^2} \sum_{j,j'} m_j G(j - j') m_{j'} - i4\pi S \sum_j m_j \mathcal{Y}_j \right) \tag{3.12}$$

where $G(r)$ is the lattice Green's function satisfying $\triangle^2 G(r) = \delta_{r,0}$. This is nothing but a plasma with integer charges m_j interacting via Coulomb interactions, and the system being charge neutral. For $d = 2$, ignoring the Berry phase term, the model has a finite-temperature phase transition from an insulator to a conductor upon increasing the temperature. In fact, this is the famous KT transition in $d = 2$. In the insulator phase, opposite charges are bound tightly to each other while in the conductor phase, the charges are free to move without pairing. For $d = 3$, the attraction between opposite charges is much weaker ($1/r$ instead of being $ln(r)$) and the system is a conductor at any finite temperature. In height models, the conductor phase is the smooth phase where the height is locked to some particular integer value; while the insulator phase is the rough phase where the integer constraint on the heights become unimportant and the surface becomes rough (being described by a pure Gaussian theory). In the $3D$ height model, the Coulomb Gas mapping implies that there is no roughening transition and the interface is always smooth. If there were no Berry phases present, the height H_j would have locked to some integer value and the interface would have been smooth. Even when the Berry phases are present, the interface remains smooth on the average despite the local corrugation in the interface configuration introduced by the offsets $2S\mathcal{Y}_j$. We will now show that any well-defined value for the average height $\bar{H}$ (H_j defined in Eqn 3.9) necessarily breaks lattice symmetry for $S = 1/2$.

The argument runs as follows [21]. Call the four sublattices of the square lattice W, X, Y, Z. Suppose we perform a 90° rotation about a direct lattice point on the square lattice, which makes $W \to Z, X \to W, Y \to X, Z \to Y$. Then we would have naively thought that the heights transform as $h_W \to h_Z, h_X \to h_W, h_Y \to h_X, h_Z \to h_Y$. However, there are different offsets present at the four different sublattice, as seen in Eq 3.9, which makes the above height transformation incorrect. The reason is simple to see. As shown in Fig 3.3, the height difference (for the total height, including the

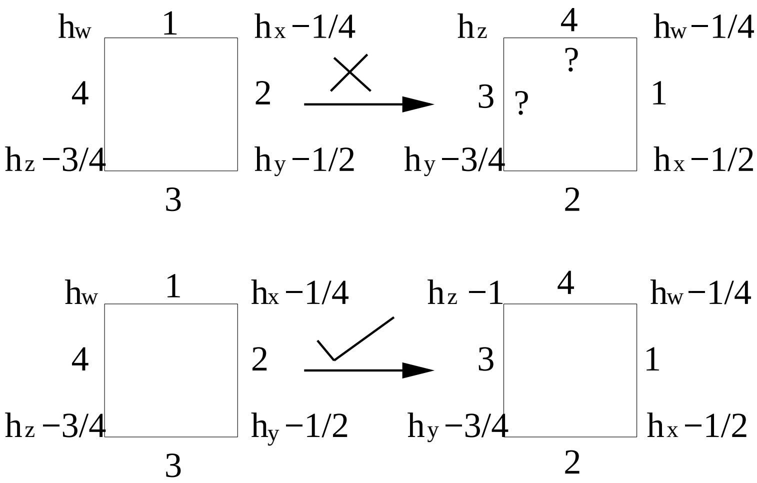

Figure 3.3: The non-trivial transformation of the h field because of the presence of different offsets on the different sublattices of the dual square lattice.

offset) transforms properly for bonds 1 and 2, but does not for bonds 3 and 4. For the height differences to transform correctly, we see that h_W transforms to $h_Z - 1$ as shown in Fig 3.3. Thus, because of the different offsets present, the transformation is $h_W \to h_Z - 1, h_X \to h_W, h_Y \to h_X, h_Z \to h_Y$ under $W \to Z, X \to W, Y \to X, Z \to Y$. This implies $\overline{H} \to \overline{H} - 1/4$ under a 90° rotation which means that there is a four-fold symmetry breaking for a smooth height phase, a scenario consistent with Hastings Theorem [24].

In gauge theory language, the VBS state corresponds to the **confined phase** of the theory. This can be understood in the following manner [26]. Consider the excitations of the quantum paramagnet. Excitations are formed by breaking a valence bond, which leads to a three-fold degenerate state with total spin $S = 1$, as shown in Fig 3.4(a). This broken bond can hop from site to site, leading to a triplet quasiparticle excitation. The spin-1 excitation is composed of two spin $1/2$ spinons. Let us now try to separate the two spinons, see Fig3.4(b). This causes a rearrangement of valence bonds along the ”string” connecting the two spinons. These valence bonds form a line defect with respect to the underlying VBS order (see Fig 3.4(b)) and the ”string” connecting the spinons cost a finite energy per unit length. This means that the $S = 1/2$ spinons are always bound together into $S = 1$ excitations and are hence confined in the VBS side. Thus, the ‘string tension’ of the confining potential is provided by the spontaneous VBS order. We should note the dual role played by the monopole configurations of the gauge field (hedgehogs). When they proliferate, the Néel order cannot survive. At the same time their proliferation induces broken lattice symmetry.

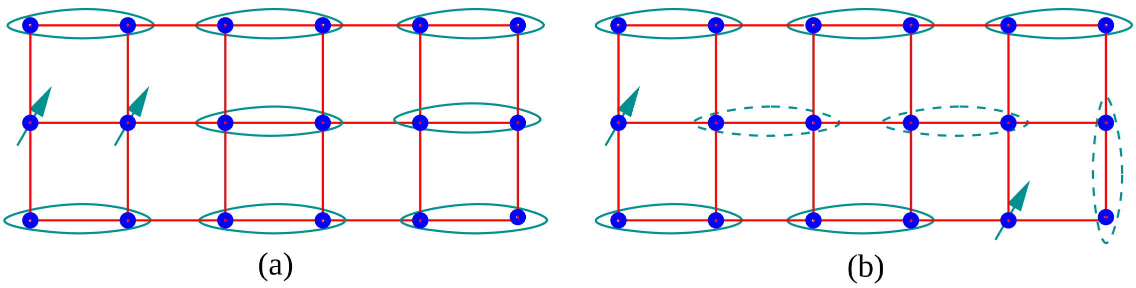

Figure 3.4: (color online). (a) Picture of the bosonic $S = 1$ excitation in the quantum paramagnet. (b) Fission of the $S = 1$ excitation into two spin $1/2$ spinons. The spinons are ”connected” by a string of valence bonds (denoted by dashed ovals) which lie on *weaker* bonds, this string costs a finite amount of energy per unit length and leads to the confinement of the spinons.

3.2 VBS from proliferation of hedgehogs

After the rather abstract proof of the symmetry breaking in the VBS state, we look at the symmetry breaking in the paramagnet from another point of view. In the Néel phase, the monopole events (hedgehogs in spin language) are suppressed at low energies. However, in the quantum paramagnet, the space-time configurations of the Néel field must be riddled with monopoles. This can be formally thought of by saying that the spinons interact with a compact gauge field A_μ, due to which there is also a term in the Lagrangian which creates or destroys monopoles of the gauge field:

$$\mathcal{L}_{mp} = \sum_{n=1}^{\infty} \lambda_n(r)([\mathrm{v}_{r\tau}]^n + [\mathrm{v}^\dagger_{r\tau}]^n) \tag{3.13}$$

where $\mathrm{v}^\dagger_{r\tau}$ and $\mathrm{v}_{r\tau}$ insert monopoles of strength 2π and -2π at the space-time point (r, τ), respectively. Then in the paramagnetic phase, we have a ‘condensation’ of the skyrmion number changing operator v. Now, the non-trivial transformation of this operator under lattice symmetry operations (which are due to the Berry phases) leads to broken lattice symmetry in the paramagnet -this may be identified as VBS order (this argument is due to Senthil *et. al.* [1]). Let us see how.

Firstly, the skyrmion number is a topological index and hence, is unchanged under global $SU(2)$ rotations. Hence the skyrmion number changing operator $\mathrm{v}^\dagger$ is also a $SU(2)$ scalar. Likewise the VBS order parameter is also a $SU(2)$ scalar. We now consider the effect of lattice transformations on the operator $\mathrm{v}^\dagger$. Under $\pi/2$ rotations in the counterclockwise direction about a direct lattice site, the Berry phase associated with a skyrmion creation event changes by $\exp(i\pi S)$. Specializing to $S = 1/2$, we have

$$R_{\pi/2} : \mathrm{v}^\dagger \to i\mathrm{v}^\dagger \tag{3.14}$$

Now consider lattice translation operations $T_{x,y}$ corresponding to translations by one unit along x, y

directions along the lattice. Firstly,

$$\begin{aligned} T_x : \hat{n}_r &\rightarrow -\hat{n}_{r+\hat{x}} \\ T_y : \hat{n}_r &\rightarrow -\hat{n}_{r+\hat{y}} \end{aligned} \quad (3.15)$$

because of the staggering implicit in the definition of $\hat{n}$. Now, the skyrmion number Q is odd under $\hat{n} \rightarrow -\hat{n}$. Consequently, $T_{x,y}$ converts $\mathrm{v}^\dagger$ to v. Furthermore, due to the difference in Berry phase factors for monopoles centered on adjacent plaquettes on the direct lattice, there is a phase factor introduced by the translation. Calculating it, we get:

$$\begin{aligned} T_x : \mathrm{v}_r^\dagger &\rightarrow -i\mathrm{v}_{r+\hat{x}} \\ T_y : \mathrm{v}_r^\dagger &\rightarrow +i\mathrm{v}_{r+\hat{y}} \end{aligned} \quad (3.16)$$

Thus a paramagnetic state with a uniform non-zero expectation value of $\mathrm{v}^\dagger$ breaks $R_{\pi/2}, T_x, T_y$ and can be identified to VBS order.

Chapter 4

Critical Theory

From the previous sections, we saw that an effective field theory which captures both the Néel state and the VBS state can be written in terms of spinons interacting with a compact $U(1)$ gauge theory in the following manner:

$$\mathcal{Z} = \prod_{j\mu} \int_0^{2\pi} \frac{dA_{j\mu}}{2\pi} \prod_{j\alpha} \int dz_{j\alpha} \prod_j \delta(|z_{j\alpha}|^2 - 1) \exp\left(\frac{1}{g} \sum_{j\mu} (z^*_{j\alpha} e^{-iA_{j\mu}} z_{j+\mu,\alpha} + c.c.) + i2S \sum_j \epsilon_j A_{j\tau} \right) \quad (4.1)$$

For small g, the Néel state is found and corresponds to the Higgs phase in this language, while for large g, we obtain a four-fold symmetry breaking VBS state which corresponds to the confined phase of the gauge theory. Now, we turn to describe the novel physics at the critical point seperating the Néel and the VBS states.

What is the expectation about the critical behaviour from the *classical* Landau-Ginzburg-Wilson (LGW) approach? Here, we need to identify the order parameter fields and construct a free energy as an expansion in powers of the order parameter fields and gradients of those fields. There are two order parameter fields in the Néel-VBS transition, the Néel field $\hat{n}$ and the VBS order parameter field ψ_{VBS}. These two order parameters are apparently independent in that the Néel order parameter describes broken spin rotation symmetry while the VBS order parameter describes broken lattice symmetry. A LGW description of the competition between such two kinds of orders would then generically predict either a first-order transition, or an intermediate region of coexistence where both orders simultaneously exist, or an intermediate region with neither order. A direct continuous transition between these two broken symmetry phases would seem to require fine-tuning to a ”multicritical” point. However, as was shown in recent work [1], in the specific case of a Néel-VBS transition on the square lattice, the transition **can generically be continuous** without any fine-tuning, due to subtle quantum interference effects that invalidate the Landau analysis.

The problem with trying to write down a local Landau theory with the Néel and the VBS order parameter fields is the following. As we saw in the last chapter, the topological defects of the Néel order parameter (hedgehogs) have a non-trivial structure. When the defects proliferate, not only do they kill the long-range Néel order (which is expected) but also induce the broken symmetry of the VBS phase. To construct a theory of a continuous transition between these two phases in terms of these order parameters, it would be necessary to associate the VBS order parameter with the hedgehogs of the Néel order parameter. This implies that the two order parameter fields will have long-ranged ”statistical” interactions with each other. Consequently, a local theory which includes only the two order parameter fields but no other field is highly unlikely to describe the physics of the critical point [1].

Recent work by Senthil et al. [1] has proposed the following picture for the Néel to VBS T=0 phase transition for $S = 1/2$ spins on the square lattice in 2d. First, contrary to the predictions of the LGW theory, a generic continuous phase transition between the Néel state and the VBS paramagnet is indeed possible. The theory of such a quantum critical point is obtained simply by taking a naive continuum limit of $\mathcal{Z}$ in Eq 4.1 while ignoring both the compactness of the gauge field and the Berry phases. Remarkably, these complications of the lattice model $\mathcal{Z}$, which we saw from previous chapters is essential for the complete theory, have effects which cancel each other out, but **only** at the critical point. Note that compactness on its own is a relevant perturbation which cannot be ignored (as we will see shortly in a later example), i,.e., without Berry phases, the compact and non-compact lattice CP^1 model have distinct critical theories. However, as noted by Senthil et al. [1], *the non-compact CP^1 model has the same critical theory as the compact CP^1 model with $S = 1/2$ Berry phases*. Taking the naive continuum limit of $\mathcal{Z}$ in Eq 4.1 and softening the hard-constraint on $z_{j\alpha}$, we obtain the proposed theory for the confined critical point between the Néel state and the VBS paramagnet for $S = 1/2$ [1]:

$$\mathcal{Z}_{deconfined} = \int \mathcal{D}z_\alpha(r,\tau)\mathcal{D}A_\mu(r,\tau)\exp\left(-\int d^2r d\tau\left[|(\partial_\mu - iA_\mu)z_\alpha|^2 + s|z_\alpha|^2 + \frac{u}{2}(|z_\alpha|^2)^2 + \kappa(\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda)^2\right]\right) \tag{4.2}$$

We have also included included a kinetic term for the gauge field above, and one can imagine this to be generated by integrating out large momentum $z_{j\alpha}$. On its own, $\mathcal{Z}_c$ describes the transition from a magnetically ordered phase with $z_{j\alpha}$ condensed at $s < s_c$, to a disordered state with a gapless $U(1)$ photon at $s > s_c$, where s_c is the critical point of Z_c. The $s < s_c$ phase corresponds to the Néel phase of $\mathcal{Z}$ (Eq 4.1) for $g < g_c$. However, the $s > s_c$ phase does not obviously correspond to the $g > g_c$ bond ordered, fully gapped, paramagnet of $\mathcal{Z}$. This is repaired by accounting for the compactness of the gauge field and the Berry phases: it is no longer possible to neglect them, while it is safe to do so at $g = g_c$. The *combined* effects of compactness and Berry phases are therefore *dangerously irrelevant* at $g = g_c$ [a dangerously irrelevant perturbation is irrelevant at the critical point, but relevant in the ordered phase].

We will illustrate this conspiracy between the compactness of the gauge field and the Berry phases at the critical point by considering a simpler problem of only one kind of matter field z_j interacting with the gauge field instead of two kinds of fields $z_{j\uparrow}$ and $z_{j\downarrow}$, following Ref [21].

4.1 Simpler Problem: Lattice Model at $N = 1$

Consider the $S = 1/2$ antiferromagnet in the presence of a staggered magnetic field (say in the z direction). Such a field would clearly prefer $z_\uparrow$ over $z_\downarrow$ because n_x and n_y would be close to zero. We can then write the z_j field as $\exp(i\theta_j)$ to satisfy the unimodular constraint and then get the following simplified theory:

$$\mathcal{Z}_s = \prod_j \int_0^{2\pi} \frac{d\theta_j}{2\pi} \int_0^{2\pi} \frac{dA_{j\mu}}{2\pi} \exp\left(\frac{1}{e^2} \sum_\Box \cos(\epsilon_{\mu\nu\lambda}\triangle_\nu A_{j\lambda}) + \frac{1}{g} \sum_{j,\mu} \cos(\triangle_\mu\theta_j - A_{j\mu}) + i2S \sum_j \epsilon_j A_{j\tau} \right) \tag{4.3}$$

We will now be concerned with the behaviour of the critical point of the above theory. However, rather than attack $\mathcal{Z}_s$ directly, we will consider a sequence of simpler models, to illustrate how compactness alone is a relevant perturbation in the theory but is *neutralized* by the Berry phases at the critical point [a good discussion of all this is given in [21]].

4.1.1 Non-compact $U(1)$ gauge theory without Berry phase

Dropping both compactness and Berry phases, $\mathcal{Z}_s$ reduces to

$$\mathcal{Z}_{s,1} = \prod_j \int_0^{2\pi} \frac{d\theta_j}{2\pi} \int_{-\infty}^{\infty} dA_{j\mu} \exp\left(-\frac{1}{2e^2} \sum_\Box (\epsilon_{\mu\nu\lambda}\triangle_\nu A_{j\lambda})^2 + \frac{1}{g} \sum_{j,\mu} \cos(\triangle_\mu\theta_j - A_{j\mu}) \right) \tag{4.4}$$

We will now show that the model is dual to the $3D$ XY model, as was shown first by Dasgupta and Halperin [27]. Firstly, we use the Villain form for the cosine term in the action and a Hubbard-Stratonovich field for the term $\exp(-\frac{1}{2e^2}\sum_\Box(\epsilon_{\mu\nu\lambda}\triangle_\nu A_{j\lambda})^2)$. Thus

$$\begin{aligned} \exp\left(\frac{1}{g} \sum_{j,\mu} \cos(\triangle_\mu\theta_j - A_{j\mu}) \right) &\rightarrow \sum_{J_{j\mu}} \exp\left(\frac{-g}{2} \sum_{j,\mu} J_{j\mu}^2 + i \sum_{j,\mu} J_{j\mu}(\triangle_\mu\theta_j - A_{j\mu}) \right) \\ \exp\left(-\frac{1}{2e^2} \sum_\Box (\epsilon_{\mu\nu\lambda}\triangle_\nu A_{j\lambda})^2 \right) &\rightarrow \int_{-\infty}^{+\infty} dP_{j\mu} \exp\left(-\frac{e^2}{2} P_{j\mu}^2 - iP_{j\mu}\epsilon_{\mu\nu\lambda}\triangle_\nu A_{j\lambda} \right) \end{aligned} \tag{4.5}$$

where $J_{j\mu}$ is an integer-valued field and $P_{j\mu}$ is real valued. Then we can write $\mathcal{Z}_{s,1}$ as

$$\begin{aligned} \mathcal{Z}_{s,1} &= \prod_j \int \frac{d\theta_j}{2\pi} \int dA_{j\mu} \sum_{J_{j\mu}} \int dP_{j\mu} \exp[-\frac{e^2}{2} \sum_{j,\mu} P_{j\mu}^2 - \frac{g}{2} \sum_{j,\mu} J_{j\mu}^2 + i \sum_j J_{j\mu}(\triangle_\mu\theta_j - A_{j\mu}) \\ &- i \sum_\Box \epsilon_{\mu\nu\lambda} P_{j\mu} \triangle_\nu A_{j\lambda}] \end{aligned} \tag{4.6}$$

In this form, the integrals over θ_j and $A_{j\mu}$ can be performed easily and give the following constraints:

$$\begin{aligned} \triangle_\mu J_{j\mu} &= 0 \\ J_{j\mu} &= \epsilon_{\mu\nu\lambda}\triangle_\nu P_{j\lambda} \end{aligned} \tag{4.7}$$

We "solve" these constraints by writing:

$$\begin{aligned} J_{j\mu} &= \epsilon_{\mu\nu\lambda}\triangle_\nu b_{j\lambda} \\ P_{j\mu} &= b_{j\mu} - \triangle_\mu \phi_j \end{aligned} \tag{4.8}$$

where $b_{j\lambda}$ is an integer-valued field and ϕ_j is a real field. Then we have

$$\mathcal{Z}_{s,1} = \prod_j \int_{-\infty}^{+\infty} d\phi_j \sum_{b_{j\mu}} \exp\left(-\frac{e^2}{2}\sum_{j,\mu}(b_{j\mu} - \triangle_\mu\phi_j)^2 - \frac{g}{2}\sum_{\square}(\epsilon_{\mu\nu\lambda}\triangle_\nu b_{j\lambda})^2\right) \tag{4.9}$$

The "hard" integer constraint on $b_{j\mu}$ can then be softened in the following manner,

$$\mathcal{Z}_{s,1} = \prod_j \int_{-\infty}^{+\infty} d\phi_j \int_{-\infty}^{+\infty} db_{j\mu} \exp\left(-\frac{e^2}{2}\sum_{j,\mu}(b_{j\mu} - \triangle_\mu\phi_j)^2 - \frac{g}{2}\sum_{\square}(\epsilon_{\mu\nu\lambda}\triangle_\nu b_{j\lambda})^2 + t\sum_{j,\mu}\cos(2\pi b_{j\mu})\right) \tag{4.10}$$

where $t > 0$. Now, $b_{j\mu} = \triangle_\mu\phi_j + P_{j\mu}$. Clearly $P_{j\mu}$ is a massive field and can be integrated out by doing a saddle point integration about $P_{j\mu} = 0$. Thus, we finally get

$$\mathcal{Z}_{s,1} = \prod_j \int_{-\infty}^{+\infty} d\phi_j \exp\left(t\sum_{j,\mu}\cos(2\pi\triangle_\mu\phi_j)\right) \tag{4.11}$$

This is nothing but the 3D XY model, which can be equally written using the complex scalar ψ ($\psi = \exp(i\phi)$), in the form

$$\mathcal{Z}_{s,1} = \int \mathcal{D}\psi(r,\tau) \exp\left(-\int d^2r d\tau(|\partial_\mu\psi|^2 + s|\psi|^2 + \frac{u}{2}|\psi|^4)\right) \tag{4.12}$$

where the two phases are $\langle\psi\rangle \neq 0$ corresponding to ferromagnetic ordering of the XY spins and $\langle\psi\rangle = 0$ corresponding to the paramagnetic state. Thus, the critical point of $\mathcal{Z}_{s,1}$ is in the 3D XY universality class.

4.1.2 Compact $U(1)$ gauge theory without Berry phase

Now we put the further complication of compactness into our theory. Thus we have

$$\mathcal{Z}_{s,2} = \prod_j \int_0^{2\pi} \frac{d\theta_j}{2\pi} \int_0^{2\pi} \frac{dA_{j\mu}}{2\pi} \exp\left(\frac{1}{e^2}\sum_{\square}\cos(\epsilon_{\mu\nu\lambda}\triangle_\nu A_{j\lambda}) + \frac{1}{g}\sum_{j,\mu}\cos(\triangle_\mu\theta_j - A_{j\mu})\right) \tag{4.13}$$

We can repeat the manipulations of the last section here. Introduce two Villain forms for the cosines and carrying out a similar analysis, we get the same form as Eqn 4.9 but with both $b_{j\mu}$ and ϕ_j being integer fields now. Again, softening the integer constraint, we get:

$$\mathcal{Z}_{s,2} = \prod_j \int_{-\infty}^{+\infty} d\phi_j \int_{-\infty}^{\infty} db_{j\mu} \exp\left(-\frac{e^2}{2}\sum_{j,\mu}(b_{j\mu} - \triangle_\mu\phi_j)^2 - \frac{g}{2}\sum_{\square}(\epsilon_{\mu\nu\lambda}\triangle_\nu b_{j\lambda})^2 + t\sum_{j,\mu}\cos(2\pi b_{j\mu}) + y_m\sum_j\cos(2\pi\phi_j)\right)$$

(4.1

Again, we see that $P_{j\mu}$ is a massive field and can be integrated out. Then we get that

$$\mathcal{Z}_{s,2} = \prod_j \int_{-\infty}^{+\infty} d\phi_j \exp\left(t \sum_{j,\mu} \cos(2\pi \triangle_\mu \phi_j) + y_m \sum_j \cos(2\pi \phi_j) \right) \tag{4.15}$$

Physically, this the the $3D$ XY model placed in a magnetic field, which can again be written in terms of $\psi(= \exp(i\phi))$ as

$$\mathcal{Z}_{s,2} = \int \mathcal{D}\psi(r,\tau) \exp\left(- \int d^2 r d\tau (|\partial_\mu \psi|^2 + s|\psi|^2 + \frac{u}{2}|\psi|^4 - y_m(\psi + \psi^*) \right) \tag{4.16}$$

However, this model has no phase transition as $\langle\psi\rangle \neq 0$ for all s. Thus, making the gauge field compact is a strongly relevant perturbation in itself.

4.1.3 Compact $U(1)$ gauge theory with Berry phase

Now we turn to the full theory with both compactness and Berry phases included.

$$\begin{aligned} \mathcal{Z}_{s,3} &= \sum_{Q_{a\mu}} \prod_{j,\mu} \int_0^{2\pi} (\frac{dA_{j\mu}}{2\pi})(\frac{d\theta_j}{2\pi}) \exp[-\frac{1}{2e^2} \sum_{j,\mu} (\epsilon_{\mu\nu\lambda} \triangle_\nu A_{j\lambda} - 2\pi Q_{a\mu})^2 + \frac{1}{g} \sum_{j,\mu} \cos(\triangle_\mu \theta_j - A_{j\mu}) \\ &+ 2\pi i \sum_j \mathcal{Y}_a \triangle_\mu Q_{a\mu}] \end{aligned} \tag{4.17}$$

We again use the trick on introducing a Villain form for the cosine term in the action (introduce integer valued fields $J_{j\mu}$ for it) and introduce a Hubbard-Stratonovich field $P_{j\mu}$ for the $\exp[-\frac{1}{2e^2} \sum_{j,\mu} (\epsilon_{\mu\nu\lambda} \triangle_\nu A_{j\lambda} - 2\pi Q_{a\mu})^2]$. Then, we can easily perform the sum over the integer valued fields $Q_{a\mu}$. This gives the following constraint:

$$P_{j\mu} - \triangle_\mu \mathcal{Y}_a = B_{j\mu} \tag{4.18}$$

where $B_{j\mu}$ is integer valued. Also, doing the integration over θ_j gives

$$\triangle_\mu J_{j\mu} = 0 \tag{4.19}$$

, which can be solved by putting $J_{j\mu} = \epsilon_{\mu\nu\lambda} \triangle_\nu b_{j\lambda}$ where $b_{j\lambda}$ is an integer valued field. Putting these two constraints into the action, we get

$$\begin{aligned} \mathcal{Z}_{s,3} &= \sum_{B_{j\mu}, b_{j\mu}} \int \frac{dA_{j\mu}}{2\pi} \exp[-\frac{e^2}{2} \sum_{j\mu} (B_{j\mu} + \triangle_\mu \mathcal{Y}_a)^2 - i \sum_{\square} B_{j\mu} (\epsilon_{\mu\nu\lambda} \triangle_\nu A_{j\lambda}) \\ &- \frac{g}{2} \sum_{j,\mu} (\epsilon_{\mu\nu\lambda} \triangle_\nu b_{j\lambda})^2 - i \sum_{j,\mu} (\epsilon_{\mu\nu\lambda} \triangle_\nu b_{j\lambda}) A_{j\mu}] \end{aligned} \tag{4.20}$$

Integrating out $A_{j\mu}$, we get the constraint $\epsilon_{\mu\nu\lambda} \triangle_\nu b_{j\lambda} = \epsilon_{\mu\nu\lambda} \triangle_\nu B_{j\lambda}$. We can solve this by putting $B_{j\mu} = b_{j\mu} + \triangle_\mu \chi_a$ where χ_a is a integer field. Thus, we get

$$\mathcal{Z}_{s,3} = \sum_{b_{j\mu}, \chi_a} \exp\left(-\frac{e^2}{2} \sum_{j,\mu} (b_{j\mu} + \triangle_\mu (\chi_a + \mathcal{Y}_a))^2 - \frac{g}{2} \sum_{j,\mu} (\epsilon_{\mu\nu\lambda} \triangle_\nu b_{j\lambda})^2 \right) \tag{4.21}$$

We then relax the integer constraint on $b_{j\mu}$ and χ_a and get

$$\begin{aligned}\mathcal{Z}_{s,3} &= \int \mathcal{D}b_{j\mu}\mathcal{D}\chi_a \exp[-\frac{e^2}{2}\sum_{j,\mu}(b_{j\mu} + \triangle_\mu(\chi_a + \mathcal{Y}_a))^2 - \frac{g}{2}\sum_{j,\mu}(\epsilon_{\mu\nu\lambda}\triangle_\lambda b_{j\lambda})^2 + t\sum_{j\mu}\cos(2\pi b_{j\mu}) \\ &+ \sum_{j,\mu}\sum_n \lambda_n \cos(2\pi n\chi_a)] \end{aligned} \tag{4.22}$$

Then we do the following shifts in the fields:

$$\begin{aligned}\tilde{\chi}_a &= \chi_a + \mathcal{Y}_a \\ \tilde{b}_{j\mu} &= b_{j\mu} + \triangle_\mu\tilde{\chi}_a\end{aligned} \tag{4.23}$$

Then, clearly $\tilde{b}_{j\mu}$ is a massive field and we can integrate it out by doing a saddle point integration about $\tilde{b}_{j\mu} = 0$. Doing this, we get the following result

$$\mathcal{Z}_{s,3} = \int \mathcal{D}\tilde{\chi}_a \exp\left(t\sum_{j,\mu}\cos(2\pi\triangle_\mu\tilde{\chi}_a) + \sum_{j,\mu}\sum_n \lambda_n \cos(2\pi n(\chi_a - \mathcal{Y}_a))\right) \tag{4.24}$$

Thus the model reduces to the $3D$ XY model with various n-fold anisotropies of strengths λ_n. Now, the shift by $\mathcal{Y}_a$ leads to rapid spacial oscillations of these anisotropy terms, which do not survive the continuum limit unless n=0 (mod 4). Thus, the leading anisotropy is at n=4 !

Hence, the critical properties of the model are that of the $3D$ XY model with a four-fold anisotropy term λ_4.

$$\mathcal{Z}_{s,3} = \int \mathcal{D}\psi(r,\tau)\exp\left(-\int d^2r d\tau(|\partial_\mu\psi|^2 + s|\psi|^2 + \frac{u}{2}|\psi|^4 - \lambda_4(\psi^4 + \psi^{*4})\right) \tag{4.25}$$

It is known from previous work [28] that the λ_4 perturbation is irrelevant at the $3D$ XY critical point. Thus, the universality class of the critical point of the full theory is the same as that of a theory where both compactness and Berry phases are neglected.

4.2 $N = 2$ critical point

What happens in the case of $N = 2$ which is relevant for us here? Consider a generalized CP^{N-1} model of an N-component complex field z that is coupled to a compact $U(1)$ gauge field with the same Haldane Berry phases as in the $N = 2$ case of interest. We already saw above that at $N = 1$, the model displays a continuous transition between a Higgs phase and a paramagnetic VBS phase with confined spinons. Also, the instanton events are irrelevant at the critical point due to the quadrupling caused by the Berry phases. Now consider the case where N is large. The scaling dimension of the q-monopole operator was computed by Murthy and Sachdev [29] and their results give a dimension

$\propto N$. For large N this is much larger than $D = 3$, and hence the $q = 4$ monopoles are strongly irrelevant for large N. (However, unlike the $N = 1$ case, the single monopole operator is irrelevant even without the Berry phases for large N) Thus, by continuity, one expects the $q = 4$ monopole events to be irrelevant for the $N = 2$ case too.

From the above considerations, we arrive at the following picture of the critical point. The two phases of the theory are the Néel and the VBS phase. In the Néel phase, the monopoles (or, hedgehogs) are energetically costly and are gapped. In the gauge theory language, this phase corresponds to the Higgs phase. On the VBS side, the monopoles proliferate and destroy the Néel order. Also, because of the Berry phase they carry, the VBS state breaks lattice symmetry. This phase corresponds to the confined phase of the gauge theory and here the presence of monopoles is essential both to explain the symmetry breaking of the state and the confinement of the $S = 1/2$ spinons into spin 1 excitations. Importantly, the Berry phases carried by the monopoles is different on the four sublattices of the square lattice, which leads to destructive interference between different tunneling paths for single monopoles. This interference effectively kills all monopole events unless they are quadrupled, corresponding to a skyrmion number change of ± 4 (we have already seen this happen in the $N = 1$ model). This quadrupling makes the monopole tunneling events irrelevant at the critical point (more precisely, it can be shown explicitly for $N = 1$ and large N and *should* hold for $N = 2$).

The irrelevance of the monopole tunnelings implies that the hedgehogs are absent at low energies at the QCP. This leads to the conservation of the skyrmion number Q at the critical point because the hedgehogs, responsible for changing the skyrmion number, are absent at low energies at the critical point. This **emergent conservation** of

$$Q = \frac{1}{4\pi} \int d^2 r (\hat{n} \cdot \partial_x \hat{n} \times \partial_y \hat{n})$$

provides a precise notion of **deconfinement** at the QCP [26]. In gauge theory language, because of the irrelevance of the monopole events, the gauge flux $\int d^2 r(\partial_x A_y - \partial_y A_x)$ is conserved, and the gauge theory can be thought to be deconfined for all low-energy properties.

It is useful to compare the behaviour of the Néel-VBS QCP with the $3D$ $O(3)$ critical point which would have been obtained if we had ignored the Berry phases in the problem through the usual mapping of a d dimensional quantum system to some $d+1$ dimensional classical system. It is known [30] that there is a finite density of "free" hedgehogs at the $D = 3$ $O(3)$ critical point. Contrast the critical behaviour of the hedgehogs with a well known and familiar example: vortices in the $2D$ XY model which exhibits the Kosterlitz-Thouless (KT) transition. Imagine we are examining a model with a short-distance momentum cutoff, Λ. Let the mean density of vortices be $\bar{\rho}_v$, and a dimensionless measure of this is $\bar{\rho}_v \Lambda^{-2}$. Now we perform an RG transformation, integrating out tightly bound dipoles of vortices, and gradually reduce the value of Λ. It is known that at the KT critical point the vortex fugacity ultimately flows to zero [31], i.e., as we scale Λ to smaller values, the dimensionless vortex density, $\bar{\rho}_v \Lambda^{-2}$ ultimately scales to zero. This is the precise form of the statement that there are no free vortices at the KT critical point. However, the behaviour of the density of hedgehogs at the $D = 3$ $O(3)$ critical point is dramatically different. $\bar{\rho}_h \Lambda^{-3}$ remains a finite number [30] of order unity even after RG scaling to the longest length scales. On the other hand, the deconfined QCP has $\bar{\rho}_h \Lambda^{-3}$ flowing to zero as the hedgehogs become irrelevant at the QCP.

4.3 Consequences of deconfined QCP

- Since the critical theory (see Eq 4.2) is isotropic in spacetime (2+1 dim), we immediately get that the dynamical critical exponent $z = 1$ for the deconfined QCP ($\xi_\tau \sim \xi^z$).

- The difference between this transition and the Heisenberg transition in $3D$ is most clearly brought out by comparing the anamolous dimension of the Néel order η in both the cases. For the Heisenberg transition, the value of $\eta \approx 0.033$. However, for the deconfined QCP, the value of η is significantly larger and is found to be $\eta \approx 0.65$ numerically [32]. In Ref [32], both the non-compact $U(1)$ theory interacting with charged spinons (Eq 4.2) and the Heisenberg model with suppression of *free* hedgehogs were studied numerically. In both the models, a continuous phase transition was obtained and the critical exponents agreed reasonably well with each other, after suitable identification of observables in the spin language to the observables in the gauge theory. Because of the conservation of the skyrmion number Q at the critical point, we immediately know that the scaling dimension of the gauge field A_μ is -1. Thus, the spinons interact with a potential $V(R) \sim 1/R$ at large distance R, which implies that they are not confined at the critical point and ”emerge” as good degrees of freedom. At the tree level, treating the spinons as free, the two-point z_α correlator will decay at the critical point as

$$\langle z^*_\alpha(r) z_\alpha(0)\rangle \sim \frac{1}{|r|^{D-2}} \tag{4.26}$$

  where $D = 3$ is the dimension of space-time. In the same approximation, we then obtain the correlations for the Néel order parameter to be

$$\langle \hat{n}(r) \cdot \hat{n}(0)\rangle \sim \langle z^*_\alpha(r) z_\alpha(0)\rangle^2 \sim \frac{1}{|r|^{2(D-2)}} \tag{4.27}$$

  Identifying the right hand side of the above equation with $|r|^{-(D-2+\eta)}$, we obtain $\eta = 1$. So, already at the Gaussian level, the deconfined critical point has a large value of η [26]. It is obviously changed because of the ignored interactions and Monte-Carlo simulations [32] show that $\eta \approx 0.65$.

- The conservation of the skyrmion number Q also fixes the scaling dimension of the flux density (or Néel skyrmion density $\hat{n}\cdot(\partial_x \hat{n} \times \partial_y \hat{n})$ in terms of the spin variables) operator $f_0 = (\partial_x A_y - \partial_y A_x)$.

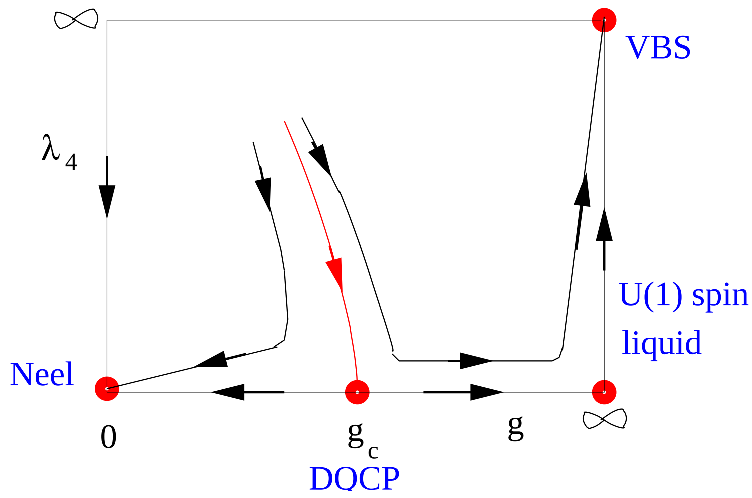

Figure 4.1: Schematic RG flows for the $S = 1/2$ square lattice quantum antiferromagnet. The theory $\mathcal{Z}_{deconfined}$ in Eqn 4.2 describes only the line $\lambda_4 = 0$, it is thus a theory for the phase transition between the Néel state and the $U(1)$ spin liquid with a gapless 'photon' state. However, the lattice antiferromagnet always has a non-zero bare value of the monopole fugacity λ_4 because the gauge field is compact. As discussed, the λ_4 perturbation is irrelevant at $g = g_c$. However, the $g \to \infty$ $U(1)$ spin liquid fixed point is unstable to λ_4, and the paramagnet is therefore a gapped VBS paramagnet.

At criticality, this conservation lae implies that the flux-flux correlator $\langle f_0(R) f_0(0) \rangle \sim R^{-4}$ at long distances.

- The presence of the dangerously irrelevant perturbation which we denote by λ_4, the bare monopole fugacity (more precisely, the quadruple-hedgehog fugacity), implies that there are two distinct length scales which diverge [1, 26] as we approach the critical point from the VBS side. This may be understood in the following manner. We look at the schematic RG flow for the Néel-VBS quantum phase transition in Fig 4.1. We can identify four fixed points in the flow diagram- the Néel fixed point, the $U(1)$ spin liquid fixed point, the Deconfined QCP and the VBS fixed point. When λ_4 is set to zero by hand, i.e., the monopoles are suppressed, we get the theory $\mathcal{Z}_{deconfined}$ (Eqn 4.2). As we commented earlier, the paramagnetic phase of this theory does not break lattice symmetry and has a 'photon' mode because of the deconfined nature of the gauge field. Because of the presence of photons, the flux-flux correlators of this phase, $\langle f_0(R) f_0(0) \rangle \sim R^{-3}$ for large R. This power law decay of the flux correlator is absent in an ordinary paramagnet. This phase corresponds to the $U(1)$ spin liquid. This explains the RG flow for the $\lambda_4 = 0$ line. Also, because the $U(1)$ spin liquid is unstable to the insertion of monopoles, the fixed point is unstable in the λ_4 direction. By continuity, any flow line starting with $g > g_c$ and $\lambda_4 \neq 0$ will initially flow towards the $U(1)$ spin liquid fixed point, and only later will turn and flow to the ultimate VBS fixed point. Thus the initial flow away from the critical fixed point is not towards the stable paramagnet but towards the unstable $U(1)$ spin liquid state. RG flows

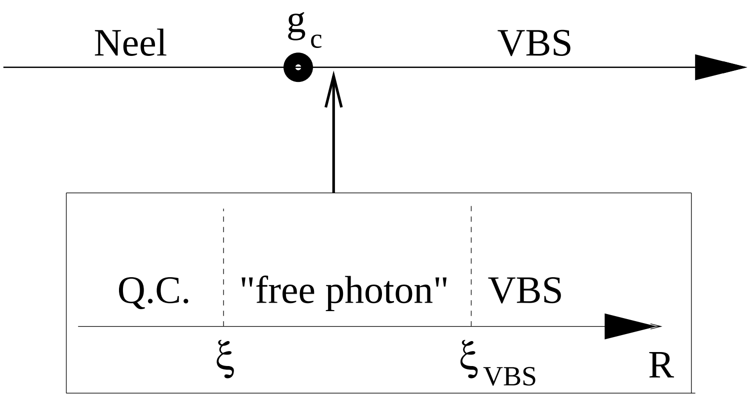

Figure 4.2: Structure of correlations on approaching the critical point from the VBS side. Two diverging length scales, ξ and and a much longer lengthscale ξ_{VBS}, are present. As usual, for length scales R shorter than ξ, quantum critical (Q.C.) correlations are observed-e.g. spin-spin correlators are power law and flux-flux correlators fall off as $\sim R^{-4}$. At intermediate length scales $\xi \ll R \ll \xi_{VBS}$, spin correlators are exponentially decaying while flux-flux correlators take on the free photon form $\sim R^{-3}$. At the longest length scales, only VBS order is present.

with this structure have the general consequence of having two distinct diverging length or time scales (or equivalently two vanishing energy scales). Consider the paramagnetic side close to the transition (see Fig 4.2).

First there is the spin correlation length ξ whose divergence is described by $\mathcal{Z}_{deconfined}$. At this scale there is a crossover from the critical fixed point to the unstable paramagnetic $U(1)$ spin liquid fixed point which has the free photon. However the instability of this spin liquid fixed point to VBS order and confinement occurs at a much larger scale ξ_{VBS} which diverges as a power of ξ. Thus, on approaching the critical point from the VBS side, for length scales $R \ll \xi$, we get quantum critical correlations as usual, where for example the spin-spin correlators show power law decay, while the flux-flux correlations have the R^{-4} form described above. At intermediate length scales, $\xi \ll R \ll \xi_{VBS}$, the spin-spin correlations fall off exponentially, but the flux-flux density correlators are power law but now decay as R^{-3} which is characteristic of flux correlators in the presence of photons. Finally at the longest length scales $\xi_{VBS} \ll R$, VBS order is established and the photon mode is destroyed.

How is ξ_{VBS} related to ξ ? On scaling grounds, we would expect that

$$\xi_{VBS} \sim \xi f(\lambda_4 \xi^{3-\triangle}) \tag{4.28}$$

where f is a scaling function and $3 - \triangle$ is the RG eigenvalue of λ_4. Because λ_4 is assumed to be irrelevant at the critical point, therefore $\triangle > 3$ ($D = 2 + 1$). For length scales $\xi \ll R \ll \xi_{VBS}$, we can regard the VBS phase as XY ordered in ψ_{VBS}, though with a weak four-fold anisotropy λ_4. Hence, the low energy variation of the phase θ of the VBS order parameter $\psi_{VBS} \sim |\psi| \exp(i\theta)$ is described by the energy [1]

$$E(\theta) = \int d^2x \left(\frac{\tilde{K}}{2} |\triangle\theta|^2 - \tilde{\lambda}_4 \cos 4\theta \right) \tag{4.29}$$

where $\tilde{K}$ and $\tilde{\lambda}_4 \propto \lambda_4$ are renormalized parameters on the scale of the correlation length ξ. Now, we can easily estimate the length scale beyond which the anisotropy term would dominate over the gradient term in Eq 4.29. Consider producing a slow twist in the θ field of the form $\theta = \frac{\pi}{2} \cos\left(\frac{\pi x}{2L}\right)$ where the phase of ψ_{VBS} twists from $\pi/2$ at $x = 0$ to 0 at $x = L$. Then the length L beyond which the energy cost due to the anisotropy term dominates over the gradient term scales as $\sqrt{\tilde{K}/\tilde{\lambda}_4}$, which implies that $\xi_{VBS} \sim \lambda_4^{-1/2}$. This requires that $f(x) \sim x^{-1/2}$ immediately giving us

$$\xi_{VBS} \sim \xi^{(\triangle-1)/2} \tag{4.30}$$

Thus ξ_{VBS} grows more rapidly than ξ as the quantum critical point is approached from the VBS side [1, 26].

Chapter 5

Discussion

In this thesis, we discussed at length the physics of the recently proposed ”deconfined critical point” [1]. The deconfined critical point has an emergent topological conservation law which makes the use of the terminology ”deconfined” precise for such critical points. Moreover, the critical theory is most naturally expressed in terms of fractionalized degrees of freedom. The order parameter fields characterizing the phases on either side of the critical point emerge as composites of the fractionalized fields. The particular example we studied was the Néel-VBS quantum phase transition for $S = 1/2$ moments on a $2d$ square lattice. These type of critical points clearly violate the standard LGW paradigm, because the order parameters are not directly related to the critical modes. We also found that these QCP's have large anomalous dimensions for the order parameter fields, unlike the usual critical points where the anomalous dimension is typically small. There may be other such examples of deconfined QCP's in strongly correlated electron systems, which might go some way in explaining various experimental puzzles associated with such systems. For example, it should be interesting to see whether a similar scenario exists for quantum critical points in doped Mott insulators, which might then lead to a strongly non-Fermi liquid like behaviour in the quantum critical region of such critical points and help understand the physics of the cuprate superconductors.

Since the deconfined critical point scenario has yet to receive experimental verification, it would be very useful to construct *toy models* which can then be analyzed analytically or numerically to check for the presence of such critical points. Continuous $T = 0$ transitions between two ordered phases had been suggested before the theory of deconfined critical points was formulated in Ref [33, 34]. However, more detailed studies failed to confirm their existence. Instead, many studies have pointed to a weakly first-order antiferromagnetic-VBS transition [35, 36, 37, 38, 39] or other scenarios inconsistent with deconfined criticality [40]. However, recent quantum monte carlo studies on a particular model by Sandvik [41] shows a Néel-VBS phase transition consistent with the deconfined quantum critical point scenario. However, given the current status, more work needs to be done to establish the correctness of this novel idea.

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