Letter

Nonadiabatic dynamics across a first-order quantum phase transition: Quantized bubble nucleation

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Metastability is a quintessential feature of first-order quantum phase transitions, which is lost either by dynamical instability or by nucleating bubbles of a true vacuum through quantum tunneling. By considering a drive across the first-order quantum phase transition in the quantum Ising chain in the presence of both transverse and longitudinal fields, we reveal multiple regions in the parameter space where the initial metastable state loses its metastability in successive stages. The mechanism responsible is found to be semidegenerate resonant tunnelings to states with specific bubble sizes. We show that such dynamics of *quantized* bubble nucleations can be understood in terms of Landau-Zener transitions, which provide quantitative predictions of nucleation probabilities for different bubble sizes.

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Introduction. Nonequilibrium aspects of many-body quantum systems are at the heart of understanding the fundamentals of statistical and condensed matter physics as well as of quantum field theory [1–9]. On the theoretical front, the analysis of the dynamics of nonintegrable systems has soared drastically during the last two decades due to the advancement and development of efficient numerical tools such as various tensor network methods [10–12]. Moreover, with the recent breakthroughs in quantum simulations [13–19], studying the nonequilibrium features of complex quantum systems on table-top experiments has become a reality, especially in substrates such as cold atoms on optical lattices [20–25] or trapped ions [26–33].

One promising avenue of work in this ubiquitous facet of fundamental physics has been to investigate nonadiabatic excitations due to quenches across a continuous quantum phase transition [34,35] under the unifying framework of the quantum version [6,36–40] of the classic Kibble-Zurek (KZ) mechanism [41–46]. However, the question that has been asked less frequently is regarding the consequence of a slow drive across a first-order quantum phase transition (FOQPT) [47,48] and whether it is possible to find any similar universal dynamical features akin to quantum KZ theory.

FOQPTs exhibit metastability on a drive across the transition, i.e., the system tends to persist in the local minimum due to the presence of a potential barrier. In the traditional language of continuous field theory, the state gets stuck in a false vacuum, that is stable against small fluctuations, and cannot tunnel to the true vacuum easily. However, on a dynamical quench across FOQPT, the false vacuum may become dynamically unstable and the true vacuum may develop due to the disappearance of the potential barrier far beyond the FOQPT point. Under such scenarios, several recent studies reported KZ scaling laws for the dynamics across certain first-order phase transitions—both classical as well as quantum [49–57]. Another more generic mechanism, through which such metastability can evaporate, is the continual creation of bubbles of the true vacuum driven by the quantum fluctuations inside the false vacuum. The aim of the present Letter is to thoroughly investigate the breakdown of metastability by the nucleation of bubbles in a many-body quantum setting—going beyond the paradigm of dynamical instability and the corresponding KZ mechanism.

We consider the generic one-dimensional (1D) quantum Ising chain in the presence of both transverse and longitudinal fields. The model possesses a FOQPT between two ferromagnetic phases of opposite orientations driven by the longitudinal field. On slow tuning of the longitudinal field across the FOQPT line, we detect a multitude of special (resonant) points/regions where the nucleation of bubbles of the true vacuum inside the metastable false vacuum becomes energetically favorable. Moreover, these tunneling processes are *quantized* in the sense that only a specific size of bubbles, pertaining to a specific perturbative order, can nucleate around the corresponding resonant value of the longitudinal field. We provide accurate quantitative explanations of these nonadiabatic changes by means of the archetypal Landau-Zener (LZ) theory [58–61].

Model. The quantum Ising model in the presence of a transverse field in 1D is one of the prototypical models used for several decades to understand the quantum phase transition at zero temperature [34,35]. In the presence of an additional longitudinal field the Hamiltonian reads

$$H = -\sum_{n=1}^{N}\left[\sigma_n^z\sigma_{n+1}^z + h_x\sigma_n^x + h_z\sigma_n^z\right], \tag{1}$$

where we assume a transverse field $h_x > 0$ for definiteness. Apart from having a rich phase diagram, this model, although being simple, has become a test bed for fascinating equilibrium as well as out-of-equilibrium phenomena, such as

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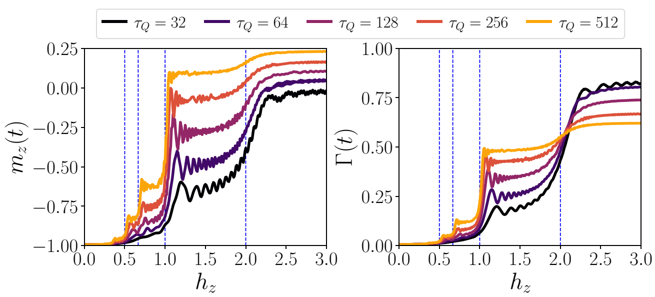

FIG. 1. The average magnetization $m_z(t)$ (left) and the density of kinks $\Gamma(t)$ (right) tracked dynamically by varying the parallel field h_z according to Eq. (2) for a wide range of quench times τ_Q. Here, we set $h_x = 0.2$ and $h_z^{\rm in} = -4.0$.

weak thermalization [62], dynamical confinement [63–66], the existence of quantum many-body scars [67–69], or fracton dynamics [70]. For the longitudinal field $h_z = 0$, this model has a continuous quantum phase transition at $h_x = 1$ separating the ferromagnetic phase ($h_x < 1$) from the paramagnetic one ($h_x > 1$). An FOQPT exists separating two ordered ferromagnetic phases along the so-called Ising line ($h_z = 0$). In this Letter, we will mostly stay in the regime of a small transverse field, $h_x \ll 1$, where, with the exception of some special regions, it can be considered as a source of small quantum fluctuations in a classical Ising chain.

Linear ramp and special regions. To initiate, we prepare the system in the ground state of the Hamiltonian (1) in one of the ordered phases ($h_x < 1$) and perform a slow ramp of the longitudinal field h_z across the first-order transition. We choose a protocol akin to what is usually used in studies of the KZ mechanism, where we ramp the field as

$$h_z(t) = h_z^{\rm in} + \frac{t}{\tau_Q}. \tag{2}$$

We start at time $t = 0$ when the initial state $|\psi(t = 0)\rangle = |\psi_{\rm in}\rangle$ is the ground state of the Hamiltonian (1) with $h_z^{\rm in} < 0$, and then ramp the field up to a final value $h_z^{\rm fin} > 0$ in the opposite ordered phase. The total ramp time is proportional to τ_Q. The dynamics is simulated by using the time-dependent variational principle (TDVP) [12,71–73] based on a matrix-product state (MPS) [10,11] ansatz with an open boundary condition.

To start, we use the average longitudinal magnetization $m_z = \frac{1}{N}\sum_n \langle\sigma_n^z\rangle$, and the longitudinal density of kinks $\Gamma = \frac{1}{2}[1 - \frac{1}{N-1}\sum_n \langle\sigma_n^z\sigma_{n+1}^z\rangle]$ as our *bona fide* observables. Deep in the ferromagnetic phase, for $|h_z^{\rm in}| \gg h_x$, the initial state has $m_z \approx -1$ and $\Gamma \approx 0$ as the state is highly polarized:

$$|\psi_{\rm in}\rangle \approx |\downarrow\downarrow\cdots\downarrow\rangle. \tag{3}$$

During the ramp, we observe that the initial state remains metastable against small quantum fluctuations driven by the transverse h_x for a long time after crossing the FOQPT point. The crucial feature in this scenario is that the system departs from the metastable state at several *special occasions* during the ramp (see Fig. 1). Deep into the positive ferromagnetic phase ($h_z > 0$), the average magnetization $m(t)$ and the density of kinks $\Gamma(t)$ get jolted up in several steps and finally saturate although with visible small oscillations. We shall show that these special regions exist around points where the initial metastable state is semidegenerate with bubbles of the true vacuum. Below, we provide a heuristic explanation first.

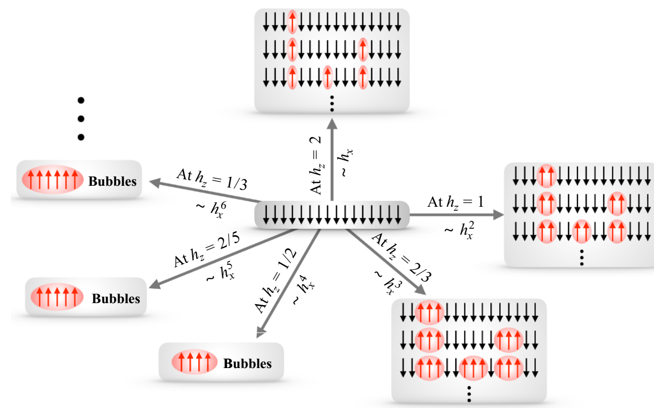

FIG. 2. Diagram showing the possible nucleation processes and their perturbative orders in h_x. At $h_z = 2/n$ the metastable initial state, with all spins pointing down, is semidegenerate with states containing size-n bubbles with spins up. They are connected by an nth-order process in h_x.

Without quantum fluctuations, when the knob is set to $h_x = 0$, any spin flips in the fully polarized initial state (3) increases the ferromagnetic energy—a domain or bubble of n consecutive $\uparrow$ spins increases the ferromagnetic energy by 4, regardless of its size. Overall, taking into account the local longitudinal fields, such a bubble of size n changes the total energy by $4 - 2nh_z$, which becomes zero when

$$h_z = 2/n. \tag{4}$$

As a result, we have *quantized* values of the longitudinal field $h_z = 2, 1, 2/3, 1/2, \ldots$, where the initial metastable state becomes degenerate with states having bubbles of sizes $n = 1, 2, 3, 4, \ldots$, respectively. These are the four major quantized values of the longitudinal magnetic field that correspond to the jolts clearly seen in Fig. 1.

When $h_x > 0$, operators σ_n^z are no longer good quantum numbers. For a generic h_z, the initial state (3), dressed with quantum fluctuations of second order in h_x, remains an approximate eigenstate. This is not the case at the special quantized values of h_z, where the initial state becomes semidegenerate with bubbles of size n—connected by anticrossings—and even a tiny h_x is enough to mix them. Each of these *resonant points* in h_z corresponds to a particular order in perturbation theory with respect to h_x. For instance, only nucleations of bubble size 1 can happen near $h_z = 2$. As this requires a single spin to be flipped, the tunneling between the degenerate states is first order in h_x. In general, tunneling at $h_z = 2/n$ between the polarized initial state and a state with an n-bubble is an nth-order process. For a schematic viewpoint, see Fig. 2.

Landau-Zener (LZ) nucleation theory. We begin with $n = 1$ near $h_z = 2$. For a low density of flipped spins, we can consider flipping an isolated spin at site j:

$$|\downarrow\cdots\downarrow\downarrow_j\downarrow\cdots\downarrow\rangle \xleftrightarrow{h_x} |\downarrow\cdots\downarrow\uparrow_j\downarrow\cdots\downarrow\rangle. \tag{5}$$

The tunneling is driven by the term $-h_x\sigma_j^x$. In the two-dimensional subspace, the Hamiltonian reads

$$H_{\mathrm{eff}}^{(1)} = E_0(h_z) + \begin{bmatrix} 0 & -h_x \\ -h_x & 4-2h_z \end{bmatrix}, \tag{6}$$

where $E_0(h_z) = -(N-1) + Nh_z$ is the energy of the metastable state. With the linear ramp (2) this becomes the LZ problem [58–61] with an anticrossing when $h_z = 2$. The LZ probability to flip the spin is $p_1 = 1 - \exp(-\pi\tau_Q h_x^2)$. Beyond the two-dimensional subspace, this formula is accurate only when $p_1 \ll 1$ or, equivalently, for fast quenches with $\pi\tau_Q h_x^2 \ll 1$. Otherwise, the density of flipped spins becomes large and we cannot consider flipping spin j in isolation from flipping other spins.

More generally, bubbles of n spins are nucleated near $h_z = 2/n$. For a low total density of bubbles we can consider flipping n consecutive spins $j, \dots, j+n-1$ by an nth-order process:

$$|\downarrow\cdots\downarrow\downarrow_j\cdots\downarrow_{j+n-1}\downarrow\cdots\downarrow\rangle$$
$$\xleftrightarrow{h_x^n} |\downarrow\cdots\downarrow\uparrow_j\cdots\uparrow_{j+n-1}\downarrow\cdots\downarrow\rangle. \tag{7}$$

For such a process the effective Hamiltonian reads

$$H_{\mathrm{eff}}^{(n)} \approx E_0(h_z) + \begin{bmatrix} 0 & -c_n h_x^n \\ -c_n h_x^n & 4-2nh_z \end{bmatrix}. \tag{8}$$

Here, c_n is a combinatorial factor. In general, it can be derived for any order n by treating the transverse field perturbatively and obtaining the low-energy effective Hamiltonian through the Schrieffer-Wolff transformation [74]. For particular perturbative orders, we will concentrate on $c_1 = c_2 = 1$ and $c_3 = 81/64$ in this Letter [75]. After the anticrossing at $h_z \approx 2/n$ the LZ probability to nucleate the n-bubble reads [75]

$$p_n = 1 - \exp\left(-\frac{c_n^2}{n}\pi\tau_Q h_x^{2n}\right) \approx \frac{c_n^2}{n}\pi\tau_Q h_x^{2n}. \tag{9}$$

It is accurate for $\tau_Q h_x^{2n} \ll 1$ only. In order to verify the LZ formula, we consider the density of n-bubbles:

$$\lambda_n = \left\langle P_i^{\downarrow}\left[\prod_{j=1}^{n} P_{i+j}^{\uparrow}\right] P_{i+n+1}^{\downarrow}\right\rangle. \tag{10}$$

Here, $P_j^{\uparrow,\downarrow} = (1 \pm \sigma_j^z)/2$ is a projector onto spin-$\uparrow$ ($\downarrow$) at site j and $\langle\cdots\rangle$ refers to averaging over all sites except for the ends of the chain to avoid the boundary effects. In Fig. 3 we plot λ_1 and λ_2 obtained with TDVP as a function of $\tau_Q h_x^{2n}$ for several values of h_x such that the low-density condition $\tau_Q h_x^{2n} \ll 1$ is satisfied. Plots for different h_x collapse to a straight line with a slope consistent with the simple LZ theory.

Nucleation versus hopping. In the second-order perturbation in h_x, the n-bubble at sites $j, \dots, j+n-1$ can hop to the right/left by one lattice site. In order to hop to the right, spin $j+n$ can be flipped upwards, followed by a downward flip of spin j, or the other way around. The net hopping rate is $\gamma = h_x^2/h_z$.

The LZ formula cannot be taken for granted if the nucleated bubble can hop away before the LZ tunneling is completed at time $t_{\mathrm{LZ}} \approx \sqrt{\tau_Q/2n}$ [36] after the anticrossing at $h_z = 2/n$. Therefore, the hopping should be irrelevant when

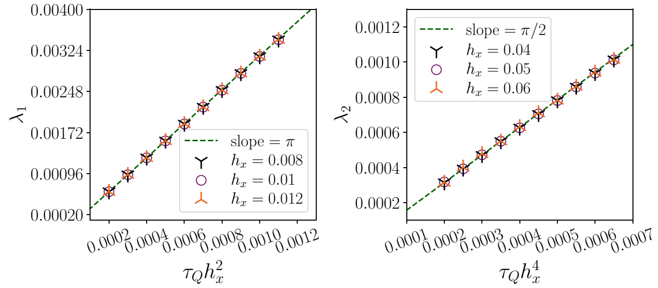

FIG. 3. The density of 1-bubbles, λ_1 (left), and 2-bubbles, λ_2 (right), are shown as functions of scaled τ_Q for several strengths h_x of quantum fluctuations. The different h_x collapse to straight lines with slopes π and $\pi/2$ for $n = 1, 2$, respectively. The collapse demonstrates the accuracy of the simple Landau-Zener theory for a low density of nucleated bubbles.

$\gamma t_{\mathrm{LZ}} \ll 1$ or, equivalently,

$$\tfrac{1}{8}n\tau_Q h_x^4 \ll 1. \tag{11}$$

For 1-bubbles this condition is satisfied with a safe margin in their low-density regime where $\pi\tau_Q h_x^2 \ll 1$. For 2-bubbles it is identical with low density. However, for 3-bubbles and bigger it is stronger than low density. For 3-bubbles the hopping is a second-order process while the LZ tunneling is formally a weaker third-order effect.

In order to demonstrate the interplay between the nucleation of 3-bubbles and their hopping we simulate a ramp from $h_z^{\mathrm{in}} = -6$ to $h_z^{\mathrm{fin}} = 0.8$. The density of 3-bubbles is shown in Fig. 4 as a function of the scaling variable deep in the low-density regime, where $\tau_Q h_x^6 \ll 1$. With increasing $\tau_Q h_x^6$ there is a crossover from the pure LZ nucleation to the regime where the hopping becomes relevant. In the former we can see good agreement with the LZ theory, demonstrated by the collapse, while in the latter the curves begin to diverge slowly.

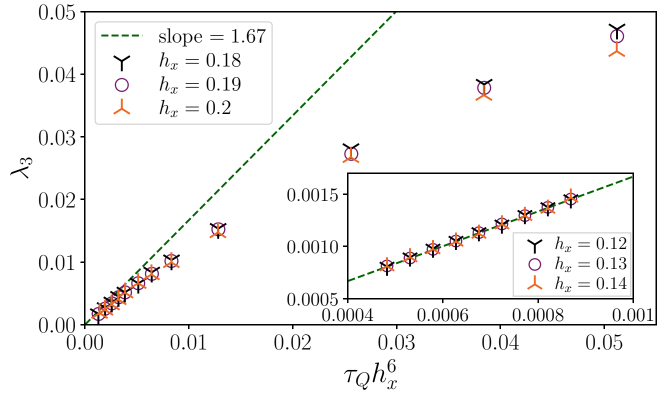

FIG. 4. Density of 3-bubbles, λ_3, as a function of the scaling variable $\tau_Q h_x^6$ for different values of h_x. Here, $\tau_Q h_x^6 \ll 1$ is deep in the low-density regime but, according to condition (11), the hopping remains irrelevant at most up to $\tau_Q h_x^6 \approx h_x^2 \approx 0.03$. To the left of this point the plots collapse to a single curve that tends to a line with the predicted slope $\frac{1}{3}(81/64)^2\pi = 1.67$ (see the inset). To the right the plots begin to diverge, demonstrating the breakdown of the simple LZ theory.

Beyond low density. Up to now, we have seen that bubble nucleations at low densities are accurately described by two-level LZ problems. Moreover, for $n = 1, 2, 3$, $\tau_Q h_x^{2n}$ is the scaling variable when the hopping is not relevant. The next natural questions are (1) if it remains such beyond the low-density regime, and (2) whether we can also treat bubble nucleations at high densities as LZ transitions. To answer these questions, we consider again the nucleation of 1-bubbles near $h_z = 2$ but this time in a full range of $\tau_Q h_x^2$. In order to isolate the 1-bubble nucleation in full TDVP simulations, we have to keep irrelevant not only the hopping (11) but also the 3- and 2-bubble nucleation at $h_z = 2/3, 1$, respectively. This requires very small h_x^2 that makes τ_Q rather long, making TDVP intractable for $\tau_Q h_x^2 \gg 1$.

In order to get perfect isolation and additionally get some analytical insights, first we consider an effective Hamiltonian by projecting the original Hamiltonian (1) into the 1-bubble subspace. On a periodic chain of N sites the subspace is spanned by the initial metastable state $|0\rangle = |\psi_{\rm in}\rangle$ in (3), the translationally invariant (TI) one 1-bubble state, $|1\rangle = \frac{1}{\sqrt{N}}\sum_j |\downarrow\cdots\downarrow\uparrow_j\downarrow\cdots\downarrow\rangle$, the TI two 1-bubble state $|2\rangle$, up to the TI state with $N/2$ 1-bubbles $|N/2\rangle = \frac{1}{\sqrt{2}}(|\downarrow\uparrow\downarrow\uparrow\cdots\rangle + |\uparrow\downarrow\uparrow\downarrow\cdots\rangle)$. It turns out that the resulting $(N/2+1)$-dimensional effective Hamiltonian can be constructed iteratively (see Ref. [75]), and for our purpose we can consider up to $N = 44$ using a standard 64-bit machine.

Similarly as (6), the resulting Hamiltonian is a linear combination of two terms [75],

$$H_{\rm eff} = \tilde{E}_0 + \frac{t}{\tau_Q} H_z + h_x H_x, \tag{12}$$

with $\tilde{E}_0 = \langle 0|H(h_z = 2, h_x = 0)|0\rangle$. This structure allows us to rewrite the Schrödinger equation $i\frac{d|\psi\rangle}{dt} = H_{\rm eff}|\psi\rangle$ as $i\frac{d}{dt'}|\psi'\rangle = (\frac{t'}{\tau_Q h_x^2} H_z + H_x)|\psi'\rangle$. Here, $t' = h_x t$ and $\tilde{E}_0$ was absorbed in the phase of $|\psi'\rangle$. This demonstrates that the final density of 1-bubbles must depend on $\tau_Q h_x^2$ as a single scaling variable.

The dependence, obtained by a simulation with the effective Hamiltonian, is plotted in Fig. 5(a). The same figure compares results from full TDVP simulations. Unlike the low-density regime, the generic problem now is that of a $(N/2+1)$-level LZ transition, which again in the low-density regime reduces to the local two-level LZ scenario. To describe such a multilevel LZ problem, we consider two transition probabilities:

$$p_{0\to 0} = \lim_{t\to\infty} |\langle 0|\psi(t)\rangle|^2,$$
$$p_{0\to\frac{N}{2}} = \lim_{t\to\infty} |\langle N/2|\psi(t)\rangle|^2. \tag{13}$$

Following Ref. [76], the former one has the exact form

$$p_{0\to 0} = \exp\left[-2\pi\tau_Q h_x^2 \sum_{n=1}^{N/2} \frac{|\langle n|H_x|0\rangle|^2}{|\langle n|H_z|n\rangle - \langle 0|H_z|0\rangle|}\right], \tag{14}$$

which translates into $p_{0\to 0} = \exp[-N\pi\tau_Q h_x^2]$ [75]. Figure 5(b) shows the profile of $p_{0\to 0}$ for different values of N that perfectly matches the analytical prediction. Moreover, for $\tau_Q h_x^2 \ll 1$ only transitions between $|0\rangle$ and states $|n\rangle$ with low density, $n \ll N$, become relevant. The total probability of these transitions is $1 - p_{0\to 0}$. Therefore, in this regime the density of 1-bubbles $\lambda_1 = \frac{1}{N}(1 - p_{0\to 0}) \approx \pi\tau_Q h_x^2$, confirming the earlier analysis again.

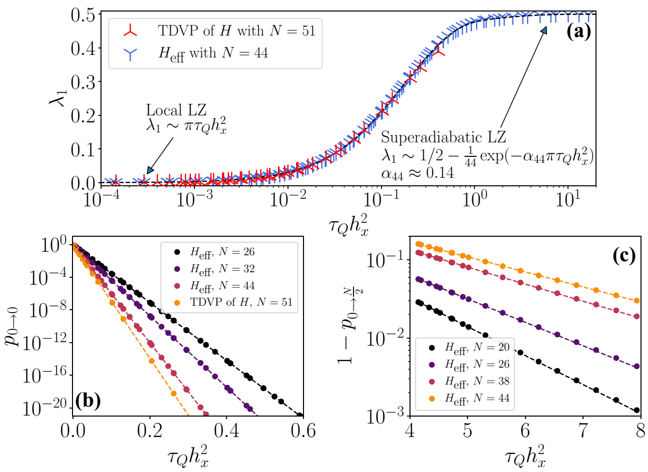

FIG. 5. (a) Density of 1-bubbles λ_1 as a function of $\tau_Q h_x^2$ after a ramp across $h_z = 2$. Here, the effective Hamiltonian (12) is benchmarked against a direct TDVP simulation. The curve crosses over from the low-density linearized LZ formula (9) with $n = 1$ to the high-density LZ profile (16). (b) The multilevel LZ transition probability $p_{0\to 0}$ as as function of $\tau_Q h_x^2$ for different system sizes N. The dashed line is the analytical formula $p_{0\to 0} = \exp[-N\pi\tau_Q h_x^2]$. (c) The superadiabatic transition probability $p_{0\to\frac{N}{2}}$ as a function of $\tau_Q h_x^2$ for different N fitted with the exponential function $p_{0\to\frac{N}{2}} = 1 - \exp[-\alpha_N\pi\tau_Q h_x^2]$.

On the other hand, when the curve in Fig. 5(a) reaches the superadiabatic regime, $\tau_Q h_x^2 \gg 1$, there is only one relevant LZ anticrossing. The initial metastable state $|0\rangle$ crosses over to the final state $|N/2\rangle$ with probability $p_{0\to\frac{N}{2}}$ and $(1 - p_{0\to\frac{N}{2}})$ becomes a small excitation probability to the state $|N/2 - 1\rangle$. An analytical derivation of $p_{0\to\frac{N}{2}}$ from the multilevel LZ problem is beyond the scope this work. However, we find the following form,

$$p_{0\to\frac{N}{2}} = 1 - \exp\left[-\alpha_N\pi\tau_Q h_x^2\right], \tag{15}$$

where the coefficient α_N decreases with N [75] [see Fig. 5(c)]. Therefore, the 1-bubble density in this regime is

$$\lambda_1 = \frac{1}{N}\left[\frac{N}{2} p_{0\to\frac{N}{2}} + \left(\frac{N}{2} - 1\right)\left(1 - p_{0\to\frac{N}{2}}\right)\right]$$
$$= \frac{1}{2} - \frac{1}{N}\left(1 - p_{0\to\frac{N}{2}}\right), \tag{16}$$

which is in good agreement with Fig. 5(a).

Conclusion and outlook. We have shown that the metastability pertained to FOQPT in the quantum Ising model under transverse and longitudinal fields is lost in successive stages in quenches across the FOQPT point, that occurs due to the *quantized* nucleation of bubbles. Specifically, we have identified special resonant regions in the longitudinal field ($h_z = 2/n$), where the metastable state can easily tunnel to nucleate bubbles of a specific size n, which are nth-order perturbative processes in the transverse field h_x. Moreover, we have unified this entire nonadiabatic process under the umbrella of

Landau-Zener theories—the low-density nucleations can be understood through two-level Landau-Zener transitions, while at higher densities the situations translate to the multilevel Landau-Zener problems.

Furthermore, our work can be easily generalized to higher dimensions, where the special resonant points become $h_z \propto S/V$. Here, S is the surface area and V the volume of a bubble, each of them taking discrete values. The physical implementation of the transverse Ising model with a chain of Rydberg atoms provided a spectacular demonstration [25] of the quantum Kibble-Zurek mechanism. Within 2 years following this breakthrough, the number of Rydberg atoms increased from 50 in 1D [25] to a few hundred in 2D/3D structures [77,78]. Such marvelous achievements on the experimental front make it possible to explore regimes where the nucleation of bubbles manifests a quantized nature, not only in 1D but also in higher dimensions.

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