Quantum Phase Transitions

G. H. Lai

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Abstract

A quantum phase transition (QPT) is a zero-temperature, generically continuous transition tuned by a parameter in the Hamiltonian at which quantum fluctuations of diverging size and duration (and vanishing energy) take the system between two distinct ground states [4]. This short review discusses the characteristic aspects of QPT and illustrates possible applications in physics and biology.

Contents

1 What are quantum phase transitions?

A phase transition is a fundamental change in the state of a system when one of the parameters of the system (the order parameter) passes through its critical point. The states on opposite sides of the critical point are characterized by different types of ordering, typically from a symmetric or disordered state, which incorporates some symmetry of the Hamiltonian, to a broken-symmetry or ordered state, which does not have that symmetry, although the Hamiltonian still possesses it.

As we approach the phase transition, the correlations of the order parameter become long-ranged. Fluctuations of diverging size and duration (and vanishing energy) take the system between two distinct ground states across the critical point. When are quantum effects significant? Surprisingly, all non-zero temperature transitions are considered "classical", even in highly quantum-mechanical systems like superfluid helium or superconductors. It turns out that while quantum mechanics is needed for the existence of an order parameter in such systems, it is classical thermal fluctuations that govern the behaviour at long wave-lengths. The fact that the critical behaviour is independent of the microscopic details of the actual Hamiltonian is due to the diverging correlation length and correlation time: close to the critical point, the system performs an average over all length scales that are smaller than the very large correlation length. As a result, to correctly describe universal critical behaviour, it should suffice to work with an effective theory that keeps explicitly only the asymptotic long-wavelength behaviour of the original Hamiltonian (for instance, the phenomenological Landau-Ginsburg free-energy functional).

So far, we have shown that classical theory suffices. However, consider what happens when the temperature around the critical point is below some characteristic energy of the system under consideration [2]. For example, the characteristic energy of an atom would be the Ryberg energy. We see a characteristic frequency ω_c and it follows that quantum mechanics should be important when $k_b T < \hbar\omega_c$. In the same spirit, if $k_b T >> \hbar\omega_c$ close to the transition, the critical fluctuations should behave classically. This argument also shows that zero-temperature phase transitions, where $T_c = 0$, are qualitatively different and their critical fluctuations have to be treated quantum mechanically.

In such zero-temperature or quantum phase transitions (QPT), instead of varying the temperature through a critical point, we tune a dimensionless coupling constant J in the controlling Hamiltonian $H(J)$. Generically [1], the ground state energy of $H(J)$ will be a smooth, analytic function of g for finite lattices. However, suppose we have the Hamiltonian $H(J) = H_0 + JH_1$, where H_0 and H_1 commute. This means that H_0 and H_1 can be simultaneously diagonalized and the eigenstates of the system will remain the same even though the eigen-energies will vary with J. A level crossing is possible where an excited level crosses the ground energy level at some coupling constant J_c, creating a point of non-analyticity in the ground state energy as a function of J, which manifests as a quantum phase transition.

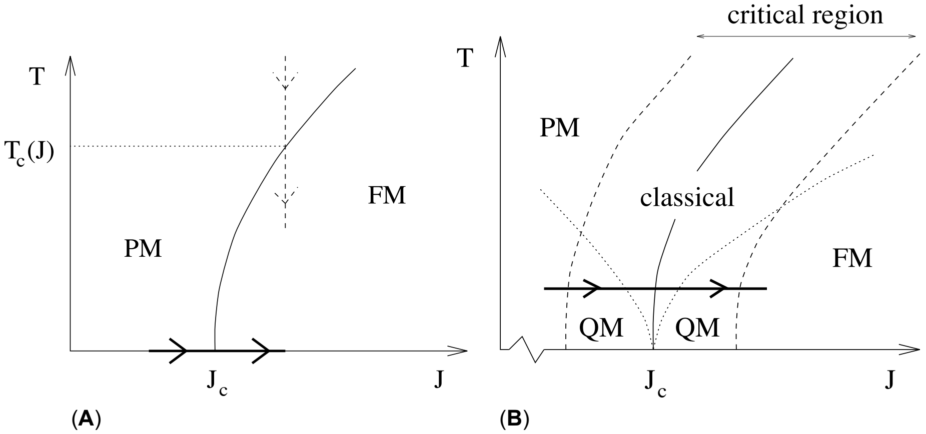


Figure 1: (A) Schematic phase diagram showing a paramagnetic (PM) and a ferromagnetic (FM) phase. The dotted path represents a classical phase transition while the solid line indicates a quantum phase transition. (B) Vicinity of the quantum critical point $(J = J_c, T = T_c)$. Indicated are the critical region, as well as the regions dominated by the clasical and quantum mechanical critical behaviour(QM) [2].

2 Features of a quantum phase transition

To illustrate the concepts, we consider the example of a metallic or itinerant ferromagnet [2]. Figure 1A shows a schematic phase diagram in the $T - J$ plane, with T the temperature and J the strength of the exchange coupling that is responsible for ferromagnetism. The coexistence curve separates the paramagnetic phase (large T, small J) from the ferromagnetic phase (small T, large J). For any given J, there is an associated Curie temperature T_c and classical phase transition occurs if we vary the temperature through T_c. On the other hand, imagine changing J at zero temperature, for instance, by alloying/doping the magnet with some non-magnetic material. Here, we encounter a quantum phase transition between the paramagnet and the ferromagnet at the critical value J_c.

The behaviour at the $T = 0, J = J_c$ is very different from $T \neq 0$. In order to understand what happens in the vicinity of a QPT, a special mathematical trick which allows us to connect QPT with classical statistical mechanics is needed [3]. Consider the partition function of a d-dimension classical system governed by a Hamiltonian H,

$$Z(\beta) = \operatorname{Tr} e^{-\beta \hat{H}} \tag{1}$$

which can be written, via Feynman's path integral formulation, as a function integral of the form (generalized for quantum many-body systems)

$$Z = \int D[\bar{\psi}, \psi]\, e^{S[\bar{\psi},\psi]}. \tag{2}$$

Here, we let $\hat{H}$ be the Hamiltonian operator and S is the action of the system,

$$S[\bar{\psi}, \psi] = \int d\mathbf{x} \int_0^{\frac{1}{k_B T}} d\tau\, \bar{\psi}(\mathbf{x}, \tau)[-\frac{\partial}{\partial \tau} + \mu]\psi(\mathbf{x}, \tau) - \int_0^{\frac{1}{k_B T}} d\tau\, H(\bar{\psi}(\mathbf{x}, \tau), \psi(\mathbf{x}, \tau)). \tag{3}$$

$\bar{\psi}$ and ψ are the conjugate fields isomorphic to the creation and annihilation operators in the second quantized formulation of the Hamiltonian. We have sneaked in the trick of Wick rotation: analytically continuing the inverse temperature β into imaginary time τ via $\tau = -i\hbar\beta$, so that the operator density matrix of Z, $e^{\beta \hat{H}}$, looks like the time-evolution operator $e^{-i\hat{H}\tau/\hbar}$. The end result is seen in the action, which looks like that of a $d+1$ Euclidean space-time integral, except that the extra temporal dimension is finite in extent (from 0 to β). As $T \to 0$, we get the same (infinite) limits for a $d+1$ effective classical system. This equivalent mapping between a d-dimension quantum system and a $d+1$-dimensional classical system allows for great simplifications in our understanding of QPT.

Since we know that the quantum transition is related to a classical analog in a different spatial dimensionality, and since changing the dimensionality usually means changing the universality class, the critical behaviour at the quantum critical point J_c should be different from that observed at any other point along the coexistence curve in Figure 1.

Also, another interesting aspect of QPT is that dynamics and thermodynamics(i.e. statics, as thermodynamics is very much a misnomer) cannot be independently analyzed, unlike the case for classical statistical mechanics. This loss of freedom is due to the non-commutability of coordinates and momenta in the quantum problem. As a result, both the form of the Hamiltonian as well as the equations of motion are required, meaning that one cannot solve the thermodynamics without also solving the dynamics –

a feature that makes quantum statistical mechanics much harder to solve. Hence, even though it was mentioned in the earlier paragraph that a quantum transition can, in some fashion, be mapped into a classical thermodynamic transition, information about the correlations in excited states which drive the system out of the ground state cannot be extracted from this map.

3 Relevance in experimental Physics and Biology

Quantum phase transitions attract intense attention because they are relevant to a host of experimental issues, despite the fact that $T = 0$ cannot be achieved experimentally. This is because associated with the quantum critical point, there is a sizable region where quantum critical behaviour is observable (labeled QM in Fig. 1B). Some examples are:

- Anderson-Mott models and metal-insulator transitions [4],
- superconductor-insulator (SI) transition in granular superconductors [5],
- transitions between quantum hall states [3],
- the physics of vortices in the presence of columnar disorder [6].

Besides the above, knowledge of dissipative effects [7] on quantum coherence and QPT is essential to assess the reliability of mesoscopic quantum devices in performing tasks that strongly depend on their ability to maintain entanglement (for instance, in quantum computation). Among quantum devices widely used, many are based on a collection of regularly arranged or single small Josephson junctions (JJ). A Josephson junction comprises two superconductors linked by a very thin insulating oxide barrier and the current that tunnels through the barrier is the Josephson current. Josephson junction arrays also constitute a particularly attractive testing ground for the superconducting-insulating (SI) transition, because all parameters are well under control and are widely tunable. Cooper pairs of electrons are able to tunnel back and forth between grains and hence communicate about the quantum state on each grain. If the Cooper pairs are able to move freely from grain to grain throughout the array, the system behaves like a superconductor. If the grains are very small, a large charging energy is incurred to

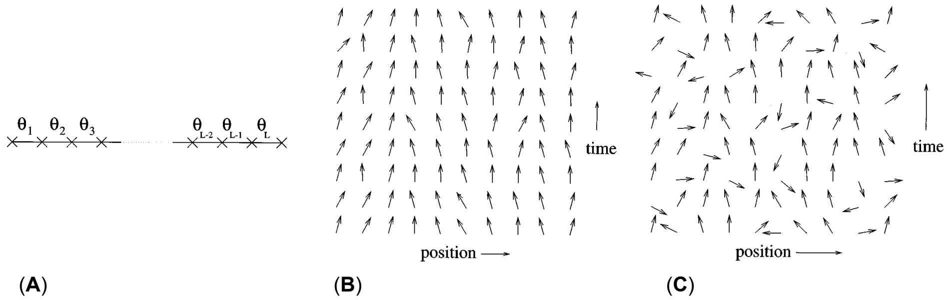
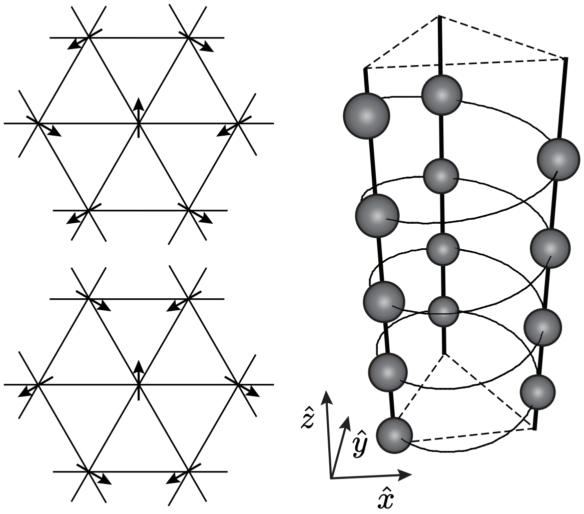


Figure 2: (A) Representation of a 1D Josephson Junction array. Crosses represent junctions between superconducting segments, and θ_i are the phases of the superconducting order parameter. (B) Typical path or time history of the 1D JJ array. Notice it is equivalent to the configuration of a 1+1D classical XY model. The long-ranged correlations are typical of the ordered (superconducting for 1D JJ) phase. (C) Typical path or time history of the 1D JJ array in the insulating phase (or disordered phase for 1+1D XY) [3].

move an excess Cooper pair onto a grain. When this energy is large enough, Cooper pairs cannot propagate and becomes confined on individual grains, leading to the quenching of the collective superconducting phase.

As an example, we consider a one-dimensional array of identical JJs (Fig. 2). The essential degrees of freedom are the phases of the complex superconducting order parameter on the metallic segments connected by the junctions and their conjugate variables, the charges (excess Cooper pairs, or equivalently the voltages) on each grain. Even without doing further math, from Fig. 2B and 2C, one can draw an analogy between our system and a 2-D classical XY model. It turns out that, in an approximation that preserves the universality class of the system, we can indeed map our 1D JJ array into a 2D X-Y system [3], with our dimensionless coupling constant $K \sim \sqrt{E_c/E_J}$ playing the role of the temperature in the classical analog, where $E_c = (2e)^2/C$ is the capacitive charging energy and E_J the Josephson coupling in the array. This equivalence generalizes to d-dimensional arrays and $d+1$-dimensional classical X-Y models. Among the systems studied, two-dimensional ones are most interesting as no true long-range order is possible at finite temperatures while a genuine QPT occurs at $T = 0$. Moreover, 2D samples can be easily fabricated and experimentally characterized.



(a) (b)

Figure 3: Correspondence between polyelectrolyte bundle and $T = 0$ 2D JJ array. (A) The two degenerate, chiral ground states of the antiferromagnetic XY model on a triangular lattice. The helical ordering around a triangular plaquette of the bundle lattice is shown in (B), where the dark black lines depict the polymer backbone while the spheres depict peaks in the condensed charge density [9].

free-energy functional, $\beta F[\phi]$	imaginary-time action, $\hbar^{-1}\mathcal{S}[\phi]$
height along polymer, z	imaginary time, $\tau = it$
longitudinal phonon (or phase) stiffness, βC	inverse grain charging energy, $\hbar E_c^{-1}$
electrostatic, inter-rod coupling, βE_{ij}	Josephson inter-grain coupling, $\hbar^{-1} E_J$
shear strain, $2G\epsilon_{\perp z}$	vector potential, $(2\pi/\Phi_0)\mathbf{a}_\perp$
elastic response, $G_{xzxz}(q_z)$	current response, $-C_{xx}(-i\omega)$

Figure 4: Correspondence between $d = 3$ classical polyelectrolyte system (**left**) and $d = 2 + 1$ quantum frustrated JJ array system (**right**) [9].

In biology, nature has a small range of temperatures to play with, due to the protein nature of life chemistry, and most phase transitions occur with the variation of a parameter other than temperature. I hypothesize that it may be possible to draw analogies with QPTs, where the temperature is fixed (at $T = 0$) and some other parameter is varied, and hence tap into the immerse theoretical and experimental work that has been done on JJ arrays. Although i do not have anything solid to back up my statement, the field of polyelectrolyte condensation may show some promise. Polyelectrolyte chains naturally repel each other, but will nevertheless form condensed bundles in the presence of oppositely charged counterions beyond a certain valency (depending on the nature of the polyelectrolyte). Examples include DNA and F-actin. In fact, polyelectrolytes condense above a certain counterion concentration and dissociate above another counterion concentration. It has become clear that this condensation results from some form of organization of the counterions, either dynamical (correlated charge density fluctuations) or essentially static, in the form of a counterion lattice (positional correlations between condensed counterions).

Some theoretical work on the counterion ‘melting’ transition suggest that the melting transition (i.e. the bundle-to-individual polyelectrolyte transition) is continuous and can be shown to be in the universality class of the three-dimensional XY model [8]. In another work [9], researchers managed to establish a mapping between a model for hexagonal polyelectrolyte bundles and a two-dimensional, frustrated Josephson-junction array (Fig.3). They found that the $T = 0$ SI transition of the quantum system corresponds to a continuous liquid-to-solid transition of the condensed charge in the finite temperature classical polyelectrolyte system. Moreover, the role of the vector potential in the JJ system is played by elastic strain in the classical system (Fig. 4). The general conclusion of this work relates the elastic constants of polyelectrolyte bundles to the phase behaviour of the counterions, which is significant as elastic constants are easier to measure than the scattering amplitudes of counterion charge modulation.

4 Further work

Due to constraints, much experimental and theoretical details have been left out. There are interesting instances of quantum phase transitions in two dimensional quantum magnets which cannot be predicted with an order parameter using the GLW (Ginzburg-Landau-Wilson) formalism that we have adopted in this study [10]. Also, studies on the dynamics of QPTs are still active and a quantum counterpart for the classical Kibble-Zurek mechanism of second order thermodynamic phase transitions was recently proposed [11, 12, 13]. It appears that both experimentalists and theorists have their work cut out for them!

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