Chapter 1

Introduction

The aim of study of many body systems is to understand its different types of phases and the transitions between these phases [1–7]. The phase transitions are thus investigated extensively in different systems for last several decades. A phase transition occurs between two states of a system with different symmetries as the temperature or some other parameter is varied. Below the critical parameter, a symmetry of the system is broken whereas the same is preserved above that critical parameter [3–5]. In general, the phase transitions are characterized by an order parameter which becomes zero above the critical point whereas it has a non-zero value below the point. These phase transitions are classified by different orders. The order of a transition can be defined by observing the nature of change of the order parameter close to the critical point as the system is tuned with a parameter. The transition is first order if the order parameter jumps discontinuously from a non-zero value to zero at the critical point. In the similar fashion, it becomes second order if the order parameter changes continuously from a non-zero value to zero with the tuning parameter. The phase transitions that are observed in our everyday life occur at finite temperature and those are called thermal or classical phase transitions driven by thermal fluctuations. The ice-water transition is a very well known example of a first order classical transition. On the other hand, the transition between the ferromagnetic and paramagnetic phases of a magnetic system is of second order. There is also a other class of phase transitions, the so-called quantum phase transitions (QPTs), that occur at zero temperature when a non-thermal parameter of the quantum many body Hamiltonian drives the system from one phase to another [4–7]. In this thesis our main focus will be on studying the continuous QPTs only.
Chapter 1

1.1 Quantum phase transitions

This thesis can be divided into two general parts. In first part, we will focus on studying some quantum information theoretic measures for quantum spin models in the context of characterizing QPTs involving both equilibrium and non-equilibrium situations. In second part of the thesis we discuss two problems related to the quenching dynamics of quantum states. The first problem deals with the dynamics of a Majorana edge state in a $p$-wave superconducting chain following sudden and slow changes of a parameter of the Hamiltonian across quantum critical points (QCPs). The second one is a study of quantum annealing of Sherrington-Kirkpatrick (SK) spin glass model with the tuning of both transverse and longitudinal fields. In the next section, we shall briefly discuss the behaviors of equilibrium QPTs.

1.1 Quantum phase transitions

A quantum phase transition is a zero temperature transition of a quantum many body system driven by a non-commuting term of the quantum Hamiltonian [4-8]. This non-commutativity actually introduces the quantum fluctuation that causes transitions at zero temperature in contrast to the thermal fluctuation in classical phase transitions. As the system is at zero temperature it will prefer to stay in the ground state for different values of the parameters. In two sides of a transition point the structures of the ground state wavefunctions are qualitatively different. The different phases of the system separated by the phase boundaries can be obtained by varying the parameters of the Hamiltonian.

We shall now discuss about some measurable quantities which show singular behavior at the QCP and the nature of these singularities is dictated by the critical exponents. These critical exponents actually characterize a QCP. At a QCP, the ground state energy of the system is a non-analytic function of a non-thermal parameter. An avoided level-crossing between the ground state and first excited state energies occurs for second order transitions, whereas actually the energy levels cross at first order transition point [5]. At a second order transition point, the energy gap $\Delta_\lambda$ between the ground state and first excited state vanishes for a infinite size system. For a quantum system with the Hamiltonian $H(\lambda) = H_0 + \lambda H_1$ where $H_0$ and $H_1$ do not commute, $\Delta_\lambda$ vanishes with the parameter $\lambda$ as it approaches $\lambda_c$:

$$\Delta_\lambda \propto |\lambda - \lambda_c|^\nu z, \quad (1.1)$$

where $\lambda_c$ is the critical point and $\nu$ and $z$ are the critical exponents associated with it. $\nu$ and $z$ are the correlation length and dynamical exponents respectively. In a continuous phase transition, the system has two length scales: one is the length of system and other is called correlation length $\xi$. The correlation length is a measure of length over which
the system is spatially correlated. The correlation length governs the exponential decay of the equal time two-point correlation in the ground state as a function of distance. The equal time correlation function of the order parameter \( O \) is defined as

\[
G(r) = \langle O(0, t)O(r, t) \rangle - \langle O(0, t) \rangle \langle O(r, t) \rangle \propto \frac{e^{-r/\xi}}{r^{d-2+\eta}},
\]

(1.2)

where \( d \) is the dimensionality of space and \( \eta \) denotes the Fisher exponent associated with the critical point. This function determines the spatial correlation between two order parameters at two different points separated by a distance \( r \) and it contains important information about a phase transition. The correlation length diverges with the critical exponent \( \nu \) as the system approaches to the critical point

\[
\xi \propto |\lambda - \lambda_c|^{-\nu}.
\]

(1.3)

The correlation function then depends only on the power law part (see Eq. 1.2) which does not carry any characteristic length. In addition to equal time correlations in space there are analogous equal space correlations in time that define a time scale \( \xi_\tau \). Similar to \( \xi \), close to the critical point the correlation time \( \xi_\tau \) diverges as

\[
\xi_\tau \sim \Delta^{-1}_\chi \propto \xi^z \propto |\lambda - \lambda_c|^{-\nu z}.
\]

(1.4)

As mentioned before, \( z \) is the dynamical exponent. This exponent does not come in the critical analysis of thermal phase transitions of classical systems because they have no intrinsic dynamics. One can see from the above equation that in contrast of classical phase transitions, space and time are interconnected to each other for QPTs. Also these characteristic length and time scales are in general different for \( z \neq 1 \). This property of QPT makes it an interesting area of research. We now define an another important critical exponent that determines how the order parameter becomes zero as the system crosses the QCP from the symmetry broken phase. The order parameter characterizing a QPT is given by

\[
\mathcal{O} \propto (\lambda_c - \lambda)^2 \text{ for } \lambda < \lambda_c \\
= 0 \text{ for } \lambda \geq \lambda_c.
\]

(1.5)

We now define some more quantities which also diverge as the critical point is approached. The specific heat \( C \) for a quantum system at zero temperature is defined as the change in ground state energy due to a small change in the parameter \( \lambda \). Close to the critical point the specific heat diverges as \( C \propto |\lambda - \lambda_c|^{-\alpha} \), where \( \alpha \) is a real number. On the other hand, susceptibility which is directly related to the fluctuations of the order parameter diverges as \( \chi \propto |\lambda - \lambda_c|^{-\gamma} \) close to the critical point. Interestingly, in general all these
critical exponents are not independent, i.e., those are connected by few relations. As an example, the classical continuous phase transitions such as magnetic transitions have seven critical exponents which are connected by four scaling relations resulting only three independent exponents [2, 3]. The set of the critical exponents for a particular phase transition characterize its critical behavior fully. The most fascinating feature of a continuous phase transition is the concept of universality classes. This implies that the values of the critical exponents for different physical systems with same universality class are same. These universality classes are only determined by the symmetries of the Hamiltonian and spatial dimensionality of the system and insensitive to the microscopic details of the Hamiltonian.

The another important property of the phase transitions is the scale invariance of the system at the critical point [2]. The correlation length $\xi$, the only characteristic length scale of a system at the vicinity of critical point, diverges as the critical point is approached. This makes the system invariant under scale transformations near that point. As a result, all the measurable quantities defined above show power law behavior close to the critical point.

In condensed matter physics mean-field theory is a powerful concept which provides exact critical exponents atleast for systems with higher dimensions or systems with infinite range interactions [2, 3]. One can define a upper and a lower critical dimensions for a short-range interacting system according the relevance or irrelevance of order parameter fluctuations. As the spatial dimension of the system increases the fluctuations become less important. Finally above the upper critical dimension $d_u^c$, the critical exponents of the system are identical with the predicted values from the mean-field theory. Whereas below the lower critical dimension $d_l^c$, fluctuations become so strong that they completely destroy the ordered phase, i.e, there is no phase transition. For example, $d_u^c$ of the classical Ising model is 4 and $d_l^c = 1$. Thus interestingly the critical behavior of a classical Ising model with $d \geq 4$ is same as obtained from mean-field theory of the model.

Although we here consider phase transitions at zero temperature only, for the sake of completeness we must discuss the effect of finite temperature on QPTs. At a finite temperature there are two types of fluctuations, i.e., quantum and classical fluctuations in a quantum system. Therefore there exists an interplay between these two types of fluctuations and finally the nature of transitions is determined by the fluctuation of larger strength. Let us assume the system is at temperature $T$ and introduce the characteristic frequency $\omega_c$ associated with the relaxation time $\xi_T$. As discussed above, the energy corresponding to the frequency $\omega_c$ vanishes as

$$\hbar \omega_c \propto |\lambda - \lambda_c|^{\nu_z},$$

(1.6)
Figure 1.1: Schematic of two possible phase diagrams close to a quantum critical point. Fig. (a) represents the case where a non-vanishing order parameter exists only at $T = 0$, for example, the one-dimensional transverse field Ising model (TFIM) with $\lambda$ defining as the transverse field. The other case is shown in Fig. (b) representing that order can exist even at finite temperature, for example, the two-dimensional TFIM. The solid curve in Fig. (b) corresponds to the phase boundary between the ordered and disordered phases. The phase transitions of such systems are determined by the classical fluctuations except at $T = 0$ where quantum phase transition occurs at $\lambda = \lambda_c$.

when the system approaches to the critical point. Quantum fluctuations will be important if the above energy scale in Eq. (1.6) is larger than the thermal energy $k_B T$. In the opposite case the phase transition is indeed determined by the thermal fluctuations and that can be described with classical picture.

At the finite temperature, we can then get a phase diagram of a system in the $T - \lambda$ plane. There are two types of phase diagrams of the quantum systems depending upon the existence of thermal phase transitions in those systems [5, 7]. The phase diagram of the systems which have ordered state only at $T = 0$ has been shown in Fig. 1.1(a). As an example, the transverse field Ising model (TFIM) in one dimension has phase transition only at $T_c = 0$ with $\lambda = \lambda_c$. Therefore, this case can not be realized in a real experiment performed at finite temperature. Irrespective of that, one can divide the phase diagram in Fig. 1.1(a) in three distinct regions depending upon whether the behavior is determined by thermal or quantum fluctuations. In thermally disordered region, the symmetry of the system is preserved due to the thermal fluctuations whereas in quantum disordered state, the physics is dominated by quantum fluctuations. On the other hand, the quantum critical region is dictated by both types of fluctuations. In the second case, the systems undergo through phase transitions even at the finite temperature resulting a phase diagram which has been shown in Fig. 1.1(b). The two-dimensional TFIM is an example of such system which has ordered state at the finite temperature. There is an extra finite temperature transition line in Fig. 1.1(b) compare to the previous case which separate thermally ordered and disordered phases; the transition is dominated by the
thermal fluctuations. This leads to make a comment that the quantum phase transitions occur only at zero temperature \[5\]. In contrary, very recently we find the remarkable result that the crossover between classical and quantum fluctuation dominated critical behaviors for the SK spin glass \[9\] in transverse field \[4, 7\] occurs at a non-vanishing temperature \[10\]. In supporting our result, we give a argument, that as the energy landscape of SK spin glass is highly rugged, at low temperature and high transverse field, only the quantum fluctuations are effective to cross the high and narrow energy barriers to reach the paramagnetic state and thus the critical behavior there is determined by the quantum fluctuations \[10\].

Although, in experiments, one can not attain zero temperature but can predict the presence of QPTs at zero temperature. In last three decades many possibilities for the experimental demonstrations of QPTs have been studied. The cuprate superconductors are ideal examples to exhibit QPTs between a Mott insulating phase and a \(d\)-wave superconducting phase. There are some other examples of systems like \(\text{La}_2\text{CuO}_4\), \(\text{LiHoF}_4\) and the heavy fermion \(\text{CeCu}_6-\chi\text{Au}_\chi\) which show phase transitions at zero temperature with tuning parameter as the transverse field or the concentration \(\chi\) of a component of the materials. Theoretically the transverse field Ising model is perhaps the simplest quantum spin model which shows QPT at zero temperature. The systems \(\text{LiHoF}_4\) and its disordered version \(\text{LiHo}_\chi\text{Y}_{1-\chi}\text{F}_4\) are good candidates for realizations of TFIM with exhibiting QPTs \[11\].

In the next section we briefly discuss the zero temperature phase diagram of a one-dimensional transverse field XY model. After that, in the next two sections we take another two spin models and provide their exact solutions with their zero temperature critical behaviors.

### 1.1.1 One-dimensional transverse field XY model

In this section we review the critical behavior of a one-dimensional XY model in a transverse field. This model is exactly solvable and furthermore, has a rich phase diagram consisting of critical and multicritical points and gapless lines which makes the system and hence has been investigated extensively \[12–16\].

The Hamiltonian of the transverse field XY model in a one-dimensional lattice \[12–14\] with \(N\) spins is given by

\[
H = - \sum_{n=1}^{N} \left( J_x \sigma_n^x \sigma_{n+1}^x + J_y \sigma_n^y \sigma_{n+1}^y + h \sigma_n^z \right),
\]

where \(\sigma_n^a\)'s (with \(a = x, y, z\)) are usual Pauli matrices. \(J_x\) and \(J_y\) are ferromagnetic interactions between neighboring spins in the \(x\) and \(y\) directions respectively, with \(h\) denoting as the transverse field in \(z\) direction. In this case, the quantity \(J_x - J_y\) indeed
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Figure 1.2: The phase diagram of a one-dimensional transverse field XY model at zero temperature. The vertical blue lines, $h = \pm (J_x + J_y)$ represent two Ising critical lines which separate the ferromagnetic phase from the paramagnetic one, whereas the horizontal line with red color ($J_x = J_y$, $|h| < J_x + J_y$) denotes the phase transition between two long-ordered phases FM$_x$ and FM$_y$, with ferromagnetic ordering in the $x$ and $y$ directions respectively. $P_1$ and $P_2$ are two multicritical points where the Ising critical lines and the anisotropic critical line meet to each other.

measures the anisotropy of interactions in xy plane. For $J_x = J_y$, the Eq. (1.7) describes a Hamiltonian of the isotropic XY model in the transverse field [12]. On the other hand, with $J_y = 0$ the above model reduces to a one-dimensional transverse field Ising model [17]. The above Hamiltonian (1.7) can be expressed as a quadratic form in terms of fermionic operators following the celebrated Jordan-Wigner (JW) transformation [12–14, 17–22] from spin to fermion operators. We leave the details of this transformation for the next subsection. Then using the Fourier and Bogoliubov transformations, the energy spectrum of the Hamiltonian (1.7) can be written as

$$\varepsilon_k = 2(\hbar^2 + J_x^2 + J_y^2 + 2h(J_x + J_y) \cos k + 2J_xJ_y \cos 2k)^{1/2}. \quad (1.8)$$

The phase diagram of the above model is shown in Fig. 1.2. The energy gap, $2\varepsilon_k$, of the system vanishes at $h = \pm (J_x + J_y)$ for $k = \pi$ and 0 respectively. This signals the phase transitions from paramagnetic phase to ferromagnetically ordered phase at $h = \pm (J_x + J_y)$. It is straightforward to determine the correlation length exponent ($\nu$) and the dynamical exponent ($z$) for this model. Considering $k = \pi$ in Eq. (1.7), we get $\varepsilon_k \propto (h - (J_x + J_y))$; it turns out that $\nu z = 1$. On the other hand, by fixing the system at
h = J_x + J_z we obtain ε_k ∼ k with redefining (k−π) as k. From these two observations, we find \( \nu = z = 1 \) for this phase transition which are also the critical exponents associated to the phase transition in a one-dimensional TFIM. So this transition belongs to the universality class of the one-dimensional TFIM and therefore called “Ising transition”. As indicated in the phase diagram, the system has ferromagnetic order in the range \(|h| < J_x + J_y\), of the parameter space and this ferromagnetic region is further divided by FM_x and FM_y phases depending upon whether the long-range order is in x or in the y direction. The line \( J_x = J_y \) represents the phase boundary between the FM_x and FM_y phases and the related transition is called “anisotropic transition”. On this line the energy gap vanishes at a specific value of the wave-vector \( k = \cos^{-1}(-h/2J_x) \). The Ising transition lines and the anisotropic transition line meet at the two points denoted by \( P_1 \) and \( P_2 \) in the Fig. 1.2, are called multicritical points (MCPs). It is easy to find out that the energy gap vanishes as \( \varepsilon_k \sim k^2 \), when the system is fixed at these MCPs. Since in this case also \( \nu z = 1 \), we get \( z = 2 \) and \( \nu = 1/2 \) associated to the MCPs.

### 1.1.2 One-dimensional three-spin interacting transverse Ising model: exact solution

In the following section, we consider a one-dimensional three-spin interacting Ising system in presence of a transverse field for studying its different phases separated by quantum critical lines \([23, 24]\). It has a rich phase diagram with different critical points that have distinct critical exponents. We here discuss two different methods for exactly solving the model: the first one is applied when the system is homogeneous and the second one is a more general method which can be applied even when the system is inhomogeneous.

The Hamiltonian of the three-spin interacting Ising model in the site dependent transverse field \( h(n) \) consisting of \( N \) spins is given by

\[
H = -\frac{1}{2} \sum_{n=1}^{N} \left[ \sigma_n^z (h(n) + J_3(n)\sigma_{n-1}^x \sigma_{n+1}^x) + J_x(n)\sigma_n^x \sigma_{n+1}^x \right],
\]

(1.9)

where \( \sigma_n^x \) and \( \sigma_n^z \) are the usual Pauli spin matrices at each site \( n \), \( J_3(n) \) is the site dependent three-spin coupling strength of the spin at site \( n \) with the spins at sites \( n-1 \) and \( n-2 \) and \( J_x(n) \) is the site dependent coupling constant of the nearest neighbor ferromagnetic interaction in x direction. We impose periodic boundary condition \( \sigma_{n+N}^x = \sigma_n^x \) in this model. The Hamiltonian in Eq. (1.9) reduces to the celebrated transverse Ising model in one dimension \([17]\) when \( J_3(n) = 0 \) for each \( n \). Although the 3-spin interacting term in the Hamiltonian (1.9) makes it appear difficult to solve, the above Hamiltonian can be diagonalized using the standard JW transformation \([12–14, 17–22]\). This transformation reduces all the quartic terms of the Hamiltonian into quadratic in terms of the spinless fermions. Also by a duality transformation (dual spins are located
at the centres of the bonds of the original lattice) the system with the Hamiltonian in Eq. (1.9) can be reduced to the one-dimensional quantum XY model in a transverse field \([14, 23]\), which also has been discussed in the previous section.

We now introduce two operators \(\sigma_n^+ = (\sigma_n^x + i\sigma_n^y)/2\) and \(\sigma_n^- = (\sigma_n^x - i\sigma_n^y)/2\) which are called spin raising and lowering operators respectively. They act on the spin states as \(\sigma^+ \downarrow = \uparrow\) and \(\sigma^- \uparrow = \downarrow\). Using these operators the Hamiltonian (1.9) takes the form

\[
H = -\frac{1}{2} \sum_{n=1}^{N} \left[ h(n) \sigma_n^z + J_3(n) \sigma_n^z (\sigma_{n-1}^+ \sigma_{n+1}^- + \sigma_{n-1}^- \sigma_{n+1}^+ + \sigma_{n-1}^+ \sigma_{n+1}^- + \sigma_{n-1}^- \sigma_{n+1}^+) \right] + J_x(n) (\sigma_n^+ \sigma_{n+1}^+ + \sigma_n^- \sigma_{n+1}^- + \sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+) \right].
\]

(1.10)

It is important to note that the spin raising and lowering operators satisfy a complicated commutation relations, i.e., commute on different sites and follow anti-commutation relations on same site:

\[
\begin{align*}
[\sigma_n^+, \sigma_n^-] &= [\sigma_n^+, \sigma_n^+] = [\sigma_n^-, \sigma_n^-] = 0 \text{ for } m \neq n, \\
\{\sigma_n^+, \sigma_n^-\} &= 1, \{\sigma_n^-, \sigma_n^-\} = \{\sigma_n^+, \sigma_n^+\} = 0, \\
\end{align*}
\]

(1.11)

where \([,]\) represents commutation and \(\{,\}\) represents anticommutation relation. These bosonic nature of \(\sigma_n^+\) and \(\sigma_n^-\) for the different sites and fermionic nature for same site make the Hamiltonian (1.10) non-trivial for exact diagonalization. We shall use the JW trick to transform the spins into a set of spinless fermions which satisfy the anti-commutation relations for same and also for the different sites. The JW transformation that maps the spin-1/2’s to spinless fermions is given by

\[
\begin{align*}
\sigma_n^- &= \exp \left[ i\pi \sum_{j=1}^{n-1} c_j^+ c_j \right] c_n = \prod_{j=1}^{n-1} (-\sigma_j^z) c_n, \\
\sigma_n^+ &= \exp \left[ -i\pi \sum_{j=1}^{n-1} c_j^+ c_j \right] c_n = \prod_{j=1}^{n-1} (-\sigma_j^z) c_n, \\
\sigma_n^z &= 2c_n^\dagger c_n - 1.
\end{align*}
\]

(1.12)

where \(c_n^\dagger\) and \(c_n\) are the fermionic creation and annihilation operators respectively with usual anticommutation relations

\[
\{c_m, c_n^\dagger\} = \delta_{mn}, \quad \{c_m, c_n\} = \{c_m^\dagger, c_n^\dagger\} = 0.
\]

One can also define the inverse transformations of the above Eq. (1.12). Here, we represent an down spin as the absence of a \(c\)-particle or a vacuum state \(|\downarrow\rangle \equiv |0\rangle = c|1\rangle\)
and a up spin as a state with a single c-particle $| \uparrow \rangle \equiv | 1 \rangle = c^\dagger | 0 \rangle$. We can observe from Eq. (1.12) that the spin operators are related with the fermionic operators by a phase term, can be called a “Jordan-Wigner string”. This string actually takes care the fermionic nature of the $c$-particles for different sites. In terms of the JW fermions the Hamiltonian in Eq. (1.10) can be expressed as

$$H = -\frac{1}{2} \left[ \sum_{n=1}^{N} h(n)(2c_n^\dagger c_n - 1) - \sum_{n=2}^{N-1} J_3(n)(c_{n+1}^\dagger c_{n-1}^\dagger - c_{n+1}^\dagger c_{n+1} + H.c.) \right. \\
+ \left. J_3(1)(c_2^\dagger c_1^\dagger - c_1^\dagger c_2 + H.c.) \exp(i\pi \sum_{n=1}^{N} c_n^\dagger c_n) \right. \\
+ \left. J_3(N)(c_N^\dagger c_{N-1}^\dagger - c_{N-1}^\dagger c_1 + H.c.) \exp(i\pi \sum_{n=1}^{N} c_n^\dagger c_n) \right. \\
- \sum_{n=1}^{N-1} J_x(n)(c_n^\dagger c_{n+1} + c_n^\dagger c_{n+1}^\dagger + H.c.) + J_x(N)(c_N^\dagger c_1 + c_N^\dagger c_1^\dagger + H.c.) \exp(i\pi \sum_{n=1}^{N} c_n^\dagger c_n) \right], \\
$$

(1.13)

where all the boundary terms contain an exponential factor which is nothing but parity of the system. Parity of the system is defined as

$$P = \exp \left[ i\pi \sum_{n=1}^{N} c_n^\dagger c_n \right] = \prod_{n=1}^{N} (-\sigma_n^z).$$

One can notice from the Hamiltonian in Eq. (1.10) that the off-diagonal terms of it either exchange the state of a pair of anti-parallel spins or flip two upward spins to downward and vice versa. Therefore, the parity of the system $P$ remains unaffected by the dynamics of the Hamiltonian. On the other hand, we can see from Eq. (1.13) that the fermions are created or destroyed in pairs, i.e., the total number of fermions $N_F = \sum_{n=1}^{N} c_n^\dagger c_n$ is not a conserved quantity but the parity of $N_F$ is conserved. So, the Hamiltonian commutes with the parity operator

$$[H, P] = 0.$$ 

(1.14)

This phenomena leads to define our formalism into two disconnected sectors corresponding $P = \pm 1$, where plus and minus signs indicate sectors with even and odd number of fermions respectively. In general, the Hamiltonian can be written as

$$H = \frac{1 + P}{2} H^+ + \frac{1 - P}{2} H^-, \\
$$

(1.15)

where $\frac{1\pm P}{2}$ are the projection operators that maps the system to the states with even or odd number of spinless fermions. $H^\pm$ have the form as Eq. (1.13) with $P = \pm 1$. The boundary terms in Eq. (1.13) are taken care by considering the appropriate boundary
conditions to the spinless fermions for both the sectors: for periodic boundary conditions \( (c_{n+N} = c_n) \), \( P = -1 \) and anti-periodic boundary conditions \( (c_{n+N} = -c_n) \), \( P = 1 \). Finally both the Hamiltonians in Eq. (1.15) can be written in the compact form

\[
H^\pm = -\frac{1}{2} \sum_{n=1}^{N} \left[ \hbar(n)(2\hat{c}_n^\dagger \hat{c}_n - 1) - J_3(n)(\hat{c}_{n+1}^\dagger \hat{c}_{n-1}^\dagger - \hat{c}_{n-1}^\dagger \hat{c}_{n+1} + \text{H.c.}) \right.
\]

\[
- J_x(n)(\hat{c}_n^\dagger \hat{c}_{n+1} + \hat{c}_{n+1}^\dagger \hat{c}_n + \text{H.c.}) \right].
\]

(1.16)

For the homogeneous case \( (\hbar(n) = \hbar, J_3(n) = J_3 \text{ and } J_x(n) = J_x) \) the model in Eq. (1.16) is translationally invariant and so, momentum is a a good quantum number here. Then we can define Fourier transform of the fermion operators as

\[
c_n = \frac{1}{\sqrt{N}} \sum_k c_k e^{ink} \quad \text{and} \quad c_n^\dagger = \frac{1}{\sqrt{N}} \sum_k c_k^\dagger e^{-ink}
\]

(1.17)

where \( k \) is the momentum which takes discrete values given by \( k = 2n\pi/N \) and \( (2n + 1)\pi/N \) for \( P = -1 \) and \( P = 1 \) respectively with \( n = -N/2 \cdots 0, 1 \cdots N/2 - 1 \) assuming \( N \) is even. Using Eq. (1.17) both the Hamiltonians (1.16) can be simplified as

\[
H = -\frac{1}{2} \sum_{k>0} \left[ 2(\hbar + J_x \cos k - J_3 \cos 2k)(c_k^\dagger c_k + c_{-k}^\dagger c_{-k}) \right.
\]

\[
+ 2i(J_x \sin k - J_3 \sin 2k)(c_k^\dagger c_{-k}^\dagger + c_k c_{-k}) - \hbar \right],
\]

(1.18)

with the appropriate choice of \( k \) modes and considering both positive and negative modes such that the summation is taken over only for \( k > 0 \). The Hamiltonian in Eq. (1.18) decouples as a direct sum of independent terms for each \( k, H = \oplus_{k>0} H_k \), where \( H_k \) is a \( 2 \times 2 \) matrix that is written in a basis \( |0\rangle \) (with 0 \( c \)-fermions) and \( |k, -k\rangle = (-c_k^\dagger c_{-k}^\dagger |0\rangle) \), and has a form

\[
H_k = \begin{pmatrix}
\hbar + J_x \cos k - J_3 \cos 2k & J_x \sin k - J_3 \sin 2k \\
J_x \sin k - J_3 \sin 2k & -(\hbar + J_x \cos k - J_3 \cos 2k)
\end{pmatrix}.
\]

(1.19)

Since the Hamiltonian (1.18) is quadratic in terms of \( c \) fermions, one can diagonalize it using Bogoliubov transformation defined as

\[
c_k = \cos(\frac{\theta_k}{2})b_k + i \sin(\frac{\theta_k}{2})b_{-k}^\dagger,
\]

\[
c_{-k} = \cos(\frac{\theta_k}{2})b_{-k} - i \sin(\frac{\theta_k}{2})b_k^\dagger
\]

(1.20)

where \( b_k \)'s are Bogoliubov fermionic operators and \( \theta_k \) is defined as

\[
\tan \theta_k = \frac{J_x \sin k - J_3 \sin 2k}{\hbar + J_x \cos k - J_3 \cos 2k}.
\]

(1.21)
After Bogoliubov transformation, the diagonalized Hamiltonian can now be written as

$$H = \sum_k \varepsilon_k (b_k^\dagger b_k - \frac{1}{2})$$

(1.22)

with the corresponding eigen energy for the $k$-th mode as

$$\varepsilon_k = (h^2 + J_3^2 + J_x^2 + 2hJ_x \cos k - 2hJ_3 \cos 2k - 2J_x J_3 \cos k)^{1/2}. \quad (1.23)$$

The Hamiltonian in Eq. (1.22) represents a system of non-interacting fermions $b_k$ which are called quasiparticles. To excite a quasiparticle mode $b_k$, the system requires $\varepsilon_k$ amount of energy. The ground state $|\Psi_0\rangle$ of the model is one without any quasiparticles, i.e., the vacuum state of $b_k$ fermions

$$b_k|\Psi_0\rangle = 0, \quad \forall k. \quad (1.24)$$

It is now convenient to express $|\Psi_0\rangle$ in terms of the $c$-fermions. In this form $|\Psi_0\rangle$ is given by

$$|\Psi_0\rangle = \prod_{k>0} (b_k b_{-k}|0\rangle), \quad (1.25)$$

where $|0\rangle$ is the vacuum state of $c$-fermions satisfying $c_k|0\rangle = 0$ for each $k$. Eq. (1.25) actually represents the ground state of the system since application of annihilation operator $b_k$ on it gives in fact zero. Now considering the inverse transformations of Eq. (1.20) and imposing the normalization condition $\langle \Psi_0 | \Psi_0 \rangle = 1$ we obtain

$$|\Psi_0\rangle = \prod_{k>0} \left( \cos \left( \frac{\theta_k}{2} \right) + i \sin \left( \frac{\theta_k}{2} \right) c_+^\dagger_{-k} \right) |0\rangle. \quad (1.26)$$

We now consider QPTs in the model. To get QCPs of the system, we have to find out the mode $k_0$ at which the low energy excitation gap becomes minimum [14]. One can obtain $k_0$ considering a condition given by

$$\frac{\partial \varepsilon_k}{\partial k} \bigg|_{k=k_0} = 0. \quad (1.27)$$

Due to the symmetric nature of the energy spectrum (see Eq. (1.23)) as a function $k$, we always get two minimum energy gaps at $\pm k_0$. The solutions of $k_0$ for different parameter values are given by

$$\cos k_0 = \alpha, \quad \text{for } |\alpha| < 1 \quad \text{and } k_0 = \pi \text{ or } 0, \quad \text{for } |\alpha| > 1$$

where $\alpha = \frac{(h - J_3)J_x}{4hJ_3}$. \quad (1.27)
Figure 1.3: Phase diagram of the three-spin interacting transverse Ising model at zero temperature. The point A corresponds to one of the MCPs. The phase boundaries are marked by the three different lines as shown in the label. The boundary between the commensurate and incommensurate regions is also shown in the plot.

The phase diagram of the model for $J_3 = -1$ is shown in Fig. 1.3. It can be seen from the phase diagram of the model that the upper paramagnetic region is further divided according the different values of the ordering wave vector $k_0$. For $|\alpha| < 1$ the values of $k_0$, defined in Eq. (1.27), are incommensurate with the lattice. On the other hand, the wave vector $k_0$ for $|\alpha| > 1$ can not be defined with cos function but can take two values $k_0 = 0$ or $\pi$ which are commensurate with the lattice. The boundary between these two regions as shown in Fig. 1.3 is defined by an equation

$$h = \frac{J_x}{4 - J_x}.$$ 

The energy gap $\Delta_g = 2\varepsilon_k$ vanishes at $k = k_0$ for certain parameter values which are called QCPs. Now, from Eq.(1.23) one can easily verify that the low energy excitation gap vanishes on the critical lines $h = J_3 + J_x$ and $h = J_3 - J_x$ for the wave vectors $k = \pi$ and 0, respectively. These two lines are the critical lines separating two phases, the ferromagnetically ordered phase and the paramagnetic phase. The long-range order in the ferromagnetic phase is present only for a weak transverse field lying in the range $J_3 - J_x < h < J_3 + J_x$. There is also another phase transition at $h = -J_3$ between three-spin dominated phase and quantum paramagnetic phase. This phase transition is analogous to the anisotropic phase transition seen in the one-dimensional transverse XY model (see section 1.1.1). The ordering wave vector $k_0$ in this case is parameter
dependent and is given by
\[ \cos k_0 = \frac{J_x(h - J_3)}{4hJ_3}. \] (1.28)

On the critical line \( h = -J_3 \), the incommensurate wave vector \( k_0 \) takes a value such that
\[ \cos k_0 = \frac{J_x}{2hJ_3}, \]
describing the anisotropic transition can not occur for \( J_3 < J_x/2 \).

The two critical lines \( h = J_3 + J_x \) and \( h = -J_3 \) meet at a point, called MCP which also exists in the one-dimensional transverse field XY model (see section 1.1.1). Another MCP occurs at the intersection of \( h = -J_3 \) and \( h = J_3 - J_x \). The energy spectrum of the system at the critical points vanishes as \( \varepsilon_k \sim k^z \) where \( z \) is the dynamical exponent as defined in section 1.1. The determination of the critical exponents associated with different QCPs is very straightforward for this system. Considering \( k_0 = \pi \) the spectrum in Eq. (1.23) reduces to
\[ \varepsilon_k \propto (h - (J_3 + J_x)) \] (1.29)
where \( h = J_3 + J_x \) is a critical line. At the same time, one can fix the system at one of the critical points satisfying the line \( h = J_3 + J_x \) and expanding about \( k_0 = \pi \), \( \varepsilon_k \) is given by
\[ \varepsilon_k \sim |\pi - k|. \] (1.30)

From above two Eqs. (1.29, 1.30), we obtain \( \nu z = 1 \) and \( z = 1 \) which are also the critical exponents for a one dimensional transverse field Ising model. So, this transition is called “Ising transition”. Similarly one can obtain the critical exponents associated with the MCP. Interestingly, at the MCP the spectrum vanishes quadratically in momentum \( k \), i.e., the dynamical exponent \( z \) for this transition is 2 satisfying \( \nu z = 1 \). This makes the system interesting to study the fidelity and Loschmidt echo close to a MCP as discussed in chapter 2 [25]. In the paper [18], authors have evaluated magnetization and correlation functions and found \( \beta = 1/8, \eta = 5/4 \) for Ising transition whereas \( \beta = 1/4, \eta = 3/2 \) associated with the anisotropic transition. As already mentioned, the present model can be mapped to the XY model in transverse field. Therefore the critical exponents associated with the Ising transition and transition at \( h = -J_3 \) of three-spin interacting TFIM must be same as obtained from transverse field XY model.

On the other hand, such homogeneous systems are very rare in nature. One atleast finds some local defects, no matter how pure the material is. The general method adopted to study systems which are not homogeneous is outlined below, which we also use in this thesis (chapter 4). Following Jordan-Wigner transformation, the Hamiltonian in Eq. (1.9) can be described by a quadratic form in terms of spinless fermions \( c_n \) and \( c^\dagger_n \) [12]
\[ H = \sum_{m,n} \left[ c^\dagger_m A_{m,n} c_n + \frac{1}{2}(c^\dagger_m B_{m,n} c^\dagger_n + h.c.) \right]. \] (1.31)

Here, \( A \) is a \( N \times N \) symmetric matrix due to hermicity of \( H \) and \( B \) is a \( N \times N \) anti-
symmetric matrix which follows from the anticommutation rules of \( c_n \)'s. We rewrite the Hamiltonian in Eq. (1.31) in the following form

\[
H = \frac{1}{2} C^\dagger \mathcal{H} C,
\]

(1.32)

where \( C^\dagger = \left( c_1^\dagger, \ldots c_N^\dagger, c_1, \ldots c_N \right) \) and \( \mathcal{H} = \sigma^z \otimes A + i \sigma^y \otimes B \). Here, \( \mathcal{H} \) is a \( 2N \times 2N \) real-symmetric matrix. The elements of \( A \) and \( B \) matrices thus obtained from Eq. (1.16) are given by

\[
A_{m,n} = -\left[ J_x(m) \delta_{n,m+1} + J_x(n) \delta_{m,n+1} \right] - \left[ J_3(m) \delta_{n,m+2} + J_3(n) \delta_{m,n+2} \right] - 2h_m \delta_{m,n},
\]

\[
B_{m,n} = -\left[ J_x(m) \delta_{n,m+1} - J_x(n) \delta_{m,n+1} \right] - \left[ J_3(m) \delta_{n,m+2} - J_3(n) \delta_{m,n+2} \right].
\]

(1.33)

The above Hamiltonian (1.31) can be diagonalized in terms of the normal mode spinless Fermi operators \( \eta_q \) given by the relation [12].

\[
\eta_q = \sum_{n=1}^{N} (u_q(n) c_n + v_q(n) c_n^\dagger),
\]

(1.34)

where \( u_q(n) \) and \( v_q(n) \) are real numbers. Now, we consider a column vector \( \Upsilon^\dagger = \left( \eta_1^\dagger, \ldots \eta_N^\dagger, \eta_1, \ldots \eta_N \right) \) satisfying \( C = U \Upsilon \), where

\[
U = \begin{pmatrix}
    u & v \\
    u & v
\end{pmatrix},
\]

(1.35)

where \( u \) and \( v \) are \( N \times N \) real matrices with the elements given in Eq. (1.34). This leads to write the Hamiltonian (1.32) in the diagonal form

\[
H = \frac{1}{2} \Upsilon^\dagger U^\dagger \mathcal{H} U \Upsilon = \frac{1}{2} \Upsilon^\dagger D \Upsilon,
\]

(1.36)

where \( D \) is a \( 2N \times 2N \) diagonal matrix. The eigenvalues of \( \mathcal{H} \) come in pairs \( \pm \Lambda_q \) (where \( \Lambda_q > 0 \) and \( q = 1, 2, \ldots N \)) with eigenvectors that are complex conjugate of each other.

This can be realized by interchanging \( c_n^\dagger \) with the \( c_n \) in \( C \) (see around Eq. (1.32) that changes the sign of \( \mathcal{H} \)). Therefore, we can write the Hamiltonian (1.31) in terms of \( N \) modes only

\[
H = \sum_{q=1}^{N} \Lambda_q \left( \eta_q^\dagger \eta_q - \frac{1}{2} \right).
\]

(1.37)

These \( \Lambda_q \)'s are also given by the solutions of the eigenvalue equations,

\[
(A - B)(A + B) \Phi_q = \Lambda_q^2 \Phi_q
\]

\[
(A + B)(A - B) \Psi_q = \Lambda_q^2 \Psi_q.
\]

(1.38)
It can be shown that the elements of the eigenvectors are related to $u$ and $v$ matrices used to diagonalize the Hamiltonian as follows: $\Phi_q(i) = u_q(i) + v_q(i)$ and $\Psi_q(i) = u_q(i) - v_q(i)$.

### 1.1.3 Kitaev model on a honeycomb lattice: exact solution

In this section, we consider two-dimensional Kitaev model on a honeycomb lattice [20] which can be solved exactly using JW transformation [12]. Although the model is two-dimensional, the special topology of the model actually makes it suitable for JW transformation. This model has rich topological properties [20]. But in this thesis we use mainly the quantum critical properties of the model. We here briefly demonstrate the exact solution of the model [20, 26]. Its critical behaviors will be discussed in chapter 3 where we study Loschmidt echo for this model [27].

The Hamiltonian of the Kitaev model on a honeycomb lattice is given by

$$H = \sum_{j+l=\text{even}} \left( J_1 \sigma_{j,l}^x \sigma_{j+1,l}^x + J_2 \sigma_{j-1,l}^y \sigma_{j,l}^y + J_3 \sigma_{j,l}^z \sigma_{j+l+1}^z \right)$$

(1.39)

where $j$ and $l$ signify the column and row indices respectively of the honeycomb lattice while $J_1$, $J_2$ and $J_3$ are coupling parameters for the three bonds (see Fig. 1.4); and $\sigma_{j,l}^\alpha$, are the Pauli spin matrices with $\alpha (= x, y$ and $z)$, denoting the spin component.

![Figure 1.4: Schematic representation of the Kitaev model on a honeycomb lattice with $\vec{M}_1$ and $\vec{M}_2$ being spanning vectors of the lattice and $J_1$, $J_2$ and $J_3$, the coupling on the three bonds. Sites $a$ and $b$ represent two inequivalent sites of the lattice.](image)

We here assume the parameters $J_1$, $J_2$ and $J_3$ are all positive and confine our analysis on the plane $J_1 + J_2 + J_3 = 4$ without any loss of generality. The most exciting property of this model is that even in two dimensions it can be exactly solved using JW
transformation in terms of Majorana fermions given by

\[ a_{j,l} = \left( \prod_{i=-\infty}^{-1} \sigma_{i,l}^z \right) \sigma_{j,l}^y \text{ for even } j + l, \]

\[ a'_{j,l} = \left( \prod_{i=-\infty}^{-1} \sigma_{i,l}^z \right) \sigma_{j,l}^x \text{ for even } j + l, \]

\[ b_{j,l} = \left( \prod_{i=-\infty}^{-1} \sigma_{i,l}^z \right) \sigma_{j,l}^x \text{ for odd } j + l, \]

\[ b'_{j,l} = \left( \prod_{i=-\infty}^{-1} \sigma_{i,l}^z \right) \sigma_{j,l}^y \text{ for odd } j + l, \] (1.40)

where \( a_{j,l}, a'_{j,l}, b_{j,l} \) and \( b'_{j,l} \) are all Majorana fermion operators. They satisfy the relations

\[ a_{j,l}^\dagger = a_{j,l}, \quad b_{j,l}^\dagger = b_{j,l}, \]

\[ \{a_{j,l}, a_{m,n}\} = \{b_{j,l}, b_{m,n}\} = 2\delta_{j,m} \delta_{l,n}, \]

\[ \{a_{j,l}, b_{m,l}\} = 0. \] (1.41)

Now we shall write the Hamiltonian (1.39) in terms of the above defined Majorana operators. Let us first consider the term containing \( J_1 \).

\[
\sum_{j+l=\text{even}} \sigma_{j,l}^x \sigma_{j+1,l}^x = -i \sum_{j+l=\text{even}} \sigma_{j,l}^y \sigma_{j+1,l}^z \sigma_{j,l}^x \sigma_{j+1,l}^x = -i \sum_{j+l=\text{even}} \left( \prod_{i=-\infty}^{-1} \sigma_{i,l}^z \right) \sigma_{j,l}^y \left( \prod_{m=-\infty}^{j} \sigma_{m,l}^z \right) \sigma_{j+1,l}^x \\
= -i \sum_{j+l=\text{even}} a_{j,l} b_{j+1,l} = i \sum_{j+l=\text{even}} b_{j+1,l} a_{j,l}.
\]

Similarly we can calculate all other terms of the Hamiltonian (1.39) and then it can be re-written as

\[
H = i \sum_{j+l=\text{even}} \left[ J_1 b_{j+1,l} a_{j,l} + J_2 b_{j-1,l} a_{j,l} + J_3 (ib'_{j+1,l} a'_{j,l}) b_{j+1,l} a_{j,l} \right]. \] (1.42)

One can now change the lattice site indices \((j, l)\) of honeycomb lattice to a two-dimensional vector \(\vec{n}\), where \(\vec{n} = \sqrt{3} n_1 + \left( \frac{\sqrt{3}}{2} \hat{i} + \frac{3}{2} \hat{j} \right) n_2\) which labels the midpoints of the vertical bonds of the honeycomb lattice. Here \(n_1\) and \(n_2\) take all integer values so that the vectors \(\vec{n}\) form a triangular lattice. The Majorana fermions \(b_{\vec{n}}\) and \(a_{\vec{n}}\) are placed at the top and bottom sites respectively of the bond labeled by \(\vec{n}\). The whole lattice is spanned by the vectors \(\vec{M}_1 = \frac{\sqrt{3}}{2} \hat{i} - \frac{3}{2} \hat{j}\) and \(\vec{M}_2 = \frac{\sqrt{3}}{2} \hat{i} + \frac{3}{2} \hat{j}\), see Fig. (1.4).
Using the two-dimensional vectors, the Hamiltonian (1.42) can be expressed as

\[
H = i \sum_{\vec{n}} \left( J_1 b_{\vec{n}} a_{\vec{n} - \vec{M}_1} + J_2 b_{\vec{n}} a_{\vec{n} + \vec{M}_2} + J_3 D_{\vec{n}} b_{\vec{n}} a_{\vec{n}} \right),
\]

(1.43)

where \(D_{\vec{n}} = i b_{\vec{n}} a_{\vec{n}}^t\). It seems from Eq. (1.43) that the Hamiltonian cannot be solved exactly because of the quartic nature of the zz interaction in terms of Majorana fermions. But for this model the Hamiltonian becomes quadratic due to the conserved quantities [20, 26, 28]. The \(D_{\vec{n}}\) operators in Eq. (1.43) have eigenvalues \(\pm 1\) independently for each \(\vec{n}\) and commute with each other and also with \(H\) which makes the Kitaev model exactly solvable. Since \(D_{\vec{n}}\) is a constant of motion one can use one of the eigenvalues \(\pm 1\) for each \(\vec{n}\) in the Hamiltonian. The ground state of the model corresponds to \(D_{\vec{n}} = 1 \forall \vec{n}\). With \(D_{\vec{n}} = 1\), we can easily diagonalize the Hamiltonian (1.43) quadratic in Majorana fermions.

The Fourier transform of the Majorana operators can be defined as

\[
a_{\vec{n}} = \sqrt{\frac{4}{N}} \sum_{\vec{k}} \left( a_{\vec{k}} e^{i\vec{k} \cdot \vec{n}} + a_{\vec{k}}^t e^{-i\vec{k} \cdot \vec{n}} \right),
\]

\[
b_{\vec{n}} = \sqrt{\frac{4}{N}} \sum_{\vec{k}} \left( b_{\vec{k}} e^{i\vec{k} \cdot \vec{n}} + b_{\vec{k}}^t e^{-i\vec{k} \cdot \vec{n}} \right).
\]

(1.44)

The \(a_{\vec{k}}\)'s and \(b_{\vec{k}}\)'s are Dirac fermions which follow the fermionic anti-commutation relations \(\{a_{\vec{k}}, a_{\vec{k'}}^t\} = \delta_{\vec{k}, \vec{k'}}, \{a_{\vec{k}}, a_{\vec{k'}}\} = 0\) and similarly for \(b_{\vec{k}}\) and \(b_{\vec{k}}^t\). Here, \(N\) is the total number of sites and \(N/2\) is the number of unit cells. In the above sum given in Eq. (1.44), \(\vec{k}\) is extended over half of the Brillouin zone of the hexagonal lattice due to Majorana nature of the fermions. We recall that the full Brillouin zone on the reciprocal lattice represents a rhombus with vertices \((k_x, k_y) = (\pm 2\pi\sqrt{3}, 0)\) and \((0, \pm 2\pi/3)\). In the momentum space the Hamiltonian (1.43) takes the form

\[
H = \sum_{\vec{k}} \left( \begin{pmatrix} a^t_{\vec{k}} & b^t_{\vec{k}} \end{pmatrix} H_{\vec{k}} \begin{pmatrix} a_{\vec{k}} \\ b_{\vec{k}} \end{pmatrix} \right),
\]

(1.45)

where the reduced \(2 \times 2\) Hamiltonian \(H_{\vec{k}}\) can be expressed in terms of Pauli matrices as

\[
H_{\vec{k}} = \alpha_{\vec{k}} \sigma^1 + \beta_{\vec{k}} \sigma^2,
\]

where \(\alpha_{\vec{k}} = 2[J_1 \sin(\vec{k} \cdot \vec{M}_1) - J_2 \sin(\vec{k} \cdot \vec{M}_2)]\),

and \(\beta_{\vec{k}} = 2[J_3 + J_1 \cos(\vec{k} \cdot \vec{M}_1) + J_2 \cos(\vec{k} \cdot \vec{M}_2)]\).

(1.46)

By solving \(2 \times 2\) eigenvalue problem for \(H_{\vec{k}}\) we obtain the eigenvalues

\[
E_{\vec{k}}^\pm = \pm \varepsilon_{\vec{k}} \quad \text{with} \quad \varepsilon_{\vec{k}} = \sqrt{\alpha_{\vec{k}}^2 + \beta_{\vec{k}}^2}.
\]

(1.47)
The unitary matrix $U_\mathbf{k}$ that diagonalize the $2 \times 2$ matrix $H_\mathbf{k}$ for each $\mathbf{k}$ is given by

$$U_\mathbf{k} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -e^{i\theta_\mathbf{k}} & e^{i\theta_\mathbf{k}} \end{pmatrix},$$

(1.48)

where

$$e^{i\theta_\mathbf{k}} = \frac{\alpha_\mathbf{k} + i\beta_\mathbf{k}}{\sqrt{\alpha_\mathbf{k}^2 + \beta_\mathbf{k}^2}}.$$

Now, we can re-write the Hamiltonian (1.45) in the diagonalized form

$$H = \sum_\mathbf{k} \left( a_\mathbf{k}^\dagger b_\mathbf{k}^\dagger \right) U_\mathbf{k} U_\mathbf{k}^\dagger H_\mathbf{k} U_\mathbf{k} U_\mathbf{k}^\dagger \left( a_\mathbf{k} b_\mathbf{k} \right) = \sum_\mathbf{k} \left[ -\varepsilon_\mathbf{k} A_\mathbf{k}^\dagger A_\mathbf{k} + \varepsilon_\mathbf{k} B_\mathbf{k}^\dagger B_\mathbf{k} \right],$$

(1.49)

where the $A_\mathbf{k}$’s and $B_\mathbf{k}$’s are Bogoliubov fermionic operators defined as

$$A_\mathbf{k} = \frac{1}{\sqrt{2}} \left[ a_\mathbf{k} - e^{-i\theta_\mathbf{k}} b_\mathbf{k} \right], \quad B_\mathbf{k} = \frac{1}{\sqrt{2}} \left[ a_\mathbf{k} + e^{-i\theta_\mathbf{k}} b_\mathbf{k} \right].$$

(1.50)

We are now interested to obtain the ground state of the model in Eq. (1.43). Firstly, we find from Eq. (1.49) that the ground state must be annihilated by the $A_\mathbf{k}^\dagger$ operators and we therefore define a state

$$|S_\mathbf{k}\rangle = A_\mathbf{k}^\dagger |\Phi\rangle = \frac{1}{\sqrt{2}} \left( a_\mathbf{k}^\dagger - e^{i\theta_\mathbf{k}} b_\mathbf{k}^\dagger \right) |\Phi\rangle,$$

(1.51)

where $|\Phi\rangle$ is the vacuum state for $a_\mathbf{k}, a_\mathbf{k}', b_\mathbf{k}$ and $b_\mathbf{k}'$ operators. Secondly, since the ground state of the model corresponds $D_{\mathbf{n}} = i b_{\mathbf{n}} a_{\mathbf{n}}^\dagger = 1$ for each $\mathbf{n}$, there will be an extra term in the ground state. Using two Majorana operators $a_\mathbf{n}$ and $b_\mathbf{n}$, we can define a Dirac fermion operator $c_\mathbf{n} = \frac{1}{2} (a_\mathbf{n}^\dagger - i b_\mathbf{n})$ for each $\mathbf{n}$. Then the ground state is an eigenstate of $c_\mathbf{n}^\dagger c_\mathbf{n} = (1/2)(1 + D_{\mathbf{n}})$ with eigenvalue 1 for all $\mathbf{n}$. It implies that the ground state must be annihilated by $c_\mathbf{n}^\dagger$ operators. We take Fourier transform of $c_\mathbf{n}^\dagger$ using Eq. (1.44) and find that the ground state is annihilated by both $c_{\mathbf{k}}^\dagger = (1/2)(a_{\mathbf{k}}^\dagger + i b_{\mathbf{k}}^\dagger)$ and $c_{\mathbf{k}} = (1/2)(a_{\mathbf{k}} + i b_{\mathbf{k}}')$ operators for each $\mathbf{k}$. The corresponding normalized state therefore can be expressed as

$$|T_{\mathbf{k}}\rangle = \frac{1}{\sqrt{2}} \left( a_{\mathbf{k}}^\dagger + i b_{\mathbf{k}}^\dagger \right) |\Phi\rangle.$$

(1.52)

Hence the complete ground state of the Hamiltonian in Eq. (1.43) can be written in the product form [28]

$$|\varphi\rangle = \prod_\mathbf{k} \left[ \frac{1}{2} \left( a_{\mathbf{k}}^\dagger - e^{i\theta_\mathbf{k}} b_{\mathbf{k}}^\dagger \right) \left( a_{\mathbf{k}} + i b_{\mathbf{k}}' \right) \right] |\Phi\rangle,$$

(1.53)
where $\vec{k}$ runs over half of the Brillouin zone of the hexagonal lattice.

1.2 Quantum information theoretic measures: indicator of a QCP

In the section 1.1, we provide a brief discussion on QPTs and show exact solutions of the three-spin interacting TFIM and the two-dimensional Kitaev model on a honeycomb lattice with their quantum critical properties. In addition, we also discuss the critical behaviors of the XY model in the transverse field. The studies on QPTs and their critical behaviors have been useful in connecting various fields like quantum information theory, quantum computation and condensed matter to each other. In recent years, a plethora of studies are being carried out which attempt to bridge a connection between quantum phase transition and quantum information theory (for a review see [7, 29–31]). For example, information theoretic measures like entanglement [32], quantum fidelity [33–38], decoherence [39–42] and quantum discord [43, 44] etc., are being studied close to the QCP. These measures not only capture the singularities associated with the QCP but also show interesting scaling behavior close to that point attracting lots of attention of the scientific community towards it. This approach to quantum phase transitions is advantageous in respect of traditional methods like Landau-Ginzburg theory [3], because here we do not need any knowledge about the order parameter and symmetry-breaking of the system. In this thesis, we will be focusing on investigation of some of the quantum information theoretic measures like fidelity, fidelity susceptibility, Loschmidt echo and entanglement entropy for quantum spin systems [25, 27, 45].

1.2.1 Quantum fidelity

In this section, we briefly discuss the concept of quantum ground state fidelity and its connection with quantum critical phenomena [35, 36]. Quantum fidelity is defined as the overlap of two ground state wavefunctions at two different parameter values of a quantum Hamiltonian. Since fidelity describes the sensitivity to the dissimilarity between the states, it is related to the measure of loss of information encoded in quantum states. So, this is a very important measure in the context of quantum information theory which also successfully detects all the QCPs of a quantum many body system. In two sides of the transition point the structures of the ground state wavefunctions are qualitatively different. Therefore the fidelity of two ground states which are very close to each other in the parameter space shows a significant drop at a QCP for a finite size system ($N$). At the same time, in the thermodynamic limit $N \to \infty$, two ground states are always orthogonal to each other even if they are separated by a very small amount in parameter space. As a result, the fidelity vanishes for any parameter value of the Hamiltonian even
though one can anticipate a sharper drop in fidelity close to a QCP. This phenomena has been realized in various quantum many body systems and is known as the Anderson orthogonality catastrophe [46].

Let us consider a general Hamiltonian of $d$-dimensional quantum many body system [7, 36]

$$H(\lambda) = H_0 + \lambda H_I,$$

(1.54)

where $H_I$ is the driving term that produces quantum fluctuations in the system and $\lambda$ denotes its strength. The eigenvalue equation for the system is given by $H(\lambda)|\psi_n(\lambda)\rangle = E_n|\psi_n(\lambda)\rangle$, where $n = 0, 1, 2 \cdots$ and $|\psi_n(\lambda)\rangle$ forms a complete basis set in the Hilbert space. Then the ground state fidelity between two ground states corresponding to the parameter values $\lambda$ and $\lambda + \delta$ is defined as

$$F(\lambda, \delta) = |\langle \psi_0(\lambda) | \psi_0(\lambda + \delta) \rangle|.$$

(1.55)

In the limit of $\delta \to 0$, one can expand $|\psi_0(\lambda + \delta)\rangle$ in term of $|\psi_0(\lambda)\rangle$ using the celebrated Taylor expansion technique and the overlap is given as

$$\langle \psi_0(\lambda) | \psi_0(\lambda + \delta) \rangle = 1 + \delta \langle \psi_0(\lambda) | \frac{\partial}{\partial \lambda} | \psi_0(\lambda) \rangle + \frac{\delta^2}{2} \langle \psi_0(\lambda) | \frac{\partial^2}{\partial \lambda^2} | \psi_0(\lambda) \rangle + \cdots.$$  

(1.56)

Now following a trivial step the absolute value of the overlap, i.e., the fidelity is calculated as

$$F(\lambda, \delta) = 1 - \frac{1}{2} \delta^2 L^d \chi_F(\lambda) + \cdots,$$

(1.57)

where linear term in $\delta$ becomes zero due to the normalization condition of the wavefunction and $L$ is the linear dimension of the system with $N = L^d$. $\chi_F$ represents the fidelity susceptibility (FS) of the ground state [7, 36, 47],

$$\chi_F(\lambda) = \frac{1}{L^d} \left[ \langle \frac{\partial}{\partial \lambda} \psi_0 \bigg| \frac{\partial}{\partial \lambda} \psi_0 \rangle - \langle \frac{\partial}{\partial \lambda} \psi_0 \bigg| \psi_0 \rangle \langle \psi_0 \bigg| \frac{\partial}{\partial \lambda} \psi_0 \rangle \right].$$

(1.58)

In case the ground state wavefunction is characterized by a large number of parameters, $\chi_F$ is calculated using metric tensor [36] which will not be discussed in this thesis.

The most relevant term in Eq. (1.57) in determining the fidelity is the coefficient of $\delta^2$, i.e., the FS. It actually measures the rate at which the fidelity changes in the limit when the two parameters are close to each other. Using Eq. (1.57) and considering $\delta^2 L^d \chi_F(\lambda) \ll 1$, the FS can be obtained as

$$\chi_F(\lambda) \equiv \lim_{\delta \to 0} \frac{1}{L^d} \frac{-2 \ln F}{\delta^2} = -\frac{1}{L^d} \frac{\partial^2 F}{\partial \delta^2}.$$  

(1.59)

One can observe that fidelity itself depends on $\delta$, but $\chi_F$ depends only on $\lambda$ and insensitive to $\delta$. As the fidelity shows a dip at a QCP, $\chi_F$ shows a large peak at that point (see
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Eq. (1.59)). Thus $\chi_F$ is also able to detect the ground state singularities associated with the QPTs without making reference to an order parameter.

We here review the method by which the scaling of $\chi_F$ can be calculated [36, 48–50]. The fidelity susceptibility $\chi_F = \bar{\chi}_F / L^d$ can be defined in terms of correlation function,

$$\bar{\chi}_F = \sum_r \int \bar{\tau} G(r, \bar{\tau}) d\bar{\tau}, \quad (1.60)$$

where the ground state correlation function $G(r, \bar{\tau}) = \langle V(r, \bar{\tau})V(0,0) \rangle - \langle V(r, \bar{\tau}) \rangle \langle V(0,0) \rangle$, $H_I = \sum_r V(r,0)$ and $\bar{\tau}$ being the imaginary time. Close to a critical point the scaling transformation can be defined as $r' = ar$, $\bar{\tau}' = a^{z}\bar{\tau}$ and $V(r') = a^{-\Delta_v}V(r)$ where $\Delta_v$ is the scaling dimension of $V(r)$ and $z$ is the dynamical exponent as defined before. Under this above scaling transformation $\chi_F$ is given by

$$\bar{\chi}_F = \frac{1}{a^{d+2z-2\Delta_v}} \frac{\chi_F'}{L^d}. \quad (1.61)$$

Close to a critical point correlation length diverges, so there is only one length scale in the system which is the system size. This leads to the scaling of $\chi_F$ as

$$\chi_F \sim L^{\frac{d}{\nu} - d}, \quad (1.62)$$

where $\Delta_v = d + z - 1/\nu$. Whereas away from the QCP ($L >> |\lambda - \lambda_c|^\nu$) the scaling of $\chi_F$ is found to be

$$\chi_F \sim |\lambda - \lambda_c|^{\nu d - 2}, \quad (1.63)$$

with $\nu d < 2$. For $\nu d > 2$, contributions from high energy modes to the FS can not be ignored. However, it has been shown that for some models with $\nu d > 2$, the FS can be used to determine the critical point provided one uses twisted boundary conditions [51]. On the other hand, in the marginal case $\nu d = 2$, $\chi_F$ shows logarithmic scaling with $L$ and $\lambda$ [52].

The scaling of $\chi_F$ can also be established using the concept of finite size scaling [7]. In this case we have to choose the appropriate length scale of the problem i.e., either the correlation length $\xi$ or $L$. The scaling relations are generally determined by the shortest length scale in the problem. It can be observed from Eq. (1.57) that the term $L^d \delta^2 \chi_F$ must be dimensionless. For a system close to a QCP ($L \ll \xi$), the parameter $\delta$ scales as $\delta \sim L^{-1/\nu}$ and now considering $L^d \delta^2 \chi_F \sim L^0$, we obtain the scaling form $\chi_F \sim L^{2/\nu - d}$. In a similar fashion away from the QCP ($\xi \ll L$), one finds $\delta \sim \xi^{-1/\nu}$ and $L^d \sim \xi^d$, which give the scaling $\chi_F \sim \xi^{2/\nu - d} \sim \lambda^{\nu d - 2}$.
1.2.2  Loschmidt echo

In recent years, there have been numerous studies on decoherence (or loss of phase information) in a quantum critical system which is closely connected to the Loschmidt echo (LE) to be discussed in this section \([16, 27, 53–60]\); understanding decoherence is essential for successful achievement of the quantum computation \([29]\). The decoherence is a process through which the quantum-classical transition occurs by a reduction from a pure state to a mixed state \([39–41]\). The notion of the LE was actually introduced in connection to the quantum to classical transition in quantum chaos \([61–66]\) and now extended to various other systems undergoing a QPT like Ising model \([53]\), Bose-Einstein condensate \([67, 68]\) and Dicke model \([69]\). It has also been studied experimentally using NMR experiments \([56, 70, 71]\). The LE, the dynamical counterpart of the fidelity, is defined as the square of overlap of the two wave functions \(\langle \psi(t) | \psi_0(t) \rangle\) evolving with two different Hamiltonians \(H\) and \(H_0\), respectively, \(i.e.\),

\[
\mathcal{L}(t) = |\langle \psi(t) | \psi_0(t) \rangle|^2.
\] (1.64)

Initially, both the states are prepared in the ground state \(\ket{\psi_0}\) of \(H_0\). This reduces the LE to a simplified form given by

\[
\mathcal{L}(t) = |\langle \psi_0 | e^{-iHt} \psi_0 \rangle|^2.
\] (1.65)

The LE provides information about how small perturbations during an evolution can result to the decoherence of the state of the system, thus being an important quantity for information processing and storage. On the other hand, the LE can also be used to detect the presence of a QCP by showing a sharp dip at the QCP of the Hamiltonian when \(H\) and \(H_0\) are close to each other.

According to Eq. (1.65), the quantification of the LE requires a Hamiltonian \(H\) that makes the evolution of the ground state \(\ket{\psi_0}\) non-trivial. This Hamiltonian \(H\) can be generated considering a central spin model in which a central spin \(S\) is coupled globally to an environmental spin model \(E\) \([53]\). In this regard, we will study here the transition of the central spin \(S\) from a pure state to a mixed one induced by the criticality of the environmental spin system and show that the decay of the LE is best enhanced by the QPT of the surrounding environment (see the chapters 2 and 3). We will provide here a general formalism for calculating the LE considering a three-spin interacting TFIM defined in Eq. (1.9) as an environment \((E)\) that is coupled to a central spin-\(\frac{1}{2}\) (qubit) \(S\). We shall denote the ground state and excited state of the central spin \(S\) by \(\ket{g}\) and \(\ket{e}\).
respectively. The composite Hamiltonian can be written in the form

$$H_T(h, \delta) = -\frac{1}{2} \sum_{n=1}^{N} \left[ h(n)\sigma_n^x + \delta \sigma_n^z \sigma_n^y + J_3(n) \sigma_n^z \sigma_{n-1}^x \sigma_{n+1}^x + J_4(n) \sigma_n^z \sigma_{n+1}^x \right], \quad (1.66)$$

where $\sigma_n^x$ denotes the Pauli matrix of the qubit and $\delta$ is the coupling strength of $S$ to $E$. We shall work in the limit of $\delta \to 0$. In this case we have not considered the system Hamiltonian for the qubit and with the chosen interaction term in the Hamiltonian (1.66) one can show the commutation relation as $[\sigma_n^z, H_T] = 0$ which signify that $\sigma_n^z$ is a constant of motion. As a result the population of the ground and excited states of the qubit do not change with time, i.e., there is no exchange of energy between system and the bath [53, 54]. The above condition ensures that in this case the qubit evolution is purely decoherent.

We consider that the $S$ is initially in a generalized state $|\phi(0)\rangle_s = c_g|g\rangle + c_e|e\rangle$ (with the coefficients satisfying the condition $|c_g|^2 + |c_e|^2 = 1$), and the $E$ is initially in the ground state $|\varphi(0)\rangle_e$. Then the initial composite wavefunction is given by

$$|\psi(0)\rangle = |\phi(0)\rangle_s \otimes |\varphi(0)\rangle_e. \quad (1.67)$$

The evolution of the environmental spin model splits into two branches, given by $|\varphi_g(t)\rangle = \exp(-iH_g t)|\varphi(0)\rangle_e$ and $|\varphi_e(t)\rangle = \exp(-iH_e t)|\varphi(0)\rangle_e$; the evolution of $|\varphi_g(t)\rangle$ is driven by the Hamiltonian $H_g = H_T(h(n), 0) + V_g$ (when the $S$ is in the ground state), whereas $|\varphi_e(t)\rangle$ evolves with $H_e = H_T(h(n), 0) + V_e$, where $V_g = \delta \sum \sigma_n^z$ and $V_e = -\delta \sum \sigma_n^z$ are the effective potentials arising due to the coupling between $S$ and $E$. Therefore, the coupling of a qubit with the transverse field term of the environmental spin chain reduces to only a change in $h(n)$ at each site $n$ by the amount $\delta$ or $-\delta$. The wave function of the composite system at a time $t$ is given by

$$|\psi(t)\rangle = e^{-iH_T(h, \delta)t}|\psi(0)\rangle_s = c_g|g\rangle \otimes e^{-iH_g t}|\varphi(0)\rangle_e + c_e|e\rangle \otimes e^{-iH_e t}|\varphi(0)\rangle_e$$

$$= c_g|g\rangle \otimes |\varphi_g(t)\rangle + c_e|e\rangle \otimes |\varphi_e(t)\rangle. \quad (1.68)$$

Although the initial composite wavefunction in Eq. (1.67) is unentangled, $|\psi(t)\rangle$ is an entangled state between $S$ and $E$. At a general time $t$, the reduced density matrix of the qubit in the $\{|g\rangle, |e\rangle\}$ basis given by

$$\rho_s(t) = \text{Tr}_E|\psi(t)\rangle\langle\psi(t)| = \begin{pmatrix} |c_g|^2 & c_g c_e^* d(t) \\ c_e c_g^* d^*(t) & |c_e|^2 \end{pmatrix}, \quad (1.69)$$

where $d(t) = \langle \varphi_g(t)|\varphi_e(t)\rangle$ is the decoherence factor. During time evolution the diagonal
terms of $\rho_S(t)$ are constant in time, however, the off-diagonal terms evolve with time. Comparing Eq. (1.64) and Eq. (1.69) one can find the relation between $L(t)$ and $d(t)$ given as

$$L(t) = |d(t)|^2 = |\langle \varphi_g(t) | \varphi_e(t) \rangle|^2.$$  

(1.70)

As the value of $L(t)$ decreases from 1 to 0, the effective interaction between $S$ and $E$ increases; $L(t) = 0$ corresponds the maximum entanglement between the qubit and the environment. On the other hand, when $L(t)$ is close to 1 the effective interaction between the qubit and the environment becomes almost zero. Therefore close to a QCP of $E$ at which $L(t)$ takes minimum value, the central spin (qubit) transits from pure state to mixed state due to its maximum entanglement with the environment.

For the homogeneous case ($h(n) = h$, $J_3(n) = J_3$ and $J_x(n) = J_x$), the Hamiltonian in Eq. (1.66) is translationally invariant and so, momentum is a a good quantum number here. Following some mathematical steps with JW and Bogoliubov transformations for Eq. (1.66), we can calculate the exact expression of the LE (see Appendix A for details) which is given by

$$L(t) = \prod_{k>0} L_k = \prod_{k>0} \left[ 1 - \sin^2(2\gamma_k) \sin^2(\varepsilon_k(h + \delta)t) \right],$$  

(1.71)

where $\gamma_k = (\theta^g_k - \theta^e_k)/2$ with $\theta^g_k = \arctan((J_x \sin k - J_3 \sin 2k)/(h - \delta + J_x \cos k - J_3 \cos 2k))$ and $\theta^e_k = \arctan((J_x \sin k - J_3 \sin 2k)/(h + \delta + J_x \cos k - J_3 \cos 2k))$. $\varepsilon_k(h + \delta)$ is the energy spectrum for the transverse field $h + \delta$ as given in Eq. (1.23). We shall use the above expression of the LE for a three-spin interacting TFIM in chapter 2, to study its critical behaviors when the various QCPs are approached with generic paths.

### 1.2.3 Entanglement

The entanglement in quantum many body systems, which is the measure of quantum correlations between the two systems, has become a topic of intensive research interest for last several years [72–83]. These studies lie at the interface of condensed matter physics and quantum information theory. Entanglement is a key ingredient in quantum information processing for sending informations in novel ways [29]. On the other hand, it also characterizes a QPT in a quantum many body system with interesting scaling behaviors close to the QCP which are given in terms of the associated quantum critical exponents [73, 74]. In the last few years several measures of the entanglement have been studied extensively for the quantum many body systems using both the analytical and numerical methods. One of the quantities to measure the entanglement between the two subsystems is the von Neumann entropy [84–87].

A quantum state $|\psi\rangle$ combining two subsystems $A$ and $B$ is entangled if it can not
be written as the tensor product of individual subsystem states $|\psi_A\rangle$ and $|\psi_B\rangle$, i.e.,

$$|\psi\rangle \neq |\psi_A\rangle \otimes |\psi_B\rangle.$$  \hspace{1cm} (1.72)

Consider a bipartite system divided into two subsystems $A$ and $B$ of length $L_A$ and $L_B$ with total length $L = L_A + L_B$. If the whole system is in a quantum pure state $|\psi\rangle$ with density matrix $\rho = |\psi\rangle \langle \psi|$, then the von Neumann entropy $S_A$ of system $A$ with reduced density matrix $\rho_A = \text{Tr}_B(\rho)$ is defined as

$$S_A = -\text{Tr}(\rho_A \ln \rho_A).$$  \hspace{1cm} (1.73)

This is actually the measure of entanglement between these two subsystems which is called entanglement entropy (EE). The EE or $S_A$ increases with increasing quantum correlations (entanglement) between the two subsystems. An unentangled combined state produces zero entanglement entropy. On the other hand, $S_A$ gives a maximum value for a maximally entangled state. The EE exhibits distinct scaling relations at and close to a quantum critical point with the shortest length scale of the system. For a critical spin chain with periodic boundary conditions where the subsystem has two boundary points, the entanglement entropy scales as $S_A \sim \frac{c}{L_A}$, where $c$ is a universal quantity and given by the central charge of the conformal field theory \cite{75, 76, 79, 84}. On the other hand, away from the critical point where the correlation length $\xi \ll L_A$, entanglement entropy is given by $S_A \sim \frac{c}{3} \ln \xi$. The above scaling relations are valid for a one-dimensional homogeneous system. It is found that some modifications are required in the scaling relations of the EE when the system is inhomogeneous. Interestingly, in this case also the scaling relations remain same as the homogeneous case with a changed prefactor $c_{\text{eff}}$ which is called the effective central charge \cite{88--93}.

### 1.3 Dynamics in quantum many body systems

In the section 1.2, we discuss some of the quantum information theoretic measures like the fidelity, the FS, the LE and the EE in the context of quantum phase transitions. Now, we are interested to study the non-equilibrium dynamics of quantum many body systems driven across quantum critical points. In quantum systems an inherent dynamics is always present which is determined by the off-diagonal term of the Hamiltonian. But the explicit time dependence of a parameter of the Hamiltonian provides an extra flavour in the system specially close to a QCP that leads to very interesting non-equilibrium phenomena \cite{94, 95}. A parameter of the Hamiltonian can be varied/quenched suddenly or slowly with time. In recent years, both of the quenches are studied extensively in quantum many body systems within different approaches following interesting findings.
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[96–103]. At the same time, the recent experimental realization of non-equilibrium dynamics on ultra cold atoms trapped in optical lattices [104–106] inspires the theoretical work of quantum quenches in critical systems. Furthermore, the study of quenching dynamics is very important for addressing the questions on the thermalization of quantum systems [107–109].

As discussed above, given the recent interest in the non-equilibrium quenching dynamics of quantum many body systems across quantum critical points (for review articles see [7, 31, 110]), the studies involving quenching dynamics of a topological system [111–113] across a QCP [114–116] have emerged as a rapidly growing field of research. Especially, the quenching dynamics of a topological insulator [117] and the $p$-wave superconducting chain [118–120] have been explored in this connection. We note that the dynamical generation [121], formation and manipulation [122] of edge Majorana states for a driven system have also been studied extensively; the sudden quench of a one-dimensional Majorana chain has also been studied through its topological signature in the entanglement spectrum [123]. We note that very recently the possibility of thermalization of nonlocal topological order has been studied by tracking the time evolution of the string correlations in a spin-1 chain in its Haldane phase following a sudden quench [124]. In the chapter 5, we study the dynamics of a Majorana edge state in a one-dimensional $p$-wave superconducting chain under both sudden [118] and slow quenching [120] of a parameter of the Hamiltonian.

1.3.1 Sudden quenches

A sudden quench in the system can be performed locally or globally. In a global quench, a parameter of the Hamiltonian is changed suddenly at all the sites; whereas local quench is defined as a local change of a parameter of the Hamiltonian. Both of the quenching schemes result to a system which is far from equilibrium. As a result, immediately after the quench the quantum state is not an eigenstate of the final Hamiltonian and hence evolves in time with time evolution dictated by the final Hamiltonian. This produces excitations in the final system. Quenches close to the QCPs are especially important due to the existence of interesting scaling relations of several physical quantities of a system in terms of the scaling exponents which are expected from universality established in the same equilibrium system [49, 125, 126]. For a sudden quench across a QCP, the scaling of the defect density generated in the final state is given in terms of the magnitude of the change of the quenched parameter and the critical exponents [49, 125, 126]. In this connection, dynamical response of different physical quantities, e.g., correlation function [98, 127], Loschmidt echo [27, 53, 54, 57–59, 128], entanglement entropy [129], heat generation [126] etc. are extensively studied following the sudden quenches for several quantum systems.
The chapter provides a study of the LE and the EE for a one-dimensional TFIM following local quenching of the parameters. The details of the calculation of the LE for exactly solvable spin models with homogeneous and also inhomogeneous couplings have been provided in the Appendices A and C.1 respectively. We have already defined the EE in section 1.2.3 considering a general situation. In the non-equilibrium case with sudden quench we have two Hamiltonians, say $H_0$ for time $t < 0$ and $H$ for $t > 0$ with different parameter values. As a consequence the time evolution of the initial density matrix $\rho_A$ is determined by the final Hamiltonian $H$. The evolution of $\rho_A$ is given by

$$\rho_A(t) = e^{-iHt} \rho_A e^{iHt}. \quad (1.74)$$

The evolution of $\rho_A(t)$ is computed using time-dependent correlation matrix and that leads to calculate time-dependent the EE (see Appendix C.1 for details). In recent years, a considerable amount of focus is given to the EE in systems out of equilibrium [100, 130–136]. The experimental demonstration of such non-equilibrium dynamics using optical lattices [106] also contributes to the sudden upsurge in studies related to decoherence and entanglement in out of equilibrium systems. As defined above, one of the ways of generating such a non-equilibrium dynamics is a sudden quench. In global sudden quench, the EE generally shows a linear increase in time $t$ up to some time $t_0$ [129]. On the other hand, in a local quench a parameter of the Hamiltonian is changed locally. For example, the entanglement entropy between two critical subsystems $A$ and $B$ of a homogeneous one-dimensional chain which are disconnected for $t < 0$ and connected at $t = 0$ increases as $S \sim \frac{2}{3} \ln t$ for $t \ll L$ [100, 130, 135]; here the final chain is periodic. On the other hand, if the final chain is open, the factor 2 in the expression of $S$ is not present. Such studies are important in the context of information propagation through a quantum many body system. In this connection the concept of light-cone-like behavior in condensed matter systems has been established in some recent theoretic studies [137, 138]. The characteristic speed of the light-cone provides the maximum allowed speed with which the information can propagate in the quantum system; it is known as the Lieb-Robinson limit [139]. In the case of integrable quantum systems, this speed reduces to the maximum group velocity ($v_{\text{max}}$) of the quasiparticles produced due to the quantum quench (see also the discussion in section 1.3.3). In particular, it has been studied that the revival structure of the LE following a sudden quench, is determined by the quasiparticles moving with the speed $v_{\text{max}}$ [135, 140]. The generalization of the Lieb-Robinson for the non-integrable quantum system also has been shown by Happola et al. [140]. In section 5.1.1 of chapter 5, we discuss the revival of survival probability of an edge Majorana (which is in fact determined through the LE) under a sudden quench in the $p$-wave superconducting chain from the viewpoint of light-cone like propagation.
1.3.2 Adiabatic quenches

We here present the adiabatic or slow quenches in the quantum systems. In this process, a parameter of the Hamiltonian is varied with a finite rate from an initial value to a final value crossing a QCP. In this regard, we study the effect of such quenches on density of defects in the final state. This quantity has universal scaling relation with the quenching rate which are given in terms of the equilibrium critical exponents. For a driven quantum many body system there is two time scales associated with its dynamics. One corresponds the relaxation time which is defined as the inverse of the minimum gap of the system (see section 1.1) and the other is given by the time scale for driving the Hamiltonian. These two characteristic time scales actually determine the dynamics of the system. If the time scale associated with the changing of the Hamiltonian is larger than the relaxation time of the system, the system can follow the changes in the Hamiltonian and it remains in its instantaneous ground state. As the system passes through a critical point, the relaxation time diverges \([2, 3, 5]\) and the system is not able to follow the changes in the Hamiltonian even though the variation is very slow. As a result the dynamics becomes non-adiabatic close to the QCP and produces excitations in the system which leads to non-zero defect density in the final state that the system reaches following the quenching \([7]\). This defect density scales with the rate of quenching which is usually determined by the Kibble-Zurek (KZ) scaling relation given in terms of the rate of quenching and some of the critical exponents associated with the critical point across which the system is driven. The Kibble-Zurek scaling was first proposed for second order classical phase transitions \([141]\) and recently it has been extended to the quantum case \([15, 26, 94, 95, 142-144]\).

Let us consider that the parameter \(\lambda\) of the system is varied linearly with time \(t\) and approaches the critical point \(\lambda_c\). We can assume the linear variation of \(\lambda\) as \(g = \lambda - \lambda_c = t/\tau\) such that the QCP is crossed at time \(t = 0\) with quenching rate \(1/\tau\). As explained above, approaching of the system to the QCP makes its dynamics non-adiabatic. Let \(t'\) is the time where the dynamics of the system transits from adiabatic to non-adiabatic. Then the time scale associated with the variation of the Hamiltonian must be the order of the relaxation time \(\xi\) at \(t'\), i.e.,

\[
\frac{|g|}{g'} = t' = \xi |\nu|.
\]  

As mentioned before the relaxation time close to a QCP diverges as \(\xi \sim |\lambda - \lambda_c|^{-\nu z}\) which allows to write the Eq. (1.75) as

\[
t' \sim (\lambda - \lambda_c)^{-\nu z} |\nu| \sim \left(\frac{t'}{\tau}\right)^{-\nu z}.
\]  

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The above equation results in an expression of $t'$, given by

$$t' \sim \tau^{\frac{1}{\nu z + 1}}.$$ 

(1.77)

As shown in Fig. 1.5, the entire evolution of the system can be divided into three regions by the times $\pm t'$ [7]. For $|t| > t'$, the system is quite away from the QCP and thus it is able to respond to the changes in the Hamiltonian. Therefore, the system remains in the instantaneous ground state of the Hamiltonian in these two time regions. On the other hand, for $-t' < t < t'$ the system becomes unable to follow the changes in the Hamiltonian thereby even at time $+t'$ the state of the system is $\psi(-t')$ which is indeed the state at $-t'$ also. Thus the adiabaticity of the system breaks here that leads to excitations. For a large value of $\tau$, only the low-energy modes are affected by the diabatic evolution, whereas the high-energy modes evolve adiabatically. Using the relations $t' \sim \xi_\tau$ (see Eq. (1.75)), $\xi \sim \xi^{1/2}$ and considering that there is one defect per unit domain size of linear length scale $\xi$, the density of defects $n$ is given by

$$n \sim \frac{1}{\xi^d} \sim \tau^{-\frac{d}{(\nu z + 1)}},$$

(1.78)

where $d$ is the dimensionality of the system. In a spin system one can realize the defects as wrongly oriented spins. The Eq. (1.78) provides an important scaling relation that connects the equilibrium quantum critical exponents to the non-equilibrium dynamics. The scaling relation in Eq. (1.78) gets modified in the case of non-linear quenching [145, 146], quenching along a gapless line [147], quenching across gapless surface [26], quenching through a multicritical point [148] and quenching across anisotropic quantum critical points [149].

Figure 1.5: The entire time evolution of the system is divided in three regions. For $|t| > t'$ the evolution is non-adiabatic whereas for $|t| < t'$, it is adiabatic.
1.3.3 Semiclassical theory of quasiparticles

In this section we will discuss the semiclassical theory of quasiparticles (QPs) created after sudden change of a parameter of the Hamiltonian. When a system at zero temperature is taken away from its ground state by applying some perturbation, the state of the system undergoes a non-equilibrium evolution with respect to the final Hamiltonian. The initial state, which now is an excited state, is a source of QPs corresponding to the final Hamiltonian. Recently, such non-equilibrium dynamics have been studied using a semiclassical picture of QPs generated for global [150, 151] and local quenches [152], where excellent agreement between the numerics and the semiclassical theory were obtained. We now briefly describe this theory of QPs generated which shall be used to explain the various timescales observed in our numerical calculations in chapter 4. For global quenches from the transverse field, \( h = 0 \) to a very small \( h \) value, it can be shown that these QPs are wavepackets of low-lying excitations and discussed in details in Ref. [150]. Due to the conservation of momentum, QPs of a given momentum are always produced in pairs, the group velocity \( v_g(k) = |\partial \varepsilon_k / \partial k| \) of them being equal and opposite to each other. As discussed in Ref. [150], these QPs in the small \( h \) limit can be considered as classical particles (sharply defined QPs) which when crosses a site, simply flips the spin at that site. Though this picture is discussed for a very specific quench (a small quench), it has been verified for stronger quenches and also for quenches in the paramagnetic phase with slight modifications. It is also argued that these QPs are no longer point particles, but are extended objects as the critical point is approached due to large correlation length. In chapter 4, we shall try to explain our numerical results at least qualitatively with this point like picture of QPs for spin chains in the ferromagnetic as well as in the critical region.

1.4 Topology in condensed matter systems

In the section 1.3, we discuss the quenching dynamics in quantum many body systems and its connection with topological order. We here provide a brief introduction to the emergence of topology in condensed matter systems. In that case we have to first know: what is topology? Topology is a branch of mathematics concerned with the geometrical properties of a system which are preserved under small changes in the system. Two systems are topologically equivalent if those can be transformed continuously into each other. It is now a important task to define a quantity for a system which represents the topology of that system. This quantity is called topological invariant which takes integer values and remains fixed under small changes in the system. The topologically distinct systems must have different topological invariant values. For example, in two-dimensional parameter space one can define winding number \( W \) as a measure
of topological invariant which counts the number of times a closed curve winds around the origin in the anticlockwise direction. Clearly winding numbers do not change continuously with some small changes in the system. To change the integer value of \( W \), therefore, the curve must have to pass through the origin where \( W \) is ill-defined.

This concept of topology in mathematics has been used in condensed matter physics to define some special states of matter. In condensed matter physics, two quantum many body systems are topologically equivalent if we can continuously transform their Hamiltonians into each other. Now if we consider this as a definition for topological invariance we can face a problem since then all quantum systems would be topologically equivalent. Therefore we have to apply some constraint in the Hamiltonians of the quantum systems. The drastic change occurs when we consider the systems with an energy gap. We can now say that two gapped quantum systems are topologically equivalent if their Hamiltonians can be continuously transformed into each other without ever closing the energy gap.

In general, for condensed matter physics the different phases of a matter correspond to some broken symmetries. In last few decades, the studies of new states of matter namely topological states [153, 154] which are not associated with the broken symmetries have emerged as a rapidly growing field of research [155–157]. As a result, the distinct topological phases of a topological system can not be defined by the usual local order parameters similar to the magnetic and superconducting systems. As defined above those states of matters are represented by some topological invariants which change discontinuously across the transition. A topological condensed matter system has insulating bulk, i.e., there is a finite gap in spectrum between the ground state and the first excited state at low temperature, with the gapless states at the boundaries. These boundary states actually contribute to electric conduction. The number of these edge states is determined by the non-zero topological invariant which is calculated from the bulk band structure of a system [155]. This is called bulk-boundary correspondence that allows to creat gapless boundary modes due to the non-trivial topology of the insulating bulk [155–157].

In particular, the topological classification of condensed matter states has been first introduced in the study of quantum Hall systems [153, 154]. For such systems only the gapless edge states contribute in quntized Hall conductance. Here, the number of edge states and the quntized Hall conductance are the topological invariants which do not change under smooth deformation of the system parameters and remains constant until the system passes through quantum phase transitions. Another important example of topological system is topological insulators [158–160] which are investigated extensively in last few years with observation of these states in real materials [161–163]. A topological insulator has a finite bulk energy gap between valence and conduction bands, i.e., its bulk is insulator. On the other hand, the surface or edge states for such
systems are gapless which are governed by two-dimensional or one-dimensional Dirac equations respectively. The gapless states of the topological insulators are protected by the time-reversal symmetry of the system [155]. A one-dimensional \( p \)-wave superconductor, introduced by Kitaev [164] is also a topological system that hosts zero energy modes at the two ends of the chain whose number is a topological invariant. These end modes can be represented in terms of the second quantized operators which are Hermitian, i.e., they are real and those modes are called Majorana modes. In two dimensions a spinless \( p_x + ip_y \) superconductor exhibits Majorana edge modes at the core of vortices [165, 166] which has a close resemblance with the chiral modes in quantum Hall effect. In the chapter 5, we consider the dynamics of an edge Majorana mode following quantum quenches in the \( p \)-wave superconducting chain. We therefore provide a brief discussion about the appearance of Majorana fermions in condensed matter systems and the different topological phases of the one-dimensional \( p \)-wave superconductor in next two sections.

1.4.1 Majorana fermions and condensed matter systems

In his 1937 paper [167], Ettore Majorana introduced theoretical concept of real fermions in the context of existence of real solution of Dirac equation which are now known as “Majorana fermions”. The anti-particle of an electrically charged particle is different from the particle due to their opposite charges. The Majorana fermions are their own anti-particles which signify that those are electrically neutral. As a usual fermionic operator \( f \) is complex, it can be splitted to two real operators which are Hermitian

\[
f = \frac{1}{2} (a + ib),
\]

where \( a^\dagger = a \) and \( b^\dagger = b \). \( a \) and \( b \) are two operators corresponding to two Majorana fermions. Therefore one complex fermion provides two Majorana fermions and thus a system with \( N/2 \) fermions can be described by \( N \) Majorana fermions. These Majorana operators satisfy the following relations \( a_j^2 = 1 = b_j^2 = 1 \), \( \{a_j, a_l\} = \{b_j, b_l\} = 2 \delta_{jl} \) and \( \{a_j, b_l\} = 0 \); these imply that to one fermionic site \( j \) there is two Majorana sites or equivalently, a Majorana fermion can viewed as occupying half of a state.

Although Ettore Majorana proposed his idea in the context of high-energy physics, in parallel the condensed matter physicists recently are giving more attention to realize Majorana fermions in a large variety of condensed matter systems [168, 169]. For conventional solids made of electrons, it appears hard to observe Majorana fermions because electrons are charged and therefore different from their antimatter counterparts, i.e., the holes with opposite charges. In second quantized operator language if \( f^\dagger \) represents the creation of an electron then \( f \) creates a hole in the system. But superconductivity, on the other hand, may be an appropriate platform for realization of such exotic Majorana
excitations because it violates charge conservation and as a result quasiparticles in a superconductor are mixtures of electrons and holes [169]. In such materials, electrons form Cooper pairs and one such pair can be added or subtracted from the condensate without significant changes of its properties. As a consequence the electron number and therefore electronic charge are no longer conserved quantities for superconducting systems. In the conventional s-wave superconductors, the overall requirement of antisymmetry of a Cooper pair means that the paired electrons must have opposite spins. The quasiparticles operators for s-wave superconductors then are not Hermitian for any situation. Thus spin of the electrons prevents to emerge Majorana fermions in such superconductors. The above discussion suggests that spinless superconductors are ideal candidates for the emergence of exotic Majorana excitations. The Cooper pairing of two spinless (or spin polarized) electrons requires non-zero relative orbital angular momentum that provides odd parity state resulting $p$-wave superconductor in one dimension [164] and also $p + ip$ superconductor in two dimensions [170]. The one-dimensional spinless $p$-wave superconductor is a topological system which has zero energy edge Majorana modes as midgap excitations that are guaranteed by particle-hole symmetry of the system. The zero energy Majorana modes are indeed mixture of particles and holes in equal measure; one can call these modes as “partiholes” [168]. The superconducting pairing term of such a Hamiltonian actually induces the zero energy excitations in the system. Whereas, for $p + ip$ superconductors zero modes exist in the vortices. These $p$-wave superconductors are referred to as “topological superconductors” which host zero modes. But, in nature there are very few candidates which show $p$-wave superconductivity, e.g., $\text{He}_3$ superfluid phase [171]. On the other hand, it has been proposed that the proximity effect between the surface states of a strong topological insulator and $s$-wave superconductor can generate a two dimensional state strongly resembling a $p$-wave superconductor which can hosts Majorana states at the vortices [172, 173].

Recent experiments have also been able to detect the signature of these Majorana modes in the zero-bias transport properties of nanowires coupled to superconductors [173–177]. Additionally, it has also been demonstrated experimentally that these Majorana modes can be hybridized and be made to appear or disappear by tuning the chemical potential of a similar system across a topological phase transition [178]. There are also some discrepancies in experimental results with the theoretical predictions of Majorana fermions which has been discussed in Ref. [179].

1.4.2 Kitaev chain: Model and topological phases

The topological properties of a $p$-wave spinless superconductor has been studied from different points of views in recent years [121, 180–185]. (For a review see [169]). These studies lie at the interface of condensed matter physics, quantum information processing,
decoherence and quantum computation [186–188]. In this thesis, we shall investigate the
topological properties of the Kitaev chain in the context of quenching of the same system.
This study requires a knowledge of the equilibrium topological properties of the model.
This section provides a brief discussion on the bulk and end properties of the p-wave
superconductor model.

The p-wave superconductor is a one-dimensional fermionic lattice model which consists a
nearest-neighbor hopping amplitude $w$, a superconducting p-wave pairing term $\Delta$
that couples two nearest-neighbor electrons and an on-site chemical potential $\mu$. The
Hamiltonian of such a system of spinless (or spin polarized) fermions with system size $N$ is
given by

$$H = \sum_{j=1}^{N} [-w(f_j^\dag f_{j+1} + f_{j+1}^\dag f_j) + \Delta(f_j f_{j+1} + f_{j+1}^\dag f_j^\dag)] - \sum_{j=1}^{N} \mu(f_j f_j - 1/2), \quad (1.80)$$

where we consider that all these parameters are real and the spacing of the lattice is
chosen to unity for simplicity. The annihilation and creation operators $f_j(f_j^\dag)$ obey the
usual fermionic anticommutation relations $\{f_j, f_l\} = 0$ and $\{f_j, f_l^\dag\} = \delta_{jl}$. The periodic
boundary condition of the lattice ($f_{N+1} = f_1$) makes the Hamiltonian in Eq. (1.80)
translationally invariant and it can be then diagonalized in momentum basis, $f_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} f_j e^{-ikj}$. In the momentum space the Hamiltonian in Eq. (1.80) can be written
in the standard Bogoliubov-de Gennes form

$$H = \sum_{k>0} \left( \begin{array}{cc} f_k^\dag & f_{-k} \\ -f_{-k}^\dag & f_k \end{array} \right) H_k \left( \begin{array}{c} f_k \\ f_{-k}^\dag \end{array} \right),$$

$$H_k = -(2w \cos k + \mu) \tau^z + 2\Delta \sin k \tau^x, \quad (1.81)$$

where $\tau^y$ and $\tau^z$ are Pauli matrices in particle-hole subspace. This leads to a particle-hole
symmetric dispersion given by

$$E_k = \pm \sqrt{(\mu + 2w \cos k)^2 + 4\Delta^2 \sin^2 k}. \quad (1.82)$$

The bulk energy gap ($2E_k$) vanishes at certain values of $\Delta$ and $\mu$ for some specific $k$
modes. The phase diagram of the model with three distinct phases (denoted by I, II and
III) is shown in Fig. 1.6. The weak pairing regime ($|\mu| < 2w$) corresponds topologically
non-trivial phase (phases I and II). On the other hand, for $|\mu| > 2w$ the system forms a
topologically trivial phase (phase III). One observes that $\mu = \pm 2w$ are two quantum
critical lines with critical modes $k_c = \pi$ and $0$ (for which the energy gap vanishes),
respectively, whereas for the critical line $\Delta = 0$ (with $\mu$ lies between $-2w$ and $2w$) with
$k_c = \cos^{-1}(-\mu/2w)$. 

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Symmetries of the model:
The symmetries have a strong influence on topology. In fact discrete symmetries (e.g., particle-hole symmetry, time-reversal symmetry etc.) play important role in classification of different topological systems [189–191]. The particle-hole symmetry is represented by an anti-unitary operator, $P = \tau^x K$, where $K$ is complex conjugation which is an antilinear operator satisfying $P^2 = 1$ [155, 156]. The Hamiltonian $H_k$ in Eq. (1.81) has an intrinsic particle-hole symmetry described by

$$P H_k P^{-1} = -H_{-k}. \quad (1.83)$$

One can easily prove the above relation for the Hamiltonian $H_k$. The minus sign in Eq. (1.83) signify that the spectrum (see Eq. (1.82)) of the system must be symmetric around zero energy. Indeed, Eq. (1.83) follows that if $\psi_k = (u_k, v_k)^T$ is an eigenvector of $H_k$ with energy $E_k$ and momentum $k$ then, $P\psi_k = (v_k^*, u_k^*)^T$ is also an eigenvector of the same Hamiltonian with energy $-E_k$ and momentum $-k$. But these two energy states do not correspond to two distinct quantum states because the Bogoliubov quasiparticles associated with them follow $b_{E_k}^\dagger = b_{-E_k}$. Therefore, creating a quasiparticle at the energy state $E_k$ is same as the creating a hole at $-E_k$. Then for $E_k = 0$, $b_0^\dagger = b_0$, i.e., $b_0$ is its own anti-particle. As mentioned above, these quasiparticles are called Majorana zero modes which are protected by the bulk gap of the system. Although Majorana zero modes do not exist in periodic boundary conditions its prediction can always be done.
from the bulk properties of the system. Another important symmetry of the system is time-reversal symmetry. As our model is spinless the time-reversal symmetry of the system is given by a relation, i.e., $H^*_k = H_k$ for all $k$.

In order to explore the non-trivial topology in the weak pairing phase of the model, we represent the Hamiltonian (1.80) in terms of the two Majorana operators $a_j$ and $b_j$ at each site are defined as

$$f_j = \frac{1}{2} (a_j + ib_j), \quad f_j^\dagger = \frac{1}{2} (a_j - ib_j).$$

(1.84)

As defined in section 1.4.1, these Majorana operators are Hermitian and satisfy the anti-commutation relations $\{a_j, a_l\} = \{b_j, b_l\} = 2\delta_{jl}$ and $\{a_j, b_l\} = 0$; Then the Eq. (1.80) with an open boundary condition can be re-written as

$$H = i \frac{2}{N-1} \sum_{j=1}^{N-1} [(-w + \Delta)a_j b_{j+1} + (w + \Delta)b_j a_{j+1}] - i \frac{2}{N} \sum_{j=1}^{N} \mu a_j b_j.$$

(1.85)

The pictorial representation of various couplings of the Hamiltonian in Eq. (1.85) is shown in Fig. 1.7.

![Figure 1.7: Schematic representation of the Majorana chain with the Hamiltonian as defined in Eq. (1.85) considering a virtual ladder. It may be thought that the middle of each vertical bond here represents a fermionic site $j$ which supports two Majorana fermions $a_j$ and $b_j$ represented by red and blue filled circles respectively with their intra-site interaction $\mu$. In this representation, other two couplings are symbolized by diagonal links.](image-url)

The zero-energy modes of the Hamiltonian in Eq. (1.85) distinguish different phases (I, II and III) in the phase diagram (see Fig. 1.6). Phase I ($\Delta > 0$ and $|\mu| < 2w$) is one of the topological non-trivial phases, due to the presence of two isolated Majorana modes at the two edges of a open and long chain. It can be shown using a special condition i.e,
Figure 1.8: Schematic representation of the Hamiltonian in Eq. (1.85) with different special conditions as defined in the text. (a) $\mu \neq 0$, $w = \Delta = 0$, (b) $\mu = 0$, $w = \Delta$ and (c) $\mu = 0$, $w = -\Delta$. In (a) the pair of Majoranas at each site is connected to each other by the strength $\mu$ resulting a topologically trivial phase. (b) In this regime, there are two isolated Majorana modes $a_1$ and $b_N$ at the left end and right end respectively. (c) This regime also represents a topologically non-trivial with two isolated Majorana modes $b_1$ and $a_N$.

for $\Delta = w$ and $\mu = 0$. This condition reduces the Hamiltonian (1.85) in the form

$$H = iw \sum_{j=1}^{N-1} b_j a_{j+1},$$

(1.86)

which incorporates interaction between Majorana fermions only at adjacent lattice sites (see Fig. 1.8(b)). One can then express the above Hamiltonian in terms of the fermions combining two Majorana fermions at $j$ and $j + 1$ which is given by

$$H = 2w \sum_{j=1}^{N-1} \left( d_j^\dagger d_j - \frac{1}{2} \right),$$

(1.87)

where $d_j = \frac{1}{2}(b_j + ia_{j+1})$. From Eq. (1.87), we can observe that adding a $d_j$ fermion in the chain has cost $2w$ amount of energy. This indicates the existence of a bulk gap in the system which is also consistent with our findings using periodic boundary conditions (see discussion around Eq. (1.82)). On the other hand, as can be seen from Eq. (1.86) that the Majorana operators $a_1$ and $b_N$ do not appear in the Hamiltonian leading to two unpaired zero energy Majorana fermions $a_1$ and $b_N$ at the left and right end of
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the chain, respectively (see Fig. 1.8(b)). These two isolated Majorana fermions can be combined to produce a highly non-local complex fermion, \( f_m = \frac{1}{2} (a_1 + ib_N) \) which is the basic building block of fault-tolerant topological quantum computation [192–196]. This non-local fermion costs zero energy and thus the ground state of the system becomes two fold degenerate with opposite fermionic parity, i.e., if \( |\psi_0\rangle \) is a ground state of the system satisfying \( d_j |\psi_0\rangle = 0 \) for \( j = 1, \ldots, N - 1 \) and \( f_m |\psi_0\rangle = 0 \), then \( |\psi_1\rangle = f_m^\dagger |\psi_0\rangle \) with \( d_j |\psi_1\rangle = 0 \) for \( j = 1, \ldots, N - 1 \) is also a ground state. Similarly, for the phase II (\( \Delta < 0 \) and \( |\mu| < 2w \)) two isolated Majorana modes, \( b_1 \) and \( a_N \), exist at the two ends of the chain as shown in Fig. 1.8(c). Therefore the phase II is also a topologically non-trivial phase with two fold ground state degeneracy. We note that the phases I and II are different with respect to the nature of edge modes in two ends of the chain. While Phase I hosts \( a_1 \) (\( b_N \)) edge Majorana modes at the left (right) of the open and long chain, it is the other way round in Phase II. On the other hand, the Majorana end modes at the critical points are free to propagate through the chain since there is no bulk gap. As a result, they are no longer localized at the ends but become uniformly delocalized throughout the chain. The phase III (\( |\mu| > 2w \)) is topologically trivial with no edge Majorana modes. This can be illustrated considering the special limit \( \Delta = w = 0, \mu \neq 0 \), when all the Majorana fermions are connected pairwise for each fermionic lattice site and consequently there is no isolated edge states (see Fig. 1.8(a)). Introducing the above special limit one can note that adding a \( f_j \) fermion in the system requires a finite energy \( |\mu| \); this confirms that in this limit the system is gapped which also has been found from periodic boundary condition results. We thus find here that the system has very less boundary effects making the phase III as topologically trivial.

Although we define different phases of the system in the context of zero-energy Majorana modes using some special cases it can be shown that those modes persist even if we move from those limiting cases [164]. But then the zero energy Majorana modes can not be simply represented by isolated modes \( a_1 \) (\( b_N \)) and \( b_N \) (\( a_N \)) for phase I and phase II respectively. In this case, the end Majorana modes will not be perfectly localized at the ends of the chain, rather their wavefunctions decay exponentially into bulk of the chain (see Fig. 1.9) with the maximum probability of getting the Majoranas at the edges. The overlap of the wavefunctions gives rise a interaction between these two Majorana end modes and they moves from zero energy with the energy scale \( e^{-N/\xi} \) where \( \xi \) is the superconducting coherence length for this system [164, 169]. As a result, except \( N >> \xi \), the degeneracy between the ground states \( |\psi_0\rangle \) and \( |\psi_1\rangle \) breaks by the same energy scale defined above.

**Topological Invariant:**

The system has a topological invariant through which we can distinguish different phases; this is known as the winding number [197, 198] (see section 1.4). The Hamiltonian in Eq. (1.81) can be defined in the form \( H_k = \vec{d}_k \cdot \vec{\tau} \), where \( \vec{d}_k = (2\Delta \sin k) \hat{y} - (\mu + 2w \cos k) \hat{z} \)
is Anderson pseudospin vector $[199]$ in the $y-z$ plane. We can easily find the angle $\theta_k$ made by the vector $\vec{d}_k$ with respect to $\hat{z}$ axis; that is given by

$$\theta_k = \tan^{-1}\left(\frac{-\mu - 2w \cos k}{2\Delta \sin k}\right).$$

(1.88)

Now, the winding number $W$ that characterizes distinct phases of the model is defined as

$$W = \oint \frac{d\theta_k}{2\pi} = \int_0^{2\pi} \frac{dk}{2\pi} d\theta_k,$$

(1.89)

where the integral is performed around the one-dimensional Brillouin zone. $W$ which takes only integer values defines the number of rotations of the vector $\vec{d}_k$ in the $y-z$ plane around the one-dimensional Brillouin zone. The number of rotations becomes positive if the vector rotates in anticlockwise direction. It can be shown considering few steps that $W$ takes values $-1, 1$ and $0$ in the phases I, II and III, respectively (see Fig. 1.6). This quantity does not change until the system passes through a quantum phase transition for some value of $k$ where $W$ is ill-defined $[185]$. It is now straightforward to find a relation between the bulk invariant $W$ and the number of edge modes $N_a$ ($N_b$) of a ($b$) type Majorana modes at the left end of the open chain. The relation is given by $W = N_b - N_a$ which correctly defines the bulk-edge correspondence as already mentioned in section 1.4.

We can also describe the above discussed distinct phases in the spin-1/2 language. One can easily transform the Hamiltonian (1.85) to a spin-1/2 $XY$ model Hamiltonian with a transverse field by using the JW transformation. The Majorana fermion operators
in terms of the spin-1/2’s can be represented as

\[ a_j = \left( \prod_{n=1}^{j-1} \sigma_n^z \right) \sigma_j^x \]
\[ b_j = \left( \prod_{n=1}^{j-1} \sigma_n^z \right) \sigma_j^y, \] (1.90)

where \( \sigma_j^x \) and \( \sigma_j^y \) are the Pauli spin matrices with x and y spin components. In this case we have considered \( \sigma_j^z = 2f_j^\dagger f_j - 1 = ia_j b_j \). Therefore, in terms of spin operators the Eq. (1.85) takes the form

\[ H = -\sum_{j=1}^{N-1} (J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y) - h \sum_{j=1}^{N} \sigma_j^z, \] (1.91)

where the interaction terms follow the relations \( J_x = (w + \Delta)/2, J_y = (w - \Delta)/2 \) and \( \mu = -2h \). The above Hamiltonian corresponds to a one-dimensional spin model with anisotropic interactions in x and y directions subjected to a transverse magnetic field which already has been discussed in section 1.1.1. So, in the context of spin system Hamiltonian (1.91) phases I and II correspond to ferromagnetically ordered phases with long range order in x and y-directions respectively. Phase III is paramagnetic with no long-range order and zero spontaneous magnetization.

### 1.5 Quantum annealing

So far we discuss the dynamics of quantum systems with non-random interactions and fields in the context of quenching (see section 1.3). Whereas the nomenclature quantum annealing (QA) is usually used to study the dynamics of the disordered systems. In this section, we discuss how QA can play an effective role to find out the ground state of the disordered systems [8, 96, 200–207]. Before discussing the QA we shall briefly review the simulated annealing (SA) technique. Optimization of cost function in a system with \( N \) independent variables often becomes NP-hard, where the search time cannot be bounded by any polynomial in \( N \). Such multivariable optimization problems can be represented by a search problem for the minima in a landscape with the effectiveness of the solution or cost plotted in the y-axis and the solution (or configuration) number plotted in the x-axis. Typically, such cost function landscapes are very rugged and have many local minima with one or degenerate global minima (see Fig. 1.10) in configuration space. So, search algorithms along a valley in such a landscape are not useful, because the system ends up in a local minimum of that valley which is not necessarily a global one. Kirkpatrick et al. [208] and Cerny [209] independently suggested a method called
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1.5. Quantum annealing

Thermal annealing

Quantum annealing

Global minimum

Configuration

(a)

Cost / energy

\[ E(X) \]

Quantum annealing

Global minimum

(b)

\[ \exp(-\Delta E/T) \]

\[ \exp(-w\sqrt{\Delta E}/\Gamma) \]

\[ \Delta E \]

\[ X \]

Figure 1.10: Variation of cost energy with different configurations of a computationally hard problem like in a spin glass. The figure 1(b) is a cartoon for figure 1(a). In classical annealing case, to reach global minima the system has to overcome a large barrier $\Delta E$ of $O(N)$, $N$ being the system size (escape probability $\sim \exp(-\Delta E/T)$ at temperature $T$). In quantum annealing case, system can tunnel through the barrier; if the barrier is narrow (tunneling probability $\sim \exp(-w\sqrt{\Delta E}/\Gamma)$ for tunneling fluctuation field $\Gamma$ and barrier width $w$).

SA to solve such optimization problems. In this process, a stochastic algorithm is chosen with a tunable noise or fluctuation such that as the system gets into a local minimum (with cost $E_i$), the fluctuation permits for acceptance of higher cost value $E (= E_l + \Delta E)$ solutions with a Boltzmann like probability $\exp(-\Delta E/T)$ and the system is allowed to explore full configuration space. The global minimum (ground state; may be degenerate) of the cost function is obtained as the fluctuation is properly tuned (with an annealing schedule) down to zero. Stated more explicitly, in this procedure initially one starts with an arbitrary configuration $C_i$ with cost function $E_i$ and go the configuration $C_f$ with energy $E_f$ following some stochastic rule. If $E_f$ is less than $E_i$ then one always accepts the change, otherwise accepts the change with finite probability $\exp(-\Delta E/T)$, where $\Delta E = E_f - E_i$. So, as the temperature decreases with time ($t$) to zero, there is a finite probability that the system reaches the ground state configuration. The success of reaching the true ground state depends on the annealing schedule $T(t)$: If temperature is reduced too quickly the system may get localized in a local minimum and the obtained configuration is not that of a global minimum. In this regard, Geman and Geman have shown that if annealing schedule is taken as $T(t) \geq N/\ln t$, then the system reaches the ground state eventually [210]. In this schedule a system must reach that with minimum energy, but it may take much longer time. In practice, good annealing results can be obtained through even a faster decrease of temperature.

The SA is quite an useful technique to solve systems with many local minima in configuration space. But this technique does not give satisfactory results for a non-
ergodic system like spin glass [102, 211]. In this systems there are many local minima and the minimum energy configurations are separated by the barrier heights of order of $N$. So, with thermal dynamics at any finite temperature, the full phase space is not covered by the system and the system may get trapped in local minima (for $N \to \infty$). Finite thermal fluctuations are unable to make the system ergodic (in the $N \to \infty$ limit) and the system can not go from one local minima to another. In such situations QA can be a good choice to overcome such effects and produce better results [204, 212–214]. As argued by Ray et al. [200], the quantum tunneling (as indicated in Fig. 1.10) can help getting out of the local minima and approach the optimum state (ground state) if the energy barrier is narrow (and the phases of the turning waves from different walls do not conspire to make the system localized). In QA process one considers a time-dependent Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \Gamma(t)\mathcal{H}_I,$$

(1.92)

where $\mathcal{H}_0$ is the classical time-independent Hamiltonian whose ground state is to be found. Here, $\mathcal{H}'(t) = \Gamma(t)\mathcal{H}_I$ is the tunneling term of the total Hamiltonian $\mathcal{H}$, which is added externally and does not commute with $\mathcal{H}_0$ ($[\mathcal{H}_0, \mathcal{H}_I] \neq 0$). $\Gamma(t)$ is the time-dependent tunneling strength between different classical configurations and plays similar role as temperature in SA. The additional part of the total Hamiltonian actually gives internal dynamics in the system and allows mixing of the different stationary states of $\mathcal{H}_0$. To get the full dynamics of the system we have to solve time-dependent Schordinger equation of the total Hamiltonian

$$i\frac{\partial|\psi(t)\rangle}{\partial t} = \mathcal{H}(t)|\psi(t)\rangle,$$

(1.93)

where $|\psi(t)\rangle$ denotes the instantaneous wave function of the total Hamiltonian $\mathcal{H}$. The term $\mathcal{H}'(t)$ gives the quantum fluctuation in the system and helps the system to traverse different eigenstates (configurations) of the (classical) Hamiltonian $\mathcal{H}_0$ by tunneling through the barriers. Initially the quantum fluctuation term ($\mathcal{H}'$) is kept very large compared to the classical part ($\mathcal{H}_0$) and the dynamics is governed mainly by the fluctuation term. The fluctuation strength tuned by tuning the parameter ($\Gamma(t)$) which decreases adiabatically from high value to zero as time $t \to \infty$. If we take initial state (state at $t = 0$) as the ground state of the total Hamiltonian, then according to adiabatic theorem [215] instantaneous quantum states will be ground states at that parameter values and hence, at the end of the annealing the system is expected to attain the ground state of the classical Hamiltonian with a satisfactory finite probability. This, we can expect even for the disordered frustrated system like the spin glass systems [9].
1.6 Plan of the thesis

In chapter 2, we will study two quantum information theoretic measures like the FS and the LE in the context of characterization of quantum phase transitions. As discussed before, these measures capture the singularities associated with the ground state of the system at the QCP and successfully detect all the QCPs. They also show distinct scaling relations when the system is close to a QCP. We propose a method for calculating the FS and the LE for a generic path and verified our method considering a three-spin interacting TFIM in one dimension with a phase diagram which consists of isolated critical points, MCPs and quasicritical points. We will also discuss how the presence of quasicritical points changes the scaling of the FS when a MCP is approached along different paths. The standard method for such path dependent study require the FS tensor, whereas, our method is simpler to implement for the same study.

In chapter 3, we discuss the effect of gapless phase on the LE considering a central spin model where a two-dimensional Kitaev model on a honeycomb lattice has been chosen as an environment. In this case the central spin or the qubit is coupled globally with the environment. The LE here successfully detects the gapless phase of the Kitaev model on a honeycomb lattice. It is interesting that the LE also can capture the anisotropic nature of the quantum critical points (lying on the boundary between the gapless and gapped phases) through its short time behavior. We confirm this behavior numerically by studying the collapse and revival of the LE when the system is fixed at a QCP. Although we have not discussed our results in the perspective of decoherence, one can easily do that.

In chapter 4, we consider the dynamics of the LE and the EE for one-dimensional TFIM following local quenches of the parameters in the Hamiltonian. We here study the effect of two simultaneous local quenches on the evolution of the LE and the EE for the above mentioned system. In this work, one of the local quenches involves the connection of two spin-1/2 chains at a certain time and the other local quench corresponds to a sudden change in the magnitude of the transverse field at a given site in one of the spin chains. We numerically calculate the dynamics associated with the LE and the EE (see Appendix C) as a result of such double quenches, and discuss various timescales involved in this problem using the picture of QPs generated as a result of such quenches. We perform a detailed analysis of the probability of QPs produced at the two sites and the nature of QPs in various phases and obtain interesting results.

In the second part of the thesis, we discuss the time evolution of a Majorana edge state of a one-dimensional $p$-wave superconductor after performing both the sudden and slow quenches in the Hamiltonian. In this part we also consider the dynamics of a
transverse field SK spin glass.

The chapter 5 itself has two parts: first part deals with a sudden quenching of the $p$-wave superconducting chain and the second part provides a study of the possibility of an adiabatic passage of an edge Majorana in the same system with a complex hopping term. In first part, we consider the temporal evolution of a zero-energy Majorana edge state of a spinless $p$-wave superconducting chain following a sudden change of a parameter of the Hamiltonian. Starting from one of the topological phases that has an edge Majorana, the system is suddenly driven to the other topological phase or to the (topologically) trivial phases and also to the QCPs separating these phases. The survival probability of the initial edge Majorana as a function of time is studied following the quench. Interestingly when the chain is quenched to the QCP, we find a nearly perfect oscillations of the survival probability, indicating that the Majorana travels back and forth between two ends of the chain with a time period that scales with the system size. The generalization of the situation when there are next-nearest-neighbor hopping and superconducting pairing terms in the superconducting chain has also been studied in the same context and found that the frequency of oscillation of the survival probability gets doubled in this case. We also perform an instantaneous quenching the Hamiltonian (with two Majorana modes at each end of the chain) to an another Hamiltonian which has only one Majorana mode in equilibrium; the Majorana survival probability (MSP) shows oscillations as a function of time with a noticeable decay in the amplitude. On the other hand for a quenching which is reverse to the previous one, the MSP decays rapidly and stays close to zero with fluctuations in amplitude.

Bermudez et al. [115], addressed the question whether an adiabatic transport of an initial edge Majorana state from one topological phase to the other is possible when the hopping amplitude of the $p$-wave superconducting Hamiltonian is slowly varied in a linear fashion with time. It has been found that such an adiabatic transportation of edge Majorana is forbidden as it gets completely delocalized throughout the chain when the system reaches the QCP separating the two topological phases. In the second part of this chapter, we consider a modified $p$-wave superconducting chain with a complex hopping term which breaks the effective time-reversal symmetry (ETRS) of the model as well as generates an extended gapless phase separating two topological phases as introduced in Ref. [185]. We now ask the question that whether an edge Majorana can be transported from one topological phase to the other for a finite chain which is driven across this extended quantum critical region. Our most significant observation is that indeed there exists a finite probability for Majorana edge state, to tunnel adiabatically through the intermediate gapless region when the superconducting gap parameter is tuned in a linear fashion with a finite quenching rate. The non-zero value of the modulus square of the overlap between the final state reached after the quenching and the equilibrium Majorana state in the other topological phase provides a measure of finding an adiabatically
transported edge Majorana. We emphasize at the outset that this adiabatic transport is only possible for an optimal transit time that the system requires to traverse the gapless region which is proportional to the system size and diverges for a thermodynamically large chain. We attribute this phenomenon to the mixing of the Majorana only with low-lying inverted bulk states. Remarkably, the Majorana state always persists with the same probability even after the quenching is stopped. For a periodic chain, on the other hand, we find a Kibble-Zurek scaling of the defect density with a renormalized rate of quenching.

In chapter 6, we study the QA of SK spin glass model with the tuning of both transverse and longitudinal fields. Both the fields are time-dependent and vanish adiabatically at the same time, starting from high values. We solve, for rather small systems, the time-dependent Schrodinger equation of the total Hamiltonian by employing a numerical technique. At the end of annealing we obtain the final state having high overlap with the exact ground state(s) of classical spin glass system (obtained independently).