

Reviewers' comments:

Reviewer #1 (Remarks to the Author):

The paper describes an experimental study of the Landau-Zener transitions with a single trapped ion. In the experiment the authors prepare the qubit in the state $|0\rangle$, apply the microwaves with the time-dependent phase to "sweep" across the resonance frequency of the transition, and measure the state of the ion at the end of this experiment to find if qubit is in the state $|0\rangle$ or $|1\rangle$ at the end of the experiment.

Authors use the equivalence of the ensemble of two level systems and 1D transverse field quantum Ising model, and relate their experiment to the studies of the Kibble-Zurek mechanism in the phase transition of interacting spins. The work was motivated by the theory paper of one of the co-authors [Ref 27] and the theory part of the manuscript have substantial overlap with Ref. 27 in terms of calculations.

The "number of kink" distribution is simulated by conducting N independent experimental sequences with different parameters for the Landau-Zener transitions, The authors measure first 3 cumulants of the probability distribution for the number of kinks and observe deviations from the theoretical predictions for slow and fast quenching times, which they attribute to the dephasing and the deviations from the Landau-Zener formula respectively.

Even though the experiment is relatively simple and is done with a single two level system, the connection to the quantum simulations of the Ising model would be interesting for the readers of Communications Physics. However, presentation of the manuscript is sometimes not clear: there are misprints, important information regarding both calculations and the experimental parameters is missing. In particular:

1. All the data in the manuscript are presented as a function of $J \tau_Q$. I was not able to find in the manuscript any values for time τ_Q in absolute units. It would be very helpful to give the range of τ_Q used in the experiment, as it can allow the reader to compare it with other decoherence time scales for the ion qubit.

2. It would also be useful to provide the absolute values of the Rabi frequencies for the experiment.

3. In the main text authors use parameter $g(t)$ and the quenching rate $1/\tau_Q$ to describe the quenching dynamics. In the Methods section authors describe the microwave signal applied to the ion in terms of ν , t_1 and t_2 . What is the relationship between these parameters?

4. Figure 4: The blue and red shaded area are shown on the figure 4, however the meaning of these shaded areas is not explained. In addition, there is no error bars for the experimental points shown on the Figure 4.

5. Authors should make a clear distinction between a magnetic field applied to the ion, and a "magnetic field" parameter g in the Ising model. It is hard sometimes to distinguish between the two, for example, when authors are talking about "quantum critical dynamic induced by a ramp of magnetic field" (Page 5).

6. Equation S10 is inconsistent with equation S11, and equation S11 is not the same as used in the main text.

7. Some important statements have these reference misplaced. For example:

Page 3: "The distribution $P(n)$ has been shown to be universal and fully determined by the scaling theory of the phase transition". No references are given.

Page 3: "Our quantum simulation approach relies on the equivalence of TFQIM in one spatial dimension and an ensemble of independent two-level systems." The reference comes only 2 sentences later.

8. The "momentum space" is used several times in the manuscript, but it is never defined and no explicit references are provided. I can find out what authors mean only after reading several papers from the list of references.

9. There are numerous misprints in the Methods section. It requires careful proofreading. For example: Page 13: "In tis condition", Page 14: "preparing the state in the bright state..", etc.

In conclusion, the results presented in the manuscript look correct and the connection between the Landau-Zener transition and simulations of the Ising model is interesting. However substantial revision is necessary to improve the clarity of the presentation and add missing experimental parameters and clarify the experimental procedure before this manuscript can be published.

Reviewer #2 (Remarks to the Author):

This is an interesting paper on a topic of broad interest in the context of quantum phase transitions, namely the dynamical crossing of a quantum critical point. The dynamical crossing of a phase transition has a long history, with initial suggestions stemming in the realm of cosmology by Tom Kibble. Certain phase transitions obey a universal scaling law, in which the number of defects (kinks) formed during the dynamical crossing (when the system breaks its symmetry, associated with its inability to react instantaneously to its driven input parameter regime) follows, in the appropriate regimes, a power-law scaling with the quench rate. In this work, the authors provide an experimental study of the critical dynamics in a 1D quantum Ising chain paramagnetic-to-ferromagnetic phase transition in the context of a trapped-ion quantum simulator, characterizing the probability distribution of defects (beyond their mean value), finding excellent agreement with theoretical predictions previously reported by one of the authors in Physical Review Letters.

The explicit experimental demonstration is exciting, topical and sheds further light on quantum phase transitions. As such, I do consider this manuscript as technically sound, clearly substantiated, and of significant importance in its specific sub-field, and beyond. For these reasons, I do recommend publication in Communications Physics, after the authors have made a few suggested clarifications.

1. The authors conclude their abstract with the statement "characterize the full probability distribution of topological defects": as this would admittedly be extremely hard, they are in effect limited to the 3 lowest cumulants (still, a highly noteworthy result). However, what I am not sure of is whether their reported experimental results effectively only demonstrate agreement (in the strict sense) for only κ_1 (standard Kibble-Zurek), and κ_2 . I still find their reported measurements of κ_3 most interesting and valid (so they should of course be reported!), but I wonder whether the claim of exactly what has been experimentally observed/verified may need slight rewording.

2. (a) The authors should also clarify the extent to which the full distribution of topological defects (or related studies of the defect morphology and distribution) has been previously reported in different contexts of quenched phase transitions, both theoretically (i.e. beyond the paper by co-author del Campo) and experimentally: in particular, are there any other claims or observations of such behaviour across the broad range of physical systems exhibiting such effect, or is this the first time this has been demonstrated experimentally across any system? This is an important point that is, in my personal view, not sufficiently clarified in the manuscript, and could be improved upon. This should not be taken as a statement on the quality of work reported herein, or

its validity, but rather to ensure that this paper demonstrates full clarity of the relevance and importance of the presented results to a broader set of potential readers.

(b) A question which may be more theoretical than experimental: while it is clear that higher-order cumulants are harder to measure experimentally, are there theoretical expectations of how far this (or other similar) experimental systems may be able to push the analysis, e.g. should we ever expect clear κ_n with $n \geq 3$ to be observable? Are there ways to reduce (in this case) the “noise-induced dephasing”, or “dephasing-induced anti-KZM behavior”? (incidentally, I am not sure I like the expression “anti-KZM behavior”), and what causes “the range of quench times characterized by universal behaviour to be reduced for high-order cumulants...”? Finally, can anything more (qualitative) be said about the “non-universal corrections”?

3. Figures and units:

(a) Are there error bars in the experimental data? I assume that perhaps the error bars are much smaller than the size of the symbols used to depict the measured points, but if so the authors should explicitly state that in the relevant figure caption.

(b) In my opinion the interesting deviations in Figs. 2 and 3 are not very evident, and alternative visualizations may make these more clear, e.g. while the deviation is obvious in one of the 4 cases demonstrated in those figures, it is not clear whether the other cases agree partly, mostly, or fully.

(c) Regarding units and figures, can units be stated where relevant? I am a bit perplexed about units of $J^* \tau_Q$: are these meant to be dimensionless (as Fig. 4 might suggest, since no specific units are mentioned in the figure), or in terms of $\hbar$, as evident from various of the employed formulae, e.g., $\tau_Q \sim \hbar / (2 \pi^3 J)$. I appreciate the main result is the scaling, but it's best to be consistent throughout.

(d) The labels in Fig. 1 appear particularly small, most notably Fig. 1B. Not sure how large the final image may appear in the manuscript, but it would probably be advisable to increase font size.

4. Minor suggestions:

(a) This may already be reported in the manuscript, but are the experimental results at all sensitive to the precise details of the initial pre-quench state of the system?

(b) It would be useful to general readers if the authors would explicitly state what they mean by the “scaling limit”, beyond stating that this is “the regime of validity of the KZM”.

(c) I appreciate that this paper is based on quantum phase transitions, but I am not convinced that the references to earlier systems exhibiting Kibble-Zurek-related physics is sufficiently extensive. For example, key experiments in ultracold atoms (e.g. by the groups of Anderson, Dalibard and Yong Il-Shin) are missing: there is no requirement per se to mention those, but it is a suggestion to the authors for their consideration (I assume similar issues may apply to other physical systems I am less familiar with – for example, I wonder if Kibble-Zurek-type studies across the QCD critical point may be relevant to be mentioned here?)

(d) There are some equations within the main text that could be better converted to full in-line equations.

(e) Also, some typos:

-the authors state interchangeably “Bernoulli” and “Bernouilli”.

-"resonate" --> resonant

-"programed"--> programmed

-"In tis condition" (in Methods)

Reviewer #3 (Remarks to the Author):

J.-M. Cui and coauthors present a study of the Kibble-Zurek mechanism (KZM) probed with a single two-level system, implemented experimentally with a trapped atomic $^{171}\text{Yb}^+$ ion. The authors present a detailed and very clear theoretical introduction on the KZM and on the nearest neighbor transverse field quantum Ising model (TFQIM), which is the playground they use to investigate KZM. They then apply the well-known Jordan-Wigner transformation to describe the

TFQIM in terms of free fermionic quasi-particles characterized by the momentum quantum number k .

Then they map this system on a Bloch sphere of a two-level system (the ion) where they measure the number of topological defects as they ramp the system across the phase transition, as a function of different ramping speeds, characterizing the transition with cumulants up to the third order.

In my opinion this work lacks clarity and cannot be published in Comm. Phys. as it stands. The authors simulate a TFQIM of $N=100$ spins (as quoted in the caption of Fig. 3) mapping this model to a single vector in a Bloch sphere. However, this mapping, which is a fundamental ingredient in this work, is not clear at all and needs to be explained adequately. Do the different k modes correspond to different angles on the Bloch sphere? How the parameters in the Hamiltonian (1) relate to the $H(t)$ defined in the supplementary materials, which is the true MW+atom interaction Hamiltonian? How do the authors derive the time-dependent phase profile explained in the supplementary materials?

The only place where this mapping can be intuitively understood is Fig.1 which seems to suggest that different angles correspond to different momenta k . However, the figure is confusing and not well explained: for example the state $|\Psi_i\rangle$ is not defined anywhere.

I think the authors should:

- Clarify this mapping in the main text. Sentences like "Experimentally, the excitation probabilities p_k can be measured by probing the dynamics in each mode." or "Exploiting the equivalence between the spin and momentum representation," are a bit vague and do not explain what they are actually doing in the experiment and how the mapping works.
- Explain in detail how this mapping gives rise to the MW pulse sequence applied to the system to simulate a specific k mode.
- Improve Fig. 1 to make it more explanatory.

After these major issues are addressed the paper can be resubmitted and evaluated.

Minor changes:

- Pag. 13 This needs to be corrected to This.

Reply to R_1 's questions/comments

R_1 .(1) *The paper describes an experimental study of the Landau-Zener transitions with a single trapped ion. In the experiment the authors prepare the qubit in the state $|0\rangle$, apply the microwaves with the time-dependent phase to “sweep” across the resonance frequency of the transition, and measure the state of the ion at the end of this experiment to find if qubit is in the state $|0\rangle$ or $|1\rangle$ at the end of the experiment.*

Authors use the equivalence of the ensemble of two level systems and 1D transverse field quantum Ising model, and relate their experiment to the studies of the Kibble-Zurek mechanism in the phase transition of interacting spins. The work was motivated by the theory paper of one of the co-authors [Ref27] and the theory part of the manuscript have substantial overlap with Ref. 27 in terms of calculations.

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Answer:

We thank the reviewer for the detailed account of our work and summarizing succinctly the experiment. We take the chance to emphasize that the goal of the manuscript is to experimentally probe universal physics beyond the KZM that is manifested, e.g., in the power-law scaling of all cumulants of the defect-number distribution with the quench time. The scaling of the first cumulant (mean number) reduces to the seminal prediction of the KZM. The scaling of higher order cumulants probes physics beyond KZM. Such scaling is clearly established for the second cumulant, while the range of quench times in which the third cumulant exhibits a universal power-law scaling is reduced.

R_1 .(2) *All the data in the manuscript are presented as a function of $J\tau_Q$. I was not able to find in the manuscript any values for time τ_Q in absolute units. It would be very helpful to give the range of τ_Q used in the experiment, as it can allow the reader to compare it with other decoherence time scales for the ion qubit.*

Answer:

We thank the reviewer for this suggestion on improving the writing style of our manuscript. In the present revised version, specifically in the Supplementary Note 3 and 4 we report all experimental parameters.

The Rabi frequency in the experiment is set around 20kHz, which mainly depend on the microwave amplifier. The experiment parameter is added to the manuscript.

R₁.(3) It would also be useful to provide the absolute values of the Rabi frequencies for the experiment.

Answer:

Again, we appreciate the comment from the referee; and it has been clear in the present revised version. Both the Rabi frequency parameters are listed in the main text and figure caption.

R₁.(4) In the main text authors use parameter $g(t)$ and the quenching rate $1/\tau_Q$ to describe the quenching dynamics. In the Methods section authors describe the microwave signal applied to the ion in terms of v , t_1 and t_2 . What is the relationship between these parameters?

Answer: We appreciate this important point from R_1 and apologize for not having been explicit enough. The problem is also comes from the unclear Rabi time (or Rabi frequencies) between theory and the real experiment. In this new version of the manuscript, we have added more descriptions about the experiment parameters and rewritten some key formulas corresponding to the real experiment unit in the experiment section. We explicitly mention this important point (please see list of changes).

R₁.(5) Figure 4: The blue and red shared area are shown on the figure 4, however the meaning of these shaded areas is not explained. In addition, there is no error bars for the experimental points shown on the Figure 4.

Answer:

The shaded area indicated the range of quench time used for the power-law scaling fit. The error bars for cumulants are directly inherited from the error bars for p_k for given τ_Q given Eqs. S14-16 in the Supplemental Material. Given the logarithmic scale used to display the universal power-law scaling, error bars are

smaller than the symbols used to plot the data.

R₁.(6) Authors should make a clear distinction between a magnetic field applied to the ion, and a “magnetic field” parameter g in the Ising model. It is hard sometimes to distinguish between the two, for example, when authors are talking about “quantum critical dynamic induced by a ramp of magnetic field” (Page 5).

Answer:

We appreciate this comment from R_1 . Our present revised manuscript addresses and corrects all these concerns. It now features explicit sections with clearer explanations, making the paper easier to read and understand. We discuss these improvements in detail below in our changes list.

R₁.(7) Equation S10 is inconsistent with equation S11, and equation S11 is not the same as used in the main text.

Answer:

Thank you for pointing this out. The typo in previous S11, now S22, has been corrected. S22 follows from S21 by taking the leading term in a $1/\tau_Q$ expansion, or alternatively, by extending the upper limit of the integral from π to ∞ . We thank the referee for this comment and have now corrected this in the revised manuscript.

R₁.(8) Some important statements have these reference misplaced. For example:

Page 3: “The distribution $P(n)$ has been shown to be universal and fully determined by the scaling theory of the phase transition”. No references are given.

Answer:

This is due to unfortunate wording and the sentence has been rewritten for clarity.

Page 3: “Our quantum simulation approach relies on the equivalence of TFQIM in one spatial dimension and an ensemble of independent two-level systems.” The

reference comes only 2 sentences later.

Answer:

The subsequent sentence has been rewritten for clarity, indicating relevant references.

R_1 .(9) *The “momentum space” is used several times in the manuscript, but it is never defined and no explicit references are provided. I can find out what authors mean only after reading several papers from the list of references.*

Answer: The meaning of quantum simulation “in momentum space” is now emphasized throughout the introduction. See in particular the discussion including Eqs (2)-(4).

R_1 .(10) *There are numerous misprints in the Methods section. It requires careful proof-reading. For example: Page 13: “In tis condition”, Page 14: “preparing the state in the bright state..”, etc.*

Answer: The manuscript has been proofread a number of times by all authors to spot any such misprints, that we have corrected in this revised version.

R_1 .(11) *In conclusion, the results presented in the manuscript look correct and the connection between the Landau-Zener transition and simulations of the Ising model is interesting. However substantial revision is necessary to improve the clarity of the presentation and add missing experimental parameters and clarify the experimental procedure before this manuscript can be published.*

Answer: We are grateful to the review (R_1) for his/her opinion. We have now revised and corrected the presentation and discussion of our work. We apologize to the referee for not having been explicit enough in our original text. In the new manuscript version, we have divided the main text in four main sections: First, Introduction and theoretical background. Second, in the section *Results*: We divide this section into two subsections: Experimental design and Full probability distribution of topological defects. Finally, in the section discussions. We have also extended the discussion (see section Results and discussions in the main text) where we show the specific experimental methodology that we use to obtain our results. Note as well that emphasis has been shifted from the total distribution of defects to the distribution of pairs, which is more relevant as kinks are created in pairs by momentum conservation.

Additionally, we improved the Supplementary Information adding new and relevant information about our experiment and theoretical description. We are convinced that the new presentation of our paper improves the comprehension and highlights the relevance of our work.

We hope that this revised version can be considered suitable for publication in Communications Physics.

Reply to R_2 's questions/comments

R_2 .(1) *“This is an interesting paper on a topic of broad interest in the context of quantum phase transitions, namely the dynamical crossing of a quantum critical point. The dynamical crossing of a phase transition has a long history, with initial suggestions stemming in the realm of cosmology by Tom Kibble. Certain phase transitions obey a universal scaling law, in which the number of defects (kinks) formed during the dynamical crossing (when the system breaks its symmetry, associated with its inability to react instantaneously to its driven input parameter regime) follows, in the appropriate regimes, a power-law scaling with the quench rate. In this work, the authors provide an experimental study of the critical dynamics in a 1D quantum Ising chain paramagnetic-to-ferromagnetic phase transition in the context of a trapped-ion quantum simulator, characterizing the probability distribution of defects (beyond their mean value), finding excellent agreement with theoretical predictions previously reported by one of the authors in Physical Review Letters.*

The explicit experimental demonstration is exciting, topical and sheds further light on quantum phase transitions. As such, I do consider this manuscript as technically sound, clearly substantiated, and of significant important in its specific sub-field, and beyond. For these reasons, I do recommend publication in Communications Physics, after the authors have made a few suggested clarifications.”

Answer:

We thank the referee for expressing that “This is an interesting paper on a topic of broad interest in the context of quantum phase transitions, namely the dynamical crossing of a quantum critical point” and “the authors provide an experimental study of the critical dynamics in a 1D quantum Ising... finding excellent agreement with theoretical predictions previously reported by one of the authors in Physical Review Letters.” as well as for the the global positive evaluation of our work and recommending its publication in Communications Physics.

R_2 .(2) *“The authors conclude their abstract with the statement “characterize the full probability distribution of topological defects”: as this would admittedly be extremely hard, they are in effect limited to the 3 lowest cumulants (still, a highly noteworthy result). However, what I am not sure of is whether their reported experimental results effectively only demonstrate agreement (in the strict sense) for only κ_1 (standard Kibble-Zurek), and κ_2 . I still find their reported measurements of κ_3 most interesting and valid (so they should of course be reported!), but I wonder*

whether the claim of exactly what has been experimentally observed/verified may need slight rewording.”

Answer:

KZM predicts the scaling of the mean number of defects, this is, of the first cumulant. The aim of this paper is to establish the existence of universal signatures in the kink number distribution beyond this prediction. We have succeeded in doing so by reporting the scaling of the second cumulant, the variance. It is surprising that signatures of universality such as the ones established in this work by demonstrating the scaling of the variance have been overlooked after four decades of uninterrupted experimental efforts exploring KZM physics. Establishing the power law scaling of the variance is thus the major achievement in this work. The scaling of the third cumulant is of course of interest. Its finite value already establishes that the distribution is not normal.

Its dependence on the quench rate is consistent with a power-law scaling over a reduced range of quench times. Its behavior, is predominantly dominated by deviations from the scaling limit. At long times deviations can be expected due to finite size and would lead to a sharp suppression of the third cumulant. However, the cumulant is shown to increase, and we attribute this to the finite coherence lifetime of the qubit, which starts to experience noise induced decoherence. High order cumulants are more sensitive to deviations than low order ones. At fast quench rates, we note that the experimental parameters satisfy $2qJ\tau_Q/\hbar \gg 1$ for $q = 1, 2, 3$ and thus one expect scaling behavior (in the sense that Eqs. S17,19, 21 reduce to S18, 20, 22). Deviations are thus associated with the failure of the Landau-Zener formula to capture correctly the excitation probability in each k -mode. This is confirmed by numerical simulations with an exact solution of time-dependent Schrödinger equation, not relying on the KLZ formula, that match correctly the experimental data.

R₂.(3) “(a) The authors should also clarify the extent to which the full distribution of topological defects (or related studies of the defect morphology and distribution) has been previously reported in different contexts of quenched phase transitions, both theoretically (i.e. beyond the paper by co-author del Campo) and experimentally: in particular, are there any other claims or observations of such behavior across the broad range of physical systems exhibiting such effect, or is this the first time this has been demonstrated experimentally across any system? This is an important point that is, in my personal view, not sufficiently clarified in the manuscript, and could be improved upon. This should not be taken as a statement on the quality of work reported herein, or its validity, but rather to ensure that this paper demonstrates full clarity of the relevance and importance of the presented

results to a broader set of potential readers.”

Answer:

To the best of our knowledge this is the first study doing so. Of course, essentially all experiments done to date do measure the distribution of topological defects, but have not analyze it in the search of universal signatures beyond the KZM. In this sense, one may expect that some of these experiments are revised. An important exception in which the statistics of topological defects has been analyzed was already considered in the seminal work Ref. 4, when discussing spontaneous current formation in superconductors and superfluids. In such case the average winding number vanishes and a random walk argument was used to establish the scaling of the rms of the winding number. Experiments were performed with superconducting rings but could only probe the onset of adiabaticity (see new refs 16, 17) and the authors have reanalyzed the data with alternative interpretations (see 16, 17, J. Phys.: Condens. Matter 25 404207 (2013)).

R_2 .(4) *“(b) A question which may be more theoretical than experimental: while it is clear that higher-order cumulants are harder to measure experimentally, are there theoretical expectations of how far this (or other similar) experimental systems may be able to push the analysis, e.g. should we ever expect clear κ_n with $n \geq 3$ to be observable? Are there ways to reduce (in this case) the “noise-induced dephasing”, or “dephasing-induced anti-KZM behavior”? (incidentally, I am not sure I like the expression “anti-KZM behavior”), and what causes “the range of quench times characterized by universal behaviour to be reduced for high-order cumulants...”? Finally, can anything more (qualitative) be said about the “non-universal corrections”?”*

Answer:

In our experiment noise induces heating. In each mode, this heating increases the average fermion number occupation. In the spin representation, heating increases the kink number. These are the conclusions of the Dutta et al and account for the role of noise in our setup.

The term “anti-KZM” was not introduced by us but it is by now established in the literature, referring to deviations of KZM with opposite trend as a function of the quench rate both at fast and slow quenches.

To avoid any misunderstanding we have removed the terminology “anti-KZM” and refer to it as simply noise-induced decoherence.

R₂.(5) “Figures and units:

- (a) *Are there error bars in the experimental data? I assume that perhaps the error bars are much smaller than the size of the symbols used to depict the measured points, but if so the authors should explicitly state that in the relevant figure caption.*

Answer:

Figures have been reported for clarity indicating error bars whenever applicable.

- (b) *In my opinion the interesting deviations in Figs. 2 and 3 are not very evident, and alternative visualizations may make these more clear, e.g. while the deviation is obvious in one of the 4 cases demonstrated in those figures, it is not clear whether the other cases agree partly, mostly, or fully.”*

Answer:

Figures have been reported for clarity. In particular, we have changed the display in Fig. 3 and further discussed deviations in Fig. 2.

- (c) *Regarding units and figures, can units be stated where relevant? I am a bit perplexed about units of $J * \tau_Q$: are these meant to be dimensionless (as Fig. 4 might suggest, since no specific units are mentioned in the figure), or in terms of $\hbar$, as evident from various of the employed formulae, e.g., $\tau_Q \sim \hbar / (2\pi^3 J)$. I appreciate the main result is the scaling, but it’s best to be consistent throughout.”*

Answer:

Thanks for your suggestion. The unit of $J\tau_Q/\hbar$ is dimensionless, we have corrected the figures. We also add the description about how to connect the dimensionless parameter to a real experiment parameters in the experiment

by using the Rabi frequencies and Rabi times.

- (d) *The labels in Fig. 1 appear particularly small, most notably Fig. 1B. Not sure how large the final image may appear in the manuscript, but it would probably be advisable to increase font size.*

Answer:

Figure 1 has been redone for clarity of presentation.

R₂.(6) Minor suggestions:

- (a) *“This may already be reported in the manuscript, but are the experimental results at all sensitive to the precise details of the initial pre-quench state of the system?”*

Answer:

We simulate the transition starting in the ground state of the paramagnetic phase and work hard to avoid any regime that is already known to give deviations even from the standard KZM. A finite temperature initial state or a paramagnet close to the critical point would give rise to deviations that are not universal. But for any paramagnet prepared deeply in the high-symmetry phase, the observed behavior holds. As the experiment probes particularly long ramps and is limited by the coherence lifetime of the ion-trap qubit, we make a choice of the initial magnetic field, large enough to ensure that the initial state corresponds to a paramagnet, while keeping the quench time smaller than the coherence lifetime. As discussed, the third cumulant is already sensitive for $J\tau_Q \sim 10^2$ to the finite coherence times.

- (b) *“It would be useful to general readers if the authors would explicitly state what they mean by the “scaling limit”, beyond stating that this is “the regime of validity of the KZM”.”*

Answer:

The meaning here is the standard one in statistical mechanics regarding continuous and quantum phase transitions, characterized by power-law divergences of various quantities. Power-law behavior governed by critical exponents is the manifestation of the scaling theory in the vicinity of the critical point. KZM exploits this scaling behavior at equilibrium to make identify scaling behavior in the mean number of defects. This has been clarified in the next and the Supplementary Information. In particular, we have clarified that the scaling behavior of κ_Q requires $\tau_Q > 2\hbar/(qJ\pi^3)$ -which is always satisfied in the parameters explored- and the validity of the Landau-Zener formula. It turns out that the latter is the limiting factor for the onset of scaling behavior as the quench time is increased.

- (c) *“I appreciate that this paper is based on quantum phase transitions, but I am not convinced that the references to earlier systems exhibiting Kibble-Zurek-related physics is sufficiently extensive. For example, key experiments in ultracold atoms (e.g. by the groups of Anderson, Dalibard and Yong Il-Shin) are missing: there is no requirement per se to mention those, but it is a suggestion to the authors for their consideration (I assume similar issues may apply to other physical systems I am less familiar with -for example, I wonder if Kibble-Zurek-type studies across the QCD critical point may be relevant to be mentioned here?)”*

Answer:

It is indeed remarkable that the experimental efforts to test KZM were started soon after its conception, from the 80s to the present with sustained interest, and exploring different platforms including superfluid helium, liquid crystals, colloids, Bénard-Rayleigh cells, Josephson junctions, multiferroics, scalar and spin BEC in different geometries, bosonic atoms in lattices, Fermi gases in the continuum, ion chains, ion-trap simulators, optical simulators, Rydberg quantum simulators, D-wave machines, etc.

A fraction of these experiments is review in Ref. 1 and some of these platforms are specifically cited in the introduction and the suggested reference have been added there. We have also added refs on superconducting rings and convective fluids.

In view of these efforts, we find particularly remarkable that signatures of universality beyond the mean number of defects in the number distribution, that is collected essentially in all experiments, have been overlooked until now.

We appreciate the suggestion by the referee to consider the QCD critical point in relation to KZM. To the best of our knowledge, no experiment has been pursued in this context.

- (d) *“There are some equations within the main text that could be better converted to full in-line equations.”*

Answer:

We thank the referee for this comment and have now fully displayed some equations that previously appeared in-text. We prefer to display exclusively the most relevant equations as independent equations, to facilitate the reading of the manuscript.

- (e) *“Also, some typos: the authors state interchangeably “Bernoulli” and “Bernouilli”. - “resonate” → resonant, - “programed” → programmed, - “In tis condition” (in Methods)”*

Answer:

We apologize for the typographical errors in the previous version of our manuscript. In the present revised version they have been corrected. In addition we have reworded several sentences to improve the grammar (see list of changes below).

Reply to R_3 's questions/comments

R_3 .(1) *“J.-M. Cui and coauthors present a study of the Kibble-Zurek mechanism (KZM) probed with a single two-level system, implemented experimentally with a trapped atomic $^{171}\text{Yb}^+$ ion. The authors present a detailed and very clear theoretical introduction on the KZM and on the nearest neighbor transverse field quantum Ising model (TFQIM), which is the playground they use to investigate KZM. They then apply the well-known Jordan-Wigner transformation to describe the TFQIM in terms of free fermionic quasi-particles characterized by the momentum quantum number k . Then they map this system on a Bloch sphere of a two-level system (the ion) where they measure the number of topological defects as they ramp the system across the phase transition, as a function of different ramping speeds, characterizing the transition with cumulants up to the third order.”*

Answer:

We thank the referee for the thorough reading the manuscript and summarizing it. As clearly expounded in the text, we find fitting to emphasize that the key achievement in our work is to probe the universal physics beyond the KZM that is manifested, e.g., in the power-law scaling of all cumulants of the kink-pair number distribution with the quench time. The scaling of the first cumulant (mean number) reduces to the seminal prediction of the KZM. The scaling of higher order cumulants probes physics beyond KZM. In spite of four decades of experimental research exploring the KZM, this work established the first experimental evidence beyond the mean number of defects, this is, beyond the prediction by the KZM.

R_3 .(2) *“In my opinion this work lacks clarity and cannot be published in Comm. Phys. as it stands. The authors simulate a TFQIM of $N=100$ spins (as quoted in the caption of Fig. 3) mapping this model to a single vector in a Bloch sphere. However, this mapping, which is a fundamental ingredient in this work, is not clear at all and needs to be explained adequately. Do the different k modes correspond to different angles on the Bloch sphere? How the parameters in the Hamiltonian (1) relate to the $H(t)$ defined in the supplementary materials, which is the true MW+atom interaction Hamiltonian? How do the authors derive the time-dependent phase profile explained in the supplementary materials? The only place where this mapping can be intuitively understood is Fig.1 which seems to suggest that different angles correspond to different momenta k . However, the figure is confusing and not well explained: for example the state $|\psi_i\rangle$ is not defined anywhere.”*

Answer:

We apologize for the lack of clarity in the first version of our manuscript. Prompted by this comment, we have performed an extensive revision of the main text. The revised version includes three new section in the Supplementary Information, where we give extensive details about the map as well as its use for the experimental quantum simulation. In the Supplementary Information, Section 1, we provide details about the standard Jordan-Wigner transformation and exact diagonalization for TFQIM. Additionally, we move the previous Methods sections as a Supplementary Section 3 and 4 , and further refine the description of experimental realization. Such as state $|\psi_i\rangle$, $|\psi_f\rangle$ are also explicitly defined. In this new version, we spell out the link between the theoretical description and their experimental implementation. All experimental parameters are now provided and Figure 1 has been revised.

R₃.(3) “I think the authors should:

-Clarify this mapping in the main text. Sentences like “Experimentally, the excitation probabilities p_k can be measured by probing the dynamics in each mode.” or “Exploiting the equivalence between the spin and momentum representation,” are a bit vague and do not explain what they are actually doing in the experiment and how the mapping works.

Answer:

These sentences have been rewritten for clarity. The first one refers to the quantum simulation of the TFQIM by relying on momentum representation in terms of decoupled modes. The excitation probability in these modes is governed by a Landau-Zener crossing that can be implemented with a trapped ion qubit, The second sentence pointed out by the referee makes reference to the two equivalent representations of the TFQIM Hamiltonian, the one in terms of spins and the one in terms of free fermion. This equivalence is by now well established as it appears in many textbooks and research papers often just quote it without further explanation. However, it is key to our quantum simulation approach. To facilitate the reading of the manuscript, we have clarified the text and included new sections in the Supplementary Information detailing the steps of the mapping between the two representations.

R₃.(4) - Explain in detail how this mapping gives rise to the MW pulse sequence applied to the system to simulate a specific k mode.

Answer:

Thanks for your suggestion. We have added the description the MW pulse in manuscript and given a further detailed derivation and formulas of the MW pulse sequence in the Supplementary Material in the new version.

R₃.(5) - Improve Fig. 1 to make it more explanatory.

Answer:

Figure 1 has been replotted for clarity with additional explanations included in the caption.

R₃.(6) After these major issues are addressed the paper can be resubmitted and evaluated.

Answer:

We thank the Reviewer for all his/her suggestions. We have answered to all of these, and we have incorporated them all into the revised manuscript which includes some changes in the text and presentation. These are indicated below.

We have accordingly revised the manuscript in response to the review reports and have addressed all of his/her concerns by improving the presentation, discussions and figures, as requested by the review. We have thoroughly revised the paper by modifying the sections with results, discussion and methods. Moreover, we improved the Supplementary Information providing additional details on background theory results and the link between the theoretical description and the experimental implementation. We feel that this revised version has improved in clarity and strength and hope that the referee finds the revised manuscript suitable for publication in Communications Physics in its current form.

$R_3.(7)$ *“Minor changes: Pag. 13 Tis needs to be corrected to This.”*

Answer:

We thank the referee for pointing our this typo, that is now corrected.

List of main changes made to the manuscript:

Now we present the list of the changes made to the main text.

- C.(1) In the Abstract, we replace the word: “KINK” by “**kink pairs**”.
- C.(2) In the first paragraph of introduction we removed the word: “EVENTUALLY”.
- C.(3) In the first paragraph of introduction we change the notation: “ $\langle n \rangle$ ” by “ $\langle n^T \rangle$ ”.
- C.(4) In the first paragraph of introduction, we extend and improve the reference list. See also response review R_2 .(6)-(c).

New references: The numeration corresponds to the present revised version.

- 16. Casado, S., González-Viñas, W., Mancini, H. & Boccaletti, S. Topological defects after a quench in a Bénard-Marangoni convection system. *Phys. Rev. E* **63**, 057301 (2001).
- 17. Casado, S., González-Viñas, W. & Mancini, H. Testing the Kibble-Zurek mechanism in Rayleigh-Bénard convection. *Phys. Rev. E* **74**, 047101 (2006).
- 18. Monaco, R., Mygind, J. & Rivers, R. J. Zurek-Kibble domain structures: The dynamics of spontaneous vortex formation in annular Josephson tunnel junctions. *Phys. Rev. Lett.* **89**, 080603 (2002).
- 19. Monaco, R., Mygind, J., Aaroe, M., Rivers, R. J. & Koshelets, V. P. Zurek-Kibble mechanism for the spontaneous vortex formation in Nb-Al/Al_{ox}/Nb Josephson tunnel junctions: New theory and experiment. *Phys. Rev. Lett.* **96**, 180604 (2006).
- 20. Weir, D. J., Monaco, R., Koshelets, V. P., Mygind, J. & Rivers, R. J. Gaussianity revisited: exploring the Kibble-Zurek mechanism with superconducting rings. *Journal of Physics: Condensed Matter* **25**, 404207 (2013).
- 25. Weiler, C. N. *et al.* Spontaneous vortices in the formation of Bose-Einstein condensates. *Nature* **455**, 948-951 (2008).
- 27. Chomaz, L. *et al.* Emergence of coherence via transverse condensation in a uniform quasi-two dimensional Bose gas. *Nature Communications* **6**, 6162 (2015).
- 29. Ko, B., Park, J. W. & Shin, Y. Kibble-Zurek universality in a strongly interacting Fermi superfluid. *Nat. Phys.* (2019).

31. Gómez-Ruiz, F. J. & del Campo, A. Universal dynamics of inhomogeneous quantum phase transitions: Suppressing defect formation. *Phys. Rev. Lett.* **122**, 080604 (2019).
- C.(5) In the second paragraph of introduction. In the first and second sentences, we remove: $P(n)$.
- C.(6) In the second paragraph of introduction. we change the final sentence: “THE DISTRIBUTION $P(n)$ HAS BEEN SHOWN TO BE UNIVERSAL AND FULLY DETERMINED BY THE SCALING THEORY OF PHASE TRANSITIONS, A PREDICTION WE AIM TO VALIDATE EXPERIMENTALLY.” to **“Indeed, it has been argued that the distribution of topological defects is generally determined by the scaling theory of phase transitions and thus exhibits signatures of universality beyond the KZM³⁵. We aim at validating this prediction experimentally.”**
- C.(7) In all manuscript, now we have improved the notation of quantum operator by add hat notation: For Example in the Equation 1. $\mathcal{H} \rightarrow \hat{\mathcal{H}}$.
- C.(8) Just after the Eq.1, we added the sentence: **“that we shall consider with periodic boundary conditions $\hat{\sigma}_1^z = \hat{\sigma}_{N+1}^z$ and N even. Additionally,”...**
- C.(9) In the next paragraph to Eq.1 the sentence: “...CROSSING OF THE CRITICAL POINT $g_c = 1$ AFTER INITIALIZING...” has been transformed to **“...crossing of the critical point $g_c = -1$ after initializing...”**.
- C.(10) Just before the Eq.(2) the sentence: “THIS SEMINAL RESULT FORMS THE BASIS OF MUCH OF THE PROGRESS ON THE STUDY OF QUANTUM PHASE TRANSITIONS AND CAN BE ESTABLISHED VIA THE JORDAN-WIGNER TRANSFORMATION²⁹. THUS, THE TFQIM HAMILTONIAN CAN BE ALTERNATIVELY WRITTEN IN TERMS OF INDEPENDENT MODES AS^{28,30}” has been modified to **“This seminal result forms the basis of much of the progress on the study of quantum phase transitions and can be established via the Jordan-Wigner transformation³⁸, Fourier transform and Bogoliubov transformation³⁹. We detail these steps in the Supplementary Information, where it is shown that the TFQIM Hamiltonian can be alternatively written in terms of independent modes as^{37,40}”**. See also response reviews R_1 .(9) and R_3 .(2).
- C.(11) In the previous change, we also included a new reference (the numeration corresponds to the present revised version):
39. Barouch, E. & McCoy, B. M. Statistical Mechanics of the XY Model. II. Spin-Correlation Functions. *Phys. Rev. A* **3**, 786-804 (1971).

C.(12) We have improved the notation of the Eq.(2). The Eq.(2) now reads as

$$\hat{\mathcal{H}} = \sum_{k>0} \hat{H}_k = \sum_{k>0} \epsilon_k (g) \left(\hat{\gamma}_k^\dagger \hat{\gamma}_k + \hat{\gamma}_{-k}^\dagger \hat{\gamma}_{-k} - 1 \right),$$

See also response reviews R_1 .(9) and R_3 .(2).

C.(13) In the paragraph just after the Eq.2. In this new version, we emphasize that we use the distribution of kinks replaced by the distribution of pairs of kinks.

C.(14) In accordance with the suggestion of the referee R_1 .(6). We have improved the notation of the previous Eq.(3) by connecting closely with the experimental parameters. The new Eq.(3) now reads

$$g(t) = \frac{t}{\tau_Q} + g(0),$$

C.(15) Just after the Eq.(3), we added the sentence: **“We further choose $g(0) < -1$ in the paramagnetic phase.”**

C.(16) In the sentence, just before the Eq.(4), we added the word **“pairs”**.

C.(17) In accordance with the kink pairs. The Eq.(4) now reads as

$$\langle n \rangle_{\text{KZM}} = \frac{N}{4\pi} \sqrt{\frac{\hbar}{2J\tau_Q}},$$

C.(18) **Main organization:** The previous version of the manuscript didn't have section divisions. Now, in the present revised version, the manuscript is organized as follows: First, Introduction and theoretical background. Second, in the section *Results*: We divide this section into two subsections: Experimental design and Full probability distribution of topological defects. Finally, in the section discussions. We have also extended the discussion (see section Results and discussions in the main text). Additionally, a detailed supplementary document are appended with the manuscript. The method section in the manuscript are move to the supplementary.

C.(19) In accordance with the suggestion of the referee R_3 .(5). Figure 1 has been replotted for clarity with additional explanations included in the caption.

C.(20) In accordance with the suggestion of the referee R_2 .(5) – (b). We have changed the display in Fig. 2-3. Now, the figures have been reported for clarity.

- C.*(21) Change the $J\tau_Q$ to $J\tau_Q/\hbar$ in Fig.2-3-4, which will be consistent with the formulas in main text.
- C.*(22) In accordance with the suggestion of the referee *R*₃.(2) and *R*₃.(3), in the present version of the main text, we extend and improve the experiment description. We report all experimental parameters and we make a clear link between the theoretical and experimental description. Additionally, we extend the methods section in the supplemental information.

In response to the comments by the referees, the manuscript has been revised substantially. While these changes do not affect the main results, they have strengthen the manuscript. In view of the four decades of sustained experimental efforts exploring the Kibble-Zurek mechanism, it is surprising that signatures of universality beyond the mean number of defects have not been explored until the present work. We thus believe that our (revised) manuscript merits publication in Communications Physics based on its timeliness and originality, being of broad interest to the scientists working in condensed matter, AMOP, statistical physics and quantum science and technology.

REVIEWERS' COMMENTS:

Reviewer #1 (Remarks to the Author):

In the revised version of the manuscript authors have addressed all my comments and suggestions. As far as I am concerned, the manuscript can be published in Nature Communications, after a minor correction. In particular

Equation S15 in the supplemental information has a misprint

Page 4, SI, supplemental information: $\gamma = \kappa_2 / \kappa_2^{3/2}$. Is there any reason not to simplify this expression ?

Page 8, SI: "... driving a chirped pulse into the qubit" can be rephrased to sound more natural.

Reviewer #2 (Remarks to the Author):

Overall I am pleased with the responses and further clarifications provided by the authors, and consider this manuscript to meet the publications standards for Communications Physics.

I was however slightly disappointed that -- while the authors responded directly to the Referee criticism -- they did not appear to soften their claim (made in paper, and noted in Abstract/Conclusions) that they "characterize the full probability distribution": While the findings presented here (up to 3rd order cumulant) are no doubt significant and novel, and do point towards the characterization of the full distribution function, the actual achievement presented in this work has -- to the best of my understanding -- been limited to the 3rd order cumulant (with the results being solid primarily only up to 2nd order cumulant). I would have expected a slight change in wording to more accurately reflect the actual findings reported herein (and do not feel this would reduce the impact of this work).

I am also slightly perplexed about the decision of the authors to have no information in the "Methods" section, beyond hinting to the presence of Supplementary Materials. Personally, I find "Methods" highly relevant and do look at those when studying a manuscript -- but there are of course always further technical details that cannot (and should not) appear there, which can be deferred to the Supplementary Materials (which are typically only read by a very small number of researchers working on closely related topics). This is the approach I would have recommended (i.e. key summary of methods/points beyond main text go in "Methods" but hidden details not contained in "Methods" go into Supplementary Materials), and which probably lies closer to the intended spirit of the journal.

Reviewer #3 (Remarks to the Author):

I have read the revised manuscript and the additional supplementary information with great interest. I think the authors made a significant effort in making the paper more clear and more readable. The mapping between the different k modes and the single qubit Hamiltonian is now explained in detail in the supplementary, along with the derivation of the non-trivial phase time dependence, which is a crucial element to understand the connection between theory and experiment and to appreciate the novelty of this work.

In conclusion, I think the revised version of the manuscript is now well suited for publication in Comm. Physics as it stands.

1. Reviewer #1 (Remarks to the Author):

RC: *In the revised version of the manuscript authors have addressed all my comments and suggestions. As far as I am concerned, the manuscript can be published in Nature Communications, after a minor correction. In particular Equation S15 in the supplemental information has a misprint Page 4, SI, supplemental information: $\gamma = \kappa_2/\kappa_2^{3/2}$. Is there any reason not to simplify this expression ? Page 8, SI: "... driving a chirped pulse into the qubit" can be rephrased to sound more natural.*

AR: We thanks the referee for the comment and suggestion. In previous version of supplementary, there's a typo error in the define of γ . We have corrected it as $\gamma = \kappa_3/\kappa_2^{3/2}$. We also refined the description in Page 8, "... by applying a chirped microwave pulse to the qubit"

2. Reviewer #2 (Remarks to the Author):

RC: *Overall I am pleased with the responses and further clarifications provided by the authors, and consider this manuscript to meet the publications standards for Communications Physics.*

AR: We thanks the referee's positive comment.

RC: *I was however slightly disappointed that -- while the authors responded directly to the Referee criticism -- they did not appear to soften their claim (made in paper, and noted in Abstract/Conclusions) that they "characterize the full probability distribution": While the findings presented hear (up to 3rd order cumulant) are no doubt significant and novel, and do point towards the characterization of the full distribution function, the actual achievement presented in this work has -- to the best of my understanding -- been limited to the 3rd order cumulant (with the results being solid primarily only up to 2nd order cumulant). I would have expected a slight change in wording to more accurately reflect the actual findings reported herein (and do not feel this would reduce the impact of this work).*

AR: We thank the reviewer's comment. We have modified descriptions in the summary as "In summary, using a trapped-ion quantum simulator we have measured the full distribution of topological defects in the quantum Ising chain, the paradigmatic model of quantum phase transitions, and characterized in detail its first three cumulants as a function of the quench rate".

RC: *I am also slightly perplexed about the decision of the authors to have no information in the "Methods" section, beyond hinting to the presence of Supplementary Materials. Personally, I find "Methods" highly relevant and do look at those when studying a manuscript -- but there are of course always further technical details that cannot (and should not) appear there, which can be deferred to the Supplementary Materials (which are typically only read by a very small number of researchers working on closely related topics). This is the approach I would have recommended (i.e. key summary of methods/points beyond main text go in "Methods" but hidden details not contained in "Methods" go into Supplementary Materials), and which probably lies closer to the intended spirit of the journal.*

AR: We thank the reviewer's suggestion. We have moved some of the description in the Supplementary Materials to the "Methods" section, which is highly related to the key technical details. We hope it will make the descriptions of the main text is self-contained.

3. Reviewer #3 (Remarks to the Author):

RC: *I have read the revised manuscript and the additional supplementary information with great interest. I think the authors made a significant effort in making the paper more clear and more readable. The mapping between the different k modes and the single qubit Hamiltonian is now explained in detail in the supplementary, along with the derivation of the non-trivial phase time dependence, which is a crucial element to understand the connection between theory and experiment and to appreciate the novelty of this work. In conclusion, I think the revised version of the manuscript is now well suited for publication in Comm. Physics as it stands.*

AR: We thanks for the referee's interest and high evaluation of our work.