Nonadiabatic Phase Transition with Broken Chiral Symmetry

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We explore nonadiabatic quantum phase transitions in an Ising spin chain with a linearly time-dependent transverse field and two different spins per unit cell. Such a spin system passes through critical points with gapless excitations, which support nonadiabatic transitions. Nevertheless, we find that the excitations on one of the chain sub-lattices are suppressed in the nearly-adiabatic regime exponentially. Thus, we reveal a coherent mechanism to induce exponentially large density separation for different quasiparticles.

The separation of two slightly different types of particles is often encountered both in applied and fundamental research. One example is the apparent asymmetry between matter and antimatter in our Universe. Observations prove that the symmetry between matter and antimatter was broken, presumably early on in the history of the Universe. However, it is still unclear how the subtle CP symmetry violation could lead to the large observed differences at the cosmological scale [1]; although it is known that when the characteristic asymmetry energy scale is very small, the large density difference has to be produced during a nonequilibrium process [2].

The goal of this article is to introduce a mechanism for controlling different quasiparticles separately using exponential sensitivity of quantum nonadiabatic transitions to symmetry-breaking interactions. Namely, when parameters of a quantum system change with time adiabatically, the system remains in the instantaneous eigenstate, e.g., the ground state. However, the Kibble-Zurek mechanism [3–11] predicts that the number of nonadiabatic excitations is not suppressed exponentially if a macroscopic system passes through a quantum critical point at which the energy gap to excitations closes. Without an asymmetry of interactions, different particle species would pass through the same phase transition simultaneously. However, even a small asymmetry generally opens the gap to certain excitation types, even though the critical point is not destroyed. Thus, we can harvest the excitations of one type and suppress the others.

A broadly known quantum example that confirms the Kibble-Zurek mechanism is the model of a uniform Ising spin chain in a transverse magnetic field [12–14], with the Hamiltonian

\[ \hat{H}_u = \sum_{n=1}^{N} \left[ B \hat{\sigma}_n^z + J \hat{\sigma}_n^x \hat{\sigma}_{n+1}^x \right], \quad B = -\beta t, \tag{1} \]

where \( \hat{\sigma}_n^x, \hat{\sigma}_n^z \) are Pauli operators for the \( n \)-th spin, \( J \) is the spin-spin coupling, and \( B \) is the transverse time-dependent field that changes with rate \( \beta > 0 \). This model has two Dirac points at \( B = \pm J \), at which its spectral gaps close, and which mark boundaries between three phases. The phase with strong quantum correlations (Fig. 1 top) contains the point \( B = 0 \) with two degenerate ground states:

\[ |\rightarrow \rightarrow \rightarrow \rightarrow \rangle \quad \text{and} \quad |\leftarrow \leftarrow \leftarrow \leftarrow \rangle. \tag{2} \]

For \( B(t) = -\beta t \), the model is exactly solvable [12]. If the system starts from the fully polarized ground state

\[ |\downarrow \downarrow \downarrow \downarrow \downarrow \rangle \tag{3} \]

as \( t \to -\infty \), then in the thermodynamic limit of this...
solution, after the passage through a critical point the number of non-adiabatic excitations follows a power law:

$$\rho \sim J^{-1} g^{1/2}. \tag{4}$$

Let us now explore robustness of the Ising model predictions by considering a spin chain whose unit cell contains two different spins, with the Hamiltonian

$$\hat{H} = \sum_{n=1}^{N} \left[ -\frac{b_1 t}{2} \hat{\sigma}^z_{2n} - \frac{b_2 t}{2} \hat{\sigma}^z_{2n+1} \right] +$$

$$+ \sum_{n=1}^{N} \left[ J_1 \hat{\sigma}^z_{2n} \hat{\sigma}^z_{2n+1} + J_2 \hat{\sigma}^z_{2n+1} \hat{\sigma}^z_{2n+2} \right]. \tag{5}$$

The difference between $b_1$ and $b_2$ is due to different spin $g$-factors, and $J_1 \neq J_2$ reflects the lack of inversion symmetry at zero field. Periodic boundary condition is imposed. Figure 1 (bottom) illustrates the structure of this spin chain.

Without loss of generality, here and in what follows, we assume $b_1 > b_2$; namely, the spins on the even sites sublattice have a larger $g$-factor than those on the odd sites. We note that for weak symmetry breaking, $|J_1 - J_2| \ll |J_1 + J_2|$ and $|b_1 - b_2| \ll |b_1 + b_2|$, the ground state polarizations at $B = 0, \pm \infty$ are the same for spins with odd and even indices, and the spin excitations on different sublattices then resemble particles of two slightly different types of matter.

Via the Jordan-Wigner transformation, Hamiltonian (5) reduces to a quadratic form of fermionic operators, $\hat{c}$ and $\hat{d}$, on the even and odd sites, respectively. The details are presented in Appendix A of the Supplemental Material (SM). Thus,

$$\hat{\sigma}^z_{2n} = 1 - 2c^\dagger_n c_n, \quad \hat{\sigma}^z_{2n+1} = 1 - 2d^\dagger_n d_n. \tag{6}$$

It is convenient to work with the Fourier transformed operators

$$\hat{c}_p = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} c_n e^{-ipn}, \quad \hat{c}^\dagger_p = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} c^\dagger_n e^{ipn}, \tag{7}$$

and similarly defined $\hat{d}_p, \hat{d}^\dagger_p$. We will assume that $N$ is even, so the momentum takes discrete values $p = \pm(2k-1)\pi/N, k = 1, ..., N/2$. Hamiltonian (5) then is

$$\hat{H} = \sum_{p \neq 0} \hat{a}^\dagger_p H_p \hat{a}_p, \tag{8}$$

where $\hat{a}_p$ and $H_p$ are given by

$$\hat{a}_p = \begin{pmatrix} \hat{c}_p \\ \hat{c}^\dagger_p \\ \hat{d}_p \\ \hat{d}^\dagger_p \end{pmatrix}, \quad H_p = \begin{pmatrix} b_1 t & 0 & g & \gamma \\ 0 & -b_1 t & -g & \gamma \gamma^* \\ g^* & -g^* & b_2 t & 0 \\ \gamma & -\gamma^* & 0 & -b_2 t \end{pmatrix}. \tag{9}$$

with the couplings

$$g \equiv J_1 + J_2 e^{-ip}, \quad \gamma \equiv J_1 - J_2 e^{-ip}. \tag{10}$$

In the Heisenberg’s picture, the evolution of $\hat{a}_p$ is described by a Schrödinger-like equation:

$$i \hbar \hat{a}_p(t) = H_p(t) \hat{a}_p(t), \tag{11}$$

and the initial ground state (3) corresponds to the initially fully filled Fermi sea, for all fermions as $t \to -\infty$.

In Fig. 2, we show the time-dependent eigenvalues of the matrix $H_p$ for a broken chiral symmetry: $J_1 \neq J_2$ and $b_1 > b_2$. Figure 2(a) shows that at $p = 0$ two of the four energy levels experience exact level crossings, whereas Fig. 2(b) illustrates that this degeneracy is lifted for nonzero $p$. This means that the chiral asymmetry does not destroy the Dirac points in the spectrum, which must produce a power law density of excitations according to the Kibble-Zurek mechanism.

We will consider the evolution with the Hamiltonian (5) during the time interval $t \in (-\infty, +\infty)$. In terms of the phase diagram in Fig. 1, this means that the system passes through two phase transition points. In the adiabatic limit, the initial ground state (3) transfers, as $t \to +\infty$, into the ground state with all spins up

$$\uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow. \tag{12}$$

This is the fermionic vacuum, and the free fermions are the elementary excitations. The numbers of excitations (non-flipped spins) on the even and odd sublattices at the end of the protocol are given by, respectively,

$$N^e_{ex} = \sum_{n=1}^{N} \langle \hat{c}_n^\dagger \hat{c}_n \rangle = \sum_{p} \langle \hat{c}_p^\dagger \hat{c}_p \rangle, \tag{13}$$

$$N^o_{ex} = \sum_{n=1}^{N} \langle \hat{d}_n^\dagger \hat{d}_n \rangle = \sum_{p} \langle \hat{d}_p^\dagger \hat{d}_p \rangle. \tag{14}$$
where, in the Schrödinger’s picture, the averaging is taken over the state at \( t = +\infty \).

The Hamiltonian \( \text{(9)} \) has the form of a multistate Landau-Zener (MLZ) model, i.e., can be written as \( H(t) = A + Bt \) with hermitian matrices \( A \) and \( B \). The MLZ models have been extensively studied previously [15-17]. Our case with \( J_1 \neq J_2 \) is generally not solvable [18] but the MLZ theory provides exact formulas for some of the evolution matrix elements [19], which we will utilize.

Let us define the \( S \)-matrix
\[
S = S(p) = U^p(T, -T)_{T \to \infty},
\]
where \( U^p(T, -T) \) is the evolution matrix over the time interval \( t \in (-T, T) \) with the Hamiltonian \( H_p \). We can say that the operators at \( t = +\infty \) are related by
\[
\hat{a}_p(+\infty) = S\hat{a}_p(-\infty),
\]
where \( \hat{a}_p \equiv \hat{a}_p(-\infty) \). Hence,
\[
\dot{c}_p(+\infty) = S_{11}\dot{c}_p + S_{12}\dot{c}_p^\dagger + S_{13}\dot{d}_p + S_{14}\dot{d}_p^\dagger,
\]
\[
\dot{c}_p^\dagger(+\infty) = S_{11}\dot{c}_p^\dagger + S_{12}\dot{c}_p + S_{13}\dot{d}_p^\dagger + S_{14}\dot{d}_p.
\]
The number of excitations \( \text{(13)} \) can be evaluated in the Heisenberg’s picture, i.e., taking the average of the operators at \( t = +\infty \) with respect to the initial state \( \text{(3)} \):
\[
N_{ex}^e(+\infty) = \sum_p (|S_{11}|^2 + |S_{13}|^2).
\]
The survival amplitudes for states with the highest energy level slopes are known exactly for any MLZ model [15]:
\[
S_{11} = S_{22} = e^{-\pi|S_{12}|^2/2 - \pi|S_{13}|^2/2}. \tag{19}
\]
Another exact relation of MLZ theory is for the transition amplitudes between the levels with the two highest slopes [19]:
\[
S_{11}S_{33} + |S_{13}|^2 = e^{-\pi|S_{12}|^2/2 + \pi|S_{13}|^2/2}. \tag{20}
\]
This does not fix \( S_{13} \) because \( S_{33} \) is not known. Fortunately, model \( \text{(9)} \) has discrete symmetries leading to
\[
S_{11} + S_{22} = S_{33} + S_{44}, \quad S_{33}(-p) = S_{44}(p), \tag{21}
\]
the derivations of which are given in Appendix B of the SM. Equations \( \text{(19)} \)-\( \text{(21)} \) then predict
\[
\sum_p |S_{13}|^2 = \sum_p \left[ e^{-\pi|S_{12}|^2/2 + \pi|S_{13}|^2/2} - |S_{11}|^2 \right]. \tag{22}
\]
This formula is exact. Hence, without approximations
\[
N_{ex}^e(+\infty) = \sum_p e^{-\pi|S_{12}|^2/2 + \pi|S_{13}|^2/2}. \tag{23}
\]
As \( N \to \infty \), we replace \( \sum_p /N \to \int_{-\pi}^{\pi} dp/(2\pi) \), and find the density of excitations (per unit cell) in the thermodynamic limit
\[
\rho_{ex}^e(+\infty) = e^{-\pi|S_{12}|^2/2 + \pi|S_{13}|^2/2} I_0 \left( \frac{4\pi J_1 J_2}{b_1 + b_2} \right), \tag{24}
\]
where \( I_0(x) \) is the modified Bessel function of the first kind. In the leading order of small \( b_1 + b_2 \)
\[
\rho_{ex}^e(+\infty) \approx e^{-\frac{\pi|S_{12}|^2}{b_1 + b_2}} \frac{\sqrt{b_1 + b_2}}{2\pi \sqrt{2J_1 J_2}}. \tag{25}
\]
This is the central result of our article. For any \( J_1 \neq J_2 \) the excitations on the even-sublattice are suppressed exponentially rather than by a power-law. The latter is found only for a symmetric case with \( J_1 = J_2 \) but \( b_1 > b_1 \). Complete exact solution for this special case is presented in Appendix D of the SM. We also note that the above solutions do not smoothly carry over \( b_1 = b_2 \) point, to which our exact MLZ analysis does not apply because of the degeneracy of the time-dependent Zeeman coupling.

Equation \( \text{(25)} \) does not contradict the Kibble-Zurek mechanism because the power-law for excitation density does appear on the odd-site sublattice. Consider
\[
N_{ex}^o(+\infty) = \sum_p (|S_{33}|^2 + |S_{31}|^2). \tag{26}
\]
Here, $|S_{31}|^2$ can be obtained exactly because $|S_{31}| = |S_{33}|$. According to Eq. (22), it produces an exponentially suppressed contribution. We also prove in Appendix C of the SM that $\sum_p |S_{33}|^2 \geq \sum_p |S_{11}|^2$, so, $N_{ex}^e \geq N_{ex}^o$. Hence, only $S_{33}$ contains the information about the power-law scaling.

The exact crossings of the 2nd and 3rd adiabatic levels of $H_p$ happen at $p = 0$ and time moments

$$t_{1,2} = \mp 2\sqrt{J_1J_2/(b_1b_2)}. \quad (27)$$

We interpret $t_{1,2}$ as the moments of the phase transitions. By setting $t = t_{1,2} + \delta t$ and $p = \delta p$, with small $\delta p$ and $\delta t$, we find an effective Hamiltonian for the interactions within the subspace of $H_p$ spanned by the two eigenstates, whose energies become nearly degenerate near the critical points:

$$\hat{H}_{eff} \approx \frac{2\sqrt{J_1J_2b_1b_2}((\sqrt{J_1J_2}\delta \tau_x + \sqrt{b_1b_2}\delta t \tau_z)}{\sqrt{(b_2J_1 + b_1J_2)(b_1J_1 + b_2J_2))}}, \quad (28)$$

where $\tau_x$ and $\tau_z$ are the Pauli operators that act in subspace of two states with closest to one Dirac point energies. The Landau-Zener formula applied to Hamiltonian (28) returns the probability of a non-adiabatic excitation after a transition through one Dirac point:

$$P_{ex} = \exp \left( -\frac{2\pi(\delta p)^2(J_1J_2)^{3/2}}{(b_2J_1 + b_1J_2)(b_1J_1 + b_2J_2))} \right). \quad (29)$$

Our system passes through two Dirac points. An excitation created near the first point should remain excited after the second point. The system may also not produce an excitation during the first crossing but produce it at the second one. Generally, there is interference between such evolution paths (Stueckelberg’s oscillations). If we disregard this interference, the probabilities of the two possibilities simply sum, i.e.,

$$P_{2ex} = 2P_{ex}(1 - P_{ex}). \quad (30)$$

Integrating $P_{2ex}$ over $\delta p \in (-\infty, +\infty)$, we find that in the adiabatic limit:

$$\sum_p |S_{33}|^2 \frac{N}{2} \approx \frac{2 - \sqrt{2}}{4\pi(J_1J_2)^{3/4}} [(b_2J_1 + b_1J_2)(b_1J_1 + b_2J_2)]^{1/4}. \quad (31)$$

This is the estimate of the excitation density on the odd-site sublattice in the nearly-adiabatic limit. In Fig. 3, the numerical simulations confirm the power-law scaling trend for the parameter dependence in (31), which is modulated by fast Stueckelberg oscillations. We also note that (31) reproduces correctly the scaling prediction of the uniform chain model (4) if we set $b_1 = b_2 = 2\beta$ and $J_1 = J_2$.

Hence, as $t \to +\infty$, the remaining excitations on the odd-site sublattice are suppressed according to a power-law, in contrast to the exponential suppression on the even-site sublattice. At the intermediate moment, $t \to 0$, excitations take the form of superpositions of kinks. The asymmetry appears then too, i.e., some of the excitations are exponentially suppressed in comparison to the others but this effect does not have a simple interpretation in terms of different kink types. We leave such details to Appendix E of the SM.

Our results illustrate how the Kibble-Zurek mechanism works when a part of a system is not observable. The latter may happen in atomic gases, in which optically observable spins interact via spins of other atomic species [20]. In the asymmetric Ising chain, if the spin excitations on the odd sites are not observable, the even-site spins still create a visible ferromagnetic state at zero external field and polarize when the external field is strong. Hence, looking only at the even spins, one can expect that this system goes through the same phase transitions as the uniform Ising chain and thus produces excitations with a power-law scaling. Our solution shows, however, that all observable spin excitations are suppressed in this case exponentially. A power-law tail of the excitations is hidden then in the non-observable spins.

Summarizing, we demonstrated that small differences between interacting spins in a simple spin chain can lead to an exponentially large effect when passing slowly through a phase transition. The underlying mechanism arguably processes universalities: strong but symmetric interactions compete with each other near a critical point, where subtle interaction differences play a decisive role. As long as a symmetry breaking opens the gap for certain types of quasi-particles while not destroying the critical point, the exponentially large density separation of different quasi-particles should happen after the passage through the phase transition independently of the model’s microscopic details.

The Kibble-Zurek mechanism for Ising-type quantum phase transition has been recently studied experimentally in ultracold atoms [9]. In such systems an asymmetry can be introduced by placing atoms in a periodic potential without the inversion symmetry. If the time-linear field ramp is induced by changing the AC-frequency in the rotating-wave approximation, the sweeping of the detuning frequency across an optical resonance effectively mimics the field changes in range $B_z \in (+\infty, -\infty)$ [21, 22]. Hence, the demonstration of our effect requires only simple modification of the control protocols in already accessible for studies dynamic phase transitions.

Let us also speculate about possible applications. Different isotopes have different spin interactions in an ultracold atomic mixture [23]. Hence, an adiabatic passage through a quantum critical point can induce spin excitations in this mixture, overwhelmingly, for only one of the isotopes. One can then separate such excited atoms using the magnetic deflection approach from [24], and thus develop a technology for isotope separation. The asymmetry of matter and antimatter in our Universe may also be viewed now as a result of a hypothetical transition through a quantum critical point during cosmic inflation, when the matter could be excited from the vacuum via
quantum nonadiabatic processes [25, 26].

The dynamic phase transitions are found broadly, from cosmological models to the experiments with superconductors and ultracold atoms. They are likely responsible for the scaling of mistakes that limit the quantum annealing computation techniques [27]. Fortunately, different systems show universal behavior, which is driven by relatively simple effects near the critical point. The quasi-particle separation is one of such effects that remain relevant near the critical point and thus can be used for control of complex quantum systems.

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Appendix A: Jordan-Wigner transformation

For the model Hamiltonian

$$\hat{H} = \sum_{n=1}^{N} \left[ -\frac{b_1 t}{2} \hat{\sigma}_n^z - \frac{b_2 t}{2} \hat{\sigma}_n^x \right] + \sum_{n=1}^{N} \left[ J_1 \hat{\sigma}_{2n}^x \hat{\sigma}_{2n+1}^x + J_2 \hat{\sigma}_{2n+1}^x \hat{\sigma}_{2n+2}^x \right] \quad (A1)$$

with periodic boundary condition, we define two separate sets of Jordan-Wigner transformation for the sublattices with even and odd indices, i.e.,

$$\begin{align*}
\hat{\sigma}_n^x &= 1 - 2 \hat{c}_n^\dagger \hat{c}_n, \\
\hat{\sigma}_{2n+1}^x &= 1 - 2 \hat{d}_n^\dagger \hat{d}_n, \\
\hat{\sigma}_{2n}^x &= -(\hat{c}_n^\dagger + \hat{c}_n) \prod_{m<n} (1 - 2 \hat{c}_m^\dagger \hat{c}_m)(1 - 2 \hat{d}_m^\dagger \hat{d}_m), \\
\hat{\sigma}_{2n+1}^x &= -(\hat{d}_n^\dagger + \hat{d}_n) \prod_{m<n} (1 - 2 \hat{c}_m^\dagger \hat{c}_m)(1 - 2 \hat{d}_m^\dagger \hat{d}_m),
\end{align*} \quad (A2)$$

where

$$\begin{align*}
\{ \hat{c}_n, \hat{c}_{n'} \} &= \{ \hat{c}_n^\dagger, \hat{c}_{n'}^\dagger \} = \{ \hat{d}_n, \hat{d}_{n'} \} = \{ \hat{d}_n^\dagger, \hat{d}_{n'}^\dagger \} = 0, \\
\{ \hat{c}_n, \hat{d}_{n'} \} &= \{ \hat{c}_n^\dagger, \hat{d}_{n'}^\dagger \} = \{ \hat{c}_n^\dagger, \hat{d}_{n'} \} = \{ \hat{d}_n, \hat{d}_{n'}^\dagger \} = 0, \\
\{ \hat{c}_n, \hat{c}_{n'}^\dagger \} &= \{ \hat{d}_n, \hat{d}_{n'}^\dagger \} = 0.
\end{align*}$$

Their Fourier transforms are defined as

$$\begin{align*}
\hat{c}_p &= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \hat{c}_n e^{-ipn}, \\
\hat{c}_p^\dagger &= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \hat{c}_n^\dagger e^{ipn}.
\end{align*} \quad (A3)$$

Due to the periodic boundary condition of the spin chain, the discrete momentum takes values in the range \((-\pi, \pi),

$$\begin{align*}
p &= \pm (2k - 1)\pi/N, \quad k = 1, ..., N/2, \quad N \text{ even}; \\
p &= \pm 2k\pi/N, \quad k = 1, ..., (N - 1)/2, \quad N \text{ odd}. \quad (A4)
\end{align*}$$

In terms of the fermionic operators, the original spin chain Hamiltonian (A1) transforms to

$$\hat{H} = \sum_{p>0} \hat{a}_p^\dagger \hat{H}_p \hat{a}_p, \quad (A5)$$

where \(\hat{a}_p\) and \(\hat{H}_p\) are defined as

$$\begin{align*}
\hat{a}_p &= \begin{pmatrix} \hat{c}_p \\ \hat{c}_p^\dagger \\ \hat{d}_p \\ \hat{d}_p^\dagger \end{pmatrix}, \\
\hat{H}_p &= \begin{pmatrix} b_1 t & 0 & g & \gamma \\ 0 & -b_1 t & -\gamma & -g \\ g^* & -\gamma^* & b_2 t & 0 \\ \gamma^* & -g^* & 0 & -b_2 t \end{pmatrix},
\end{align*} \quad (A6)$$

with the couplings

$$g \equiv J_1 + J_2 e^{-ip}, \quad \gamma \equiv J_1 - J_2 e^{-ip}. \quad (A7)$$
Appendix B: Derivation of analytically exact $\sum_p |S_{13}|^2$

Consider the $S$-matrix in the 4-level Landau-Zener problem of the Hamiltonian $\hat{H}_p$, which is defined in Eq. (A6). Here, the $S$-matrix refers to the unitary matrix

$$S = S(p) \equiv U^p(T, -T)_{T \to \infty}, \quad (B1)$$

with $U^p(T, -T)$ the evolution matrix over the time interval $t \in (-T, T)$ with the Hamiltonian $\hat{H}_p$.

This model belongs to a particularly well-understood subclass of multilevel Landau-Zener problems. Namely, it contains bipartite interactions and all diabatic levels are crossing in one point in the time-energy diagram [19]. Here “bipartite” means that all states can be partitioned into two groups, such that states in one group are coupled directly only to states in the other group; and the diabatic levels are linearly time-dependent diagonal elements of the Hamiltonian. Following Ref. [19], we list here three properties of the scattering matrix that are essential for solving the exact solutions:

(i) As in all other MLZ systems, the amplitudes of surviving on the levels with the lowest and highest slopes are given by the Brundobler-Elser formula:

$$S_{11} = S_{22} = e^{-\frac{|g|^2}{4T} - \frac{|\gamma|^2}{4T}}. \quad (B2a)$$

Considering the definition of $g$ and $\gamma$ in (A7), this means also that

$$S_{11}(p) = S_{22}(p) = S_{11}(-p) = S_{22}(-p). \quad (B2b)$$

(ii) The other two diagonal elements of the scattering matrix, $S_{33}$ and $S_{44}$, can be different from each other and from Eq. (B2a), but they are real and satisfying the relations (see Eq. (21) in Ref. [19]):

$$S_{11}S_{33} + |S_{13}|^2 = e^{-\frac{2|\gamma|^2}{4T}} \quad (B3a)$$

$$S_{44}S_{22} + |S_{42}|^2 = e^{-\frac{2|\gamma|^2}{4T}} \quad (B3b)$$

(iii) Following Ref. [19], we can derive one more constraint for the diagonal elements of the $S$-matrix. Define a matrix

$$\Theta \equiv \begin{pmatrix} \hat{I}_2 & 0 \\ 0 & -\hat{I}_2 \end{pmatrix},$$

where $\hat{I}_2$ is a $2 \times 2$ identity matrix. It can be verified that Hamiltonian $H_p$ satisfies

$$\Theta H_p(-t) \Theta = -H_p(t). \quad (B4)$$

Consider the formal expression of the evolution operator

$$U(T, 0) = \lim_{dt \to 0} \prod_{n=0}^{T/dt} e^{-iH_p(t_n)dt},$$

where $t_n = ndt$ and the product is time ordered. By inserting the resolution of the identity $\mathbb{1} = \Theta \Theta$ after each factor in the product, and using relation (B4), we get

$$\Theta U(T, 0) \Theta = \lim_{dt \to 0} \prod_{n=0}^{T/dt} \Theta e^{-iH_p(t_n)dt} \Theta$$

$$= \lim_{dt \to 0} \prod_{n=0}^{T/dt} e^{iH_p(-t_n)dt} = U^\dagger(0, -T)$$

Let us take the trace of the evolution operator multiplied by $\Theta$, i.e.,

$$\text{Tr} [U(T, -T) \Theta] = \text{Tr} [U(0, -T) \Theta U(T, 0)]$$

$$= \text{Tr} [U(0, -T) \Theta U(T, 0) \Theta]$$

$$= \text{Tr} [U(0, -T)U^\dagger(0, -T) \Theta] = \text{Tr} [\Theta].$$
This implies that the $S$-matrix satisfies $\text{Tr}[S\Theta] = \text{Tr}[\Theta] = 0$, which imposes a constrain on the diagonal elements,

$$S_{11} + S_{22} - S_{33} - S_{44} = 0.$$  \hfill (B5)

(iv) Finally, the particular model (A6) has an additional symmetry. By the definition of the $S$-matrix, we have

$$\hat{d}_p(+) = S_{31}\hat{c}_p + S_{32}\hat{c}_p^\dagger + S_{33}\hat{d}_p + S_{34}\hat{d}_p^\dagger,$$

$$\hat{d}_p(-) = S_{41}\hat{c}_p + S_{42}\hat{c}_p^\dagger + S_{43}\hat{d}_p + S_{44}\hat{d}_p^\dagger.$$

Taking the Hermitian conjugate of $\hat{d}_p(+\infty)$, and replacing $p$ with $-p$, we find

$$\hat{d}_{-p}(+) = S_{31}^*(-p)\hat{c}_{-p}^\dagger + S_{32}^*(-p)\hat{c}_{-p} + S_{33}^*(-p)\hat{d}_{-p} + S_{34}^*(-p)\hat{d}_{-p}^\dagger,$$

where we used the fact that $S_{33}(-p)$ is real [19]. Comparing the above two different expressions for $\hat{d}_{-p}(+\infty)$, we find that

$$S_{33}(-p) = S_{44}(p).$$  \hfill (B6)

Relations (B2) - (B6) are still insufficient for finding all elements of the scattering matrix. Nevertheless, they allow us to find $\sum_p |S_{13}|^2$ without any approximation. Since the summation index in (18) runs over a symmetric interval $p \in (-\pi, \pi)$, we have

$$\sum_p |S_{13}|^2 \overset{(B3a)}{=} \sum_p \left[ e^{-\frac{2\pi|\gamma|^2}{\hbar^2}} - S_{11}S_{33} \right]$$

$$\overset{(B2b,B6)}{=} \sum_{p>0} \left[ 2e^{-\frac{2\pi|\gamma|^2}{\hbar^2}} - S_{11}(S_{33} + S_{44}) \right]$$

$$\overset{(B2b,B5)}{=} 2\sum_{p>0} \left[ e^{-\frac{2\pi|\gamma|^2}{\hbar^2}} - |S_{11}|^2 \right].$$  \hfill (B7)

### Appendix C: Bounds on $N_{ex}^o$

In this section, we discuss the bounds on $N_{ex}^o$, the number of non-adiabatic excitations on the odd-site sublattice.

#### 1. Lower bound

As given in the main text, the number of excitations on the odd-site sublattice is expressed in terms of the $S$-matrix elements,

$$N_{ex}^o(+\infty) = \sum_p (|S_{33}|^2 + |S_{34}|^2).$$  \hfill (C1)

The sum over the second term in the above equation can be obtained exactly using the symmetry of the transition probability matrix (Eq. (13) in Ref. [19]): $|S_{31}| = |S_{13}|$, which is given by Eq. (22) in the main text.

The exact formula for $\sum_p |S_{33}|^2$ cannot be derived because energy level 3 does not have the highest slope. Nevertheless, a lower bound can be found. Since $S_{33}$ and $S_{44}$ are both real,

$$\sum_p |S_{33}|^2 \geq \sum_{p>0} [(S_{33} + S_{44})^2 + (S_{33} - S_{44})^2]$$

$$\geq \frac{1}{2} \sum_{p>0} (S_{33} + S_{44})^2 = \sum_p |S_{11}|^2,$$

where the last equality is a consequence of Eqs. (B2) and (B5). Thus, $N_{ex}^o$ is always bounded by the number of excitations on the even-site sublattice, $N_{ex}^o \geq N_{ex}^e$. 

2. Upper bound

The upper bound for the number of excitations of the odd-site sublattice can be obtained under a special condition, namely, as a function of $p$, the sign of $S_{33}$ remains fixed in a given regime of the quenching rate. In this case, as a consequence of relation (B6), $S_{33}S_{44} > 0$. Hence,

\[ \sum_{p>0} |S_{33}|^2 = \sum_{p>0} (|S_{33}|^2 + |S_{44}|^2) \leq \sum_{p>0} (S_{33} + S_{44})^2 = \sum_{p>0} |2S_{11}|^2 = 2 \sum_{p} |S_{11}|^2, \]  

which is suppressed exponentially in the adiabatic limit. This condition is fulfilled for large quenching rate, for which $S_{33} \sim 1$. We thus conclude that for relatively large quenching rate, an exponential suppression for the non-adiabatic excitation on the second sublattice may be observed. However, in the adiabatic limit, when the value of $S_{33}$ becomes small, this condition may be broken, which makes it possible for the power-law excitation tail to appear in the nearly-adiabatic regime.

Appendix D: Exact solutions for $J_1 = J_2$

Finally, we note that the case with $J_1 = J_2$ can be fully solved, i.e., all elements of the scattering matrix can be obtained analytically. Let us group the transition probabilities into a matrix with elements $\hat{P}_{ij} \equiv |S_{ij}|^2$. For our $4 \times 4$ model at $J_1 = J_2$, they are listed in Ref. [17]:

\[ \hat{P} = \begin{pmatrix} p_1 p_2 & 0 & p_2 q_1 & q_2 \\ 0 & p_1 p_2 & q_2 & p_2 q_1 \\ p_2 q_1 & q_2 & p_1 p_2 & 0 \\ q_2 & p_2 q_1 & 0 & p_1 p_2 \end{pmatrix}, \]  

where

\[ p_1 \equiv e^{-\frac{2\pi |q|^2}{|p_1 + q_2|^2}}, \quad p_2 \equiv e^{-\frac{2\pi |q|^2}{|p_1 - q_2|^2}}, \quad q_n \equiv 1 - p_n, \]  

with restriction $b_1 + b_2 > 0$, $b_1 - b_2 > 0$. This solution can be extended to a more general condition with $b_1 \neq \pm b_2$, by permuting the levels to full fill the condition. Now, with this exact solution, the non-adiabatic excitations at $t = +\infty$ with the initial ground state $|\downarrow\downarrow\cdots\downarrow\rangle$, Eqs. (18) and (20) in the main text, can be computed as

\[ N_\text{ex}^{(a)}(+\infty) = \sum_{p} e^{-\frac{2\pi |q|^2}{|p_1 + q_2|^2}}, \quad b_1 \neq \pm b_2, \]  

which confirms our analytical predictions in the main text for the case with $J_1 = J_2$. The above solution for the nonadiabatic excitations covers the case of $b_1 = b_2$, which corresponds to the simple uniform spin chain.

Appendix E: Nonadabatic Excitation at $t = 0$

The quasi-particle excitations at $t = 0$ take the form of superpositions of kinks. Here, we look at two different types of kinks separately, namely, moving from left to right along the chain, the kinks between odd and even sites, and the kinks between even and odd sites. The corresponding operators are

\[ N_{\text{kinks}}^{\text{even}} = \frac{1}{2} \sum_{n} (1 - \hat{\sigma}_{2n}^{+} \hat{\sigma}_{2n+1}^{+}), \]

\[ N_{\text{kinks}}^{\text{odd}} = \frac{1}{2} \sum_{n} (1 - \hat{\sigma}_{2n}^{+} \hat{\sigma}_{2n}^{+}). \]  

Using the Jordan-Wigner transformation (A2) and the Fourier transformation (A3), the operators for the numbers of kinks can be expressed in terms of the fermionic operators, i.e.,

\[ N_{\text{kinks}}^{\text{even}} = \frac{1}{2} \sum_{p} 1 - (\hat{c}_{p}^{\dagger} \hat{d}_{p} + \hat{c}_{p}^{\dagger} \hat{d}_{-p}^{\dagger} + h.c.), \]

\[ N_{\text{kinks}}^{\text{odd}} = \frac{1}{2} \sum_{p} 1 - (\hat{c}_{p}^{\dagger} \hat{d}_{p} e^{-ip} + \hat{c}_{p} \hat{d}_{-p} e^{ip} + h.c.). \]
Now the evolution of the fermionic operators in the Heisenberg picture is governed by the effective Schrödinger equation with Hamiltonian \( \hat{H}_p \) in (A6). Define the \( S \)-matrix for the evolution over the time interval \( t \in (-T, 0) \), i.e.,

\[
\begin{align*}
  s &= s(p) \equiv U^p(0, -T)_{T \to \infty},
\end{align*}
\]

with \( U^p(0, -T) \) the evolution matrix with the Hamiltonian \( \hat{H}_p \). The fermionic operators in the Heisenberg picture at \( t = 0 \) admit solutions in terms of the \( S \)-matrix elements. We only list the relative quantities here:

\[
\begin{align*}
  \hat{c}_p(0)\hat{d}_p(0) &= s_{11}^p s_{31}^p \hat{c}_p \hat{d}_p + s_{13}^p s_{33}^p \hat{d}_p \hat{d}_p + \hat{O}, \\
  \hat{c}_p(0)\hat{d}_p(0) &= s_{11}^p s_{41} \hat{c}_p \hat{d}_p + s_{13}^p s_{43} \hat{d}_p \hat{d}_p + \hat{O}, \\
  \hat{c}_p(0)\hat{d}_p(0) &= s_{12}^p s_{32}^p \hat{c}_p \hat{d}_p + s_{14}^p s_{44}^p \hat{d}_p \hat{d}_p + \hat{O}. 
\end{align*}
\]

Here, the operators on the RHS are interpreted as at \( t = -\infty \) and the operator \( \hat{O} \) involves all other terms that do not contribute to the computation of the number of kinks. Namely, we will evaluate the operator expectation value with respect to the initial ground state at \( t = -\infty \), which is annihilated by \( \hat{O} \). Taking average of the operators for the number of kinks with respect to the state at \( t = 0 \), we get the number of kinks,

\[
\begin{align*}
  N_{\text{kinks}}^c &= \frac{1}{2} \sum_p \left[ 1 - (s_{11}^p s_{31}^p + s_{13}^p s_{33}^p + s_{11}^p s_{41}^p + s_{13}^p s_{43}^p + c.g.) \right], \\
  N_{\text{kinks}}^o &= \frac{1}{2} \sum_p \left[ 1 - (s_{11}^p s_{31}^p e^{-ip} + s_{13}^p s_{33}^p e^{-ip} + s_{12}^p s_{42}^p e^{ip} + s_{14}^p s_{44}^p e^{ip} + c.g.) \right].
\end{align*}
\]

The above involved \( S \)-matrix elements are represent in the diabatic basis, i.e., the eigenbasis of Hamiltonian \( \hat{H}_p \) at \( t = \infty \). One can express the \( S \)-matrix element in terms of transition amplitude to the eigenbasis at \( t = 0 \), i.e., \( \{ |\tilde{i} \rangle \}_{i=1,2,3,4} \), as labeled in Fig. E1. For instance,

\[
\begin{align*}
  s_{11} &= \langle 1 | s | 1 \rangle = \langle 1 | s \sum_i | \tilde{i} \rangle \langle \tilde{i} | 1 \rangle = \sum_i s_{1\tilde{i}} \langle \tilde{i} | 1 \rangle.
\end{align*}
\]

Here the transition probability \( s_{1\tilde{i}} \) can be solved using LZ theory. Finally, in terms of transition amplitudes, the number of kinks reads

\[
\begin{align*}
  N_{\text{kinks}}^c &= \frac{1}{2} \sum_p \left[ 1 - \frac{1}{4} \left( (e^{-ip} - 1)(s_{33}^p + s_{43}^p) - (e^{-ip} + 1)(s_{34}^p + s_{44}^p) + c.g.) \right], \\
  N_{\text{kinks}}^o &= \frac{1}{2} \sum_p \left[ 1 - \frac{1}{4} \left( (e^{-ip} - 1)(e^{-ip}s_{33}^p - e^{ip}s_{43}^p) - (e^{-ip} + 1)(e^{-ip}s_{34}^p - e^{ip}s_{44}^p) + c.g.) \right].
\end{align*}
\]

The excitation of kinks only involves transition amplitudes between the third the fourth level around the Dirac point. This, as has been shown in the main text for excitations at \( t = +\infty \) on the odd-site sublattices, results in power-law scaling.

FIG. E1. The time-dependent spectrum of the Hamiltonian \( H_p(t) \) from (A6) around the Dirac point (vertical red-dashed line), with the parameters \( p = 0.3, b_1 = 2, b_2 = 1, J_1 = 3, J_2 = 1 \).