Quench dynamics and defects formation in the Ising chain in a transverse magnetic field

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Abstract. We study quench dynamics and defects formation in the one-dimensional quantum Ising chain in a time-dependent transverse magnetic field, given by a semi-infinite pulse and as the pulse of the finite width. The system’s final state depends on the quench time and pulse amplitude, resulting in the emergence of topological defects, and consists of a mixture of ground and excited states. We obtain a new analytical expression, generalizing the Landau-Zener (LZ) and adiabatic-impulse (AI) approximation formulas for the asymptotic probability of remaining in the ground state. We show that our theoretical predictions are in good agreement with the results of the numerical simulations, even when the LZ and AI approximations fail.

1 Introduction

Quantum phase transition (QPTs), being associated with energy level crossing, are characterized by qualitative changes of the ground state of many-body systems and occur at the zero temperature \cite{1}. Since thermal fluctuations are frozen, QPTs are purely quantum phenomena driven by quantum fluctuations. Well-known examples of QPTs are the superconductor to insulator transition in high-\textit{T}\textsubscript{c} superconducting systems, the quantum paramagnet to ferromagnet transition occurring in Ising spin system under an external transverse magnetic field, and the superfluid to Mott insulator transition. One specific case of QPT is a spin crossover phenomenon that occurs in many transition metal oxides and metal–organic complexes, where cations Fe+3 or Fe+2 have several terms, for example, the high spin (HS) and the low spin (LS). Under the external pressure, these energy level crossing resulting in the QPT \cite{2} with a Berry-like phase as the order parameter. The interatomic exchange interaction transforms the QPT into the first-order phase transition and increases the critical pressure value stabilizing the HS state with magnetic order \cite{3}.

Suppose that the quantum system is initially in the ground state and experiences the QPT during its evolution. It does not matter how the system is evolved, slowly or fast. Near the critical point, non-equilibrium phenomena associated with the drastically grown quantum fluctuations can drive the system from the ground state. Its final state depends on how fast the transition occurs. If the quenching process is sufficiently fast, large numbers of topological defects are created, and the system’s state can be essentially different at the end of evolution from that obtained for slow evolution.

To illustrate these ideas, consider the Hamiltonian, \(\mathbf{H}(t) = \mathbf{H}_0 + \Gamma(t)\mathbf{H}_1\), with the external time-dependent field \(\Gamma(t)\) being a control parameter. To provide a non-trivial dynamics of the quantum system, we assume that \([\mathbf{H}_0, \mathbf{H}_1] \neq 0\). Assume that the system is initially in the ground state, and \(\Gamma(t)\) decreases from the initial value \(\Gamma_0\) to zero during the quantum evolution. If the value \(\Gamma_0\) is large enough, the ground state of \(\mathbf{H}_1\) is the initial state of the total system. The adiabatic theorem guarantees that if \(\Gamma(t)\) decreases sufficiently slow, the system remains in its ground state. One of the adiabatic theorem requirements is the presence of a finite gap between the instantaneous ground state and the first excited state. However, in typical cases, the minimal gap, \(g_m\), is exponentially small. For instance, in the commonly used quantum optimization \(n\)-qubit models, the estimation of the minimal energy gap yields \(g_m \approx 2^{-n/2}\) \cite{4–7}. It leads to the emergence of defects caused by the quantum fluctuations, and the final state of the system is different from the ground state of \(\mathbf{H}_0\). Qualitatively, the dynamics of the quantum system can be described by the Kibble–Zurek (KZ) theory of non-equilibrium phase transitions \cite{8–10}. The KZ mechanism assumes that the main contribution to the quench dynamics is made in the neighborhood of
the critical point. To depict the system’s behavior, one has to use the so-called adiabatic-impulse (AI) approximation [11–13].

This paper aims to study the quench dynamics of the quantum Ising chain in a transverse time-dependent magnetic field. We consider two cases: the magnetic field given by a semi-infinite pulse and the magnetic field as the pulse of the finite width. In the first case, we study the quench dynamics leading to the phase transition from the ferromagnetic to paramagnetic state and vice versa. While the first case is related to Landau–Zener (LZ ) problem, the second case is relevant to the St"uckelberg problem for double-passage transition probability [14–17]. Initially, in the ground state, the system’s final state depends on the quench time and may contain many topological defects (kinks). For the finite pulse, the dynamics is more complicated and, sometimes, contrary to intuition and common sense.

The main result of our study is a new analytical expression, generalizing the AI formula for the probability of remaining in the ground state. For the adiabatic evolution, our expression reduces to the Landau-Zener (LZ ) formula. We compare our theoretical outcomes with the results of the numerical simulations and show they are in excellent agreement, even when the LZ and AI approximations fail.

The paper is organized as follows. Section 2 introduces the model and discusses its main features. In Sect. 3, we study the quench dynamics for a magnetic field given by a semi-infinite pulse and the magnetic field as the pulse of the finite width. In Sect. 4, we study the quench dynamics leading to the phase transition from the ferromagnetic to paramagnetic state and vice versa. While the first case is related to Landau–Zener (LZ ) problem, the second case is relevant to the St"uckelberg problem for double-passage transition probability [14–17]. Initially, in the ground state, the system’s final state depends on the quench time and may contain many topological defects (kinks). For the finite pulse, the dynamics is more complicated and, sometimes, contrary to intuition and common sense.

The main result of our study is a new analytical expression, generalizing the AI formula for the probability of remaining in the ground state. For the adiabatic evolution, our expression reduces to the Landau-Zener (LZ ) formula. We compare our theoretical outcomes with the results of the numerical simulations and show they are in excellent agreement, even when the LZ and AI approximations fail.

The paper is organized as follows. Section 2 introduces the model and discusses its main features. In Sect. 3, we study the quench dynamics for a magnetic field defined by a pulse of a given shape. In Sect. 4, we perform the numerical simulations for the semi-finite pulse and pulse of the finite width. In Sect. 5, we describe defects formation in the Ising chain. We conclude in Sect. 6 with a discussion of our results.

### 2 Description of the model

In this section we consider in detail the one-dimensional Ising model in a transverse magnetic field governed by the following Hamiltonian:

$$\mathcal{H} = -\frac{J}{2} \sum_{n=1}^{N} (h\sigma_n^x + \sigma_n^x \sigma_{n+1}^x).$$

We assume that the periodic boundary conditions, \(\sigma_{N+1} = \sigma_1\), are imposed. The external magnetic field is associated with the parameter \(h\). Quantum phase transition (QPT) occurs in the thermodynamic limit \((N \gg 1)\) at the critical value \(h_c = 1\).

The Hamiltonian in Eq. (1) can be diagonalized using the standard Jordan–Wigner transformation, following well-known procedures described in [18–22]. The Jordan–Wigner transformation maps a spin-1/2 system to a system of spinless fermions,

$$\sigma_n^\alpha = 1 - 2c_n^\dagger c_n,$$

$$\sigma_n^\beta = i (c_n^\dagger - c_n) \prod_{m<n} (1 - 2c_m^\dagger c_m),$$

with anticommutation relations: \(\{c_m^\dagger, c_n\} = \delta_{mn}\) and \(\{c_m, c_n\} = \{c_m^\dagger, c_n^\dagger\} = 0\). Applying these transformations, we obtain

$$\mathcal{H} = -\frac{J}{2} \sum_{n=1}^{N} (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}^\dagger + c_{n+1} c_n + h(1 - 2c_n^\dagger c_n)).$$

The periodic boundary conditions imposed on the spin operators lead to the following condition for the fermionic operators:

$$c_{N+1} = -e^{i\pi S_x} c_1,$$

where \(S_x = \sum_{n=1}^{N} c_n c_n^\dagger\) being the total number of fermions. Using Eq. (2) we find that \(S_x = N/2 - S^z\), where \(S^z = (1/2) \sum_n \sigma_n^z\) is the total \(z\)-component of the spins. For the particular choice of \(S^z = 0\), we obtain \(N_F = N/2\). This yields periodic periodic (antiperiodic) boundary conditions for \(c_n\), if \(N/2\) is odd (even). Since the parity of the fermions is conserved, the imposed boundary conditions are valid for all values of the parameter \(h\).

Applying the Fourier transformations,

$$c_n = e^{-i\pi/4} \sqrt{N} \sum_k c_k e^{i\pi kn/N},$$

we find that the Hamiltonian (5) can be recast in Fourier space as

$$\mathcal{H} = \frac{J}{2} \sum_k \left( 2(h - \cos \varphi_k) c_k^\dagger c_k - h \right.$$\n
$$+ \sin \varphi_k (c_k^\dagger c_{-k}^\dagger + c_{-k} c_k) \right),$$

where \(\varphi_k = 2\pi k/N\). In what follows, we impose the antiperiodic boundary conditions for the fermionic operators, \(c_{N+1} = -c_1\). Suppose that the lattice spacing is \(a = 1\), then the wave number \(k\) takes the following discrete values:

$$k = \pm \frac{1}{2}, \pm \frac{3}{2}, \ldots, \pm \frac{N-1}{2}. $$

The Hamiltonian (8) can be diagonalized by employing the Bogolyubov transformations,

$$c_k = \cos \frac{\theta_k}{2} a_k + \sin \frac{\theta_k}{2} a_{-k}^\dagger,$$

$$c_k^\dagger = \cos \frac{\theta_k}{2} a_k^\dagger + \sin \frac{\theta_k}{2} a_{-k},$$

$$a_k = \cos \frac{\theta_k}{2} c_k + \sin \frac{\theta_k}{2} c_{-k}^\dagger,$$

$$a_k^\dagger = \cos \frac{\theta_k}{2} c_k^\dagger + \sin \frac{\theta_k}{2} c_{-k}.$$
For $h \gg 1$, the ground state is paramagnetic with all spins oriented along the $x$ axis, and from Eq. (14) we obtain $\cos \theta_k \to 1$ as $h \to \infty$. This yields $|u_-(k)\rangle \to \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $|u_+(k)\rangle \to \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. On the other hand, when $h \ll 1$ there are two degenerate ferromagnetic ground states with all spins polarized in opposite directions along the $z$ axis. In the thermodynamic limit, the system passing through the critical point ends in a superposition of up and down states with finite domains of spins separated by kinks [23].

## 3 Quench dynamics

### 3.1 Adiabatic and non-adiabatic evolution

In this section, we consider the Ising model defined by the Hamiltonian: $\mathcal{H} = \sum_k \mathcal{H}_k$,

$$\mathcal{H}_k = \varepsilon_{0k} \mathbf{1} + J \begin{pmatrix} h - \cos \varphi_k & \sin \varphi_k \\ \sin \varphi_k & -h + \cos \varphi_k \end{pmatrix},$$

(24)

with the time-dependent parameter $h = h(t/\tau_0)$ and the characteristic duration of pulse being $\tau_0$. We assume that the system is initially in the ground state.

In the adiabatic basis formed by the instantaneous eigenvectors of the Hamiltonian $\mathcal{H}_k$, the total wavefunction can be written as $|\psi\rangle = \otimes_k |\psi_k(t)\rangle$, where

$$|\psi_k(t)\rangle = \alpha_k(t) e^{i \int \varepsilon_{0k}(t) dt} |u_-(k,t)\rangle + \beta_k(t) e^{i \int \varepsilon_{0k}(t) dt} |u_+(k,t)\rangle.$$  

(25)

The requirement the wavefunction been normalized, yields $|\alpha_k(t)|^2 + |\beta_k(t)|^2 = 1$. From Eqs. (21) and (22) it follows

$$\alpha_k(t) = u_k(t) \cos \left( \frac{\theta_k(t)}{2} \right) - v_k(t) \sin \left( \frac{\theta_k(t)}{2} \right),$$

(26)

$$\beta_k(t) = v_k(t) \cos \left( \frac{\theta_k(t)}{2} \right) + u_k(t) \sin \left( \frac{\theta_k(t)}{2} \right).$$

(27)

The straightforward computation shows that the wavefunction,

$$|\Psi_k(t)\rangle = \begin{pmatrix} \beta_k(t) \\ \alpha_k(t) \end{pmatrix},$$

(28)

satisfies the Bogolyubov–de Gennes equation

$$i \frac{\partial}{\partial t} |\Psi_k\rangle = H_k(t) |\Psi_k\rangle,$$

(29)

where

$$H_k = \varepsilon_{0k} \mathbf{1} + \begin{pmatrix} \varepsilon_k & i \theta_k(t)/2 \\ -i \theta_k(t)/2 & -\varepsilon_k \end{pmatrix}.$$  

(30)
Employing (31), one can recast Eq. (36) as,

\[
\dot{\theta}_k = -\frac{\dot{h}(t) \sin^2 \theta_k(t)}{\sin \varphi_k}. \tag{31}
\]

Since different pairs of quasiparticles \((k, -k)\) evolve independently, the probability of remaining in the ground state is the product [23]

\[
P_{gs}(t) = \prod_{k>0} P_{gs}^k(t), \tag{32}
\]

where \(P_{gs}^k(t) = |\alpha_k(t)|^2\). Using the normalization condition, \(|\alpha_k(t)|^2 + |\beta_k(t)|^2 = 1\), one can recast Eq. (32) as

\[
P_{gs}(t) = \prod_{k>0} (1 - |\beta_k(t)|^2). \tag{33}
\]

The adiabatic theorem guarantees that during quantum evolution the system remains in the ground state, as long as the instantaneous ground state does not become degenerate at any time. The validity of the adiabatic theorem requires

\[
\sum_{m \neq n} \left| \frac{\langle \psi_n | \partial \mathcal{H}(t) / \partial t | \psi_m \rangle}{(E_m - E_n)^2} \right| \ll 1. \tag{34}
\]

For the quantum processes being related to the quantum phase transitions, the condition of Eq. (34) can be recast as [5, 24],

\[
\left| \frac{\langle \psi_e | \partial \mathcal{H}(t) / \partial t | \psi_g \rangle}{|E_e - E_g|^2} \right| \ll 1, \tag{35}
\]

where \(|\psi_g\rangle\) is the ground state, and \(E_e\) is the energy of the first excited state, \(|\psi_e\rangle\). This restriction is violated near the degeneracy, where the QPT occurs.

In the adiabatic basis, the requirement of the adiabatic theorem (35) take the form

\[
\max \left| \frac{d\theta_k}{dt} \right| \ll \min 2\varepsilon_k = 2J \sin \varphi_k. \tag{36}
\]

Employing (31), one can recast Eq. (36) as,

\[
|\dot{h}_c| \ll 2J \sin^2 \varphi_k, \tag{37}
\]

where \(\dot{h}_c = \dot{h}(t_c)\), and \(t_c\) denotes the moment of time when the magnetic field reached its critical value, \(h_c = 1\).

Before proceeding further, it is convenient to introduce the parameter of adiabaticity, \(\omega_k\), defined as

\[
\omega_k^2 = \tau_Q \sin^2 \varphi_k, \tag{38}
\]

where \(\tau_Q = J/|\dot{h}_c|\) is the quench time. The quench time determines a time scale staying the system in the neighborhood of avoiding energy level crossing.

Using (38) in Eq. (37), we find that for the given value of \(k\), the condition of adiabaticity can be written as \(\omega_k^2 \gg 1\). As follows from Eq. (35), for the whole system the condition of adiabaticity can be written as

\[
\omega^2 = \tau_Q \sin^2 \left( \frac{\pi}{N} \right) \gg 1. \tag{39}
\]

For \(N \gg 1\), we obtain

\[
\omega^2 = \frac{\pi^2 \tau_Q}{N} \gg 1. \tag{40}
\]

By presenting

\[
\alpha_k(t) = a_k(t) e^{i \int_0^t \varepsilon_k(t) dt}, \tag{41}
\]

\[
\beta_k(t) = b_k(t) e^{-i \int_0^t \varepsilon_k(t) dt}, \tag{42}
\]

one can show that, if the evolution begins from the ground state, the coefficient \(b_k(t)\) satisfy the following asymptotic conditions [25–33]:

\[
b_k(\infty) = \mathcal{O}\left( \exp \left( 2z_0 \int_{z_0}^{z_c} \varepsilon_k(z) dz \right) \right), \tag{43}
\]

where the critical point, \(z_c\), lies on the first Stokes line in the lower complex line defined as

\[
\Im \int_{z_0}^{z_c} \varepsilon_k(z) dz < 0. \tag{44}
\]

The critical point is determined as a solution of the equation \(\varepsilon_k(z_c) = 0\), in the complex plane obtained by analytical continuation \(t \to z\). Employing Eq. (17), we find that for the Ising model the integral in the r.h.s. of Eq. (43) can be recast as follows:

\[
\int_{z_0}^{z_c} \varepsilon_k(z) dz = \int_{z_0}^{e^{-i \varepsilon_k}} \sqrt{Z^2 - 2Z \cos \varphi_k + 1} \frac{dZ}{Z'}, \tag{45}
\]

where \(Z = h(z)\) and \(Z' = dZ/dz\).

For given \(k\), the probability remaining at the ground state at the end of the evolution is given by \(P_{gs}(t) = 1 - |\beta_k(t)|^2\). Using Eqs. (33) and (43), we obtain

\[
P_{gs}^k(\infty) = 1 - e^{4\tau_Q \int_{z_0}^{z_c} \varepsilon_k(z) dz}, \tag{46}
\]

\[
P_{gs}(\infty) = \prod_{k>0} \left( 1 - e^{4\tau_Q \int_{z_0}^{z_c} \varepsilon_k(z) dz} \right). \tag{47}
\]

It is a central result of our paper which we consider in more detail in Sects. 4 and 5.
3.2 Landau–Zener and the adiabatic-impulse approximations

To obtain the LZ approximation, we replace $Z'(z)$ in Eq. (45) by its value in the critical point, $Z'(z_c)$. Taking the integral and inserting the result in Eq. (46), we get the Landau–Zener (LZ) formula [14–16,34],

$$ P_{gs}^k \approx 1 - e^{-\pi \omega_k^2}, $$

where $\omega_k^2 = \tau Q \sin^2 \varphi_k$, and, as above, $\tau Q = J/|\dot{h}_c|$ denotes the quench time.

Let us expand $h(t)$ near of the critical point as $h(t) \approx 1 + \dot{h}_c(t - t_c)$. Then applying the LZ approximation, one can recast the Hamiltonian (24) as follows (we omit unessential diagonal contribution, $0_k$):

$$ \mathcal{H}_k(t) \approx J \left( \dot{h}_c(t - t_c) + 2 \sin^2 (\varphi_k/2) \sin \varphi_k - \dot{h}_c(t - t_c) - 2 \sin^2 (\varphi_k/2) \right). $$

Before proceeding further it is convenient to introduce new variables: $\tau = \sqrt{h|h_c|/(t - t_c)}$ and

$$ \tau_k = \text{sgn}(\dot{h}_c) \tau + 2 \sqrt{\tau Q} \sin^2 \left( \varphi_k/2 \right). $$

The transformed Hamiltonian takes the form of the LZ model

$$ \mathcal{H}_k = \begin{pmatrix} \tau_k & \omega_k \\ \omega_k & -\tau_k \end{pmatrix}, $$

with the coupling strength being $\omega_k = \sqrt{\tau Q} \sin \varphi_k$. The wavefunction, $|\psi_k\rangle$, satisfies the Schrödinger equation written in the rescaled time $\tau$ as

$$ i \frac{\partial}{\partial \tau} |\psi_k\rangle = \mathcal{H}_k(\tau)|\psi_k\rangle. $$

In the LZ model, the asymptotic probability of remaining in the ground state is given by

$$ P_{gs}(\infty) = \prod_{k>0} (1 - e^{-\pi \omega_k^2}). $$

In Sect. 4, we will show that the LZ approximation is good enough when $\omega^2 \gg 1$.

According to the KZ mechanism, the main contribution to the QPT is made in the neighborhood of the critical point [8–10]. The system evolves nonadiabatically in the vicinity of this point and experiences a mixing in the populations of the ground and first excited states. Further, one can expect that the system’s evolution will be almost adiabatic far from the critical point.

Qualitatively, the dynamics of the system can be described by using so-called the adiabatic-impulse (AI) approximation [11–13]. The AI approximation assumes that the whole evolution can be divided into three parts, and up to the phase factor of the wavefunction, $|\psi_k(t)\rangle$, can be described as follows:

$$ \tau_k \in [-\infty, -\hat{\tau}_k] : |\psi_k(\tau_k)\rangle \approx |u_-(k, \tau_k)\rangle $$

$$ \tau_k \in [-\hat{\tau}_k, \hat{\tau}_k] : |\psi_k(\tau_k)\rangle \approx |u_-(k, -\hat{\tau}_k)\rangle $$

$$ \tau_k \in (\hat{\tau}_k, +\infty) : |\langle \psi_k(\tau_k)|u_-(k, \tau)\rangle|^2 = \text{const.} $$

The time $\hat{\tau}_k$, introduced by Zurek [9], is called the freeze-out time and define the instant when the behavior of the system changes from the adiabatic regime to an impulse one where its state is effectively frozen and then back from the impulse regime to the adiabatic one. If the evolution starts at moment $\tau_i \ll \hat{\tau}_k$ from the ground state, the equation for determining $\hat{\tau}_k$ can be written as $\pi \tau_k = 1/\varepsilon_k(\tau_k)$ (for details of calculation, see reference [11]).

Its solution is given by

$$ \hat{\tau}_k = \frac{\omega_k}{\sqrt{2}} \sqrt{1 + \frac{4}{\pi^2 \omega_k^4}} - 1. $$

In the AI approximation, the probability, $P_{ex}^k$, of exciting mode $k$ at $\tau_f \gg \hat{\tau}_k$ can be calculated as follows [11,13]:

$$ P_{ex}^k \approx P_{AI}^k = |\langle u_+(k, \hat{\tau}_k)|u_-(k, -\hat{\tau}_k)\rangle|^2 = \frac{\tau_k^2}{\omega_k^2 + \hat{\tau}_k^2}. $$

Substituting $\hat{\tau}_k$ from (54), we obtain

$$ P_{ex}^k = \frac{2}{x_k^2 + x_k \sqrt{x_k^2 + 4} + 2}. $$

where $x_k = \pi \omega_k^2$. For $\omega_k^2 \ll 1$, from Eq. (56) it follows $P_{AI}^k \approx 1 - \pi \omega_k^2$. In the first order this coincides with the result predicted by exact LZ formula: $P_{ex}^k = e^{-\pi \omega_k^2}$. For the adiabatic evolution, $\omega_k^2 \gg 1$, we obtain $P_{AI}^k \approx 1/(\pi^2 \omega_k^2)$. In the thermodynamic limit, the variable $\varphi_k$ becomes continuous, and we obtain

$$ P_{ex}(\tau_Q, \varphi) = \frac{2}{x^2 + x \sqrt{x^2 + 4} + 2}, $$

where $x = \pi \tau_Q \sin^2 \varphi$. In Fig. 1 the probability of finding the system in excited state is presented. One can see that for $\tau_Q \gg 1$ the main contribution to $P_{ex}$ is occurred from the values of $\varphi \approx 0$ and $\varphi \approx \pi$. In other limit, $\tau_Q \ll 1$, the values of $\varphi \approx \pi/2$ yield the most important contribution to the probability $P_{ex}(\tau_Q, \varphi)$.

Employing (33), we find that in the AI approximation, the probability remaining at the ground state for
the whole system is given by

\[ P_{gs} = \prod_{k > 0} \left( 1 - \frac{x_k^2 + x_k \sqrt{x_k^2 + 4}}{x_k^2 + x_k \sqrt{x_k^2 + 4} + 2} \right). \]  

(58)

In Sect. 4, we will show that the AI approximation is better than the LZ approximation. It is good enough in two limiting cases \( \omega^2 \gg 1 \) and \( \omega^2 \ll 1 \).

4 Quench dynamics under shock-wave load

4.1 Semi-finite pulse

Transition from paramagnet to ferromagnet

Suppose that the system is initially in a ground state, and \( h(t/\tau_0) \) decreases from the initial value \( h_0 \gg 1 \) to zero during the quantum evolution. Since the value \( h_0 \) is large, the initial ground state is the paramagnetic one. During the evolution, the system does not remain in the ground state at all times. The quantum system becomes excited at the critical point \( h_c = 1 \), and the number of defects determines its final state. It looks like follows: \( \ldots \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \ldots \downarrow \downarrow \uparrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \ldots \).

The neighboring spins polarized in the same directions along the \( z \)-axis are separated by kinks (defects), where the polarization of spins has the opposite orientation. We specify the magnetic field as a semi-infinite pulse with the shape determined by (see Fig. 2)

\[ h = h_0(1 - \tanh(t/\tau_0)). \]  

(59)

\[ \frac{\partial}{\partial s} \langle \Psi_k(s) \rangle = \hat{H}_k(s)\langle \Psi_k(s) \rangle, \]  

(62)

where

\[ \hat{H}_k = \hat{\varepsilon}_0 k + \begin{pmatrix} \varepsilon_k & 0 \\ 0 & -i\theta_k / 2 \end{pmatrix} - \hat{\varepsilon}_k. \]  

(63)

We set \( \theta'_k = d\theta_k / ds, \varepsilon_0 k = \tau_0 \varepsilon_0 k, \) and \( \varepsilon_k = \tau_0 \varepsilon_k. \)

Let the wavefunction

\[ \langle \Psi_k(s) \rangle = \begin{pmatrix} \beta_k(s) \\ \alpha_k(s) \end{pmatrix}. \]  

(64)

be a solution of the Bogolyubov–de Gennes equation. Then the probability of remaining in the ground state for the whole system is given by

\[ P_{gs}(s) = \prod_{k > 0} (1 - |\beta(s)|^2). \]  

(65)

To estimate the asymptotic behavior of the probability at \( s \to \infty \), we use Eq. (47), writing

\[ P_{gs}^k = 1 - e^{-4\tau_0 \varepsilon_0 \int \varepsilon_k(z)dz}, \]  

\[ P_{gs} = \prod_k (1 - e^{-4\tau_0 \varepsilon_0 \int \varepsilon_k(z)dz}). \]  

(66)
Employing (59) in Eq. (45), we are performing integration to obtain

\[ 4\Im \int_{\infty}^{z_c} \varepsilon_k(z)dz = \pi J\tau_0(\sqrt{h_m^2 - 2h_m \cos \varphi_k + 1} + 1 - h_m). \]  

(67)

Substitution of this result in Eq.(66) yields

\[ P_{gs}^k = 1 - e^{-\nu_k^2}, \]  

(68)

\[ P_{gs} = \prod_{k>0} \left(1 - e^{-\nu_k^2}\right), \]  

(69)

where

\[ \nu_k^2 = \tau_0 J \left(\sqrt{h_m^2 - 2h_m \cos \varphi_k + 1} + 1 - h_m\right). \]  

(70)

For long wavelength modes with \( \varphi_k \ll \pi/4 \), we obtain

\[ \nu_k^2 \approx \omega_k^2 \approx \frac{2\pi^2 J\tau_0 k^2}{N^2} = \frac{4\pi^2 \tau_0 k^2}{N^2}, \]  

(71)

In Figs. 3, 4, we present the results of the numerical simulation performed for \( N = 32, 48, 64, 128, 256, 512 \) spins. The system is initially in the ground (paramagnet) state. Solid lines present the results based on the numerical solution of the Bogolyubov–de Gennes equation (62), and dashed lines correspond to the asymptotic formula (69). The outcomes presented in Fig. 3 show that the asymptotic formula (69) is in good agreement with the results of numerical simulations. As expected, decreasing the parameter \( \omega \) means remaining in the ground state also decreases. It implies that at the end of evolution, the quantum system does not remain in the ground state, and its final state is the superposition of blocks with the spins oriented up/down, separated by walls (kinks). As one can observe in Fig. 4, the contribution from the short wave perturbations \( (k \gg 1) \) to the transition probability from the ground state to the first excited state is negligible.
Fig. 5 Shape of pulse, $h(s)$, as a function of dimensionless time $s = t/\tau_0$ ($h_0 = 20$)

Transition from ferromagnet to paramagnet

To describe transition from ferromagnet to paramagnet, we specify the magnetic field as a semi-infinite pulse with the shape determined by (see Fig. 5)

$$ h = h_0 \left( 1 + \tanh(t/\tau_0) \right). \quad (73) $$

Suppose the system is initially in the ferromagnet ground state, then the probability remaining in the ground state at $t \to \infty$ is given by

$$ P_{gs}(\infty) = \prod_k (1 - e^{-\pi \nu_k^2}), \quad (74) $$

where

$$ \nu_k^2 = J_0 \left( \sqrt{\frac{1}{2} - 2 h_m \cos \varphi_k + 1} + 1 - h_m \right). \quad (75) $$

In Fig. 6 we present the results of numerical simulations performed for $N = 32, 64, 128, 256$ spins. Solid lines present the outcome based on the numerical solution of the Bogolyubov–de Gennes equation (62), and dashed lines correspond to the asymptotic formula (74). One can observe that as in the transition paramagnet $\rightarrow$ ferromagnet, short-wavelength excitations are essential at the critical point, at the end of evolution, their contribution to the transition probability from the ground state to the first excited state is negligible. The results presented in Fig. 6a show that the asymptotic formula (74) is in good agreement with the results of numerical simulations.

Numerical simulation: LZ formula and AI approximation

In this section, we compare LZ formula and AI approximation with the results of the numerical simulations for a semi-infinite pulse. As before, we assume that the system is initially in the ground state, then the probability remaining in the ground state at the end of evolution can be written as,

$$ \text{LZ} : P_{gs}^{LZ} = \prod_{k>0} (1 - e^{-x_k^2}), \quad (76) $$

$$ \text{AI} : P_{gs}^{AI} = \prod_{k>0} \frac{x_k^2 + x_k \sqrt{x_k^2 + 4} + 4 + 2}{x_k^2 + x_k \sqrt{x_k^2 + 4} + 4}. \quad (77) $$

where $x_k = \pi \omega_k^2$, the parameter of adiabaticity being $\omega_k^2 = \sqrt{\tau_Q} \sin \varphi_k$. For the semi-finite pulse introduced in the Secs. 4.1.2. and 4.1.3, we have

$$ \tau_Q = \frac{J_0 h_m}{2(h_m - 1)}. \quad (78) $$

In Fig. 7, we compare the predictions of LZ formula and AI approximation with the results of numerical simulations performed for $N = 32, 64, 128, 256$ spins, for the paramagnet $\rightarrow$ ferromagnet transition (Fig. 7a) and the ferromagnet $\rightarrow$ paramagnet transition (Fig. 7b). Solid lines present the results of the numerical simulations, and dash-dotted/dashed lines correspond to the asymptotic formulas (76) and (77), respectively. As expected, when the parameter of adiabaticity $\omega^2 \gg 1$ (see Eq. (39)), the LZ formula is in good agreement with the numerical results (blue curve). One can observe that AI approximation is good enough for $\omega^2 \ll 1$ (black curve) and $\omega^2 \gg 1$ (blue curve).

4.2 Pulse of finite width

Below we will consider the Ising spin chain in a transverse magnetic field defined by a pulse of finite width,

$$ h(\tau) = h_0 \left( \tanh(t/\tau_0) - \tanh(t/\tau_0 - \delta) \right), \quad (79) $$

with height being $h_m = 2 h_0 \tanh(\delta/2)$ (see Fig. 8).

Suppose that the evolution starts from the ferromagnetic ground state. Near the first critical point, the quantum system becomes excited, and after crossing the critical point, its state is determined by the number of flipped spins. According to the KZ mechanism, the system will stay in this state until reaching the second critical point. When the pulse width is relatively large, there is the intermediate asymptotic for the probability of remaining in the ground state given by

$$ P_{gs} = \prod_k (1 - e^{-\pi \nu_k^2}), \quad (80) $$

where

$$ \nu_k^2 = \tau_0 \left( \sqrt{\frac{1}{2} - 2 h_m \cos \varphi_k + 1} + 1 - h_m \right). \quad (81) $$

Comparing (81) with (75), one can conclude that the expression for the intermediate asymptotic for the probability of remaining in the ground state is identical to the semi-infinite pulse.

After crossing the second critical point, the system ends in the state with the domain structure, consisting of regions with neighboring spins polarized in the same
Fig. 6 Ferromagnet → paramagnet transition. The probability, $P_{gs}$, to remain in the ground state as a function of the dimensionless time $s = t/\tau_0$. Parameters used: $J = 1$, $\tau_0 = 500$, $h_0 = 1, 20$. Orange line ($N = 32$), green line ($N = 64$), red line ($N = 128$), black line ($N = 256$). Dashed lines correspond to the asymptotic formula (74). a $h_0 = 20$; b $h_0 = 1$

Fig. 7 The probability, $P_{gs}$, remaining in the ground state as a function of the dimensionless time $s = t/\tau_0$. Blue line ($N = 32$, $\omega = 2.4$), green line ($N = 64$, $\omega = 0.6$), red line ($N = 128$, $\omega = 0.15$), black line ($N = 256$, $\omega = 0.04$). a Paramagnet → ferromagnet transition. Dashed lines correspond to the LZ formula (76). b Ferromagnet → paramagnet transition. Dash-dotted lines depict the LZ approximation (76). Dashed lines correspond to the AI approximation (77). Choice of parameters: $J = 1$, $\tau_0 = 500$, $h_0 = 20$

Fig. 8 Finite pulse, $h(s)$, as a function of dimensionless time $s = t/\tau_0$ ($h_0 = 20$). a $\delta = 1$; b $\delta = 100$

directions along the $z$-axis and separated by kinks with the polarization of spins in the opposite directions.

In Figs. 9, 10, 11, we present the results of the numerical simulations (solid lines); dashed lines correspond to the asymptotic formula (80). One can observe good agreement between the intermediate asymptotic given by Eq. (80) and the results of numerical simulations (Fig. 10). Under a shock wave load with the quench time $\tau_0 \ll 1$ and the pulse width $\delta = 1$, the system’s final state depends on the number of spins $N$, and quench time. For $\tau_0 = 0.001$, the probability of remaining in the ground state has much variance with changing the number of spins. For $\tau_0 = 0.001$, the final state is the ferromagnetic one with a small number of defects and a slight dependence on the number of spins (Fig. 11).
Fig. 9  Shock wave load. The probability, $P_{gs}$, to stay in the ground state as a function of the dimensionless time $s = t/\tau_0$ ($h_0 = 10$, $\tau_0 = 1$). a $\delta = 1$; b $\delta = 0.1$. Blue line ($N = 32$), green line ($N = 64$), red line ($N = 128$), black line ($N = 256$).

![Fig. 9](image)

Fig. 10  The probability, $P_{gs}$, to remain in the ground state as a function of the dimensionless time $s = t/\tau_0$ ($h_0 = 10$, $\delta = 10$). a $\tau_0 = 20$. b $\tau_0 = 5$. Blue line ($N = 32$), orange line ($N = 48$), green line ($N = 64$), red line ($N = 128$). Dashed lines correspond to the asymptotic formula (80).

![Fig. 10](image)

Fig. 11  Shock wave load. The probability, $P_{gs}$, to stay in the ground state as a function of the dimensionless time $s = t/\tau_0$ ($h_0 = 10$, $\delta = 1$). a $\tau_0 = 0.01$; b $\tau_0 = 0.001$. Blue line ($N = 32$), green line ($N = 64$), red line ($N = 128$), black line ($N = 256$).

![Fig. 11](image)

5 Critical phenomena and defects formation

As discussed before, the system’s final state is determined by the number of defects (kinks). According to [23], the operator of the number of kinks is given by

$$\hat{N} = \frac{1}{2} \sum_{n=1}^{N} (1 - \sigma_n^z \sigma_{n+1}^z) = \sum_k a_k^\dagger a_k. \quad (82)$$
Employing Eqs. (10)–(13), we obtain
\[
\mathcal{N} = \frac{N}{2} + \frac{1}{2} \sum_k \left( \cos \theta_k (c_k^\dagger c_k - c_{-k}^\dagger c_{-k}) + \sin \theta_k (c_k^\dagger c_{-k} + c_{-k}^\dagger c_k) \right),
\]
Eq. (83)

The number of defects is defined by the expectation value of the operator of the number of defects, \( \mathcal{N} = \langle \mathcal{N} \rangle \). The computation yields
\[
\mathcal{N} = \frac{N}{2} - \frac{1}{2} \sum_k (|\alpha_k|^2 - |\beta_k|^2).
\]
Eq. (85)

In the adiabatic basis this formula takes a more simpler form,
\[
\mathcal{N} = \frac{N}{2} - \frac{1}{2} \sum_k (|\alpha_k|^2 - |\beta_k|^2).
\]
Eq. (87)

For the expectation value of the density of defects, we obtain,
\[
n = \frac{\mathcal{N}}{N} = 1 - \frac{1}{N} \sum_k |\alpha_k|^2.
\]
Eq. (86)

Denoting the probability to stay in the ground state as \( P_{gs}(\varphi_k) \equiv |\alpha_k|^2 \), we rewrite Eq. (86) as
\[
n = 1 - \frac{1}{N} \sum_k P_{gs}(\varphi_k).
\]
Eq. (87)

Next, using the approximated formula (46), we obtain
\[
n \approx \frac{1}{N} \sum_k e^{\alpha_0 \sum f_0^c(z) dz}
\]
Eq. (88)

When \( N \to \infty \), the sum in Eq. (87) can be replaced by integral,
\[
n = \lim_{N \to \infty} \frac{\mathcal{N}}{N} = 1 - \frac{1}{2\pi} \int_0^\pi P_{gs}(\varphi) d\varphi
\]
Eq. (89)

Substituting \( P_{gs}(\varphi) \) from Eq. (46), we find
\[
n = \frac{1}{2\pi} \int_0^\pi e^{-\nu^2(\varphi)} d\varphi,
\]
Eq. (90)

where
\[
\nu^2(\varphi) = J\tau_0(\sqrt{h_m^2 - 2h_m \cos \varphi + 1} + 1 - h_m).
\]
Eq. (91)

Using the method of steepest descent, for \( \tau_0 \gg 1/J \), we obtain
\[
n = \frac{1}{2\pi \sqrt{\tau_Q}},
\]
Eq. (92)

where \( \tau_Q = J\tau_0 h_m / 2(h_m - 1) \) is the quench time.

In other limit case, \( h_0 \gg 1 \), the computation yields
\[
n = e^{-2\pi \tau_0} I_0(2\pi \tau Q),
\]
Eq. (93)

where \( I_0 \) is the modified Bessel function. For \( \tau_Q \gg 1 \), using the asymptotic expansion of the Bessel function for large argument, we obtain
\[
n = \frac{1}{2\pi \sqrt{\tau_Q}}.
\]
Eq. (94)

It is consistent with Eq. (92) in the limit of \( h_0 \gg 1 \), and with results known from the literature [23,35].

The previous section shows that only long-wavelength modes, with the lowest \( \varphi = \pi / N \), can be excited during the slow evolution. Therefore in the adiabatic regime, \( \omega^2 \gg 1 \), one can approximate the average number of defects at the end of evolution by the LZ formula,
\[
n = 1 - e^{-\pi \omega^2},
\]
Eq. (95)

where \( \omega^2 = \pi^2 \tau_0 J / N^2 \). It is in agreement with the results reported in [23,36].

In Figs. 12, 13, 14, we compare our theoretical predictions with the results of numerical simulations performed for \( N = 32, 64, 128, 256 \) spins. In Fig. 12, the density of defects for the paramagnet \( \rightarrow \) ferromagnet and ferromagnet \( \rightarrow \) paramagnet transitions are depicted. Solid lines present the results of the numerical simulations, and dashed lines correspond to Eq. (88). One can observe that the outcomes predicted by the asymptotic formula (88) are in good agreement with the numerical calculations. Additionally, for a large number of spins, one can use Eq. (92) to estimate the density of defects. For comparison, we bring here values of the density of defects obtained from Eqs. (88) and (92), denoting them as \( n_N \) and \( n_\infty \), respectively: \( n_{128} = 0.00981689 \), \( n_{256} = 0.00993995 \), \( n_\infty = 0.0099393 \). Thus, starting with \( N > 100 \), one can apply Eq. (92) to calculate the density of defects with high accuracy.

In Figs. 13, 14, the density of defects is depicted for a pulse of finite width. One can observe good agreement between the intermediate asymptotic given by Eq. (88) and the results of numerical simulations performed for the relatively long pulse with \( \delta = 10 \) (Fig. 13). Under a shock wave load with a narrow width \( \delta = 1 \), the final state depends on the quench time \( \tau_0 \) (see Fig. 14a). A density of defects increases up to \( n \sim 0.6 \) when the adiabatic regime changes to an impulse one and decreases to its minimum value when the impulse regime returns to the adiabatic one. If the quench time is relatively large, a significant number of defects emerge and remain to the end of evolution. As can be observed, for \( \tau_0 = 0.001 \),
the defects vanish at the end of evolution, and the system remains in the ground (ferromagnetic) state. To explain this result, consider a shape of pulse depicted in Fig. 14b. For $\tau_0 = 0.001$, the pulse looks like a $\delta$-function. The system gets a kick that excites half of the spins to the paramagnetic state. Since the impulse regime immediately changes to the adiabatic one, there is not enough time for relaxation, and the system returns to the ferromagnetic ground state.

In some cases, the results are contrary to intuition and common sense. For instance, one expects that the density of defects should decrease with the increasing quench time. However, as shown in Fig. 14a, the density of defects for $\tau_0 = 5$ is larger than for $\tau_0 = 0.01$ and less than for $\tau_0 = 0.1$. 

**Fig. 12** Semi-finite pulse. Density of defects vs. $s$ ($\tau_0 = 500, h_0 = 20$). Blue line ($N = 32$), green line ($N = 64$), red line ($N = 128$), black line ($N = 256$). Dashed lines correspond to the asymptotic formula (88). a Paramagnet → ferromagnet transition. b Ferromagnet → paramagnet transition.

**Fig. 13** Finite pulse. Density of defects vs. $s$ ($h_0 = 20, \delta = 10$). Cyan line ($N = 32$), blue line ($N = 48$), green line ($N = 64$), red line ($N = 128$), black line ($N = 256$). Dashed lines correspond to the asymptotic formula (88). a $\tau_0 = 20$; b $\tau_0 = 5$.

**Fig. 14** Finite pulse. a Density of defects vs. dimensionless time. Quench time: $\tau_0 = 0.001$ (red), $\tau_0 = 0.01$ (blue), $\tau_0 = 0.1$ (gray), $\tau_0 = 0.5$ (cyan), $\tau_0 = 1$ (orange), $\tau_0 = 5$ (green), $\tau_0 = 10$ (black). b Shape of the pulse: $\tau_0 = 0.001$ (red), $\tau_0 = 0.01$ (blue), $\tau_0 = 0.1$ (gray), $\tau_0 = 0.5$ (cyan). Choice of parameters for both cases: $h_0 = 10, \delta = 1, N = 64$. 
6 Discussion and conclusion

In this paper, we have studied the quench dynamics of the quantum Ising chain in a transverse time-dependent magnetic field, given by a semi-infinite pulse or a pulse of finite width. We have found a new analytical expression, generalizing the LZ and AI formulas for the asymptotic probability of remaining in the ground state at the end of evolution. We compared our asymptotic formulas with the results of the numerical simulations for the semi-infinite pulse and have shown they are in excellent agreement, even when the LZ and AI approximations fail. In the case of the finite pulse, there is the intermediate asymptotic for the probability of remaining in the ground state when the pulse width is relatively large. There is a good agreement between the intermediate asymptotic obtained from exact results and our theoretical predictions.

For the semi-infinite pulse, leading to the phase transition from the ferromagnetic to paramagnetic state and vice versa, the system’s final state depends on how slowly or fast the system evolves in the neighborhood of the critical point. Near the critical point, topological defects may emerge and, in such a way, define the system’s final state. For the large amplitude of the pulse, in the thermodynamic limit, we have obtained a novel analytical expression for the density of defects and have shown that it is consistent with known from the literature.

For the finite pulse, the dynamics is more complicated and, sometimes, contrary to intuition. Under a shock wave load with a narrow width (δ = 1), the final state depends on the quench time $\tau_Q \sim \tau_0$ in such a way that, for $\tau_0 \lesssim 0.01$, the density of defects decreases with decreasing the quench time. However, for $\tau_0 > 0.01$, this pattern is broken. For instance, the density of defects for $\tau_0 = 5$ is larger than for $\tau_0 = 0.01$ and less than for $\tau_0 = 0.1$. This issue needs further study to explain the discrepancy.

We hope that our outcomes can be helpful for studying more complicated quantum systems, like the XY model in a transverse magnetic field, and the influence of environment on the quench dynamics.

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Author contributions

All authors contributed equally to the paper.

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