Defect generation in a spin-1/2 transverse XY chain under repeated quenching of the transverse field

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We study the quenching dynamics of a one-dimensional spin-1/2 XY model in a transverse field when the transverse field $h(=t/\tau)$ is quenched repeatedly between $-\infty$ and $+\infty$. A single passage from $h \to -\infty$ to $h \to +\infty$ or the other way around is referred to as a half-period of quenching. For an even number of half-periods, the transverse field is brought back to the initial value of $-\infty$; in the case of an odd number of half-periods, the dynamics is stopped at $h \to +\infty$. The density of defects produced due to the non-adiabatic transitions is calculated by mapping the many-particle system to an equivalent Landau-Zener problem and is generally found to vary as $1/\sqrt{\tau}$ for large τ ; however, the magnitude is found to depend on the number of half-periods of quenching. For two successive half-periods, the defect density is found to decrease in comparison to a single half-period, suggesting the existence of a corrective mechanism in the reverse path. A similar behavior of the density of defects and the local entropy is observed for repeated quenching. The defect density decays as $1/\sqrt{\tau}$ for large τ for any number of half-periods, and shows a increase in kink density for small τ for an even number; the entropy shows qualitatively the same behavior for any number of half-periods. The probability of non-adiabatic transitions and the local entropy saturate to 1/2 and ln 2, respectively, for a large number of repeated quenching.

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I. INTRODUCTION

Zero-temperature quantum phase transitions^{1,2} driven by quantum fluctuations have been studied extensively in recent years. In a quantum system, statics and dynamics are intermingled and hence a quantum critical point is associated with a diverging length scale as well as a diverging time scale called the relaxation time. The relaxation time of a quantum system is the inverse of the minimum energy gap which goes to zero at the quantum critical point. In the proximity of a quantum critical point, the spatial correlation length ξ grows as $\xi \sim |\delta|^{-\nu}$ and the characteristic time scale or the relaxation time ξ_{τ} scales with ξ as $\xi_{\tau} \sim \xi^{z}$, where δ is the measure of the deviation from the critical point, and ν and z are the critical exponents characterizing the universality class of the quantum phase transition.

When a quantum system is swept across a zerotemperature critical point^{1,2} by slowly varying a parameter of the Hamiltonian at a uniform rate, the resulting dynamics fails to be adiabatic, however slow the time variation may be. This is because of the diverging relaxation time discussed above. There exist nonadiabatic transitions which eventually lead to defects in the final state. According to the Kibble-Zurek (KZ) argument³, the non-adiabatic effects dominate close to the critical point where the rate of change of Hamiltonian is of the order of the relaxation time of the quantum system. The KZ analysis predicts that when a parameter of the Hamiltonian is quenched at a uniform rate as t/τ through the critical point, the density of defects in the final state shows a power-law behavior with the time scale of quenching τ given by $1/\tau^{\nu d/(\nu z+1)}$. Following recent experimental studies⁴ of non-equilibrium dynamics of strongly correlated quantum systems, there is an upsurge in the theoretical investigation of related non-random^{5,6,7,8} and random models⁹, and models with a gapless phase¹⁰. A generalized scaling relation for the defect density in a non-linear quench across a quantum critical point has also been proposed¹¹.

The quenching dynamics of a spin-1/2 XY chain in a transverse field, when either the transverse field⁷ or the interaction⁸ is quenched from $-\infty$ to $+\infty$ at a uniform rate t/τ , has been studied extensively in recent years, and the defect density is found to obey the KZ prediction. It should also be noted that recent studies of the two-dimensional Kitaev model indicate a generalization of the KZ prediction when quenched along a critical surface¹².

In this work, we investigate a situation where the transverse field is guenched back and forth across the quantum critical points from $-\infty$ to $+\infty$ and again from $+\infty$ to $-\infty$ and so on, with the functional form of the transverse field being given by $h = \pm t/\tau$. According to the Kibble-Zurek argument, the system fails to evolve adiabatically near the quantum critical points, where the relaxation time is very large, which results in the production of kinks (in this case, oppositely oriented spins in the final state). In our notation, n(l) corresponds to the defect density in the final state after l passages through both the Ising quantum critical points to be defined below. Thus even values of *l* signify *l* half-periods and the transverse field is brought back to the initial value $h \to -\infty$; for odd values of l, the field in the final state tends to $+\infty$. Clearly, the case of l = 1 has been extensively studied earlier^{7,8}. In all the cases, the initial value of h is large and negative so that all the spins are down, i.e., oriented antiparallel to the z-axis. If the dynamics were adiabatic for the entire span of time, one would expect all spins to be down

II. THE QUENCHING SCHEME AND RESULTS

The Hamiltonian of our model is given by

$$H = -\frac{1}{2} \sum_{n} (J_x \sigma_n^x \sigma_{n+1}^x + J_y \sigma_n^y \sigma_{n+1}^y + h \sigma_n^z), \qquad (1)$$

where the σ 's are Pauli spin matrices satisfying the usual commutation relations. The strength of the transverse field is denoted by h, and $J_x - J_y$ is the measure of anisotropy; J_x , J_y and h are all non-random variables. The Hamiltonian in Eq. (1) can be exactly diagonalized using the Jordan-Wigner transformation which maps a system of spin-1/2's to a system of spinless fermions^{13,14,15}. Diagonalizing the equivalent fermionic Hamiltonian in terms of Bogoliubov fermions, we arrive at an expression for the gap in the excitation spectrum given by^{13,15}

$$\epsilon_k = [h^2 + J_x^2 + J_y^2 + 2h(J_x + J_y)\cos k + 2J_x J_y \cos 2k]^{1/2}.(2)$$

The gap given in Eq. (2) vanishes at $h = \mp (J_x + J_y)$ for wave vectors k = 0 and π respectively, signaling a quantum phase transition from a ferromagnetically ordered phase to a quantum paramagnetic phase known as the "Ising" transition. On the other hand, the vanishing of the gap at $J_x = J_y$ for $|h| < (J_x + J_y)$ at an ordering wave vector $k_0 = \cos^{-1}(h/2J_x)$, signifies a quantum phase transition which belongs to a different universality class from the Ising transitions between two ferromagnetically ordered phases. In our quenching scheme, the system will be swept across the Ising critical points only.

Let us first briefly recall the case with $l = 1^{7,8}$. When projected to the two-dimensional subspace spanned by the state vectors $|0\rangle$ (empty state) and $|k, -k\rangle$ (two fermion state), the Hamiltonian takes the form

$$\begin{aligned} H_k(t) &= - \left[h + (J_x + J_y) \cos k \right] I_2 \\ &+ \left[\begin{array}{c} h + (J_x + J_y) \cos k & i(J_x - J_y) \sin k \\ -i(J_x - J_y) \sin k & -h - (J_x + J_y) \cos k \end{array} \right], \end{aligned}$$

where I_2 denotes the 2×2 identity matrix. Therefore, the many-body problem is effectively reduced to the problem of a two-level system, with the two levels being the states $|0\rangle$ and $|k, -k\rangle$. The general state vector $\psi_k(t)$ evolving in accordance with the Schrödinger equation $i\partial_t\psi_k(t) = H_k(t) \psi_k(t)$ can be represented as a linear superposition $|\psi_k(t)\rangle = C_{1k}(t)|0\rangle + C_{2k}(t)|k, -k\rangle$, with the initial condition $C_{1k}(-\infty) = 1$ and $C_{2k}(-\infty) = 0$. The off-diagonal term of the projected Hamiltonian, $\Delta =$ $(J_x - J_y) \sin k$, represents the interaction between the two time-dependent levels $\epsilon_{1,2} = \pm [h(t) + (J_x + J_y) \cos k]$. The Schrödinger equation given above is identical to the Landau-Zener (LZ) problem of a two-level system¹⁶ and therefore, the transition probability of excitations at the

$$n(l=1) \equiv n(1) = \int_0^{\pi} \frac{dk}{\pi} p_k \simeq \frac{1}{\pi \sqrt{\tau} |J_x - J_y|},$$
 (3)

state

in the limit of large τ . The $1/\sqrt{\tau}$ decay of the defect density is in accordance with the Kibble-Zurek prediction^{6,7}.

We shall now generalize the quenching dynamics to the case l = 2, when the system is brought back to the state with $h \to -\infty$ from the final state of the case l = 1, with the initial condition given by $|C_{1k}(\infty)|^2 = e^{-2\pi\gamma}$ and $|C_{2k}(\infty)|^2 = 1 - e^{-2\pi\gamma}$. With a view to estimating the non-adiabatic transition probability, we consider two time-dependent states $|1\rangle$ and $|2\rangle$ with energy $\epsilon_1(t)$ and $\epsilon_2(t)$, respectively where $\epsilon_1(t) - \epsilon_2(t) = \alpha t$, α being a constant and the time-independent coupling between the states being Δ . Let us also assume that the time t goes from $-\infty$ to $+\infty$ (the forward path in Fig. 1).



FIG. 1: The time-dependent energy levels of the Landau-Zener Hamiltonian. The minimum gap is 2Δ .

Defining a general state vector as $|\Psi(t)\rangle = C_1(t)|1(t)\rangle + C_2(t)|2(t)\rangle$, where $|C_1(t)|^2(|C_2(t)|^2)$ is the probability of the state $|1\rangle(|2\rangle)$ at time t, we can recast the Schrödinger equation in the form

$$\frac{d^2}{dz^2}\overline{U}(z) + (r + \frac{1}{2} - \frac{1}{4}z^2)\overline{U}(z) = 0,$$
(4)

where $z = e^{-\frac{\pi}{4}i} \alpha^{\frac{1}{2}}t$, $r = i\Delta^2/\alpha$, and $U(t) = \overline{U}(z)$ is related to $C_2(t)$ through the relation $U(t) = C_2(t)e^{i\int_{-\infty}^t dt'\epsilon_2(t')}e^{\frac{i}{2}\int_{\infty}^t dt'(\epsilon_1(t')-\epsilon_2(t'))}$. Focusing on the special case with $|C_1(-\infty)| = 1$ and $|C_2(-\infty)| = 0$, we have $\overline{U}(z) = AD_{-r-1}(-iz)$ as the particular solution of the Weber's differential Eq. $(4)^{17,18}$. We remark that the axis in the z plane which corresponds to t, is along $e^{-\frac{1}{4}\pi i}$ for t > 0, and along $e^{\frac{3}{4}\pi i}$ for t < 0. The constant A is determined from the initial condition $|C_1(-\infty)| = 1$ by taking the asymptotic expansion of $D_{-r-1}(-iz)$ along $e^{\frac{3}{4}\pi i}$ (or $t \to -\infty$ limit). This finally yields $D_{-r-1}(-iRe^{\frac{3}{4}\pi i}) \approx e^{-\frac{\pi}{4}(n+1)i}e^{-iR^2/4}R^{-n-1}$, where $R = \sqrt{|\alpha|}|t|$ and we find $|A| = \gamma^{1/2}e^{-\pi\gamma/4}$. The solution in the limit $R \to +\infty$ (or $t \to +\infty$) along z =

 $Re^{-\frac{1}{4}\pi i}$ leads to the final expression $|C_1(\infty)|^2 = e^{-2\pi\gamma}$ (a result already used for the case l = 1). The parameter $\gamma = \Delta^2/\alpha$ depends on the magnitude of the slope α of the two approaching states and the interaction Δ . Using the above results, we therefore get a recursive relation for the probabilities after the (l + 1)-th quenching (with $l \geq 0$) given as

$$|C_{1}(-(-1)^{l+1}\infty)|^{2} = e^{-2\pi\gamma}|C_{1}(-(-1)^{l}\infty)|^{2} + (1 - e^{-2\pi\gamma})|C_{2}(-(-1)^{l}\infty)|^{2}, \quad (5)$$

$$|C_{2}(-(-1)^{l+1}\infty)|^{2} = (1 - e^{-2\pi\gamma})|C_{1}(-(-1)^{l}\infty)|^{2} + e^{-2\pi\gamma}|C_{2}(-(-1)^{l}\infty)|^{2}, \qquad (6)$$

(5) and (6) look incomplete at first sight Eqs. because they do not contain any cross terms like $C_1(\pm\infty)C_2(\pm\infty)^*$ or $C_2(\pm\infty)C_1(\pm\infty)^*$. However, this is because at $t \to \pm \infty$, the coefficients $C_1(t)$ and $C_2(t)$ vary rapidly with time as $\exp[\pm(i/\hbar)\int^t dt' E(t')]^7$. Hence, the two cross terms given above vary rapidly with the initial time (which is going to $+\infty$ or $-\infty$ depending upon the number of repetitions as explained above) and independently of each other for different values of k. Their contribution to the defect density therefore vanishes upon integration over k due to the presence of terms like $\cos(T\cos k)$, T being the time at which the terms are calculated (which is $\pm \infty$ in our case). On the other hand, the terms given in Eqs. (5) and (6), namely, $|C_1(\pm \infty)|^2$ and $|C_2(\pm \infty)|^2$ have no such rapid variations, since any arbitrary large phase in $C_1(\pm \infty)$ cancels the exactly opposite phase appearing in $C_1(\pm \infty)^*$ (with a similar argument holding for $C_2(\pm \infty)$. Thus Eqs. (5) and (6) follow from an exact solution of the Landau-Zener problem with general initial conditions $C_1(-\infty)$ and $C_2(-\infty)$, once we use the fact that the phases of these initial amplitudes are rapidly varying and are therefore uncorrelated with each other. This is also the reason why we can consider the state obtained after one or more quenches as a mixed state with an entropy given by the expression in Eq. (9)below.

Using the above results, one finds the probability of a non-adiabatic transition to be

$$p_k(2) = |C_2(-\infty)|^2 = 2e^{-2\pi\gamma}(1 - e^{-2\pi\gamma}).$$
 (7)

The transition probability $p_k(2)$ (Fig. 2) is maximum for $k = \pi/2$ for small values of τ , whereas for higher values of τ , there are two maxima symmetrically placed around $k = \pi/2$ at $k_0 = \sin^{-1} \sqrt{\frac{\ln 2}{\pi \tau (J_x - J_y)^2}}$ which gradually shift to k = 0 and π for very large τ . In the limit of $\tau \to +\infty$, there is no non-adiabatic transition as the dynamics is perfectly adiabatic. The observed behavior of $p_k(2)$ also corresponds to the existence of an inherent time scale τ_0 (for $k_0 = \pi/2$) in the problem which separates the regions of small and large τ . It is interesting to note that the non-adiabatic transition probability for the forward path attains the minimum value⁷ of 1/2 at the wave vector

 $k = \pi/2$ for $\tau = \tau_0 = (\ln 2)/[\pi (J_x - J_y)^2]$, while for the reverse path, although $p_{k_0=\pi/2,\tau_0}(2)$ is once again 1/2, this is the maximum possible value of $p_k(2)$.



FIG. 2: Variation of $p_k(2)$ with k for different values of τ as obtained analytically for $J_x - J_y = 1$.

The kink density n(2), i.e., the density of the up spins in the final state with $h \to -\infty$, is again related to $p_k(2)$ as $n(2) = \frac{1}{\pi} \int_0^{\pi} dk p_k(2)$ (Fig. 3 (a)). In the limit of large τ , we find that

$$n(2) = \frac{2}{\pi\sqrt{\tau}(J_x - J_y)} (1 - \frac{1}{\sqrt{2}}).$$
(8)

Clearly, the magnitude of the defect density after a full period (l=2) case, is smaller than the l=1 case given in Eq. (3) in the limit of large τ , and also in the limit of small τ when the defect density is maximum for l = 1. This establishes the existence of a corrective mechanism during the reverse quenching process, arising from the fact that the maximum possible value of $p_k(2)$ is 1/2, which makes the area under the curve of $p_k vs k$ smaller for the l = 2 case as compared to the l = 1 case. The defect density n(2) (see Fig. 3) attains a maxima around $\tau \sim 2\tau_0$; eventually there is a $1/\sqrt{\tau}$ decay in the asymptotic limit of τ . We can explain the *n* vs τ behavior in the following way: in the limit of small τ , the system fails to evolve appreciably, and always remains close to its initial state for both l = 1 and l = 2, whereas for large τ , the system evolves adiabatically at all times except near the quantum critical points. In either situation the non-adiabatic transition probability $p_k(2)$ and hence the density of defects n(2) are small though it is larger in the intermediate range of τ .

Although the final state after a full period is a pure state, locally it may be viewed as a mixed state described by a decohered reduced diagonal density matrix with elements⁷ p_k and $1 - p_k$. The Von Neumann entropy density of the final state is given by

$$s = -\int_0^{\pi} \frac{dk}{\pi} [p_k \ln(p_k) + (1-p_k) \ln(1-p_k)].$$
(9)

s(2) shows a similar behavior with τ as n(2) (Fig. 3(b)), and the behavior can be justified along the same line of arguments as given above.



FIG. 3: (a) Variation of n(1), n(2), n(3) and n(4) with τ , and (b) variation of s(1), s(2), and s(3) with τ as obtained by numerically integrating Eqs. (9) and (10) with $J_x - J_y = 1$. In (a), n(4) denotes the defect density as obtained from the analytical expression in Eq. (11). In the limit of large τ , the numerical results match perfectly with the analytical results.

For an arbitrary number of repeated quenching, the non-adiabatic transition probability $p_k(l) = (1 - e^{-2\pi\gamma}) - (1 - 2e^{-2\pi\gamma})(1 - p_k(l-1))$. We can simplify this to obtain

$$p_k(l) = \frac{1}{2} - \frac{(1 - 2e^{-2\pi\gamma})^l}{2}.$$
 (10)

Eq. (10) shows that $p_k(l)$ increases with l for even values of l, while for odd l, this variation depends on the value of k. However, in the asymptotic limit of l, $p_k(l)$ saturates to the value 1/2 for all k which implies that every spin is up or down with an equal probability in the final state following a large number of quenches.

Using $p_k(l)$ given above for any l, we find that the defect density scales as $1/\sqrt{\tau}$ in the asymptotic limit of τ and can be put in the form

$$n(l) = \frac{1}{2\pi (J_x - J_y)\sqrt{\tau}} \sum_{w=1}^{l} \frac{l!}{w!(l-w)!} \frac{2^w}{\sqrt{w}} (-1)^{w+1} . (11)$$

Interestingly, using Eqs. (10) and (11), for two successive values of l, we find that n(l + 1) < n(l) for small values of τ if l is odd, a fact that once again emphasizes the corrective mechanism in the reverse path mentioned already. A similar result is also obtained for large τ for smaller values of l, as shown in Fig. 3 (a). On the other hand, n(l + 1) is always greater than n(l) for even l. We also find that $n(l + 1) \rightarrow n(l)$ in the asymptotic limit of l and τ for both even and odd values of l. Moreover, for any odd l, the kink-density n(l) decreases monotonically with τ , while for even l, n(l) attains a maxima around τ_0 ; in the limit $\tau \rightarrow \infty$, n(l) decays as $1/\sqrt{\tau}$ in both cases. A close inspection of the variation of n(l) with τ

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(see Fig. 3 (a)) also unravels other interesting aspects of the repeated quenching dynamics: (i) For even values of l, the characteristic scale τ^* at which the defect density is maximum shifts to higher values of τ (from $\tau^* \sim 2\tau_0$ for l = 2). At the same time we find that n(l) > n(l-2) for all values of τ so that it eventually saturates to 1/2 for all τ for asymptotic l. (ii) Similarly for odd l, n(l+2) < n(l)for small τ ; for higher τ , n(l+2) exceeds n(l) following a crossover around $\tau \sim \tau^*$. Once again n(l) saturates to 1/2 for a large number of repeated quenches. The behavior of the entropy density as a function of τ for any general value of l is shown in Fig. 3 (b). It follows from Eq. (9) that for any given τ , the local entropy density increases with l; in the limit $l \to \infty$, $p_k(l)$ tends to 1/2 and therefore the local entropy density tends to its maximum value of $\ln 2$.

III. CONCLUSION

In conclusion, we have studied the defect generation and entropy production in a transverse XY spin-1/2 chain under repeated quenching of the transverse field between $-\infty$ and $+\infty$. We have employed a generalized form of the Landau-Zener transition formula along with the concept of uncorrelated initial phases of the probability amplitudes so that the cross terms appearing in the recursion relation of probabilities vanish under integration over momentum. Using the non-adiabatic transition formula thus obtained, we evaluate the defect density in the final state after an arbitrary number of quenches.

Our results show that the defect density satisfies n(l) > ln(l+1) for small τ , if l is odd; this points to the existence of a corrective mechanism in the reverse path. The results obtained by numerical integration of the transition probability and by using the analytical expression given in Eq. (11) match perfectly in the limit of large τ . The entropy density, however, is found to increase monotonically with the number of repetitions, showing that the local disorder of the system increases monotonically with l, irrespective of the behavior of the kink density. For an odd number of repetitions, we observe a monotonic decrease of the kink density with τ , as seen previously for the widely studied l = 1 case. For even l, on the other hand, n(l) grows for small τ but eventually decreases as $1/\sqrt{\tau}$ in the large τ limit, attaining a maxima at an intermediate value of $\tau = \tau^*$; τ^* shifts to higher values of τ with increasing l. The difference in the behaviors of the defect density for an even and odd number of repetitions originates from the fact that the system is expected to come back to its initial ground state after an even value of l for a perfectly adiabatic dynamics.

As mentioned above, the local entropy increases after each half-period of quenching. In the limit $l \to \infty$, the entropy s(l) eventually saturates to its maximum possible value of ln 2 for all τ while the non-adiabatic transition probability $p_k(l)$ approaches 1/2 for all k. This result suggests that a spin remains up or down with the same probability, irrespective of the applied field after a large number of quenches. Using Eq. (10), one can also define a characteristic number of repetitions $l^*(k,\tau)$ so that for $l > l^*(k,\tau)$, the transition probability $p_k(l) \sim 1/2$; it can be shown that $l^*(k,\tau)$ attains a minima at an intermediate value of τ . We conclude by noting that the defect production due to repeated quenching can be studied in systems of atoms trapped in optical lattices¹⁹, quantum magnets²⁰ and spin-one Bose condensates²¹.

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