Defect production and quench dynamics in three-dimensional Kitaev model

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The three dimensional (3D) Kitaev model is studied in a situation where a linear drive \((J \rightarrow Jt/\tau)\) with quench rate \(\tau^{-1}\) takes the system across a quantum critical hyper-surface. Unlike 2D Kitaev model, the 3D Kitaev model is mapped into a 4-state Landau-Zener problem. This four-state Landau-Zener problem has been studied by exact numerics and found to be in good agreement with independent crossing approximation. It is found that the defect density scales as \(\tau^{-1}\) in the limit of very slow quench in consistent with the general prediction. However the asymptotic dependence of the defect density on the ratio \(J_g/J_x\) is seen to be completely different than 2d Kitaev model. It is not the critical surface on which the spectrum is gapless but the coupling \(\Delta(k_x, k_y, k_z)\) between relevant states that crosses in adiabatic evolution determines the dependency on \(J_g/J_x\). The defect correlation is found to be anisotropic due to the fact that the 3D lattice become decoupled into independent chains in the specific limits of the ratio, \(J_g/J_x\).

I. INTRODUCTION

Study of phase transition and the properties of physical system near phase transition have always attracted physicists form a long past. In particular, at low temperatures, one observes such transition when the inherent quantum fluctuations dominate over the thermal fluctuations and determine ground state properties of the system\[1–3\]. In this respect a pertinent question which generally arises is what happens, at absolute zero temperature, when the parameter of a given Hamiltonian (or physical) system is driven or varied in time and the system is taken across different phases. Recently such driven quantum system has attracted a lot of interest. It is an interesting fundamental question because one tries to find the answer whether the quantum system always remains at its instantaneous ground states or fail to do so due to diverging length and time scales of the system\[1,2\]. As a direct consequence of such divergent time scale, the system fails to remain in its instantaneous ground state when it is near the quantum critical point (QCP). The scaling law of created excitations at the asymptotic limit (at large time) says that for the generic 2nd order phase transition it is given by \(\tau^{-1-1/\nu}\)\[2,12\]. The creation of excitations as the system is taken across a gapless regime is amount to breakdown of the adiabatic limit. It is found explicitly that for low dimensional systems, the response of the system to the slow changes of the Hamiltonian parameters could be non-analytic and non-adiabatic\[14\]. Soon after, it has been shown that for a sufficiently slow quench at a rate \(1/\tau\) with quench time \(\tau >> 1\) the density of the above mentioned defect scales with the quench time as, \(n_d \sim \tau^{-1-1/\nu}\), where the quench takes the system through a \(d-m\) dimensional critical hyper-surface characterized by correlation length exponent \(\nu\) and dynamic critical exponent \(z\)\[11,13,15,16\]. Theoretical studies examining such scaling have been performed mostly on several exactly solvable models in one or infinite dimensions where all the higher excited states can be known a-priory\[11\]. However reference\[15\] and\[16\] established the above scaling law of defect production for the two-dimensional (2D) Kitaev model\[17\].

Kitaev model has been a test bed of numerous theoretical studies revealing many interesting and insightful aspects of condensed matter many body systems, for example, quantum computations\[28\], topological phase transition, topological degeneracy, fractionalisation of spins, quantum spin liquid, entanglement study etc\[18–20\]. The novelty of the Kitaev model and its subsequent enthusiasm to work on it have culminated in discovering the presence of Kitaev like interactions in certain materials namely Iridiate system\[29,32\]. Though the original Kitaev model was proposed on Honeycomb lattice, various extensions of the Kitaev model was observed in other three co-ordinated lattice in two as well in three dimensions\[3,9\]. The theoretical extension of the Kitaev model to three dimensions soon found material realisation as well\[30,36\]. The 3D Kitaev model differs from its 2D counter part in regard to some key properties for example, it becomes a four sublattice structure, dispersion being gapless in a contour, fermionic and bosonic non-local excitations\[27\] etc. All these fact motivates us to study for the first time the quench dynamics in a three dimensional spin model, viz., the spin-1/2 3D Kitaev model on the hyper-honeycomb lattice. This model can be solved exactly by mapping it into a theory of non-interacting Majorana fermions in the background of a static Z2 gauge field\[33\]. The phase diagram consists of a gapped phase and a gapless one, similar to the 2D case\[33\]. Although the phase boundaries are identical, the nature of the excitations are distinctly different from its...
2D counterpart, and accordingly we expect qualitatively distinct behaviours in resulting defect density, correlation function, and entropy generated in quench dynamic studies of 3D Kitaev Model. Another motivation for this study is that 3D Kitaev model is mapped into a 4-state Landau-Zener (LZ) model. Such a 4-state LZ model has been studied recently [37,38] in the context of a model Hamiltonian. However Kitaev model being an example of more physically interesting and realizable model, we find it as a natural setting to expand the scope of study of quench dynamics to a multilevel LZ model and a 3 dimensional gapless system.

The paper is organized as follows. In section II we have introduced the basics of 3 dimensional Kitaev model and mapped it to a 4 level LZ problem. In section III we have explained in details the formalism employed in this article to solve this 4 level LZ problem. We discuss two complementary methods which makes our study self contained. First we discuss the so called ”independent crossing approximation” (and its applicability) which is a first step to counter any multilevel LZ problem and then present exact numerical procedure carried out. Sections IIIA and IIIB describe the results corresponding to the calculations of defect density, defect correlation and entropy respectively. We finally conclude in section IV and discuss several important aspects of our results. In the Appendix A we have dealt with the issue of dynamic phases in the transition probability associated semi-classical trajectory and justified the ”independent crossing approximation”.

II. THE MODEL

The three dimensional (3D) Kitaev model is defined on a hyper-honeycomb lattice with lattice coordination number ‘3’ as shown in the left upper panel of Fig. 1

Any spin on a particular lattice site interacts with its three nearest neighbours through three different links, viz., x-link, y-link, and z-link which only exhibit interaction between the corresponding spin components [33].

The spin Hamiltonian on the hyper-honeycomb lattice has the form,

$$H = -J_x \sum_{x-\text{link}} \sigma^x_i \sigma^x_j - J_y \sum_{y-\text{link}} \sigma^y_i \sigma^y_j - J_z \sum_{z-\text{link}} \sigma^z_i \sigma^z_j.$$

(1)

The unit cell on the hyper-honeycomb lattice contains four sites with the basis vectors given by, $a_1 = 2x$, $a_2 = 2y$, and $a_3 = (x + y + 2z)$ [33]. Following Kitaev’s original prescription corresponding to the 2D model, the above Hamiltonian can be Fermionized to have a non-interacting Majorana Fermion hopping problem in the presence of conserved $Z_2$ gauge fields defined on every links. These $Z_2$ gauge fields can take values ±1. For each configuration of this $Z_2$ gauge field, one obtains a fermionic spectrum. It is found that [33], the ground state sector lies for the configuration when all the $Z_2$ gauge fields are taken uniformly one. In the ground state sector the effective Majorana fermion hopping problem reduces as,

$$H = \sum_{\mathbf{r}} \left[ J_x c_{1a}(\mathbf{r}) c_{2b}(\mathbf{r} - \mathbf{a}_1) + J_y c_{1a}(\mathbf{r}) c_{2b}(\mathbf{r} - \mathbf{a}_2) + J_z c_{1a}(\mathbf{r}) c_{2b}(\mathbf{r} - \mathbf{a}_3) \right].$$

(2)

where $\mathbf{r} = n_1 a_1 + n_2 a_2 + n_3 a_3$ is a position vector of a lattice point [33]. Owing to the bipartite nature of the lattice, in the above Hamiltonian, we conveniently introduced two indices to label the sites within a unit cell; $\mu = 1, 2$, denotes the dimer to which a site belongs and $\alpha = a, b$, denotes the sub lattice indices [33]. One can easily find the spectrum of the Hamiltonian given in Eq. (2) and one finds that the spectrum is gapless in the shaded region as shown in the right panel of Fig. 1. In our quench study, we take the $J_z$ to be linearly dependent on time $t$ as $J_z = Jt/\tau$. To implement the quench study in an effective four level LZ problem, we rewrite the Hamiltonian in Eq. (2) by introducing the complex fermions $\psi$ and $\phi$ by regrouping the two Majorana fermions at two $z$-bonds of the unit cell as given below,

$$\psi_1 = c_{1,1a} + i c_{1,1b}, \quad \phi_1 = c_{1,2a} + i c_{1,2b}.$$

(3)

After employing the above transformation and a subsequent Fourier transform, we obtain,

$$H = \sum_{\mathbf{k}} \Psi^\dagger_k h(\mathbf{k}) \Psi_k,$$

(4)

where

$$h(\mathbf{k}) = \begin{pmatrix}
2J_z & -\Delta_{2k}^* & 0 & -\Delta_{1k}^* \\
-\Delta_{2k} & 2J_z & \Delta_{1k} & 0 \\
0 & -\Delta_{1k}^* & -2J_z & -\Delta_{2k}^* \\
-\Delta_{1k} & 0 & -\Delta_{2k} & -2J_z
\end{pmatrix}.$$

(5)

FIG. 1. In the left, we have shown a basic building block of 3 dimensional lattice on which 3 D Kitaev model is defined. The phase diagram of the 3D Kitaev model in the parameter space $(J_x, J_y, J_z)$ has been shown. Point P corresponds to $J_x = 1$ and $J_y = J_z = 0$, Q corresponds to $J_y = 1$ and $J_x = J_z = 0$, and R corresponds to $J_x = 1$ and $J_z = J_y = 0$. The gray shaded region corresponding to the inverted triangle in the middle is the gapless phase.
and \( \Psi_k = (\psi_k^i, \phi_k^i, \psi_{-k}^i, \phi_{-k}^i)^T \) where \( \Delta_{1k} = e^{i\delta_{1k}} + \delta_{2k}, \) and \( \Delta_{2k} = e^{-i\delta_{1k}} - \delta_{2k}^* \) where \( \delta_{i,k} = J_y + J_x e^{i \theta} \) with \( i = 1, 2. \) Next we diagonalize the upper (or lower) 2 \times 2 part of the matrix \( \hat{h}(k) \) using the following unitary transformation,

\[
U_k = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{-i\theta_{2k}} & e^{-i\theta_{2k}} \\ 1 & 1 \end{pmatrix}
\]

where \( e^{i\theta_{2k}} = \frac{\Delta_{2k}}{\Delta_{2k}} \) which gives two eigenvalues, \( \epsilon_{1k} = 2J_z + |\Delta_{2k}| \) and \( \epsilon_{2k} = 2J_z - |\Delta_{2k}|. \) Finally we obtain a transformed Hamiltonian whose matrix representation is given by,

\[
\tilde{h}(k) = \begin{pmatrix} \epsilon_{1k} & 0 & g_k & -\gamma_k \\ 0 & \epsilon_{2k} & \gamma_k & -g_k \\ -g_k & \gamma_k & -\epsilon_{1k} & 0 \\ -\gamma_k & g_k & 0 & -\epsilon_{2k} \end{pmatrix}
\]

where \( g_k = -i|\Delta_{1k}| \sin \theta_{12k} \) and \( \gamma_k = -|\Delta_{1k}| \cos \theta_{12k}, \) and \( \epsilon_{1k} = 2J_z + |\Delta_{2k}| \) and \( \epsilon_{2k} = 2J_z - |\Delta_{2k}|. \) For each \( k \)-mode the above Hamiltonian matrix corresponds to the form of a 4-state Landau Zener model. If \( \alpha_{i,k} (i = 0, 1, 2, 3) \) denotes annihilation operators corresponding to the four states, we have the following relation between the old and new basis,

\[
\begin{pmatrix} \alpha_{3k} \\ \alpha_{2k} \end{pmatrix} = U_k \begin{pmatrix} \psi_k \\ \phi_k \end{pmatrix}, \quad \begin{pmatrix} \alpha_{0k} \\ \alpha_{1k} \end{pmatrix} = U_k \begin{pmatrix} \psi_{-k}^T \\ \phi_{-k}^T \end{pmatrix}
\]

We now apply the quench \( J_z(t) = Jt/\tau \) at a fixed rate \( 1/\tau, \) from \(-\infty \) to \( \infty, \) keeping \( J \) fixed and considering \( J_x = J \cos \alpha \) and \( J_y = J \sin \alpha \) fixed at some non-zero value such that \( J_x = \eta = \tan \alpha. \) In the limit of \( t \to \pm \infty \) the dominating terms in the \( (7) \) are the diagonal terms where we retain a very small non-zero value of \( |\Delta_{2k}|, \) owing to the fact that \( J_z(\eta) \) have infinitesimal but non-zero values. This helps us to avoid the obvious degeneracy (which otherwise originates from the fact that two of the diagonal elements of the above matrix become equal) in the limit \( t \to \pm \infty, \) in the same spirit of removing the ground state degeneracy of a spin-\( S \) Ferromagnetic Heisenberg model with an infinitesimally small symmetry breaking field. In the limit of \( t \to -\infty \) the ground state is gapped, and the corresponding eigenvalue is given by, \( \epsilon_{2k} = -2J_z - |\Delta_{2k}| \) with \( |\Delta_{2k}| \) very small so that the adiabatic levels are well separated at distant past or future, as plotted in Fig.2(a). According to our convention, at \( t \to -\infty, \) the eigenstates corresponding to \( \epsilon_{2k}, \epsilon_{1k}, -\epsilon_{1k}, \) and \( -\epsilon_{2k} \) denote the level \( |0_k, 1_k, 2_k \), and \( 3_k \) respectively. The diabatic ground-state in this time limit is given by, \( |G_{-\infty} \rangle = (0, 0), \) whereas in the limit \( t \to +\infty \) the diabatic ground state is \( |G_{+\infty} \rangle = (0, 0) \). The corresponding adiabatic levels are plotted in Fig.2(b). It may be mentioned that in usual many body sense the ground state is constructed by populating both the negative energy states for available \( k \)-values. However once one does this, the subsequent quench dynamics makes it a 6 level LZ problem and makes the quench dynamics computationally more demanding. In the present case by ground state we mean that the initial state is constructed by filling the most negative energy states. However the outcome of the quench dynamics should not differ fundamentally as the underlying properties of the physical model in question are same.

![FIG. 2.](attachment:fig2.png)

**III. FORMALISM AND RESULTS**

There are studies of quench dynamics on various model systems which in essence reduces to a two level LZ problem \( \text{[12, 14, 16]} \) which can be analytically examined in relatively easy way. However the system we are interested is mapped to a 4-state LZ model and thus poses a difficulty in terms of complete analytical investigation. In this circumstances one is compelled to resort to numerically estimate the evolution of the system under quench and determine the long time behaviour of the system. Another alternative useful approximation to deal with the 4-state LZ problem is the independent crossing approximation (ICA) \( \text{[37]} \) which essentially examines the possibility.
whether in the presence of more than two level in question, the transition probability from a given state to another given state can be reduced to an effective two level problem without worrying about existence of the rest of the levels. We have investigated the quench dynamics of 3D Kitaev model by exact numerical evaluation as well as within the ICA and found excellent agreement between the two. For this reason we first elaborate in detail our scheme of ICA and then discuss the numerical details. We use the ICA to figure out the scattering matrix $S$ whose elements’ squared $|S_{ij}|^2$ represent the transition probabilities from $i$’th state at $-\infty$ to $j$’th state at $+\infty$. In order to apply the ICA we must have the avoided level crossing points far from each other, and this is indeed satisfied in our case as shown in Fig. 2(b). Within the ICA one follows the diabatic levels, as illustrated in Fig.2(a) and apply 2-level LZ formula at each crossing point along the path [37–39]. The most necessary criteria for the applicability of such an approximation is the cancellation of dynamic phase (gained along the path of evolution) in the expression of the transition probabilities [37–39]. It indeed turns out that the dynamic phases gained along all the possible trajectories corresponding to the transitions from the ground state |0⟩ get cancelled in the expression of the probability density. Here the probability density is the square of the modulus of the transition amplitude. The same is true for all possible transitions from the ground state at $t = \infty$. However, in the case of trajectories forward in time, for all the transitions from the states |1⟩ and |2⟩ exhibit the effects of the dynamic phases, as explained in Appendix A. It is worthwhile to point out that the above approximation is semi-classical because this does not allow a flow backward in time. Therefore transitions from |0⟩ to state |1⟩, and from |3⟩ to state |2⟩ are not possible. Details of the calculations of the transition amplitudes in semi-classical approximations are given in Appendix A. The probability that the system remains in the ground state defines the defect density, calculation of which is one of the main aims of this paper. In the following we first calculate the same.

A. Defect density

Analytical calculations: Within the formalism of independent crossing approximation the defect density can be calculated by using the following formula,

$$n_d = \frac{1}{\Omega_{HBZ}} \int_{HBZ} d^3k p_k,$$

(9)

where the area of the half Brillouin zone (HBZ) is given by $\Omega_{HBZ} = \pi^3/2$ and the integration is performed over the HBZ as indicated above. In the above equation, the quantity $p_k$ is the probability of defect which is given by the probability of the system to remain in the ground state after the complete quench, i.e., $p_k = P_{00} = \exp\left(-\frac{|\Delta_{1k}|^2}{2}\right)$ where $|\Delta_{1k}|^2$ is given by,

$$|\Delta_{1k}|^2 = 4J^2 \left[ (\cos^2 \alpha) \cos^2 \left(\frac{k_x + k_y + 2k_z}{2}\right) + (\sin^2 \alpha) \cos^2 \left(\frac{k_x + k_y - 2k_z}{2}\right) 
+ 2 \sin(2\alpha) \cos \left(\frac{k_x - k_y}{2}\right) \cos \left(\frac{k_x + k_y + 2k_z}{2}\right) \cos \left(\frac{k_x + k_y - 2k_z}{2}\right) \right].$$

(10)

In Fig. 3 the defect density is plotted as a function of quench rate $J\tau$, where both the results corresponding to numerical and numerically evaluated analytical expressions corresponding to (9) are indicated. It is easy to see that for sufficiently slow quench $J\tau >> 1$, the quantity $p_k$ is exponentially small for all values of $k$ except on a contour dictated by $|\Delta_{1k}|^2 = 0$. If a generic point on the above mentioned contour are given by $(k^0_x, k^0_y, k^0_z)$, we can assume that the contribution to the momentum integrals come from values of $k$ close to these points. It is straightforward to see that the condition $\text{Min}(|\Delta_{1k}|^2) = 0$, leads to the following parametric surface in the $k$-space,

$$\tan(k_x) \tan(k_z) = \frac{1 + \tan \alpha}{1 - \tan \alpha} k_x = k_y + 2n\pi.$$

(11)

where $\alpha = J_x/J_y$. The above equation indeed represents a critical line for each value of $\alpha$. However, the above conditions are valid only for all the values of $\alpha$ except $\alpha = 0$, and $\pi/2$. For these two values of $\alpha$ the minimum conditions can be obtained directly from Eq. (11). It is therefore possible to make a Taylor expansion of the function $|\Delta_{1k}|^2$ around the points $(k^0_x, k^0_y, k^0_z)$ situated on the above mentioned surface. Implementing such an expansion up to leading order we obtain,

$$|\Delta_{1k}|^2 = \frac{1}{2} \sum_{i,j=x,y,z} \left[ \frac{\partial^2(|\Delta_{1k}|^2)}{\partial k_i \partial k_j} \right] (k_i - k^0_i)(k_j - k^0_j).$$

(12)

where the quantity $\left[ \frac{\partial^2(|\Delta_{1k}|^2)}{\partial k_i \partial k_j} \right]$ is the $ij$th element of the precision matrix $(3 \times 3)$ of a Multivariate Gaussian. Since the function $p_k$ corresponding to Eq. (9) is prac-
tically vanishingly small for all values of $k$ except the points near $(k_0^x, k_0^y, k_0^z)$ the limit of $k$-integration can be extended from 0 to $\infty$, which makes the expression of the defect density a Gaussian integral. Use of the condition $k_x = k_y + 2\pi, i.e., k_x$ and $k_y$ are related to each other by a constant shift makes the differences $k_x - k_0^x = k_y - k_0^y$ and thereby reduces the above mentioned $3 \times 3$ precision matrix to a $2 \times 2$ which leads Eq. (12) to simplify as,

$$|\Delta_{1k}|^2 = \frac{1}{2}(4J^2)[4f_{xz}(k_x - k_0^x)^2 + 4f_{xz}(k_x - k_0^y)(k_z - k_0^y) + f_{zz}(k_z - k_0^z)^2] \tag{13}$$

where we have rewritten $\frac{\partial^2|\Delta_{1k}|^2}{\partial k_x \partial k_z} = 4J^2f_{ij}(\alpha)$. After the integration as explained, we have the expression for defect density as,

$$n_d = \frac{\pi}{\Omega_{HBZ}} \left( \frac{1}{(J\tau)^{\sqrt{|f_{ij}(\alpha)|}}} \right), \tag{14}$$

where $|f_{ij}(\alpha)| = 4[f_{xx}f_{zz} - (f_{xz})^2]$ is the determinant of the $2 \times 2$ precision matrix, which must be positive definite. It turns out that for $\alpha = 0$ and $\pi/2$ the above mentioned determinant vanish and therefore we can’t apply the Gaussian integral, and therefore, we have evaluated the corresponding integral numerically within the HBZ. Thus our analytical calculation using ICA establishes the defect density to scales as $(J\tau)^{-1}$ in the limit of very slow quench. Now it is customary to compare the above results with the prediction [15] that defect density crucially depends on the dimensionality of the critical hyper-surface through which the system passes during the quench. The quantities which are of importance are $z$ which tells how the energy dispersion of a given system depends on momentum at low energy, the dynamical exponent $\nu$ which determines the asymptotic dependence of two point correlation function at large distance and $m$ which tells how the system becomes gapless in momentum space. In the case of the 3D Kitaev model considered here with, it can be checked easily that $\nu = z = 1$. The dispersion of 3d Kitaev model discussed here is such that dispersion vanishes in a contour which constitute a 2 dimensional critical hyper-surface under the action of quench yielding $m = 2$. Keeping in mind that our system is a 3 dimensional with $d = 3$, substituting the above values of $(z, \nu, d, m)$ in the expression of defect density $n_d = \tau^{-1}$, we obtain $n_d \equiv \tau^{-1}$. In Fig. 3 we have plotted defect density with respect to $J\tau$ which conforms the above scaling. A very good agreement with the exact numerical calculation with that obtained in independent crossing approximation is remarkable. Before we elaborate on the discussion of $n_d$, let us take a small detour on the numerical procedure followed to calculate the exact defect density.

**Numerical calculations:** The main characteristic features of studying the quench dynamics of 3d Kitaev model which makes it an important case is two fold. First the model is mapped to a four level L-Z model for each $k$ as evident from Hamiltonian given in Eq. (7). Secondly it serves a critical gapless system where the spectrum is gapless on a contour unlike at isolated points of 2D Kitaev model. The final outcome of quench is a result of intricate effect of those two aspects mentioned. For this reason we think it is necessary to write the coupled equations that one needs to solve for determining the exact time-dependence of states. The obtained coupled equations are given by,

$$i\frac{d|1(t)\rangle}{dt} = \epsilon_1|1(t)\rangle + g_1|2(t)\rangle - \gamma_1|3(t)\rangle$$
$$i\frac{d|0(t)\rangle}{dt} = \epsilon_2|0(t)\rangle + \gamma_1|2(t)\rangle - g_1|3(t)\rangle$$
$$i\frac{d|2(t)\rangle}{dt} = -\gamma_1|1(t)\rangle + \gamma_0|0(t)\rangle - \epsilon_1|2(t)\rangle$$
$$i\frac{d|3(t)\rangle}{dt} = -\gamma_1|1(t)\rangle + \gamma_0|0(t)\rangle - \epsilon_1|3(t)\rangle, \tag{15}$$

where the notation of the states $|0\rangle, |1\rangle, |2\rangle$ and $|3\rangle$ are consistent with the same appearing in Fig. 2. Unlike two state LZ coupled problem, the exact solution of the above set of equations are non-trivial and one invariably needs to resort to numerical means. However the evolution of time dependent quantum state numerically needs a careful algorithm otherwise a large error might result in producing non-physical outcome. We use a numerical algorithm which capture the time evolution from an arbitrarily large time in past to an arbitrarily large time in future and proceeds in a discrete but small steps $dt$. The unitary operator describing the time evolution for each $k$ mode is given by,

$$\hat{U}(k,t) = \left(\hat{I} + \hat{h}(k,t)\frac{dt}{2}\right)\left(\hat{I} - \hat{h}(k,t)\frac{dt}{2}\right)^{-1} \tag{16}$$

where $\hat{h}(k,t)$ is the Hamiltonian matrix (7) with the quench protocol mentioned earlier, and $\hat{I}$ is a $4 \times 4$
Identity matrix. Such a time evolution operator has been used to study 4-state L-Z model in the context of model Hamiltonian \[ H = J_x S_x S_y + J_y S_y S_z + J_z S_z S_x. \] This evolution operator is equivalent to a true evolution operator in the limit of \[ dt \to 0. \] Use of this procedure also reduces error to \[ \frac{(dt)^2}{4} \] at \( O(dt^2) \). In this paper we have found the following quantities, \( \langle 0 | \hat{U}(k, t) | 0 \rangle \) and \( \langle f | \hat{U}(k, t) | 0 \rangle \) where \( |f\rangle \) are the final states except the ground state itself. The quantity \( \langle 0 | \hat{U}(k, t) | 0 \rangle \) is equivalent to \( p_{k0} = p_k \) and further use of Eq. \( 9 \) determines numerically the defect density \( n_d \). The red dots in the Fig. 4 are the numerically obtained defect density. At this point we must mention that the results corresponding to the independent crossing approximation exactly matches with those obtained by exact numerical calculations. This signifies the success of the independent crossing approximation in describing the quench dynamics corresponding to the linearly driven 3D Kitaev model. Furthermore, we also need the other transition probabilities corresponding to \( P_{10}, P_{20}, \) and \( P_{20} \) for the calculation of entropy. The results remain same if we would have started at \( t \to \infty \), with \( |2\rangle \) being the corresponding ground state.

It is instructive to compare our results with that of 2d Kitaev model where one have \( n_d = \tau^{-0.5} \). One more interesting fact that differentiate the asymptotic behaviour of defect density of 2d KM model to that of 3d KM is the dependence of \( n_d \) on \( \alpha \). As the \( \alpha \) is varied from 0 to \( \pi/2 \), the defect density increases monotonically up to \( \alpha = \pi/4 \) and then decreases monotonically such that it is symmetric with respect to \( \alpha = \pi/4 \). For 3d Kitaev model the asymptotic behaviour for large \( \tau \) is symmetric with respect to \( \alpha = \pi/4 \) but unlike 2d Kitaev model, it is maximum at \( \alpha = 0 \) and decreases monotonically and then again reaches a local maxima at \( \alpha = \pi/4 \) as shown in Fig. 4. To explain this unusual fact we look back to the expression of \( p_k \) appearing in the expression of \( n_d \) in Eq. \( 9 \) in subsection III A. We observe that the factor \( \Delta_k \) explicitly appearing in the integral. Thus it is reasonable to define an effective density of states corresponding to the the variable \( \Delta_k \) and investigate it near \( \Delta_k = 0 \) as near this vanishing values of \( \Delta_k \), the integral is going to receive more contribution.

From the (effective) DOS plot in Fig. 5 we can see that DOS corresponding to \( \Delta_k = 0 \) for various values of \( \alpha \) is such that it is maximum at \( \alpha = 0, \pi/2 \) and decreases initially as it approaches toward \( \alpha = \pi/4 \). However after some values of \( \alpha \), the DOS start increasing and produces a local maxima at \( \alpha = \pi/4 \). This explains the variation of asymptotic values of \( n_d \) with respect to \( \alpha \). Thus we come to the conclusion that for multilevel LZ problem, the gapless condition for the complete spectrum need not appear explicitly at the expression of defect density, rather it is the coupling between relevant two level system which determines the asymptotic behaviour. This points out to the fact of possibility that the asymptotic dependence of \( n_d \) may be determined by the effective part of the total system.

![FIG. 4. Plot of defect density \( n_d \) as a function of \( \alpha \) where \( \alpha = \arctan(J_y/J_x) \) for \( J_T \gg 1 \). The red dotted points are results corresponding to exact numerical calculations, and the surface plot is the result corresponding to the Independent crossing approximation. A hump at \( \alpha = \pi/4 \) signifies a local maximum](image)

![FIG. 5. Effective Density of States (DOS) as a function of \( \alpha \) where \( \alpha = \arctan(J_y/J_x) \) at the gapless phase.](image)

**B. Correlation functions**

As we have already mentioned that the quenching a system effects a quantum system in various ways though they are intimately related to each other. In this section, we will discuss the effect of quench in correlation function of the system and how does it related to the defect production. We note that the true quantum ground state of 3d Kitaev model is supposed to be a quantum spin liquid where the spin-spin correlation function is short range and anisotropic as well. The two spin-correlation is non-zero only for nearest neighbour spins for all values of the model parameter system. Thus it remains a matter of great interest how the correlation functions develop non-locality as a result of such quench. For simplicity we consider here a two spin correlator given by,

\[
\mathcal{O}^{3D}(r) = \sigma_\mathbf{R} \cdot \sigma_{\mathbf{R}+\mathbf{r}}
\]

(17)

which is nothing but a product of spin operators from a site \( \mathbf{R} \) at \( b \) sub-lattice to a site \( \mathbf{R}+\mathbf{r} \) at \( a \) sub-lattice.
The quantity $O^{3D}(r)$ is only non-zero for $r = 0$ and this fact remains the same for all parameter values. In the Majorana Fermion representation the above correlation function takes the form $O^{3D}(r) = ic_{1a}(R)c_{2b}(R + r)$. In the following we study the evolution of this two fermion correlator rather than the spin-spin correlation. Thus the object of our interest is

$$C^{3D}(r) = ic_{1a}(R)c_{2b}(R + r). \quad (18)$$

After doing a Fourier transform, the ground state expectation value of the two fermion correlation takes the following form,

$$\langle C^{3D}(r) \rangle = \pm \frac{1}{2N} \sum_{k \in HBZ} \cos(k \cdot r), \quad (19)$$

where + and - sign refers to the ground state corresponding to $J_z = -\infty$ and $\infty$ respectively and $\langle C^{3D}(r) \rangle$ is indeed $\pm \sigma_{r,0}$. In the state after quench there exists a mixture of ground state with probability $p_b$ and other excited states corresponding to $J_z \to \infty$ with the corresponding probabilities, viz. $(1 - u^2_x)$, and $u^2_y(1 - u^2_y)$ respectively (see (A7)). In this case the correlation function takes the form,

$$\langle C^{3D}(r) \rangle = -\sigma_{r,0} + \frac{1}{\Omega_{HBZ}} \int d^3k p_b \cos(k \cdot r), \quad (20)$$

where the second term in the above equation is a measure of defect correlation and henceforth will be analysed. In the limit $J_z \to -\infty$ the system is in the ground state where nearest-neighbor spins are anti-ferromagnetically aligned, and as the system passes through the quench, the state of the system deviates from the ground state configuration and defects are produced. We evaluate the second term of the above equation by expanding the defect probability $p_b$, obtained within the independent crossing approximation, in the limit of very slow quench corresponding to $J_T >> 1$. As usual the dominant contribution comes from contour dictated by $|\Delta \kappa| = 0$ which is given by (11). Doing the relevant Gaussian integrals, as has been done for the defect density in the previous section, we find,

$$\langle C^{3D}(r) \rangle = \frac{\pi}{\Omega_{HBZ}} \left( \frac{1}{(J\tau)\sqrt{||f_{ij}(\alpha)||}} \right) \exp \left[ -\frac{(N_x + N_y)^2f_{xz} + 4N_x^2f_{xx} - 4(N_x + N_y)N_xf_{xz}}{4\pi J\tau ||f_{ij}(\alpha)||} \right] \times \cos \left[ k_x^0(N_x + N_y) + k_y^0N_z \right]. \quad (21)$$

The above equation shows the asymptotic behaviour of the defect correlation as a function of $J_T$, and

$$\langle C^{3D}(r) \rangle \sim \tau^{-1} \exp(-A\tau^{-1}), \quad (22)$$

where $A = \frac{(N_x + N_y)^2f_{xz} + 4N_x^2f_{xx} - 4(N_x + N_y)N_xf_{xz}}{4\pi J\tau ||f_{ij}(\alpha)||}$, and $N_x = 2n_1 + n_3$, $N_y = 2n_2 + n_3$, and $N_z = 2n_3$.

After having the asymptotic analytic expression of defect correlation function as given in Eq. (21) it is instructive to analyse it in different directions and plane to gain more understanding into how the defect correlation actually behaves. In order to do that we evaluate the equation (20) numerically in various directions. We note that any arbitrary point on the lattice is given by $r = n_1a_1 + n_2a_2 + n_3a_3$. In Fig. 6 we have plotted the spatial variation of the defect correlation as a function of $n_1$, $n_2$, and $n_3$ for $J_x = J_y = J = 1$. From Fig. 6a and 6b it is easy to recognize that the spatial variation of the defect correlation is isotropic in the $a_1 - a_2$-plane. However, it is not isotropic in the $a_1 - a_3$-plane as evident from Figs. 6c and 6d. Furthermore, owing to the symmetric nature of it in the $a_1 - a_3$-plane the spatial variation of the defect correlation in the $a_1 - a_3$-plane is same as that of the $a_2 - a_3$-plane. Therefore, it is expected to have the spatial anisotropy too for arbitrary values of coupling constants corresponding to $J_x \neq J_y$. In order to investigate the above mentioned anisotropic nature of the correlation in space when the ratio $J_y/J_x$ is varied from 0 to $\infty$ while maintaining $J^2_x + J^2_y = 1$ we have plotted in Fig. 7 the correlation $\langle O^{3D}(r) \rangle$ as a function of $\alpha = \tan^{-1}\frac{J_y}{J_x}$. Here the quantity $\langle O^{3D}(r) \rangle$ has been obtained by numerically evaluating the second term of Eq. (20) where $p_b$ has been obtained using both the independent crossing approximation and exact numerical calculations explained in the previous section. From the plots it is easy to recognize that the results corresponding to independent crossing approximations and that corresponding to numerical calculations match exactly. Furthermore, we find that as $\alpha$ is varied from 0 to $\pi/2$, correlation along the $n_1$ (x-) direction increases from its zero value at $\alpha = 0$ to a maximum value at $\alpha = \pi/2$, and again decays to its zero value at $\alpha = \pi/2$. Due to symmetric nature of the defect correlation in the and $n_1 - n_2$-plane, the above mentioned finding is true for $n_2$-direction also. In the $n_3$-direction however, the defect correlation is maximum at $\alpha = 0$ and decays to its zero value at $\alpha = \pi/2$. From Fig. 7 we further see that in the $n_1 - n_3$-plane the defect correlation become maximum at an arbitrary value $J_x$ and $J_y$ for which $0 < \alpha < \pi/4$. Owing to the symmetry correlation along $n_2 - n_3$-plane has the same behaviour. On the
FIG. 6. Plot of defect correlation $\langle C^{3D}(r) \rangle$ as a function $n_1, n_2$ and $n_3$, i.e., as a function of spatial coordinate $r$. The spatial variation of the defect correlation in the $a_1-a_2$-plane (a) when $n_3 = 0$ and (b) when $n_3 = 1$. The spatial variation of the defect correlation in the $a_1-a_3$-plane (c) when $n_2 = 0$ and (d) when $n_2 = 1$. See text for explanations.

FIG. 7. Plot of defect correlation $\langle C^{3D}(r) \rangle$ as a function of $\alpha$ where $\alpha = \arctan(J_y/J_x)$. $n(1,0,0)$ and $n(0,0,1)$ are obtained from exact numerical calculations and others are obtained from independent crossing approximation.

The above mentioned typical behaviour of the defect correlation as function of $\alpha$ can be readily understood by looking at the lattice structure of the 3D Kitaev model. We have drawn different configurations of the 3D lattice corresponding to the cases of arbitrary $\alpha$ in Fig. (a), $\alpha = 0$ in Fig. (b), and $\alpha = \pi/2$ in Fig. (c). In the case when $\alpha = \pi/4$ we can see from Fig. (a) that we have $J_x = J_y$ and the lattice is a pure 3D structure. In this situation the correlation in x-direction $(1,0,0)$, y-direction $(0,1,0)$ and in general in the xy-plane $(n_1 -$ $n_2$ plane) starts increasing as one starts varying $\alpha$ from zero, and becomes maximum at $\alpha = \pi/4$ because in this case the correlation in x-direction $(1,0,0)$, y-direction $(0,1,0)$ and in general in the xy-plane $(n_1 -$ $n_2$ plane) starts increasing as one starts varying $\alpha$ from zero, and becomes maximum at $\alpha = \pi/4$ because in this
case all the nearest available dimer bonds reside on the $n_1 - n_2$ plane (i.e., $a_1 - a_2$-plane). When $\alpha = 0$ and $\pi/2$, the lattice no longer remains a 3D structure, instead it converts into several decoupled chains. At $\alpha = 0$ it turns out that correlation along $a_3$ direction or equivalently (0,0,1) direction is maximum because in this direction one dimer finds another to be located on the same chain (see Fig. 9(b)). However, correlation along x-direction (or (1,0,0 direction)), y-direction (or (0,1,0 direction)), and in general through the xy-plane vanishes because in this plane two dimers reside on two different chains. On the other hand, when $\alpha = \pi/2$ corresponding to the case of Fig. (8c), correlation vanishes along all the available directions (as plotted in Fig. 7) because the decoupling of chains take place in such a way that every dimer finds another one to be located on a different chain.

One can determine a sum rule for the correlation function by evaluating $O_{\text{total}} = \sum_r |O_r|$. Considering the fact that $\sum_r e^{i k \cdot r} = (\Omega_{BZ})^{\delta(3)}(k)$ the sum rule can be evaluated to be $O_{\text{total}} = -1 + 2p_0 = 1$. Therefore, the total correlation is normalized to unity.

C. Entropy

It may be noted that at time $t = -\infty$, the ground state is a trivial product states of dimers on $z$-links. In the dimer the two spins are anti-ferromagnetically aligned. When the system is now quenched such that effective $J_z \rightarrow \frac{J}{\tau}$, the instantaneous ground state deviates from the initial trivial dimer-states. The quenched states will now find a non-zero probability to occupy other excited states which are highly entangled. We may remember that in its course of time evolution from $t = -\infty$ to $t = \infty$, the instantaneous ground states pass through gapped states and gapless states as depicted in Fig. 1. Though, the states at the beginning and end is a trivial product states, it does travel through all the possible states whose time averaged signature could be examined by noticing that for each momentum $k$, the state of the system after quench is given by,

$$|\psi\rangle = \sqrt{P_{00}} e^{-iE_{0,k}t}|0\rangle + \sqrt{P_{02}} e^{-iE_{2,k}t}|2\rangle + \sqrt{P_{03}} e^{-iE_{3,k}t}|3\rangle,$$

where the eigenvalues $E_{n,k}$ are essentially constants at $t = \pm \infty$. However, the final density matrix of the system still remains diagonal [42] owing to the fact that all the off-diagonal terms vary so rapidly that their effect on any physical quantity is zero. The density matrix of the entire system is then given by, $\rho = \otimes \rho_k$, since each $k$ modes are independent. Therefore, it is easy to evaluate the von-Neumann entropy which is given by,

$$s = -\frac{1}{\Omega_{BZ}} \int_{HBZ} d^3k [P_{00} \ln P_{00} + P_{02} \ln P_{02} + P_{03} \ln P_{03}]$$

where the quantities $P_{ij}$ are the matrix elements of the transition matrix [A7]. In the above equation $P_{00} = p_k = (u_\gamma u_\gamma)^2$, where $u_\gamma = \exp\left(-\frac{\pi |\gamma|^2 J_z}{4J_t}\right)$ and $u_\gamma = \exp\left(-\frac{\pi |\gamma|^2 J_z}{4J_t}\right)$, and $P_{02} = (1 - u_\gamma^2)$ and $P_{03} = u_\gamma^2 (1 - u_\gamma^2)$. In the limit of very small $\tau$, i.e., $\tau \rightarrow 0$, $P_{00} \rightarrow 1$ and $P_{02} = P_{03} = 0$, the entanglement entropy is zero. We note that at $t \rightarrow -\infty$ the initial state $\Psi$ is a product state of dimers defined on each $z$-bonds where the spins on the each dimers are ferromagnetically aligned and the correlation $\langle O_0 \rangle = 1$. In terms of fermions constructed out of two Majorana fermions on a given dimer, the state $\Psi$ can be written as,

$$|\Psi_{t = -\infty}\rangle = \prod_{i_z} |00\rangle_{i_z}$$

where $|00\rangle_{i_z}$ denotes a state with no fermion at the dimer $i_z$. The instantaneous ground state at time $t$ (when $J_z \rightarrow Jt/\tau$) can be obtained easily by diagonalizing Eq. 2 and filling up the negative energy states for all momentum $k$. As we started with a state having lowest negative energy states to be occupied, the quenching will lead a transition to excited states which contains the informations of instantaneous Hamiltonian with $J_z \rightarrow Jt/\tau$. The entanglement content of this state is much more than the initial state [25]. However the probability of excitations depends on the rate of quenching $\tau$. If the $\tau$ is very small, it is expected that very small transition would happen causing little entanglement generation. However as we increase $\tau$ it is expected that entanglement will increase. But this increment will eventually be saturated owing to the simple fact that the total probability of finding the states in different $k$-mode is constant. It is the relative ratio of probability that defines overall quantitative value of entanglement. Physically as we increase $\tau$, at the intermediate values of $\tau$, it is possible for the initial ground state to receive correct amount of energy to make transition to excited states. However at very large values of $\tau$, the drive is so rapid that the initial state does not find time to respond to external drive. Thus we find

**FIG. 9.** Plot of von Neumann entropy as a function of $J\tau$ and $\alpha$.
that at $t = \infty$, the entanglement goes to zero again. In Fig. [2] we have given a 3D plot of entanglement entropy in $J\tau$ and $\alpha$ plane. We notice that for a given $\alpha$, the entanglement entropy reaches maximum at certain values of $J\tau$ and then goes to zero asymptotically.

IV. CONCLUSIONS AND DISCUSSIONS

To summarize, we have studied the quench dynamics and defect production in the spin-1/2 three dimensional Kitaev model by mapping it into a 4-state Landau-Zener (LZ) model. We have investigated the nature of the defect density as a function of quench time as well as $\alpha = \tan^{-1}(J_y/J_x)$. Both exact numerical calculations, and analytical calculations using the independent crossing approximation have been performed. Results from both the methods match exactly. Although the LZ model corresponding to our 3D Kitaev model doesn’t satisfy all the criteria for the integrability, for transitions from ground state corresponding to both $t = \pm \infty$ to other excited states does not involve any dynamic phase affect originated from the area swept by the diabatic levels in the energy-time plane. This is because the dynamic phases get cancelled when one takes the square of the modulus of the transition amplitude in the corresponding transition probabilities. Therefore, our results corresponding to defect density do not get affected by the dynamic phase.

We have found that in the limit of very slow quench, viz., $\tau >> 1$ the defect density $n_d$ scales as $\tau^{-1}$ with the quench time $\tau$ which satisfy the general scaling law $n_d = \tau^{\alpha - m\nu}$, with $m = 2$, and $\nu = z = 1$, where $\nu$ is the critical exponent of the correlation length, and $z$ is the dynamic critical exponent. However, the variation of the defect density for a fixed $\tau$ is different from its counterpart in the 2D Kitaev model. It turns out that the defect density here is maximum at $\alpha = 0$ and $\pi/2$, and at $\pi/4$ it has a local maximum. This behaviour originates form the nature of the density of states corresponding to the ground state in the gapless phase. The system spends maximum amount of time in the gapless phase at $\alpha = 0$ and $\pi/2$. On the other hand time spent by the system in the same gapless phase at $\alpha = \pi/4$ is locally maximum.

We have further calculated the defect correlation function both analytically and numerically, and studied its spatial anisotropy. In the limit of very slow quench the defect correlation function scales as $\tau^{-1}e^{-A/\tau^z}$ with the quench rate $\tau$. We have found that the correlation function is spatially isotropic in the xy-plane or equivalently in the $n_1 - n_2$ plane, and anisotropic in the other two planes. It turns out that when either $J_x$ or $J_y$ vanishes, the lattice becomes a set of decoupled chains and only those correlations survive for which a dimer can be found in another dimer in the same chain. Moreover, when $J_x = J_y$ the lattice retains it 3D structure and the nearest neighbour dimers are placed along the $a_1$ and $a_2$ directions. This makes the correlation in the $n_1 - n_2$ plane to become dominant in this situation. Lastly, we have computed the von-Neumann entropy generated in such processes and have found that the entropy peaks approximately at values of the quench rate $\tau$ within the range $0 < \tau < 1$, for which the defect correlation changes from $-1$ to 1.

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Appendix A: Transition amplitudes

In order to calculate the transition amplitudes, we first consider all possible semi-classical paths corresponding to Fig. [11](a). As mentioned in section [11] the ground state at $t = -\infty$ is $|0\rangle$. First we note that there are four crossing points, viz.,

$$
|0\rangle \rightarrow |3\rangle : \text{with coupling constant} : g_k \\
|3\rangle \rightarrow |0\rangle : \text{with coupling constant} : -g_k \\
|1\rangle \rightarrow |2\rangle : \text{with coupling constant} : -g_k \\
|2\rangle \rightarrow |1\rangle : \text{with coupling constant} : g_k \\
|3\rangle \rightarrow |1\rangle : \text{with coupling constant} : -\gamma_k \\
|0\rangle \rightarrow |2\rangle : \text{with coupling constant} : \gamma_k 
$$

We apply the LZ formula by using the above coupling constants corresponding to the respective crossing points. We note that whenever a state crosses another state with coupling constant $g_k$ (as well as $-g_k$), the probability amplitude that the system remains in the same state is given by $u_g = \exp \left( -\pi i g_k^2 |J_{xy}| / \tau \right)$. Therefore, the probability amplitude that the system makes transition is $i\xi \sqrt{1 - (u_g)^2}$, where $\xi = 1$ when the sign of the coupling constant is positive.
and $\xi = -1$, when negative. These expressions for the crossing points with coupling $\gamma_k$ are same except $|g_k|$ shall be replaced by $|\gamma_k|$. In the following let us write down the transition amplitudes $S_{ij}$ for all the semi-classically allowed paths. In writing such paths we need to consider the effect of the dynamic phase $e^{i\phi_{ij}^d(\nu)}$ in a given path $\nu$ which is given by,

$$
\phi_{ij}^d(\nu) = \int_{-\infty}^{+\infty} dt \epsilon_{\nu k}(t); \text{ with } 0, 1, 2, 3, \quad (A2)
$$

where $\epsilon_{\nu k}(t)$ are the diabatic energy levels participating in the trajectory. This dynamic phase is nothing but the area under the trajectory $\nu$ under consideration. All the transition amplitudes corresponding to the transitions from the state $|0\rangle$ to the rest of the states are given by,

$$
|0\rangle \rightarrow |0\rangle : S_{00} = u g u \gamma
$$

$$
|0\rangle \rightarrow |1\rangle : S_{01} = 0, \text{ not an allowed transition}
$$

$$
|0\rangle \rightarrow |2\rangle : S_{02} = i \sqrt{1 - u^2} \gamma
$$

$$
|0\rangle \rightarrow |3\rangle : S_{03} = i u \gamma \sqrt{1 - u^2} \quad (A3)
$$

In the above equation the dynamic phases in the respective trajectories get cancelled when the square of the modulus of the transition amplitudes are taken. Therefore we have dropped the term $e^{i\phi_{0j}^d(\nu)}$ corresponding to the dynamic phase. Similarly, all the transition amplitudes corresponding to the transitions from $|1\rangle$ to the rest of the states can be written down. Here, while considering all the semi-classical trajectories we need to consider the effects of the dynamic

![Diagrams](image-url)

**FIG. 10.** Diabatic levels corresponding to the Hamiltonian $H$ (a) the semi-classical trajectories showing the possible paths along which a transition from the state $|1\rangle$ to the state $|0\rangle$ can take place. Similar trajectories corresponding to the transitions from (b) the state $|1\rangle$ to the state $|3\rangle$, (c) the state $|2\rangle$ to the state $|0\rangle$, (d) the state $|2\rangle$ to the state $|3\rangle$ are shown. The blue dashed and red solid trajectories shall henceforth be called trajectory (2) and (1) respectively. The gray shaded region is the dynamic phase difference between the said trajectories.
phases on the transition amplitude in the corresponding trajectories.

\[
\begin{align*}
\langle 1 \rangle & \rightarrow \langle 1 \rangle : S_{11} = u_g u_\gamma \\
\langle 1 \rangle & \rightarrow \langle 0 \rangle : S_{10} = u_g \sqrt{(1 - u_g^2)(1 - u_\gamma^2)} [e^{i\phi_d^{(1)}(1)} - e^{i\phi_d^{(2)}(1)}] \\
\langle 1 \rangle & \rightarrow \langle 3 \rangle : S_{13} = i \sqrt{1 - u_\gamma^2} \left[ (1 - u_g^2) e^{i\phi_d^{(1)}(1)} - u_g^2 e^{i\phi_d^{(2)}(1)} \right] \\
\langle 1 \rangle & \rightarrow \langle 2 \rangle : S_{12} = i \left( \sqrt{1 - u_\gamma^2} \right) u_g,
\end{align*}
\]  
(A4)

where in the above equation \(e^{i\phi_d^{(1)}(1)}\) and \(e^{i\phi_d^{(2)}(1)}\) are the dynamic phases corresponding to the trajectories (1) and (2) respectively, and phase difference is given by, \(\Delta \phi_d = \phi_d^{(2)}(1) - \phi_d^{(1)}(1) = 4J_z T^2 + |\Delta g_k| T\), which is the area in the \(\epsilon - t\) plane bounded by both the trajectories. \(\pm T\) are the points on the \(t\)-axis where the diabatic levels cross each other and the time axis too. It is easy to recognize from FIG. 10 that the phase difference is same for all the four transition amplitudes where the dynamic phase plays its role. Likewise, all the transition amplitudes corresponding to the transitions from \(\langle 2 \rangle\) are given by,

\[
\begin{align*}
\langle 2 \rangle & \rightarrow \langle 2 \rangle : S_{22} = u_g u_\gamma \\
\langle 2 \rangle & \rightarrow \langle 3 \rangle : S_{23} = -S_{10} \text{ (from symmetry)} \\
\langle 2 \rangle & \rightarrow \langle 0 \rangle : S_{20} = -S_{13} \text{ (from symmetry)} \\
\langle 2 \rangle & \rightarrow \langle 1 \rangle : S_{21} = i \left( \sqrt{1 - u_\gamma^2} \right) u_\gamma,
\end{align*}
\]  
(A5)

Lastly, all the transition amplitudes corresponding to the transitions from the state \(\langle 3 \rangle\) are given by,

\[
\begin{align*}
\langle 3 \rangle & \rightarrow \langle 3 \rangle : S_{33} = u_g u_\gamma \\
\langle 3 \rangle & \rightarrow \langle 2 \rangle : S_{32} = 0, \text{ not an allowed transition} \\
\langle 3 \rangle & \rightarrow \langle 1 \rangle : S_{31} = -i \sqrt{1 - u_\gamma^2} \\
\langle 3 \rangle & \rightarrow \langle 0 \rangle : S_{30} = -iu_\gamma \sqrt{1 - u_\gamma^2}.
\end{align*}
\]  
(A6)

Therefore the transition probability matrix is given by,

\[
P = \begin{pmatrix}
(u_g u_\gamma)^2 & 0 & (1 - u_\gamma^2) & u_\gamma^2 (1 - u_\gamma^2) \\
|S_{10}|^2 & (u_g u_\gamma)^2 & u_\gamma^2 (1 - u_\gamma^2) & |S_{13}|^2 \\
|S_{13}|^2 & u_\gamma^2 (1 - u_\gamma^2) & (u_g u_\gamma)^2 & |S_{10}|^2 \\
(u_\gamma^2 (1 - u_\gamma^2) & (1 - u_\gamma^2) & 0 & (u_g u_\gamma)^2 \\
\end{pmatrix},
\]  
(A7)

where the matrix elements of the above matrix is given by, \(P_{ij} = S_{ij}^* S_{ij}\), and

\[
\begin{align*}
P_{10} &= |S_{10}|^2 = 4u_\gamma^2 (1 - u_\gamma^2) (1 - u_\gamma^2) \sin^2 \left( \frac{\Delta \phi_d (2, 1)}{2} \right) \\
P_{13} &= |S_{13}|^2 = \left[ 1 - 4u_\gamma^2 (1 - u_\gamma^2) \right] (1 - u_\gamma^2) \cos^2 \left( \frac{\Delta \phi_d (2, 1)}{2} \right).
\end{align*}
\]  
(A8)

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