I
An Introduction to Quantum Phase Transitions, Information and Dynamics

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Quantum Phase Transitions

1.1 Aim and Scope of this Book

A plethora of systems exhibit phase transitions as the temperature or some other parameter is changed. Examples range from the ice-water phase transition observed in our daily life to the loss of ferromagnetism in iron or to the more sophisticated Mott insulator-superfluid phase transition observed in optical lattices [343]. The last five decades have witnessed a tremendous upsurge in the studies of phase transitions at finite temperature [727, 149, 333, 136, 494, 541, 556]. The success of Landau-Ginzburg theories and the concepts of spontaneous symmetry breaking and the renormalization group [27, 410, 821, 578] in explaining many of the finite temperature phase transitions occurring in nature has been spectacular.

In this book, we will consider only a subclass of phase transitions called quantum phase transitions (QPTs) [154, 658, 725, 799, 185, 63, 62, 66, 141, 744] and we will discuss these mainly from the view point of recent studies of information and dynamics. QPTs are zero temperature phase transitions which are driven by quantum fluctuations and are usually associated with a non-analyticity in the ground state energy density of a quantum many-body Hamiltonian. We will focus on continuous QPTs where the order parameter vanishes continuously at the quantum critical point (QCP) at some value of the parameters which characterize the Hamiltonian. We will not discuss first order quantum phase transitions associated with an abrupt change in the order parameter. Usually, a first order phase transition is characterized by a finite discontinuity in the first derivative of the ground state energy density. A continuous QPT is similarly characterized by a finite discontinuity, or divergence, in the second derivative of the ground state energy density, assuming that the first derivative is continuous. This is of course the classical definition; we will later mention some QPTs where the ground state energy density is not necessarily singular.

The central theme of the book is quantum phase transitions in transverse field models, (namely, Ising and XY models in a transverse magnetic field) which are paradigmatic models exhibiting zero temperature continuous QPTs, and the recent studies (both experimental and theoretical) of dynamics and information involving these models. In the process, we shall also discuss some related models for the sake of completeness clearly indicating the relevance of those models in the present context.

To the best of our knowledge, the one-dimensional version of the transverse Ising model (TIM) first appeared in the context of the exact solution of the two-dimensional nearest-neighbor ferromagnetic (NN FM) classical Ising model; the row-to-row transfer matrix of the two-dimensional model can be mapped to a transverse Ising chain in some limit [482]. The exact solution of this one-dimensional version of the model soon followed [426]. Shortly thereafter, the model was invoked to mimic the order-disorder transitions in Potassium Dihydrogen Phosphate (KDP) ferroelectrics [211]. Our book will attempt to highlight the aspects of the TIMs for which these models and their variants continue to be enormously useful, even more than fifty years after their first appearance, in understanding QPTs, non-equilibrium dynamics of quantum critical systems, and connections between QPTs, dynamics and quantum information, and finally, in possible experimental and theoretical realizations of quantum annealing. Moreover, experimental realizations of these transverse Ising models have opened up new vistas of research.

Before presenting the chapter-wise plan of this book, let us first discuss in what sense it would be useful to the community. The plan of the book is to cover the most recent theoretical as well as experimental studies of QPTs in transverse field models, pointing to the open problems wherever possible. For example, a very recent experimental study of the exotic low-lying spectrum of the transverse Ising systems in a longitudinal field [180] has been discussed in this book at some length mentioning the corresponding theoretical prediction of the same made decades ago. Even when discussing some conventional topics, which have been reviewed elsewhere, we emphasize recent developments and debates; for example, we allude to recent studies of matrix product states and their connection to quantum information and dynamics. The correspondence between QPTs and classical finite-temperature phase transitions (in a model with one added dimension) is well studied for these models, but the possible breakdown of this established scenario in the context of the spin-boson model is relatively less familiar; we include this in the book. Although the novel features associated with random quantum Ising transitions have been reviewed previously, we mention the most generalized model introduced in connection to quantum information theory (more precisely, to the entanglement entropy, to be defined in Section 2.1) and point to the recent debate on the possibility of a generalized c-theorem. Similarly, the long-standing debate concerning the width of the floating phase in the phase diagram of a one-dimensional transverse Ising model with regular frustrations is highlighted. A recent realization of the traverse field Ising model for an eight-qubit chain using tunable Josephson junctions [412] has been discussed at some length. This represents a significant breakthrough because it also permits experimental examination of quantum annealing (adiabatic quantum computation) with unprecedented detail.

The chapters of the book are broadly divided in five parts: the first part provides an introduction to the topics to be discussed within a generic framework, while in parts two and part three we illustrate the generic theories enunciated in the first part using the example of transverse Ising and other related models. In part four we present at length the experimental developments of transverse Ising models; we would like to emphasize that this is the first time that these developments are being placed together within the same book. Part five is dedicated to the studies of quantum annealing (or adiabatic quantum computations).

Let us also mention at the outset that some other models which are closely connected to the transverse field model will be dealt with at some length in the present book. Although the main emphasis is on the transverse Ising and XY models, we also briefly dwell on other one-dimensional exactly solvable models (closely related to the Ising and XY models) for example, the transverse Ising model with a dimerized interaction and field, and also the one-dimensional and the two-dimensional Kitaev models. All these models are exactly solvable via the Jordan-Wigner (JW) transformation which maps spin-1/2's to spinless fermions. In that sense, this book covers the entire gamut of JW solvable models, especially from the viewpoint of quantum information and dynamics. Moreover, Appendix B provides a discussion on the method of bosonization and QPTs in Tomonaga-Luttinger liquids which go beyond JW solvable models. In addition, we have added a section on the one-dimensional ($1D$) p-wave superconducting chain. Here, a long chain with an open boundary condition is known to host zero energy edge Majorana modes; consequently the model is of immense theoretical and experimental relevance because of the possibility of using the Majorana modes as quantum bits which are topologically protected and hence robust against perturbations. Thanks to the JW transformation, this model is also closely related to a transverse XY spin chain and has an identical phase diagram. Dirac Hamiltonians are of great relevance due to their wide range of applicability in understanding the physics of graphene and topological insulators. On the other hand, there have been numerous studies of quantum information and quenching dynamics which exploit the inherent 2×2 nature of these Hamiltonians enabling us arrive at exact analytical results in higher than one dimension. For example, Dirac Hamiltonian in two dimensions represents an ideal marginal situation for the scaling of the quantum fidelity; the semi-Dirac point on the other hand, provides an ideal example of an anisotropic quantum critical point(AQCP).

In the first chapter, we shall briefly present the phenomenology of a QPT and introduce the transverse field models. These discussions are intended to help a beginner to navigate through the more involved topics discussed in subsequent chapters. We shall briefly introduce QPTs and critical exponents. We then introduce the transverse Ising models in one and higher dimensions. This is followed by a discussion of a XY spin chain which is a generalized version of the Ising chain with XY-like interactions. The anisotropic version of the XY spin model has the same symmetry (Z_2) as the TIM and both the models are exactly solvable in one spatial dimension. However, the transverse XY chain exhibits a richer phase diagram with critical, multicritical points and gapless critical lines. Transverse Ising models have been extended to n-component quantum rotor models which are in fact quantum generalizations of classical n-vector models; we also briefly touch upon quantum rotor models which are closely connected to an array of Josephson junctions.

Another useful aspect of the TIMs is their connection to classical Ising models in the sense of the universality class which we briefly mention in the first chapter; we summarize the essential idea here. The zero temperature transition of a d-dimensional TIM with NN FM interactions belongs to the same universality class as the thermal phase transition of a classical Ising model with similar interactions in $(d+1)$-dimensions; this equivalence can be established using a Suzuki-Trotter formalism and through the imaginary time path integral formalism of the quantum model where the additional dimension is the Trotter direction or imaginary time direction. Similarly, starting from the transfer matrix of the two-dimensional Ising model, one can arrive at the quantum Ising chain in a limit which is known as the τ-*continuum limit*. The underlying idea in both cases is that the extreme anisotropy in interactions along different spatial directions does not alter the universality class, i.e., the critical exponents. The quantum-classical correspondence holds even when the interactions in the quantum model are frustrated or random; in this case interactions along d spatial dimensions of the higher-dimensional classical models become frustrated or random as in the original quantum model but the interactions in the Trotter (time) direction remain ferromagnetic and nearest-neighbor. Therefore, one ends up with a classical model with randomness or frustration correlated in the Trotter direction. The quantum-classical correspondence turns out to be useful for several reasons: (i) since classical models are well studied, one can infer some of the critical exponents of the equivalent quantum model beforehand. For example, one can immediately conclude that the upper critical dimension for a short-range interacting quantum Ising model would be three since this is equivalent to the thermal transition of a four-dimensional classical Ising model. (ii) Secondly, this mapping renders quantum Ising models ideal candidates for quantum Monte Carlo studies, and to understand the quantum transitions one has to study a classical Ising model with one additional dimension. Although an equivalent classical model exists for many quantum spin models (though not all), one usually ends up with a classical model with complicated interactions. Therefore, this equivalence is a unique property of TIMs which has been exploited intensively to gain a better understanding of QPTs in random models. In a similar spirit, one can show that the QPT in a quantum rotor model is equivalent to the thermal transition in a classical n-vector model with one additional dimension. However, this traditional notion has been challenged in the context of the spin-boson model that we discuss later (Section 5.3). Although, we shall retain $\hbar$ explicitly in chapter 1, it will be set equal to 1 in subsequent chapters.

In chapter 2, we will discuss some connections between quantum information theoretic measures and QPTs. It is interesting that these quantum information theoretic measures can capture the ground state singularities associated with a QPT. The quantum correlations of a state can be quantified in terms of bipartite entanglements; one such measure is concurrence. We also discuss the generic scaling for the entanglement entropy close to a QCP. Subsequently, we review the notion of quantum fidelity which is the modulus of the overlap of two ground state wave functions with different values of the parameters of the Hamiltonian. Although the fidelity vanishes in the thermodynamic limit, for a finite system it shows a dip at the QCP and hence is an ideal indicator of a QCP. We discuss the concept of fidelity susceptibility valid in the limit when two parameters under consideration are infinitesimally close to each other; this fidelity susceptibility shows a very interesting scaling behavior close to a QCP which can be verified analytically for transverse field spin chains. In the process, we comment on the quantum geometric tensor defined on a multi-dimensional parameter space. Very recently, the fidelity has been studied for a large system (which means that the linear dimension of the system is the largest length scale of the problem) when the difference in the parameters characterizing two ground state wave functions is finite; this is referred to as the fidelity in the thermodynamic limit. A scaling of fidelity has been proposed in this limit also.

When a quantum system is driven across a quantum critical point by changing a parameter of the Hamiltonian following some protocol, defects are generated in the final state. This is due to the diverging relaxation time close to the QCP; no matter how slowly the system is quenched[1] the dynamics fails to be adiabatic. The scaling of the density of defects in the final state is given by the rate of change of the parameter and some of the exponents of the QCP across which the system is driven. What is exciting about this problem is that the defects are generated through a non-equilibrium dynamics but the scaling of the defect density is dictated by the equilibrium quantum critical exponents. This scaling is known as the Kibble–Zurek scaling which is the central theme of our discussion in chapter 3. We discuss in some detail adiabatic perturbation theory in order to arrive at the Kibble–Zurek scaling law; we also discuss the counterpart of this law in the limit when a parameter of the Hamiltonian is suddenly changed by a small amount starting from the QCP. We discuss how the scaling of the defect density following a sudden or adiabatic quench can be related to a generalized fidelity susceptibility.

Part II of the book deals with the static properties of transverse field and related models mentioned above. The possible exact solutions in different limits are discussed at length. In chapter 4, we present some mean field theoretical studies of the transverse Ising and XY models which are useful in higher dimensions where no exact result is available.

The integrability of the transverse Ising and XY chains with nearest-neighbor interactions has possibly attracted the attention of the physicists the most[2]. In Section 5.1, we will see how these spin models can be solved exactly using the JW transformation. The reduced

[1]In this book, we shall use the term "quenching" to denote both sudden and slow changes referring them as "slow quench" and "sudden quench", respectively.

[2]We will discuss later what integrability means; here the expression implies that all the eigenfunctions and energies can be exactly obtained.

Hamiltonian in the Fourier space gets decoupled into 2×2 Hamiltonians; this two-level form eventually turns out to be extremely useful in calculating the defect density following a sweep of the spin chain across a QCP as we shall discuss in chapter 10. Moreover, the ground state takes a direct product form of qubits; this simple form of the ground state wave function is extremely helpful in understanding the behavior and scaling of information theoretic measures close to a QCP which we shall discuss in chapter 12. Finally, we will briefly discuss the connection of various one-dimensional models to conformal field theory and show how the scaling dimensions of different operators can be extracted from the conformal properties of the equivalent action at the QCP. This information turns out to be useful, e.g., for the transverse Ising chain in the presence of a longitudinal field that destroys the integrability of the model.

There are some variants of transverse Ising and XY spin chains which can be exactly solved and show rich phase diagrams (and are being studied extensively), e.g., the transverse XY spin chain with alternating interactions and fields, and a transverse Ising chain with three-spin interactions. The latter model is known to have a matrix product ground state and undergoes a quantum phase transition which has some unconventional properties as explained in Section 1.8. There are also QPTs which cannot be characterized by a local order parameter and the ordered phase is characterized by a topological invariant. In this regard, we discuss Kitaev models in one and two dimensions, p-wave superconducting chain, the Dirac-like Hamiltonians appearing in Graphene and topological insulators; we also present a discussion on the energy spectrum of the Bernevig-Hughes-Zhang (BHZ) Hamiltonian in a ribbon geometry. The Kitaev model, on a honeycomb lattice, in particular, is one of the very few models which are exactly solvable in two dimensions; the solution employs a mapping of spin$-1/2$'s to Majorana fermions through a JW transformation. Hence the model has been widely used to understand non-equilibrium dynamics of quantum critical systems as well as in quantum information studies which we shall refer to in subsequent sections. We shall introduce the Kitaev model, the appropriate JW transformation and the phase diagram of the model in Section 6.4.

It is well known that the presence of disorder or randomness in interactions or fields deeply influences the phase transition occurring in a classical system, often wiping it out completely. A modified Harris criterion points to a stronger dominance of randomness in the case of a zero temperature quantum transition. Although the quantum versions of classical Ising and n-vector spin glasses have been studied in the last four decades and their quantum counterparts were introduced in the early eighties, the experimental results for $LiHoF_4$ and its disordered version $LiHo_xY_{1-x}F_4$ which are ideal realizations of TIMs with long-range dipolar interactions led to a recent upsurge in exploring the QPT in quantum Ising spin-glasses which are briefly mentioned in chapter 7. The most exciting features associated with low-dimensional random quantum critical systems are the prominence of Griffiths-McCoy (GM) singular regions close to the QCP and the activated quantum dynamical scaling right at the QCP. We shall argue that these off-critical singularities are more prominent in transverse Ising models than in the rotor models due to the Ising symmetry in the former. These singular regions arise due to locally ordered large 'rare' clusters, which can be viewed as a giant spin. If the spins are Ising-like, this giant spin can flip only through the barrier tunneling which is an activated process thereby leading to prominent GM regions. These issues and the contrast with the $O(n)$ symmetric quantum rotor models will be discussed in Section 7. 3 where we allude to the effect of a random longitudinal field on the quantum Ising transitions. Experimental signatures of this GM phase are also discussed later. The role of these GM singularities in the quantum information theoretic measures and dynamics of disordered spin chains will be discussed in appropriate sections.

In chapter 8, we shall introduce a version of the classical Ising model with competing interactions in which in addition to the NN FM interactions along all the spatial directions, there is a next-nearest-neighbor antiferromagnetic interactions along a particular direction, called the axial direction. This model is known as the axially anisotropic next-nearest-neighbor Ising (ANNNI) model which is the simplest model with non-trivial frustration and exhibits a rich phase diagram that has been studied for the last three decades. We focus on the bosonization study of the equivalent quantum model in one dimension. We show that different numerical studies and the bosonization studies contradict each other and whether a floating phase of finite width exists in the phase diagram of the one-dimensional transverse ANNNI is not clearly established till today. To make a connection with bosonization studies, we present the main ideas of bosonization and its applications to one-dimensional spin systems in Appendix B. In this context, we refer to the quantum rotor models with ANNNI-like frustrations and mention theoretical and experimental studies of the quantum Lifshitz point which appears in the phase diagram of these rotor models.

In chapter 9, we illustrate the generic scaling behavior of quantum information theoretic measures enunciated in chapter 3 for transverse field and other models introduced in chapter 6. While the entanglement is a measure of the correlation based on the separability of two subsystems of the composite system, the quantum discord is based on the measurement on one of the subsystems. Both the concurrence and quantum discord show distinctive behaviors close to the QCP of a one-dimensional transverse XY spin model and interesting scaling relations which incorporate the information about the universality of the associated QPT. We elaborate on these scaling relations for transverse field spin models. Similar studies are presented for for the entanglement entropy and fidelity. Moreover, one finds surprising results for the fidelity susceptibility close to a multicritical point. The discussion here also point towards the close connection between the fidelity susceptibility and the geometric phase. Finally, we comment on the decoherence of a qubit (spin-1/2) or a central spin coupled to an environment which is conveniently chosen to be a transverse Ising/XY spin chain. Due to the interaction between the qubit and the environment, the initial state (chosen to be the ground state) of the spin chain evolves with two different Hamiltonians and the corresponding Loschmidt echo is measured. The echo shows a sharp dip close to the QCP and shows a collapse and revival there which can be taken to be an indicator of quantum criticality. The sharp dip in the echo at the same time indicates a complete loss of coherence of the qubit which reduces from the initial pure state to a mixed state. The connection between the static fidelity and the dynamic Loschmidt echo is also mentioned. We have illustrated the role of marginality in the scaling of fidelity using the example of $1D$ and two-dimensional ($2D$) Dirac Hamiltonian in Section 9.7, while in Section 9.8, we present a special case where fidelity susceptibility can be used to detect the QCP by application of a twist in a situation where the conventional approach fails.

In chapter 10, we study in detail many aspects of the Kibble–Zurek scaling for the quenching dynamics of quantum systems across quantum critical points or lines, using the integrability of the transverse field spin chains and the Landau-Zener (LZ) transition formula for the non-adiabatic transition probability. We indicate how to calculate the defect density following a quench across the critical points for the transverse XY spin chain. When the system is quenched across a multicritical point (MCP) or a gapless critical line of the transverse XY spin chain or an extended gapless region of the Kitaev model, the traditional Kibble–Zurek scaling is non-trivially modified that we review at some length. Interesting results are obtained for non-monotonic variations of parameters and also when the spin chain is coupled to a bath. The effect of randomness in the interactions on the quenching is also discussed to indicate the role of GM singular regions (discussed in chapter 8) in modifying the Kibble–Zurek scaling relations. We also discuss about recent studies of Kibble–Zurek mechanism in space. It is natural to seek an optimized rate of quenching that minimizes defects in the final state within a fixed time interval ($-T$ to T). This knowledge would be extremely useful for the adiabatic evolution of a quantum state; related studies are also discussed in this chapter.

In chapter 11, we go beyond the Kibble–Zurek scaling and address different questions: like what happens when a parameter of the Hamiltonian is changed suddenly or locally; it so happens that in that case, one finds an interesting time evolution of the correlation function following the quench which can be visualized within the framework of a semiclassical theory. We also discuss how does topology influence the quenching dynamics taking the examples of edge Majorana of a superconducting chain and the edge state of a topological insulator.

In chapter 12, we embark on establishing the connection between the non-equilibrium quantum dynamics and quantum information discussed in Chapters 2 and 9, respectively. As mentioned above, a sweep across a QCP generates defects in the final state which in turn generate non-zero quantum correlations; interestingly the scalings of the concurrence, negativity, entanglement entropy and other measures of entanglement are also dictated by the scaling of the defect density at least for transverse field models. Remarkably, the time evolution of the entanglement entropy following a quench of an integrable model is oscillatory in time that can be interpreted in terms of the Loschmidt echo.