Full Counting Statistics of Topological Defects after Crossing a Phase Transition

Fernando J. Gómez-Ruiz[©], ^{1,*} Jack J. Mayo, ^{1,2} and Adolfo del Campo[©], ^{1,3,4,†}

¹Donostia International Physics Center, E-20018 San Sebastián, Spain

²University of Groningen, 9712 CP Groningen, Netherlands

³IKERBASQUE, Basque Foundation for Science, E-48013 Bilbao, Spain

⁴Department of Physics, University of Massachusetts, Boston, Massachusetts 02125, USA

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We consider the number distribution of topological defects resulting from the finite-time crossing of a continuous phase transition and identify signatures of universality beyond the mean value, predicted by the Kibble-Zurek mechanism. Statistics of defects follows a binomial distribution with $\mathcal N$ Bernouilli trials associated with the probability of forming a topological defect at the locations where multiple domains merge. All cumulants of the distribution are predicted to exhibit a common universal power-law scaling with the quench time in which the transition is crossed. Knowledge of the distribution is used to discuss the onset of adiabatic dynamics and bound rare events associated with large deviations.

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In a scenario of spontaneous symmetry breaking, the dynamics of a system across a continuous phase transition is described by the Kibble-Zurek mechanism (KZM) [1–4]. When the transition is driven in a finite quench time τ_O , the KZM predicts the formation of domains of volume $\hat{\xi}^D$, where D is the spatial dimension of the system. Specifically, the KZM uses as input the equilibrium value of the correlation length ξ and the relaxation time τ . By varying a control parameter λ across the critical value λ_c both quantities exhibit a power-law divergence as a function of the distance to the critical point $\epsilon = (\lambda - \lambda_c)/\lambda_c$,

$$\xi = \xi_0 |\epsilon|^{-\nu}, \qquad \tau = \tau_0 |\epsilon|^{-z\nu}.$$
 (1)

Here, ν is the correlation-length critical exponent and z denotes the dynamic critical exponent. Both are determined by the universality class of the system. By contrast, ξ_0 and τ_0 are microscopic constants. The KZM states that when the phase transition is driven in a timescale τ_Q by a linear quench of the form $\epsilon = t/\tau_Q$, domains in the broken symmetry phase spread over a length scale

$$\hat{\xi} = \xi_0 \left(\frac{\tau_Q}{\tau_0} \right)^{\frac{\nu}{1+z\nu}}.$$
 (2)

In D spatial dimensions, the KZM predicts the mean number of topological defects to scale as

$$\langle n \rangle \propto \left(\frac{\tau_0}{\tau_O}\right)^{\frac{D\nu}{1+z\nu}}.$$
 (3)

This power-law behavior with the quench time, initially derived for classical systems, similarly describes the

dynamics across a quantum phase transition [5–7]. In this context, the scaling is generally studied in the residual mean energy and the number of quasiparticles, which generally differs from the number of topological defects [8–10]. The KZM has also been extended to a variety of scenarios, including nonlinear quenches [11–13], long-range interactions [14–19], and inhomogeneous phase transitions in both classical [7,20–25] and quantum systems [13,26–30]. The KZM has been experimentally investigated in a wide variety of platforms reviewed in [7], with recent tests being performed in trapped ions [31–33], colloidal monolayers [34], ultracold Bose and Fermi gases [35–39], and quantum simulators [17,40–43].

Despite this progress, features of the counting statistics of defects other than the mean number have received scarce attention. An exception concerns scenarios of U(1) symmetry breaking leading to, e.g., the spontaneous current formation in a superfluid confined in a toroidal trap or a superconducting ring [3,4,44–47]. While the average circulation vanishes, it was shown that its variance is consistent with a one-dimensional random walk model in which the number of steps is predicted by the circumference of the ring divided by the KZM length scale $\hat{\xi}$ [3,4]. It is, however, not clear how to extend this argument to higher dimensions [8]. Not long ago, the distribution of kinks formed in a quantum Ising chain driven from the paramagnetic to the ferromagnetic phase was studied both theoretically [48] and in the laboratory [49,50].

In this Letter, we focus on signatures of universality beyond the mean number of topological defects and show that the full counting statistics of topological defects is actually universal. In particular, we argue that (i) the defect number distribution is binomial, (ii) all cumulants are proportional to the mean and scale as a universal power law with the quench rate, and (iii) this power law is fixed by the conventional KZM scaling. This knowledge allows us to characterize universal features regarding the onset of adiabatic dynamics (probability for no defects) and deviations of the number of kinks away from the mean value.

Number distribution of topological defects.—To estimate the defect number distribution we assume that the number of domains in the total system is set by

$$\mathcal{N}_D = \frac{\text{Vol}}{\hat{\xi}^D},\tag{4}$$

where Vol denotes the volume of the system. Topological defects may form at the interface between multiple domains. For instance, the formation of vortices has been demonstrated by merging independent Bose-Einstein condensates [51]. The same principle is at the core of phase-imprinting methods for soliton formation [52]. Disregarding boundary effects, the number of locations where a topological effect may be formed is approximately given by $\mathcal{N} = \mathcal{N}_D/f$, where f takes into account the average number of domains that meet at a point. Alternatively, f can be considered a fudge factor.

We next propose that, at the merging between multiple domains, a topological defect forms with a probability p. Similarly, no topological defect will be formed at any such location with probability 1-p. The formation of topological defects at different locations is assumed to be independent and, in each case, the event of formation can be associated with a Bernouilli random variable. We thus propose that the number distribution of topological defects can be approximated by the binomial distribution with parameters $\mathcal N$ and p. This is the discrete probability distribution for the number of successes (number of topological defects formed) in a sequence of $\mathcal N$ independent trials,

$$P(n) \sim B(n, \mathcal{N}, p) = \binom{\mathcal{N}}{n} p^n (1 - p)^{\mathcal{N} - n}.$$
 (5)

Thus, P(n) is centered at

$$\langle n \rangle = \frac{p \text{Vol}}{f \hat{\xi}^D} = \frac{p \text{Vol}}{f \xi_0^D} \left(\frac{\tau_0}{\tau_Q} \right)^{\frac{D\nu}{1+z\nu}}, \tag{6}$$

in agreement with the KZM scaling. Further, its variance is set by

$$\operatorname{Var}(n) = \langle n^2 \rangle - \langle n \rangle^2 = \frac{\operatorname{Vol}}{f\hat{\xi}^D} p(1-p) \propto \tau_Q^{\frac{D\nu}{1+z\nu}} \tag{7}$$

and is always proportional to the mean, as $Var(n) = (1-p)\langle n \rangle$.

High-order cumulants.—To further characterize the number distribution of defects, it is convenient to introduce the Fourier transform $\tilde{P}(\theta)$ of P(n), satisfying [53]

$$P(n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \tilde{P}(\theta) \exp[-i\theta n]$$
 (8)

and known as the characteristic function $\tilde{P}(\theta) = \mathbb{E}[e^{i\theta n}]$. Its logarithm is the cumulant generating function. Specifically, cumulants κ_q of P(n) are defined using the expansion

$$\log \tilde{P}(\theta) = \sum_{q=1}^{\infty} \frac{(i\theta)^q}{q!} \kappa_q. \tag{9}$$

For the binomial distribution, the cumulant generating function reads

$$\log \tilde{P}(\theta) = \langle n \rangle \log(1 - p + pe^{i\theta}), \tag{10}$$

whence it follows that all cumulants are proportional to the mean and thus scale universally with the quench time

$$\kappa_q \propto \left(\frac{\tau_0}{\tau_Q}\right)^{\frac{D\nu}{1+2\nu}}.$$
(11)

They satisfy the recursion relation $\kappa_{q+1} = p(1-p)d\kappa_q/dp$ and those with q > 2 signal non-normal features of the distribution. For instance, $\kappa_3/\langle n \rangle = p(1-p)(1-2p)$ and $\kappa_4/\langle n \rangle = p(1-p)(1-6p+6p^2)$.

However, it follows from the central limit (de Moivre–Laplace) theorem that for large \mathcal{N} with p constant the distribution becomes asymptotically normal [53], i.e.,

$$P(n) \sim \frac{1}{\sqrt{2\pi(1-p)\langle n\rangle}} \exp\left[-\frac{(n-\langle n\rangle)^2}{2(1-p)\langle n\rangle}\right],$$
 (12)

where $\langle n \rangle$ is given by (6) in agreement with the KZM and we have used that the variance is proportional to the mean, according to Eq. (7).

Nonuniform probabilities for defect formation.—We have assumed at the interface between multiple domains that topological defects form with constant probability p. One can generally expect this not to be the case. For instance, according to the geodesic rule, the probability for defect formation depends on the number of domains that merge at the location of interest [1,51,54,55]. One may wonder how the defect number distribution is affected when the probability for formation of topological defect is not fixed but varies at different locations. Keeping the assumption that the events of formation of topological defects are independent, the number of defects formed is thus given by the sum of independent Bernouilli trials, in which the probabilities for defect formation are $\{p_1, p_2, ..., p_{\mathcal{N}}\}\$. The resulting distribution is the so-called Poisson binomial distribution with characteristic function $\tilde{P}(\theta) = \prod_{j=1}^{\mathcal{N}} (1 - p_j + p_j e^{i\theta})$, mean $\langle n \rangle = \sum_{j=1}^{\mathcal{N}} p_j$, and variance $Var(n) = \sum_{j=1}^{N} p_j (1 - p_j)$. This probability distribution actually describes the distribution of the number of pairs of quasiparticles in quasifree fermion models (one-dimensional Ising and XY chains, Kitaev model, etc.) [48,49]. Clearly, the mean $\langle n \rangle = \mathcal{N}\bar{p}$, where the average formation probability $\bar{p} = \sum_{j=1}^{\mathcal{N}} p_j/\mathcal{N}$. Similarly, it is known that $\mathrm{Var}(n) = \mathcal{N}[\bar{p}(1-\bar{p})-s_p^2]$, where $s_p^2 = \sum_{j=1}^{\mathcal{N}} (p_j - \bar{p})^2/\mathcal{N}$ is the variance of the distribution $\{p_1, p_2, ..., p_{\mathcal{N}}\}$ [56]. Assuming the latter to be small, for large \mathcal{N} , both $\mathrm{Var}(n)$ and $\langle n \rangle$ are proportional to \mathcal{N} and inherit a universal power-law scaling with the quench time.

Onset of adiabaticity.—Many applications in statistical mechanics, condensed matter, and quantum science and technology require the suppression of topological defects. This is the case in the preparation of novel phases of matter in the ground state or the suppression of errors in classical and quantum annealing. Strict adiabaticity can be associated with the probability to have no defects at all, i.e., P(0). The latter is given by

$$P(0) = (1 - p)^{\frac{\text{Vol}}{f\hat{\xi}^D}} \approx \exp\left[-\frac{\text{Vol}}{f\hat{\xi}^D}p\right] = \exp(-\langle n \rangle), \quad (13)$$

where the last term holds for small p. In this case, the probability for zero defects decays exponentially with the mean number of defects, i.e., $\langle n \rangle = p \operatorname{Vol}/f \hat{\xi}^D$. As a result,

$$\log[P(0)] = -\frac{p\text{Vol}}{f\xi_0^D} \left(\frac{\tau_0}{\tau_Q}\right)^{\frac{D\nu}{1+z\nu}},\tag{14}$$

a prediction we shall test below.

Relaxed notions of adiabaticity, not based in P(0), can be imposed by considering the cumulative probability in the tails of the distribution, for which explicit expressions can be found with the binomial model and its normal approximation; see Supplemental Material [57]. It is also possible to find robust bounds, e.g., by considering the tails of the distribution associated with high kink numbers. For example, using the Chernoff bound the upper tail is constrained by the inequality $P(n \ge \langle n \rangle + \delta) \le \exp[-(\delta^2)/(2\langle n \rangle + \delta/3)]$ [57].

Numerical results.—For the sake of illustration, we consider the breaking of parity symmetry in a second-order phase transition [58]. Specifically, we analyze a one-dimensional chain exhibiting a structural phase transition between a linear and a doubly degenerate zigzag phase. This scenario is of relevance to trapped ion chains [23,59], confined colloids, and dusty plasmas [60], to name some relevant examples. In the course of the phase transition, parity is broken and kinks form at the interface between adjacent domains. To describe the dynamics, we consider a lattice description in which each site is endowed with a transverse degree of freedom ϕ_i and the total potential reads

$$V(\{\phi_i\}, t) = \sum_{i} \frac{1}{2} [\lambda(t)\phi_i^2 + \phi_i^4] + c \sum_{i} \phi_i \phi_{i+1}, \quad (15)$$

where $\{\phi_i\}$ are real continuous variables and i=1,...,N. As the coefficient $\lambda(t)$ is ramped from a positive initial value to a negative one, the local single-site potential evolves from a single well to a double well. The nearest-neighbor coupling favors ferromagnetic order when c<0 and antiferromagnetic otherwise. The evolution across the critical point λ_c is described by Langevin dynamics

$$\ddot{\phi}_i + \eta \dot{\phi}_i + \partial_{\phi_i} V(\{\phi_i\}, t) + \zeta = 0, \quad i = 1, ..., N, \quad (16)$$

where $\eta > 0$ accounts for friction and $\zeta = \zeta(t)$ is a real Gaussian process with zero mean. Equations (15) and (16) account for the Langevin dynamics of a ϕ^4 theory on a lattice. This system is well described by Ginzburg-Landau theory and is characterized by mean-field critical exponents $\nu = 1/2$ and z = 2 in the overdamped regime [23,58]. The dynamics is induced by a ramp of $\lambda(t)$ from the value $\lambda(0) = \lambda_0$ to $\lambda(\tau_Q) = \lambda_f$ in the quench time τ_Q according to $\lambda(t) = \lambda_0 + |\lambda_f - \lambda_0|t/\tau_Q$ across the critical point $\lambda_c = 2c$ (see [57,61] for details).

Full counting statistics of kinks is built by sampling over an ensemble of 15 000 trajectories; see Fig. 1 and Supplemental Material [57] for lower sampling. The mean

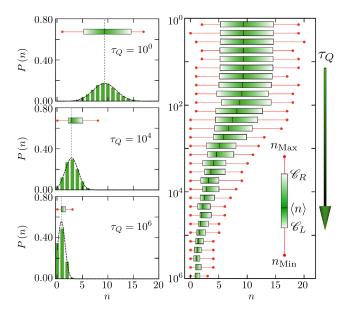


FIG. 1. Characterization of probability distribution of topological defects. (Left) Probability distribution of the number of kinks P(n) generated as a function of the quench time τ_Q . The numerical histograms are compared with the normal approximation (12) and the dashed vertical line denotes the mean value $\langle n \rangle$. (Right) Total distribution of kinks in a box-and-whisker chart, for different quench times and a chain of N=100 sites, using 15 000 trajectories. \mathcal{C}_R and \mathcal{C}_L denote the cumulative probability above and below the mean.

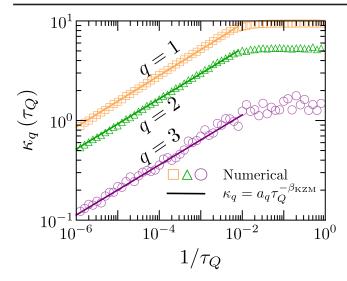


FIG. 2. Universal scaling of the cumulants κ_q of the kink number distribution. From top to bottom, the mean kink density (q=1), its variance (q=2), and the third centered moment (q=3) are shown as a function of the inverse quench time τ_Q for a chain of N=100 sites and 15 000 trajectories. Symbols represent numerical data, while solid lines describe the analytical approximation derived in the scaling limit, with $\beta_{\rm KZM} = \nu/(1+z\nu)$.

and width of the distribution are reduced for increasing quench times. Histograms for P(n) are shown to be well reproduced by the normal approximation (12) away from the onset of adiabatic dynamics when the value of P(0) is significant.

The universal power-law scaling of the cumulants as a function of the quench time is shown in Fig. 2. A fit to the mean number of kinks yields $\kappa_1 = (30.838 \pm 0.297) \tau_Q^{-0.251 \pm 0.001}$, in good agreement with the KZM, which predicts the power-law exponent $\beta_{\rm KZM} = \nu/(1+z\nu) = 1/4$ for mean-field values $\nu = 1/2$, z=2. Signatures of universality beyond the KZM are evident from the scaling of higher-order cumulants. Non-normal features of the distribution are signaled by the non-zero value of κ_q with $q \ge 3$. The variance scales as $\kappa_2 = (16.948 \pm 0.217) \tau_Q^{-0.252 \pm 0.001}$, while the third cumulant is fitted to $\kappa_3 = (3.621 \pm 0.281) \tau_Q^{-0.251 \pm 0.011}$. Power-law exponents are thus found as well in excellent agreement with the theoretical prediction in Eq. (11).

We note, however, that there is an infinite number of distributions in which cumulants exhibit a universal scaling with the quench rate of the form $\kappa_q = a_q \tau_Q^{-\beta_{\rm KZM}}$. According to our model for the full kink counting statistics, the ratio between any two cumulants is independent of the quench time and fixed by the probability p for kink formation at the merging between adjacent domains. In particular, $\kappa_2/\kappa_1 = 1 - p$ and $\kappa_3/\kappa_1 = (1-p)(1-2p)$. Figure 3 shows the ratio between the first three cumulants as a function of the quench rate. The numerical results are in excellent agreement with the theoretical prediction. In

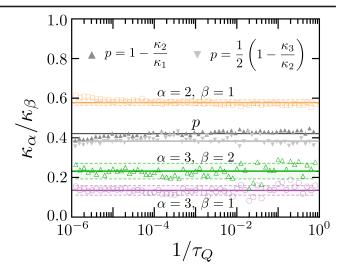


FIG. 3. Ratio between the first three cumulants as a function of the quench rate. The numerical results (symbols) for the ratio between the cumulants κ_{α} and κ_{β} , where $\alpha > \beta$ and $\alpha, \beta \in \{1,2,3\}$, are depicted as function of the inverse quench time τ_Q . The solid line corresponds to the average of the ratio $\kappa_{\alpha}/\kappa_{\beta}$ and the shadow region between two dashed lines corresponds to the uncertainty associated with each cumulant ratio. Additionally, we show the numerical (symbols) and mean value (solid lines) of p calculated according to the plot legends.

particular, it is found that the observed cumulant ratios $\kappa_2/\kappa_1 = 0.578 \pm 0.014$, $\kappa_3/\kappa_1 = 0.134 \pm 0.023$, and $\kappa_3/\kappa_2 = 0.232 \pm 0.040$ are consistent with a single well-defined value of the probability for kink formation $p = 0.422 \pm 0.014$; see Supplemental Material [57].

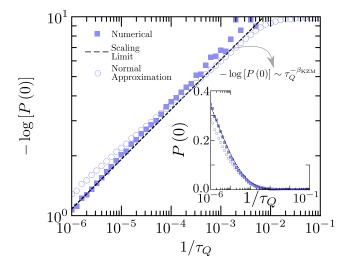


FIG. 4. Universal scaling of the probability for no kinks P(0) as a function of quench time. The dashed lines show the universal scaling of the probability for no kinks, as predicted by Eq. (14), plotted as a reference with $\beta_{\text{KZM}} = \nu/(1+z\nu)$. Numerical data (squares) are in excellent agreement with the theoretical prediction. Additionally, using Eq. (12) with n=0, we show the normal approximation for large \mathcal{N} (circles) with the fitted value of p in Fig. 3.

As further evidence for our model, we analyze the probability for no kink formation P(0) as a function of the quench time in Fig. 4. Its numerical value estimated from the histogram constructed with the ensemble of trajectories follows the theoretical prediction (14). Thus, Fig. 4 confirms that P(0) decays exponentially with the mean number of kinks, which exhibits a universal power-law scaling. At fast quenches, P(0)approaches zero, the comparison is limited by the finite sampling, and the saturation of κ_1 in Fig. 2 due to finite-size effects. The normal approximation P(0) = $[1/\sqrt{2\pi(1-p)\langle n\rangle}] \exp[-\langle n\rangle/2(1-p)]$ works well for moderate quench rates when P(n) is symmetric and in absence of finite-size effects, losing accuracy at the onset of adiabaticity, when P(0) is significant. This is shown in Fig. 4 for the estimated $p = 0.422 \pm 0.014$ extracted from the mean number of kinks (e.g., in Fig. 2). As with P(0), we note that other notions of deviations away from the mean are also shown to be constrained by KZM scaling, as shown in the Supplemental Material [57].

Summary.—When a continuous phase transition is traversed in a finite timescale τ_O , topological defects form. The average number scales with the quench time τ_O following a universal power-law scaling predicted by the Kibble-Zurek mechanism. The same scaling describes the density of excitations in the quantum domain as well. Given a system whose critical dynamics is described by the KZM, we have argued that the full number distribution of topological defects is universal and described by a binomial distribution. This model assumes that, in the course of the critical dynamics, the system size is partitioned in domains of length scale given by the KZM correlation length. The event of topological defect formation at the interface between multiple domains is associated with a discrete random variable with a fixed success probability. A testable prediction is that all cumulants of the distribution are proportional to the mean and thus inherit a universal powerlaw scaling with the quench time, while cumulant ratios are constant and uniquely determined by the probability for kink formation. Other quantities such as the probability for no defects and the deviations away from the mean also exhibit a universal dependence on the quench time. Our findings motivate the quest for universal signatures in the counting statistics of topological defects across the wide variety of experiments used to test KZM dynamics, using, e.g., convective fluids [62,63], colloids [34], cold atoms [35–39], and trapped ions [31–33].

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- *fj.gomez34@dipc.org
 †adolfo.delcampo@dipc.org
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