Quenches and dynamical phase transitions in a non-integrable quantum Ising model

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We study quenching dynamics of a one-dimensional transverse Ising chain with nearest neighbor antiferromagnetic interactions in the presence of a longitudinal field which renders the model non-integrable. The dynamics of the spin chain is studied following a slow (characterized by a rate) or sudden quenches of the longitudinal field; the residual energy, as obtained numerically using a t-DMRG scheme, is found to satisfy analytically predicted scaling relations in both the cases. However, analyzing the temporal evolution of the Loschmidt overlap, we find different possibilities of the presence (or absence) of dynamical phase transitions (DPTs) manifested in the non-analyticities of the rate function. Even though the model is non-integrable, there are periodic occurrences of DPTs when the system is slowly ramped across the quantum critical point (QCP) as opposed to the ferromagnetic (FM) version of the model; this numerical finding is qualitatively explained by mapping the original model to an effective integrable spin model which is appropriate for describing such slow quenches. Furthermore, concerning the sudden quenches, our numerical results show that in some cases, DPTs can be present even when the spin chain is quenched within the same phase or even to the QCP while in some other situations they completely disappear even after quenching across the QCP. These observations lead us to the conclusion that it is the change in the nature of the ground state that determines the presence of DPTs following a sudden quench.

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Following the remarkable advancement of the experimental studies of ultracold atoms trapped in optical lattices 1,[2], there is a recent upsurge in the studies of non-equilibrium dynamics of closed quantum systems, in particular from the viewpoint of quantum quenches across a quantum critical point (QCP). 3–4. The relaxation time of the quantum system diverges at the QCP resulting in a non-adiabatic dynamics and proliferation of topological defects in the final state reached after the quench.

According to the Kibble-Zurek (KZ) scaling relation 5–6, generalized to quantum critical systems 7–8, when a d-dimensional quantum system, initially prepared in its ground state, is driven across an isolated QCP, by changing a parameter of the Hamiltonian in a linear fashion as $t/\tau$, the density of defect satisfies the KZ scaling $\tau^{-d\nu/(z\nu+1)}$; here, $\nu$ and $z$ are the correlation length and the dynamical exponent associated with the QCP respectively 9–11. Subsequently several modifications of the scaling have been proposed 12–14. Similarly when the system is quenched to the gapless QCP, the residual energy (the excess energy over the ground state of the final Hamiltonian) scales as $\tau^{-(d+z)\nu/(z
u+1)}$; on the contrary, when quenched to the gapped phase, the residual energy follows a scaling relation identical to that of the defect density. Similar scaling relations for the residual energy and the defect density have also been derived using an adiabatic perturbation theory for a sudden quench of small magnitude 15. (See review articles 16–18).

It is well established that the phase transition in a thermodynamic system is marked by the non-analyticities in the free-energy density whose information can be obtained by analyzing the zeros of the partition function in a complex temperature plane as proposed by Fisher 19. These zeros of the partition function coalesce into a line (or area 20) in complex temperature plane, crossing the real axis in the thermodynamic limit; these crossings mark the non-analyticities in the free-energy density. A similar observation was made earlier by Lee-Yang 21 for a complex magnetic plane. In a similar spirit, a recent work by Heyl et al. 22 introduced the notion of dynamical phase transitions (DPTs) in connection to quantum quenches probing the non-analyticities in the dynamical free energy in the complex time plane. The idea stems from the similarity between the canonical partition function

$$Z(\beta) = \text{Tr} \ e^{-\beta H},$$

of an equilibrium system (where $\beta$ is the inverse temperature) and that of the overlap amplitude (the Loschmidt overlap (LO)) defined at an instant of time $t$ as

$$G(t) = \langle \psi_0 | e^{-iHt} | \psi_0 \rangle,$$

where, in the above equation, $H$ is the final Hamiltonian of the system reached through a sudden quenching of parameters, while $|\psi_0\rangle$ is the ground state of the initial Hamiltonian. Generalizing to the complex time ($z$) plane, one can define the dynamical free energy, $f(z) = -\ln G(z)$; one then looks for the zeros of the $G(z)$, known as Fisher zeros, and can claim the occurrence of DPTs (at real times) when the lines of Fisher zeros cross the imaginary axis. These DPTs are manifested in sharp non-analyticities in the rate function ($I(t) = -\ln |G(t)|^2/N$) at those instants of time. This usually happens when the
system is quenched across the QCP [23]. The initial observation by Heyl et al. [22] for a transverse Ising chain led to a series of works for both integrable and the non-integrable spin chains [24][26] where DPTs were observed for sudden quenches across the QCP. Although, a later work [27] showed that DPTs can occur even when the system is quenched within the same phase. These studies have also been generalized to two-dimensions [28] where topology may play a non-trivial role [28].

A pertinent question at this point is how does the DPT depend on the integrability of the model under consideration or the nature of driving (slow or sudden)? Is quenching across a QCP essential to observe this? In this letter, we shall address these issues in the context of a specific non-integrable model. We note in passing that the LO is also connected to the work-statistics [34–37] and has been generalized to finite temperature [38]. The LO is also connected to the work-statistics [39] and the entropy generation following a quench [40].

The model we consider here is a one-dimensional Ising model with a nearest neighbor antiferromagnetic (AFM) interaction $J$ (scaled to unity in the subsequent discussion) subjected to a transverse field (Γ) as well as a longitudinal field ($h$). This is described by the Hamiltonian [11]

$$H = \sum_i \sigma_i^z \sigma_{i+1}^z - \Gamma \sum_i \sigma_i^x - h \sum_i \sigma_i^z,$$

where $\sigma_i$'s are Pauli matrices. For $h = 0$, the model is integrable with QCPs at $\Gamma = \Gamma_c = \pm 1$, while any non-zero value of $h$ renders the model non-integrable. Furthermore, since the AFM interaction and the field $h$ compete with each other, there is a QPT from AFM ordered phase to the disordered phase at a particular value of $\Gamma_c(h)$ for a given value of $h$. As a result, one finds a phase diagram in the $\Gamma - h$ plane (separating the ordered from the disordered paramagnetic phase, see the supplementary material (SM)) starting from the integrable QCP ($\Gamma_c = 1$, $h = 0$) at one end and terminating at first order transition points at $\Gamma = 0$, $h = \pm 2$ on the $h$-axis.

In this letter, we shall restrict our attention to the case when $\Gamma$ is fixed to $\Gamma_c = 1$ so that the system is at the QCP when $h = 0$; $h$ is driven slowly (i.e., defined by a rate $\tau^{-1}$) or suddenly in the vicinity of the QCP when the system is always initially prepared in its ground state. In the presence of a small $h$, a gap ($\Delta E$) opens up in the energy spectrum and a perturbation theoretic calculation, valid for small $h$, yields $\Delta E \sim h^{\nu_h} = h^2$ [11], where $\nu_h$ is the correlation length exponent associated with the relevant perturbation $h$ and $z$ is the dynamical exponent associated with the QCP at $\Gamma = 1$. Noting that $z = 1$, one concludes that the exponent $\nu_h = 2$. We note that a similar study was reported in reference [42] for a ferromagnetic (FM) Ising chain in a skewed field (having both $\Gamma$ and $h$); however, the universal behavior associated with the FM case is different.

Our results establish that for a sudden quench starting from the QCP as well as a slow quench up to the QCP, numerically obtained residual energies per spin exhibit scaling relations which perfectly match earlier predictions. On the contrary, there is a series of interesting and unexpected results concerning the scenario of DPTs following these quenches which are not reported before. Even though the model is non-integrable, we find prominent existence of DPTs when the longitudinal field is slowly ramped across the QCP. This is remarkable, given the fact that in the FM case [42] sharp
non-analyticities are present in \( I(t) \) in the integrable case for \( h = 0 \) when \( \Gamma \) is ramped across the QCP; on the contrary, those get smoothened out when the skewed field is quenched through the QCP at \( \Gamma = 1 \) so that the system is always non-integrable except at the QCP. On the other hand, for sudden quenches the DPTs are found to occur whenever there is a difference in the nature of the ground states of the initial and the final Hamiltonians irrespective of the fact whether the system is quenched across a QCP or not.

Let us first consider the situation when the field \( h \) is ramped linearly to the QCP \((h = 0)\) as \( h = -t/\tau \) fixing \( \Gamma = 1 \). Denoting the final Hamiltonian \( H_f \) with ground state energy \( E_f^0 \), and final wave function of the system (of length \( N \)) reached after the quench as \( |\psi_f\rangle \), the residual energy per spin is defined by \( \epsilon_{\text{res}} = \langle (\psi_f|H_f|\psi_f) - E_f^0 \rangle /N \). Using the t-DMRG calculations with an open boundary condition, we find \( \epsilon_{\text{res}} \sim \tau^{-4/3} \) (see main part of the Fig. (1)). This is in perfect agreement with the KZ scaling prediction, \( \epsilon_{\text{res}} \sim \tau^{-\nu(d+2)/(\nu+2)} \) with \( \nu = \nu_h = 2 \) and \( z = 1 \) (see the discussion in the SM). We now turn our attention to the sudden quench, in which the system is initially at the QCP and suddenly a small longitudinal field \( h \) is switched on: in this case, numerically we find \( \epsilon_{\text{res}} \sim \hbar^2 \) (Inset, Fig. (1)). According to the prediction of the adiabatic perturbation theory [15], for such a sudden quench of small magnitude starting from the QCP, \( \epsilon_{\text{res}} \) should scale as \( \hbar^{2(d+2)/3} \), as long as the exponent does not exceed 2; this is indeed true in the present case and as a result the exponent saturates to 2.

Having established the scaling of \( \epsilon_{\text{res}} \) for both slow and sudden quenches, we now probe the scenario of possible DPTs. The Loschmidt overlap at an instant \( t \) (where the initial time \( t = 0 \) is set immediately after the quenching is complete) is given by \( G(t) = \langle \psi_f|\exp(-iH_f t)|\psi_f \rangle \) and consequently one defines the rate function \( I(t) = -\ln |G(t)|^2/N \), and investigates its temporal evolution to probe the signature of possible DPTs (namely, the non-analyticities in \( I(t) \)). Results obtained for the slow and sudden quenches obtained by using t-DMRG are presented in Figs. 2 and 3; we below analyze the remarkable findings.

We first analyze the slow-quenching of the model (3) with \( h \sim -t/\tau \), where \( h \) is varied from a large positive to a large negative value. Referring to the Fig. 2 we find that \( I(t) \) shows non-analyticities which appear at regular (and periodic) intervals when \( \tau \gg 1 \) in contrast to the FM case [42]. To analyze this, we recall that for a sufficiently slow driving the dynamics is always adiabatic except in the vicinity of the QCP \((h \ll 1)\) where the relaxation time diverges. Remarkably, the non-integrable Hamiltonian (3) can be mapped to an effective integrable model for \( h \ll 1 \), described the Hamiltonian:

\[
H_{\text{eff}} = (1 - bh^2) \sum_i \tau_i^x \tau_{i+1}^x - \sum_i \tau_i^z, \tag{4}
\]

where \( \tau_i^x \)'s are Pauli spin matrices and \( b \) is a constant which in our case can be chosen to be of the order of unity: this mapping to the model (4) is shown to exactly describe the low-lying excitations of the Hamiltonian (3) in the thermodynamic limit [41]. Consequently so far as the slow quenching is concerned, when the dynamics is non-adiabatic only in the vicinity of a QCP, one can work with the effective Hamiltonian (4) which represents an AFM transverse Ising chain and is equivalent to a FM transverse Ising chain by a simple gauge transformation. Both the models are exactly solvable by Jordan-Wigner transformation. Focussing only at the QCP at \( h = 0 \) and considering a slow ramp of \( h \) from a large positive value to a large negative value with the system initially in its ground state, one can derive the final wave function by numerically integrating the corresponding Schrödinger equation; the rate function thus obtained indeed shows occurrences of the DPTs thereby qualitatively explaining the phenomena we observe here (see the SM for details).

Interestingly, the mapping to the effective Hamiltonian (4) also enables us to explain the absence of DPTs following a sudden quench of small amplitude across the QCP of the original model as presented above in Fig. (3a) be-
cause the interaction term in the equivalent Hamiltonian does not change sign which implies that this quenching does not take the system across the QCP of Hamiltonian $H_2$. This explains the absence of DPT in this case though there is a crossing of QCP in the original model. Though the mapping to the equivalent Hamiltonian is strictly valid for $h \ll 1$, in Fig. 3(a), we show this argument can be extended to explain the absence of DPTs when $h$ is quenched from $+0.7$ to $-0.7$ crossing the QCP at $h = 0$.

Analyzing the original Hamiltonian $H_3$, we note that the ground state is paramagnetic with all spins polarized in the direction of $h$, when $h \gg 1$; on the contrary, it is a quantum paramagnet with majority of spins orienting in the direction of $\Gamma$ when $h \ll 1$. The change in the nature of the ground state is reflected in DPT, irrespective of the fact whether the system crosses the QCP in the process of quenching. In Fig. 3(b), we find a prominent presence of DPTs when $h$ is quenched from 3 to 0.2; here, even though the quenching does not take the original Hamiltonian across a QCP, the nature of ground state changes. Similar DPTs are observed when quenched to the QCP also (Fig. 3(c)). No such DPT is found to occur when the nature of the ground state is the same (e.g., when $h$ is changed from 3 to 2). Finally, when $h$ is suddenly quenched from $+3$ to $-3$ across the QCP, one finds a regular (but not periodic as shown in Fig. 2 occurrence of DPTs (see Fig. 3(d)). This is a generic feature of a sudden quench across the QCP as also observed in the FM case [24] (while the periodic pattern is only a characteristic of the integrability of the underlying Hamiltonian). In this case, the initial and final ground states are nearly fully polarized states with their overlap being exponentially small with the system size; this difference of the ground states results in observed DPTs. When the quench amplitude is further increased (e.g., $h = +5$ to $-5$; see the inset of Fig. 3(d)), both the initial and final Hamiltonians essentially reduce to an assembly of non-interacting spins; in such situations DPTs are rounded off leading to Rabi oscillations between two fully polarized states.

Finally, we summarize the results: we have established that $\epsilon_{\text{res}}$ satisfies universal scaling relations for both sudden and slow quenches. Furthermore, for the slow quenches, the model $H_3$ provides a unique example where one can work with an equivalent integrable model for $\tau \gg 1$. This mapping enables us to explain the KZ scaling and also a periodic occurrence of DPTs for a slow quenching across the QCP. This is remarkable in the sense that, to the best of our knowledge, the presence of DPTs following a slow quench of a non-integrable model has not been reported earlier; in the FM situation, these non-analyticities get smoothened out [12]. Concerning the sudden quench, we also present some remarkable observations: in some cases, DPTs do not occur even when the system is quenched across the QCP; but they may appear when the system is quenched within the same phase (even to the QCP). For very large amplitude quench of $h$ across $h = 0$, DPTs get rounded off. These observations lead us to the conclusion that concerning the sudden quenches, it is the change in the nature of the ground state that is responsible for DPTs.

We would like to conclude with the note that the Hamiltonian $H_3$ has been experimentally studied using Bose atoms in an optical-lattice [43], with $\Gamma \ll h$. The field $\Gamma$ of the equivalent spin chain is determined by the hopping amplitude $t$ of the Bose atoms and is given by $\gamma/2t$; $\Gamma$ is necessarily kept small to stabilize the Mott state necessary for the realization of a spin system. On the other hand, a quantum Monte-Carlo study [14] shows that in one dimension it should be possible to achieve a field $\Gamma \approx 1$. Therefore it should be possible to verify some of the situations of the present study in experimental systems.

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Supplementary Material on “Quenches and dynamical phase transition in a non-integrable quantum Ising model”

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In this supplementary material, we shall illustrate how to derive the Kibble-Zurek scaling relation of the residual energy of the original Hamiltonian

\[ H = \sum_i \sigma_i \sigma_{i+1} - \Gamma \sum_i \sigma_i - h \sum_i \sigma_i, \] \quad (S1)

when the longitudinal field \( h \) is quenched as \(-t/\tau\), and also show how the behavior of the Fisher zeros in the complex time plane dictates the occurrence of DPTs for such a slow quench. The transverse field \( \Gamma \) is always set to unity so that the system is at the integrable quantum critical point (QCP) when \( h = 0 \). The phase diagram of the model and the quenching path are shown in Fig. S1.

\[ \text{FIG. S1: The schematic phase diagram of the model given in Eq. (S1); the solid line extending from (0, h = 2) to (0, h = -2) through (1, h = 0) separates the antiferromagnetic (AFM) phase from the paramagnetic (PM) phase. The points (0, h = ±2) denote the first order transition while (1, h = 0) corresponds to the integrable quantum critical point. Throughout this paper, \( \Gamma \) is set equal to 1 and \( h \) is quenched along the dashed line shown with an arrow.} \]

THE KIBBLE-ZUREK SCALING

As emphasized in the main text, so far as the slow quenching of the longitudinal field \( h \) is concerned (especially, for large \( \tau \)), one can equivalently work with the effective integrable Hamiltonian given by

\[ \hat{H}_{\text{eff}} = (1 - b h^2) \sum_i \tau_i \tau_{i+1} - \sum_i \tau_i, \] \quad (S2)

where \( b \) is a constant \textsuperscript{[S1]} which is inessential in the argument below, and hence set equal to unity hereafter. Using a gauge transformation (which flips the spins of alternate sites) and a duality transformation \textsuperscript{[S2]}, the Hamiltonian in Eq. (S2) can be mapped to an equivalent dual Hamiltonian with a nearest neighbor ferromagnetic (FM) interactions:
\[ \hat{H}_{\text{eff}} = -\sum_i \tilde{\tau}_i^z \tilde{\tau}_{i+1}^z - (1 - h^2) \sum_i \tilde{\tau}_i^x \]
\[ = -\sum_i \tilde{\tau}_i^z \tilde{\tau}_{i+1}^z - \sum_i \tilde{\tau}_i^x + h^2 \sum_i \tilde{\tau}_i^x \] (S3)

which is a FM transverse Ising Hamiltonian in an effective transverse field \( \Gamma_{\text{eff}} = 1 - h^2 \). We note that \( \hat{H}_{\text{eff}} \) with \( h = 0 \) represents a critical Hamiltonian. Using the Fourier transformation followed by the Jordan-Wigner transformation, the model can be reduced to a two-level problem in the basis \(|0\rangle \) (no fermion state) and \(|k, -k\rangle \) (a state with a pair of fermions with quasi-momenta \( k \) and \(-k \), respectively) \([S3] \); the reduced \( 2 \times 2 \) Hamiltonian is then given by

\[ H_k(h) = 2 \left( \begin{array}{cc} (1 - h^2) - \cos k & -i \sin k \\ i \sin k & -(1 - h^2) + \cos k \end{array} \right). \] (S4)

Analyzing the spectrum, \( \epsilon_k = 2 \sqrt{\{(1 - h^2) - \cos k\}^2 + \sin^2 k} \), it is straightforward to show that the model (S3) has three QCPs: the energy gap \( (2\epsilon_k) \) vanishes at critical points at \( h = 0 \) and \( h = \pm \sqrt{2} \), with the corresponding critical wave vector (for which the energy gap vanishes) \( k_c = 0 \) and \( \pi \), respectively. We are however interested in the transition at \( h = 0 \) which is the only relevant QCP to the context of the original Hamiltonian (S1). To focus on the critical point at \( h = 0 \), we expand the Hamiltonian (S1) in the vicinity of \( k = 0 \) to arrive at the Hamiltonian

\[ H_k(h) = 2 \left( \begin{array}{cc} -h^2 + \frac{k^2}{2} & -ik \\ ik & h^2 - \frac{k^2}{2} \end{array} \right), \] (S5)

which shows only one quantum critical point at \( h = 0 \). Analyzing the simplified form of the spectrum \( \epsilon_k = \sqrt{(h^2 - k^2/2)^2 + k^2} \), one immediately finds for \( h = 0 \), the gap \( (\Delta E_k = 2\epsilon_k) \sim k \), yielding \( z = 1 \) and for \( k = 0 \), gap scales as \( h^2 \) yielding \( \nu z = 2 \), and hence \( \nu = 2 \) (referred to as \( \nu_h \) in the main text).

Let us now point out that the quenching \( h = -t/\tau \), with \( t \) going from \( -\infty \) to \( 0 \), in the original Hamiltonian is equivalent to driving the reduced Hamiltonian (S5) from \( h \rightarrow \infty \) to the QCP at \( h = 0 \) by a non-linear protocol \((t/\tau)^2\); in both the cases the system is initially prepared in its ground state. Even though the non-adiabatic transition probability for the mode \( k \) \((p_k)\) cannot be calculated directly using the Landau-Zener formula for such a non-linear protocol, one can make appropriate rescaling in the corresponding Schrödinger equations \([S3, 4, 0]\) to argue that it would be a function of the dimensional combination of \( k^2 \tau^{4/3} \), i.e., \( p_k = \mathcal{F}(k^2 \tau^{4/3}) \) where \( \mathcal{F} \) is an unknown scaling function. Since the gapless QCP is characterized by gapless excitations \( k \), the scaling of the residual energy can be obtained as \( \epsilon_{\text{res}} \sim \int dk \mathcal{F}(k^2 \tau^{4/3}) \sim \tau^{-4/3} \); this matches perfectly with the KZ prediction with \( d = z = 1 \) and \( \nu = 2 \) and the numerical result presented in the main text.

**SLOW QUENCHING AND NON-ANALYTICITIES IN THE RATE FUNCTION**

We shall now calculate the nature of the Fisher zeros of the effective partition function \([S7]\) obtained from the Loschmidt overlap (LO) when the parameter \( h \) of the Hamiltonian (S3) is quenched from a large positive to a large negative value following the protocol \( h = -t/\tau \); this is equivalent to the slow quenching of the longitudinal field \( h \) in the original Hamiltonian (S1). But there is a subtle difference that needs to be emphasized: the field \( h \) contributes a quadratic \( h^2 \) term to the transverse field of the equivalent model (S3), thus as \( h \) is linearly changed from a large positive value to the negative value in model (S1), the parameter \( h^2 \) changes from a positive initial value to zero (i.e., the QCP) and returns to the original initial value at the final time; this in a sense is a reverse quenching of the transverse field of the Hamiltonian (S3) as studied in [S8] in a non-linear fashion.

To calculate the Loschmidt overlap of a system of length \( N \) defined by \( f(z) = -\ln \langle \psi_f | \exp(-H_f z) | \psi_f \rangle / N \), where \( z \) is the complex time, \( H_f \) is the final Hamiltonian and \( | \psi_f \rangle \) the state reached following the quantum quench, we focus on the reduced \( 2 \times 2 \) Hamiltonian (S3). Summing over the contributions from all the momenta mode, a few lines of algebra leads us to the expression \([S9]\)

\[ f(z) = -\int_0^\pi \frac{dk}{2\pi} \ln \left( (1 - p_k) + p_k \exp(-2\epsilon_k^* z) \right) \] (S6)
where $p_k$ is the non-adiabatic transition probability for the mode $k$. The zeros of the “effective” partition function (where $f(z)$ is non-analytic) are given by:

$$z_n(k) = \frac{1}{2\epsilon_k} \left( \ln\left( \frac{p_k}{1 - p_k} \right) + i\pi(2n + 1) \right),$$

where $n = 0, \pm 1, \pm 2, \cdots$. For a non-linear reverse quenching protocol, the expression for $p_k$ can not be exactly determined using the LZ formula (though an exact form can be obtained for the linear case [S8]). However, it can be argued $p_k = \mathcal{G}((k - k_0)^2\tau^{4/3})$, where $k_0$ is the wave vector for which $p_k$ is maximum which shifts to $k = 0$ for large $\tau$ and $\mathcal{G}$ is an unknown function. We find from Eq. (S7) Fisher zeros cross the imaginary axis for a particular value of $k_*$ for which $p_{k_*} = 1/2$ [S9, 10] and the rate function shows sharp non-analyticities at $t_n^* = \pi(n + \frac{1}{2})/\epsilon_{k_*}^t$.

For the present case, to calculate the Fisher zeros and especially the rate functions $I(t)$ we shall use the form of the Hamiltonian near $k = 0$ given in Eq. (S5) (to avoid the influence of the QCP at $h = \sqrt{2}$), when $h$ is quenched from $+3$ to $-3$. Numerically integrating the Schrödinger equation describing the dynamics of the Hamiltonian (S5) with the initial condition that the system is in the ground state of the initial Hamiltonian, we obtain the value of $p_k$ which is then substituted in the expression of the rate function:

$$I(t) = -\int_0^\pi \frac{dk}{2\pi} \log \left( 1 + 4p_k(p_k - 1) \sin^2 \epsilon_k^t \right).$$

As shown in Fig. S2 this qualitatively explains the periodic occurrence of DPTs presented in Fig. 2 in the main text.

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