Quantum Phase Transitions Outside the Wilson Landau Ginzburg Paradigm

Rahul Biswas

May 8, 2004

Abstract

We review certain aspects of quantum phase transititions. We then report on certain recent theoretical advances in the study of quantum phase transitions in the context of two dimensional quantum magnets, which do not fit into the Ginbzburg-Landau-Wilson (GLW) formalism usually used to study phase transitions.

1 Introduction

A macroscopic system is built out of microscopic building blocks, which interact according to certain laws. However, the results of experiments conducted on the macroscopic system do not depend on all the microscopic details of the system. As the experimental measurements made are typically on time and length scales much larger than the corresponding scales of various microscopic processes, a large number of quantities that would be relevant from a microscopic point of view get averaged over space and time. Consequently, a macroscopic system can be described completely in terms of a few relevant macroscopic parameters which survive the averaging process. This is the general intuition for the feasibility of a thermodynamic or an effective description. It is, of course, obvious that success of such a thermodynamic description of physics crucially depends on the correct identification of the macroscopic parameters.

Of the numerous scenarios well described by thermodynamics, an extremely important one is the physics of phase transitions [2],[3]. This is mainly because phase transitions are very common in nature. Further, with the available thermodynamic understanding we are able to deal with phase transitions in very diverse systems. The modern theory of phase transitions was developed with important contributions from Landau, Ginzburg, and Wilson, and will be refered to here as the Landau-Ginzburg-Wilson Paradigm (LGW).

Following [3],[1],[8], we will try to review certain ideas of phase transitions, focussing on distinctive characteristics where quantum effects are important. Such phase transitions are called quantum phase transitions (QPT). We will then specialize to the specific example of QPT in two dimensional quantum magnets, where experiments and numerical simulations seem to contradict predictions of the LGW paradigm. We will then look into the recent work

of [5],[6], to try and understand what could invalidate LGW, and discuss modifications of LGW that could provide a suitable theoretical framework to study these QPT.

2 Phase Transitions

Phase transitions involve a sudden change of well defined properties (phases) of a system with the change of a control parameter. A more precise definition follows from the understanding that the idea of "well defined properties" of the system stems from a smooth free energy $F = -\frac{1}{\beta}\ln Z(\beta)$, where Z is the partition function of the system. Z may be calculated by using the usual ideas of statistical mechanics, with a Hamiltonian modelled phenomenologically at the relavant spatial and temporal length scale. As previously emphasized details of microscopic behaviour do not enter the Hamiltonian, and hence the free energy. The relevant degree of freedom that enters the free energy is called the order parameter. (In some cases we may have to deal with more than one order parameter). Further, the Hamiltonian would be built out of effective interactions and have effective coupling constants as parameters. In such a system then, phase may be described as a a region in parameter space over which the free energy F is analytic. Phase transitions occur a parameter (either a coupling constant or the temperature) is changed such that the system moves across points in paramater space where F is non analytic.

In LGW, the physics of critical phenomena is captured by the order parameter. The system tends to minimize its free energy. In order to do so, it may undergo a phase transition by jumping across a region of non analyticity in parameter space. In the process its order parameter changes. If the order parameter changes in a discontinuous fashion, the phase transition is said to be of first order. If the order parameter changes continuously, the phase transition is said to be a continuous phase transition. Here, we will mainly concern ourselves with continuous phase transitions. Near the critical point for such phase transitions, the correlation length and the correlation time diverge as power laws with irrational exponents, known as critical exponents. The critical behaviour has two aspects: statics, which determines which phase the system lives in as it must minimize the free energy; and the dynamics, which determines how the phase transition actually proceeds with the change of control parameters. The dynamics is roughly determined by spatial averages of local fluctuations that cause a change in phase locally. In general, these are uncorrelated and hence do not change the total phase of the system. However, near the critical phenomena, these fluctuations get correlated over the large correlation length leading to the phase transition.

We would like to address the question of whether quantum effects are important for phase transitions. Even when quantum mechanics plays a dominant role in determining the properties of the different phases of materials, they may or may not determine the physics of fluctuations near the critical point. Since, we require fluctuations correlated over a large length scale in critical phenomena, the fluctuations that bring about phase transitions must have enough energy to change the phase over the correlated region. Now, the system has a characterestic energy scale for quantum fluctuations, The energy scales of thermal fluctuations on the other hand is determined by $k_B T$, where T is the temperature of the system. Hence, it can be seen that at high temperatures, thermal effects dominate strongly

over quantum effects. In fact, the quantum energy scale vanishes near a critical point. This is true because near a critical point both the correlation length ξ^{-1} and time (related inversely to the characterestic energy δ) diverge according to the relations

$$\xi^{-1} \ \Lambda|g - g_c|^{\nu}, \qquad \delta \ J|g - g_c|^{z\nu} \tag{1}$$

where Λ is a an inverse length of the order of lattice spacing. Hence, phase transitions taking place at temperatures above zero Kelvin are dominated completely by classical effects. In such cases, even though quantum mechanics may be instrumental in determining the phases themselves, the critical behaviour can be modelled and studied using classical statistical mechanics. On the other hand, phase transitions at temperatures at absolute zero have quantum effects. Of course, no experiments are performed at exactly zero temperatures. However, the physics of substances in a region near the critical point $(g_c, T = 0)$ are strongly influenced by quantum phase transitions. Hence, more than the quantum critical point itself, one is interested in the quantum critical region which is accesible in the low temperature experiments. The idea is that a study of QPT would enhance our understanding of this region. Such phase transitions should be studied using quantum statistical mechanics.

In quantum statistical mechanics, the expectation values of an operator $\hat{O}$ is calulated by

$$\langle \hat{O} \rangle = \frac{1}{Z(\beta)} \mathrm{Tr}(\hat{\mathrm{O}} \exp(-\beta \mathrm{H})).$$

It is easy to see that in the limit of zero temperature, the free energy becomes the ground state energy, while any statistical averages of any other operator is given by the ground state expectation value of that operator. Thus minimization of the free energy becomes a question of minimization of the ground state energy. As discussed, QPT occur at zero temperature, due to changing the dimensionless coupling constants of the Hamiltonian. Generically, for a finite sized system the Hamiltonian H(g) would be a smooth function of the coupling g, and one would not expect non analytic behaviour to arise out of this. However, consider the Hamiltonian to be

$$\mathrm{H(g)} = \mathrm{H_0} + \mathrm{gH_1},$$

where $\mathrm{H_0}$ and $\mathrm{H_1}$ commute. Thus, as one varies g, the states remain the same, while their energy eigenvalues change as a function of g. For a suitable choice of the Hamiltonian, one can get the phenomena of level crossing, ie. at some point in the parameter space (say at $\mathrm{g_c}$) a state that was an excited state for the initial value of g becomes the ground state. Thus, non analytic behaviour can arise in finite sized systems. In infinite systems, an avoided level crossing too would lead to non analyticity in the ground state energy.

A distinctive property of QPT is the inablitly to separate the statics from the dynamics. While in classical thermal fluctuation driven phase transitions, one can study the statics and dynamics quite separately, this is not easily possible in QPT. Heuristically, it is easy to undertand the reason. The energy scales that determine the statics are also related to the time scales of fluctutation by Heisenberg's uncertainty, thereby carrying information about the dynamics of the system as well. At T=0, a quantum system in d dimensions can be exactly mapped to a classical system in d+1 dimensions. This equivalence is clearest if one

looks at the quantum partition function at β as a path integral, in which case it can be seen that it is formally the same as a classical statistical mechanics partition function of dimensions d+1. The only difference is that while the d+1 dimensional partition function has spatial integrals with infinite limits, the imaginary time integral in the quantum partition function has limits from 0 to β. So setting the temperature to zero gives us the same limits. This result is important as it allows us to use ideas of classical statistical mechanics in QPT.

So far we have only noted that under certain conditions QPT are possible. We end this section by emphasizing that QPT are not merely a theoretical possibilty, but in fact they play a dominant role in a number of condensed matter systems.

3 Quantum Magnets in Two Dimensions

In this section, we specialize to the example of quantum magnets in two dimensions. Consider a model system of spins $S = \frac{1}{2}$ at the sites of a two dimensional square lattice. If the spin at the lattice site r is labelled by $\vec{S_r}$, then the model anti ferromagnetic Hamiltonian is

$$H = \frac{-J\tilde{g}}{2} \sum_r \hat{L}_r^2 + H_{int} \tag{2}$$

$$H_{int} = J \sum_{\langle r,r' \rangle} \vec{S_r} \cdot \vec{S_{r'}} + ... \quad , \qquad J > 0 \tag{3}$$

(We will not be considering the effects of an external magnetic field). and $\langle rr' \rangle$ implies nearest neighbour sites, the condition $J > 0$ tells us that the material is antiferromagnetic rather than ferromagnetic. The ground states of this quantum mechanical system have been studied in detail, and they have different symmetry properties from the Hamiltonian, which has explicit rotational symmetry in the spin space, and discrete translational symmetry in the lattice space. Different ground states are possible in this model, depending on the value of the coupling constant. There are anti-ferromagnetic ground states with long range magnetic order, as well as paramagnetic ground states with no long range magnetic order.

A simple example of an anti-ferromagnetic ground state is the Néel state (see Figure 1) where the spins are collinear (though they may point in opposite directions. On the two dimensional square lattice with the lattice sites labelled by $r = \{x, y\}$, the spin at the site r is given by $\vec{S_r} = \epsilon_r \vec{N_r}$, with $\epsilon_r = (-1)^{(x+y)}$. Thus, the Néel state lowers the energy by antialligning nearest neighbout spins. Thus, it is characterised by $\langle \vec{N_r} \rangle \neq 0$, and this expectation value is also independent of the lattice site r. It is also evident that by choosing a direction (along which the spins are alligned), it breaks the spin rotational symmetry.

There are also a number of paramagnetic states like the Valence Bond Stas (VBS) or the Resonating Valence Bond States. We will be interested in the simple example of VBS. In the VBS phase (See Figure 2), a spin pairs up with neighbouring spins to form a singlet. Here the dot products of neighbouring spins in a two dimensional square lattice is give by

$$\vec{S_r} \cdot \vec{S}_{r+x} = \mathrm{Re}(\psi_{\mathrm{VBS}})(-1)^{\mathrm{x}}, \qquad \tilde{\mathrm{S}}_{\mathrm{r}} \cdot \tilde{\mathrm{S}}_{\mathrm{r+y}} = \mathrm{Im}(\psi_{\mathrm{VBS}})(-1)^{\mathrm{y}}$$

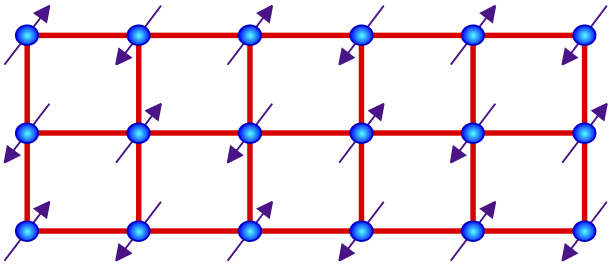

Figure 1: The Neel State (picture taken from [5])

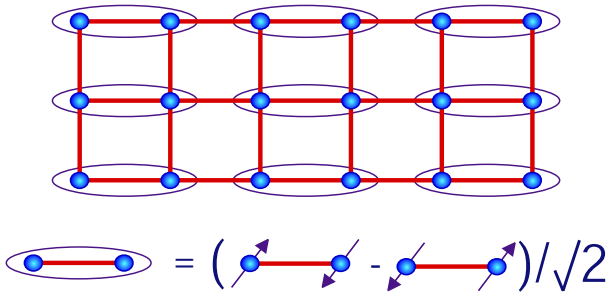

Figure 2: The Valence Bond State (picture taken from [5]

where ψ_{VBS} is a complex order parameter. It can be seen that this leads to different patterns of short range order. For example, if the order parameter is such that $(\psi_{VBS})^4$ is real and positive , then one gets columnar order (Figure 3a) ie. the two neighbouring spins are correlated along a particular direction (either x or y depending in whether the phase is actually π or $\frac{\pi}{2}$ modulo 2π) to form singlets. If $(\psi_{VBS})^4$ is real and negative, one gets plaquette ordering (Figure 3b), ie. four spins on the vertices of a lattice square are correlated to form the singlets. These short range correlations between neighbouring spins are referred to as valence bonds. Thus, this ground state is is invariant under spin rotational symmetry, but breaks lattice translational symmetry.

We will be concerned with transitions between these phases. To study the fluctuations of these phases one needs to use a free energy involving the order parameter for the phase in question. However, the order parameter of the Néel state is a unit vector $\hat{n}$ in three dimensions, while the order parameter of the VBS phase is a complex number ψ_{VBS}. The fact that they are very different is a reflection of the fact that the two phases have different broken symmetry properties, rather than being distinguished by broken or unbroken symmetry of only one kind as is usual in continuous phase transitions. A Landau Free Energy used to study phase transition from the Néel to VBS phase should then have terms involving both the order parameters. This situation typically would predict a competition between these terms that would result in a first order phase transition. Alternatively, it could predict a very finely tuned multicritical point, where the transition proceeds through a phase where

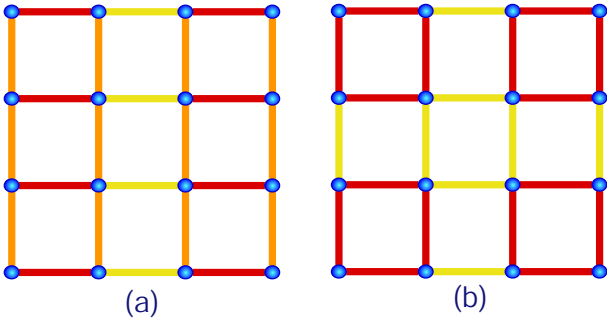

Figure 3: (a)Columnar and (b)Plaquette Order: The 'valence bonds' are represented by the red lines. (picture taken from [5])

both the translational and spin rotation symmetry are either broken or unbroken, but a direct transition to VBS is observed because the region in parameter space corresponding to the intermediate stage is too small. In other wordsthere could be actually two transition that take place so close to one another that it becomes hard to distinguish them.

The surprise is that it appears that a direct continuous transition *can* occur between two states of different broken symmetries. This indication comes from certain numerical calculations. There is also evidence from experiments looking at the onst of magnetic order in a class of rare earth metals, as stated in [5]. As explained in the previous paragraph, this is in conflict with expecations of LGW. It is then important to ask if this is a result of misinterpretation of the numerical simulataions and experiment (for example could this actually be coming from the fine tuning mentioned above) or if the LGW does not hold in such cases. If it turns out that LGW is invalid, then ir would be worth asking what specifically ivalidates LGW, and attempt to identify classes of problems where LGW is not invalidated by this mechanism, and how LGW can be modified in order to deal with these problems. Here, we will not attempt to review the question of misinterpretation of the data or numerical analysis of [9],[10] but follow [5],[6] in their proposed theory which can account for the phase transitions.

4 Flucutations of the Néel State

To study the fluctuations [4] in the vicinity of the Néel state, one must write out an effective theory for the quantum mechanical excitations about this ground state. As noted before, the Néel state breaks a continuous symmetry, namely the spin rotational symmetry. This implies the existence of massless transverse excitations, but the amplitude fluctuations must be suppressed. Assuming a minimum number of derivative terms, one finds that the simplest coarse grained effective lagrangian with these properties is an Euclidean continuation of an O(3) non-linear sigma model of the order parameter $\hat{n}$:

$$S_0 = \frac{1}{2\tilde{g}} \int d\tau \int d^2r \left[(\frac{\partial \hat{n}}{\partial \tau})^2 + (\nabla_r \hat{n})^2 \right] \tag{4}$$

with the constraint that $|\hat{n}| = 1$. However, it was known that the in the limit when the number of spin components tend to a large number (instead of the three considered), the non linear sigma model has a finite correlation function. Thus, if it were the long wavelegth limit of the quantum magnets under discussion, they would not have critical behaviour for large spins. Actually, in order to correctly describe the physics this action must be augmented by a topological Berry's phase term S_b [4],[7].

$$S_b = iS \sum_r \epsilon_r \mathcal{A}_r \tag{5}$$

$$S_n = S_0 + S_r \tag{6}$$

Following Haldane [7], we will try to give a feel for why this is true. First, consider a system with only one spin. In calculating the quantum partition function, one takes a trace of $exp(-\beta H)$ over quantum states (as indicated before) by treating the temperature as an imaginary time split into infinitesimal (imaginary) time intervals, and inserting complete sets of states. This can be done using any complete set of states. In particular we may use the spin coherent states (though they are actually overcomplete) which are actually described by $|\hat{n}\rangle$. While we get the usual effective field theory terms as described by S_0 from the Hamiltonian, we also get en exponent which comes from propagating the $|\hat{n}\rangle$ and coming back to itself (because of the trace). This is the origin of the Berry's phase term. The quantity $\mathcal{A}$ is the area swept out on the surface of a sphere of unit radius by the tip of the vector $\hat{n}$ moving in a closed loop. There is an ambiguity regarding the value of the area as the sphere is a boundaryless surface. Hence the area may be calculated in two ways. The difference of the two (taking into account orientation) is 4π. When we consider all the lattice points, terms of the kind mentioned for one spin are added with a factor of ϵ in order to keep track of the orientation of the spins in the Néel state. This is a topological term and as such will not pick up corrections from a large S computation if we go through one.

We may well ask if this new term is important everywhere, ie. our description of Néel state in terms of the order parameter $\hat{n}$ was incorrect throughout. We will show, that insofar as we consider only low energy properties of the Néel state, or fluctuations about it that leave it smooth this term has no effect on the physics. However, it is crucially important in the critical regime. In fact, the central idea of [5],[6] is that in this regime this term has the capacity to capture the description of the paramagnetic VBS state too.

If we consider smooth configurations of the Néel vector, we are considering a three dimensional vector at each point of the two dimensional spatial lattice. If one could coarse grain spatial lattice to a smooth manifold, then one has a topolgical invariant which we will here called the total skyrmion number defined by

$$Q = \frac{1}{4\pi} \int dxdy \epsilon_{ijk} \hat{n}_i \partial_x \hat{n}_j \partial_y \hat{n}_k \tag{7}$$

which is conserved as it is integral and continuous. On the other hand, by expanding the Berry phase about the classical Néel state (as shown in in figure 1) it can be written as a sum of dynamical quantities (like $\hat{L}$, which may be further elimninated to find some quantity

proportional to the standard non linear sigma model lagrangian) and a residual topological term which sums to

$$2\pi S \sum_n (-1)^n Q(t) \tag{8}$$

. But, if Q remains a constant, then this term vanishes due to the oscillatory factor. We may interpret this as destructive interference of a quantum mechanical parameter. In fact, this is probably an example of the fact that microscopic quantities do not usually survive spatial and temporal averaging. On the other hand, we should remember that the 'microscopic' model we started with was defined on a lattice, not a smooth manifold. Hence, Q can change by integral quantities. Such processes are called tunneling processes or alternatively monopole or hedghehog processes.

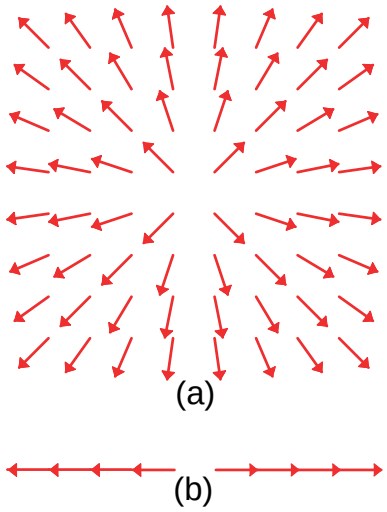

Figure 4: Monopole process (picture taken from [5])

In fact, such processes too interfere destructively, unless they change Q by four. This is seen from the sum of the monopole events which turns out to be

$$\Pi_n exp(i\frac{\pi}{2}\zeta_n \Delta Q_n) \tag{9}$$

Here, ΔQ_n is either +1 or -1 and its sum must be zero due to periodic boundary conditions on the time axis, and the integer ζ_n can take on values 0,1,2,3 depending on the dual lattice coordinate n. Thus, the phase again destructively interferes to zero for single monopole events, but is non zero for events which are characterized by $\Delta Q_n = 4$. In fact, such quadrupling events that change the phase should be included in the path integral. Taking the changes of the skyrmion numbers, one can write creation and annhilation operators for the skyrmions. If these have the same symmetry properties as the VBS order parameters, they can be identified with the order parameter for the VBS phase ψ_{VBS}. It can be checked

that the skyrmion annhilation operator v has the same properties under both spin rotation symmetry and lattice translation symmetry as ψ_{VBS} if we make the identification:

$$\psi_{VBS} \equiv e^{\frac{-i\pi}{4}} \psi_{VBS} \tag{10}$$

5 Conclusions

Here we have seen that direct conitnuous phase transitions between the Néel state and the VBS phase are possible, even though the classical LGW paradigm did not predict it. Thus, we come to an exciting juncture, and we may ask if these methods applied to other scenarios give interesting new phenomena as well.

References

[1] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, England, 1999)

[2] L. D. Landau, E. M. Lifshitz, and E. M. Pitaevskii, *Statistical Physics* (Butterworth-Heinemann, New York, 1999)

[3] N. Goldenfeld, *Lectures on Phase Transitions and the Renormalization Group* (Westview Press, Boulder, 1992)

[4] E. Fradkin, *Field Theories in Condensed Matter Systems* (Addison-Wesley Publishing Company, Redwood City, California, 1991)

[5] T. Senthil, A. Vishwanath L.Balents, S. Sachdev, and M. Fisher, Science **303**, 1490 (2004)

[6] T.Senthil, Leon Balents, Subir Sachdev, Ashvin Vishwanath, and Matthew P.A. Fisher, http://arxiv.org/abs/cond-mat/0312617

[7] F. Haldane, Phys. Rev. Lett. **61**, 1029 (1988)

[8] S. Sondhi., S. Girvin, J. Carini, and D. Shahar, Review of Modern Physics, **69**, 315 (1997) http://arxiv.org/abs/cond-mat/9609279

[9] P. Coleman, C. Pepin, Q. Si, and R. Ramazashvili, Journal of Physics: Condensed Matter **13**, 723 (2001) http://arxiv.org/abs/cond-mat/0105006

[10] G. Stewart, Review of Modern Physics 56, 755 (1984)