Quantum Phase Transitions

Seyyed Mohammad Hassan Halataei

Phase Transitions and Renormalization Groups

Professor Nigel Goldenfeld

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Abstract:

This essay describes what a quantum phase transition is and one way of proving its very existence for an Ising Model. Quantum-classical mapping is discussed and showed that quantum problem in d spatial dimension can be reduced to classical problem in (d+z) effective dimension. The existence of an exact solution for one dimensional quantum Ising model is cited and it is compared to the previous estimates for density of kinks.

Introduction and Background.

This paper studies quantum phase transitions and describe them based on the knowledge we have obtained in the class. As an example I focus on Quantum Phase transitions for an Ising Model and also give a real example of it in nature. Studying Classical phase transitions in vast details motivated some physicists to do the same for Quantum Phase Transitions. After all, the systems of interest are governed by Quantum rules in microscopic level and when temperature approaches to zero it seems reasonable that the role of Quantum fluctuations can in principle become important compared to thermal fluctuations which are responsible for Classical phase Transitions.

The first task is to show that Quantum phase transitions exist. This can be done by looking at two different regimes of a system and check that if there is one state or at least two. If there are two then at zero temperature and in the absence of thermal fluctuations one could argue that somewhere there should be a nonanalytic transition between these two phases and since the system is in absolute zero temperature, the transition is a quantum phase transition. I show this approach for the Ising Model by studying the two states of it in two extremes: (1) when a coupling constant for spin interactions are so large compared to the external field, (2) when the coupling constant is so small compared to the field.

Doing Quantum mechanics is usually a bit harder than doing classical physics for large systems. Particularly, in the case that physicists in this field are interested in, the Hamiltonian of the system are composed of a kinetic part and a potential part. In Classical physics these two Hamiltonian commute and hence the partition function factorizes, however in Quantum physics they don't necessarily commute and as a result the partition function bears time dimension evolution with itself. This motivated the authors of this field to think about some possible mapping between Quantum phase transitions and classical phase transitions. They were successful in this investigation and could find some mapping and analogy between the two physics. I devote parts of this paper to show a mapping between the Quantum phase transitions and Classical ones and their dimensional relations.

Solving any problem in approximation and in asymptotic limits is always useful and gives us some feeling about the physics of the problem and its qualitative behavior in general. However, it can't be a replacement for an exact solution. Fortunately, the Quantum Ising model is solvable in 1D. I devote a brief part to asserting this fact. 1-dimensional Quantum Ising model is of essential interests in this field, quantum phase transitions, and Sachdev[1], on of a pioneers in the field, recognized that as one of the two prototypical models on which understanding of quantum phase transitions is based[2].

I am interested in Quantum physics. Whatever topic that I encounter to I would like to figure out the physics of it in quantum regime and see how the reality of world is really revealed in microscopic level. What is the very nature of nature and how can this problem in particular help me and open a new window for me to understand it? That is my general motivation in physics which reduces to any specific case and make my direction in any part of physics that I study.

Singularities discussed in Quantum phase transitions are in ground states and hence at absolute zero temperature whereas almost all experiments are in nonzero temperatures. That brings this question up that what is the impotency of studying quantum phase transitions? Sachdev [1] answers this question that although the system might not reach the critical point in terms of temperature and coupling constants, the thermodynamic and dynamic properties of many systems near the critical point can be understood upon understanding the physics of the system at the critical point. In addition, for some systems one can argue that there is a quantum critical point which is physically inaccessible to the system; nevertheless the physics in vicinity of it can be derived from the quantum phase transitions discussions.

What is a quantum phase transition?

Continuous or second order phase transitions which occur at ground state of a system and at absolute zero temperature due to quantum fluctuations which come from Heisenberg's uncertainty principle are called quantum phase transition [1,4].

Following [1] , let us study quantum phase transition definition more formally. Assume a lattice with Hamiltonian $H = H_0 + g H_1$ where g is a dimensionless coupling constant. In general for a finite lattice H(g) is analytic. However, if H_0 and H_1 commute i.e. if they correspond to conserved quantities then they can be diagonalized with the same eigenvectors which are independent of g, although eigenvalues are still functions of g. In this case a level-crossing can possibly happen at some $g = g_c$ the ground state and an exited state reach the same value and make a nonanalytic point for the ground state (see Fig 1)[1].

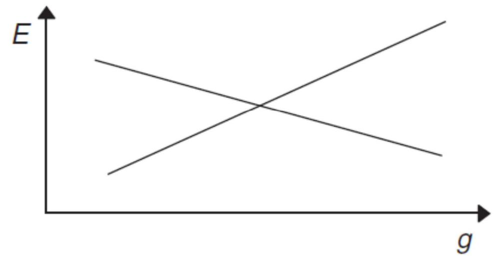

Fig 1. Eigenvalues, E, of Hamiltonian H(g) vs g. Level-crossing may occur for an infinite lattice when H_0 and H_1 commute.(Credit to [1])

Level-crossing usually occurs in infinite lattice. When the system is finite what most likely happens is an avoided level crossing (see Fig 2) instead of level-crossing.

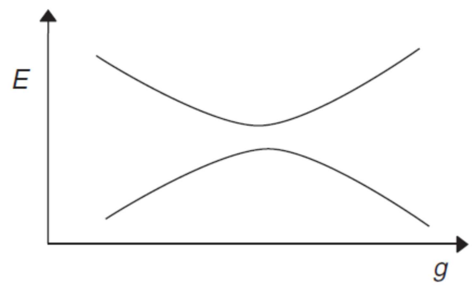

Fig 2. Avoided level crossing for a finite lattice. (Credit to [1])

However as the size of the system gets larger the avoided level crossing becomes sharper and leads to a nonanalyticity at $g = g_c$. No matter what is the origin of the nonanalyticity and where it occurs, in a finite system or infinite one, we consider it as a *quantum phase transition* when it appears in the ground state energy of a system.

Here my focus is on second order quantum phase transitions. It can be put in this way, loosely speaking, that the fluctuation characteristic energy Δ in these transitions vanishes as the coupling constant g approaches its critical value. This vanishing is usually modeled as power law [1] :

$$\Delta \sim J|g - g_c|^{z\nu},$$

where J is the energy scale of a characteristic microscopic coupling. There is also a correlation length scale in this theory which diverges as g approaches g_c. This correlation length scale can be the length scale which determines the exponential decay of correlations at equal time in the ground state [1]:

$$\xi^{-1} \sim \Lambda|g - g_c|^{\nu},$$

where Λ is a momentum cutoff. Now, using the last two proportionalities one obtains,

$$\Delta \sim \xi^{-z}$$

The exponent z is called dynamic critical exponent and as it will be discussed it appears in the relation between dimensions of quantum system and classical system in quantum-classical mapping. Having introduced basic concepts and notations, I go to the next topic which considers the possibility of existence of quantum phase transitions.

There exists a quantum phase transition: Quantum Ising Model

To be specific I focus on quantum Ising model and show that there are two different states for this model for two extremes of the coupling constant and hence there should be a transition. At the end, I introduce a real example of this model which exists in nature.

The Hamiltonian of the quantum Ising model is [1]

$$H_I = -Jg \sum_i \hat{\sigma}_i^x - J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z .$$

Here J is the positive exchange constant which determines the microscopic energy scale and g is a positive dimensionless coupling which is used to carry the system through its different phases. The spin operators above are the usual Puali matrices which act on site i of a d-dimensional lattice and the sum in the second term is a nearest neighbor summation.

I want to study two extremes g << 1 and g >> 1 . Let's start with g >> 1. In this case the first term in the Hamiltonian dominates and to the leading order in 1/g , the ground state is

$$|0\rangle = \prod_i |\rightarrow\rangle_i ,$$

That is a product of eigenstates of the Pauli matrix in x-direction. More formally in terms of the eigenstates of $\hat{\sigma}_i^z$ [1],

$$|\rightarrow\rangle_i = (|\uparrow\rangle_i + |\downarrow\rangle_i)/\sqrt{2},$$
$$|\leftarrow\rangle_i = (|\uparrow\rangle_i - |\downarrow\rangle_i)/\sqrt{2},$$

Now notice that the eigenvalues of the Pauli matrices in z-directions are uncorrelated in the above ground state for large g. Hence,

$$\langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle = \delta_{ij}$$

That's when the corrections from the perturbation have not been considered. Adding them to the leading term one expects the correlation still remain short-range and be of the form [1]

$$\langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle \sim e^{-|x_i - x_j|/\xi}$$

where $|x_i - x_j|$ is the spatial distance between site i and j. Now I like to find the correlation of $\hat{\sigma}_i^z$ in small g and see if there is a way to start from the above relation and get to the other one. So let's consider the case g << 1. In this case the second term in the Hamiltonian dominates. For g = 0 the spins are either all up or all down [1] :

$$|\uparrow\rangle = \prod_i |\uparrow\rangle_i \quad \text{or} \quad |\downarrow\rangle = \prod_i |\downarrow\rangle_i \, .$$

For small g some of the spins flip. Let call the ground state obtained by the perturbation theory from the above states for a small g, |0>. The nature of the above two states, all up or all down, suggests that in this case [1]

$$\lim_{|x_i - x_j| \to \infty} \langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle = N_0^2,$$

where N_0 is the spontaneous magnetization of the ground state. Looking at the above correlation relation and the one introduced for large g, one would realize that there is no way for states that satisfy these two relationships to transform into each other analytically as a function of g [1]. As a result there must be a critical value $g = g_c$ at which the spin correlator for large distances changes from on to the other function above. This is the location of quantum phase transition. Therefore I conclude that there exists a quantum phase transition for an Ising Model. A physical realization of this Ising model in experiment is $CoNb_2O_6$ which have been studied by Coldea and collaborators [6]. Opposed to $LiHoF_4$ which has long range interactions, $CoNb_2O_6$ has nearest neighbor interactions which is what required for our example in this section.

Quantum-Classical Mapping

It will be so interesting if we find out that we can solve the quantum phase transition problems by tools of Classical phase transition that we have already built. Looking at literatures you figure out that this is really possible. Riger and Young [5] studied quantum phase transitions for Ising spin glass in a transverse field in 2D and indeed used an effective classical system in 2+1 dimensions and Monte Carlo simulations to deal with their problem. They found z = 1.5 and ν =

1.0. So our observation tells us at least in some cases there are classical analogs for the quantum problem. The question is why such a correspondence exists and how different quantities are related in this analogy. In this section I briefly answer these questions.

Following [3] I first look at the partition function which is a generator function for thermodynamics properties

$$Z = \mathrm{Tr}\, e^{-H/k_B T}$$

Where the Hamiltonian composed of

$$H = H_{\mathrm{kin}} + H_{\mathrm{pot}}$$

a kinetic part plus a potential part. As mentioned in the introduction in Classical system these two parts commute and hence the partition function factorizes

$$Z = Z_{\mathrm{kin}} Z_{\mathrm{pot}}$$

The kinetic part does not make any singularity in the free energy because it comes from some Gaussian integrals. So the study of a Classical system is reduced to a study of a static time independent system which lives in d dimensions.

Quantum problems, in contrast, do not let us in general to have decoupled kinetic and potential parts, the partition function does not factorize and indeed the static and dynamic are usually coupled. The density operator, exp(-H/kT) looks like a time evolution operator in imaginary time $\tau = 1 / k\, T = -i2\, \pi\, \theta / h$ where θ is the real time here. When T = 0, time ranges from zero to infinity and an extra dimension naturally adds to the system. For a classical system, say a classical ferromagnet, with reduced temperature t and external magnetic field B close to the critical point the singular part of the free energy scales as

$$f(t, B) = b^{-d} f(t\, b^{1/\nu}, B\, b^{y_B}).$$

where y_B is a critical exponent and b is positive scale factor. At zero temperature it turns out that for a quantum phase transition the singular part of the free energy scales as

$$f(t, B) = b^{-(d+z)} f(t\, b^{1/\nu}, B\, b^{y_B})$$

where $t = |g - g_c| / g_c$. The reason is that the extra parameter, the imaginary time, scales as the length to the power z. Now we observe that a quantum phase transition in d dimensions is related to a classical phase transition in *(d+z)* dimensions [3] near the critical point at zero temperature. It is a well-known fact [1, 4, 7, 8, 9, 10, 11, 12] that the quantum statistical problem in d-dimensions at zero temperature can be converted to the classical problem in d+1 dimensions. What I showed above is a bit different though. The above argument showed that for the critical properties the effective dimension of the system is *d+z* instead of d+1 [4]. Here z is the dynamical exponent and it can be an integer like 1 or even a fractional number. As a result the effective dimension of a quantum system near the critical region may even become greater than the upper critical dimension of the system. That has its own consequences. Fig 3. shows the effect of such a phenomenon for the phase transition in the antiferromagnet $MnCl_2.4H_2O$ where the value of the critical exponent β varies with temperature and at zero temperature reaches its mean field theory value[4,13] as a consequence of this effect.

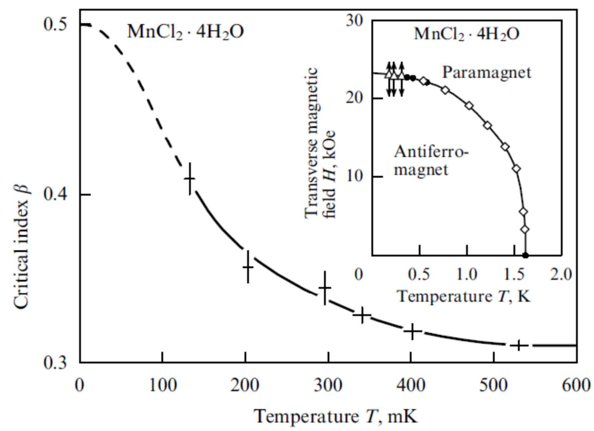

Fig 3. Dependence of critical exponent β to temperature. (Credit to [4])

Up until now we did not use any exact solution for the obtained result. However such a solution for 1D Ising model exists which make the topic of last section of this paper.

Existence of an exact solution for 1D Quantum Ising Model

I like to end this paper by asserting that an exact solution for one dimensional quantum Ising model exists. Dziarmaga [2] found this solution and showed that the problem is solvable exactly. Moreover, the exact result is not far from the approximation that had been made before that. Following [2] let's visit the problem briefly here. The phase transition for one and two dimensional Ising model occurs at g = 1. When g is small and the system is infinite it is impossible to pass the critical point without exciting the system. Therefore, the system winds up in a quantum superposition of up and down states with finite domains of up-spins and down-spins which are separated by kinks. A kink is the first place in which a spin flips. Average density of these kinks depends on the transition rate [2].

We approximate g(t) which derives the system to the critical point as a linear function of time $g(t) = t / \tau_Q$ where τ_Q is the transition time. Ref. [14] estimated density of kinks based on the linear assumption for dependence of the coupling constant in time as

$$n \simeq \left(\frac{\hbar}{2J\tau_Q}\right)^{1/2}$$

Dziarmaga [2] shows that doing formal calculations and finding the exact result, the above estimate will change by a factor of $(1/2\pi) = .159$. That shows the estimate was good enough. The other good news is that numerical simulations also confirm the prefactor of .16 in calculating the density of the kinks [2] which is a verification of the correctness of the exact solution.

Conclusion

In conclusion, I visited the phenomenon of quantum phase transition in this paper. It was defined that what a quantum phase transition is. What its underlying physics can be and how critical quantities are related to each other in the critical region through power laws. A nonanalyticity in ground state of a system which occurs at zero temperature as a result of quantum fluctuations, i.e. a quantum phase transition, then acquired a proof for its existence in nature. I showed a proof of it for quantum Ising model by avoiding unnecessary technical details in this paper and mentioned one observable example of it which has already been studied. An interesting analogy between quantum phase transition and classical phase transition exists that I reviewed briefly in this paper and mentioned that the quantum Ising model is essentially solvable and was indeed solved and the results show good agreement with simulations.

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