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Large deviations and universality in quantum quenches

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We study the large deviations statistics of the intensive work done by changing globally a control parameter in a thermally isolated quantum many-body system. We show that, upon approaching a critical point, large deviations well below the mean work display universal features related to the critical Casimir effect in the corresponding classical system. Large deviations well above the mean are, instead, of quantum nature and not captured by the quantum-to-classical correspondence. For a bosonic system we show that in this latter regime a transition from exponential to power-law statistics, analogous to the equilibrium Bose-Einstein condensation, may occur depending on the parameters of the quench and on the spatial dimensionality.

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Introduction – Recent experimental progresses in the physics of trapped ultracold atomic gases have stimulated a growing interest in the non-equilibrium behavior of thermally isolated quantum many-body systems [1]. A number of aspects are presently being investigated experimentally, ranging from the propagation of correlations after quenches [2] to relaxation and pre-thermalization inferred from the statistical fluctuations of the interference contrast of split condensates [3]. On the theoretical side, a compelling issue under investigation is that of the role played by universality in the non-equilibrium dynamics [1], since predictions independent of microscopic details make the comparison with experiments a particularly stringent test. Universal behavior can be investigated by studying either the time dependence of correlation functions [4, 5], in particular close to criticality, or their statistical fluctuations [6]. In this context, a number of studies have focused on macroscopic, thermodynamic variables such as work [7–12] and entropy [13], exploring the emergence of universality in their statistical fluctuations.

Statistical fluctuations are known to provide insight into the physics of classical equilibrium and non-equilibrium systems [14]. The statistics of macroscopic *extensive* variables exhibits a first, obvious form of universality associated to typical, "small" fluctuations, which is however rather insensitive to the underlying properties of the system [14]. Indeed, as the mean of a generic extensive quantity W_N (e.g., the magnetization in a spin system) grows proportionally to the number N of degrees of freedom, the one of the associated *intensive* variable $w_N \equiv W_N/N$ (i.e., the magnetization per unit volume) approaches a finite value $\bar{w}$. The central limit theorem (when applicable) suggests that the typical fluctuations of w_N are suppressed $\sim 1/N^{1/2}$ and have a Gaussian distribution around $\bar{w}$. On the other hand, large fluctuations, though rare, are capable of probing the specific details of the physical system [14] and they might provide valuable information on its universal behavior. In order for a large fluctuation to occur, an extensively large number of microscopic fluctuating variables (i.e., the spin, in our example) has to deviate significantly from their corresponding means and this happens with a probability which is exponentially small in the size N. Accordingly, for large N, one expects w_N to be distributed according to a probability density $p(w) \sim \exp[-NI(w)]$, where the so-called *rate function* $I(w)$ is non-negative, vanishes for $w = \bar{w}$, and characterizes the statistics of both large deviations and Gaussian fluctuations.

Here we show that the statistics of large deviations of the intensive work w done during a global quench of a thermally isolated quantum many-body system provides insight into its universal properties. For a global quench one heuristically expects $p(w)$ to feature a prominent Gaussian peak centered at a finite mean $\bar{w}$. By focusing on the tails of this distribution, we demonstrate that there is a clear distinction between large deviations well below ($w \ll \bar{w}$) and well above ($w \gg \bar{w}$) the mean. The former are determined by the excess free energy f_{ex} of the $d+1$ dimensional classical correspondent in a film [5, 9] and acquire universal features close to a possible critical point. The latter, instead, are genuinely quantum features, beyond the quantum-to-classical correspondence, which may, however, maintain some tracts of universality. Our analysis encompasses as examples the cases of quenches in the quantum Ising chain [7] and in a free bosonic system [15]. In addition, we show that, depending on the space dimensionality, the large deviation statistics of bosonic systems displays a so-called *condensation transition* (see, e.g., Ref. [16]), analogous to the Bose-Einstein condensation.

Statistics of the work – Consider a quantum system with N interacting degrees of freedom and Hamiltonian $H(g)$. The extensive work W_N performed on the system during the quench $g_0 \to g$ is determined by the initial state, typically the ground state $|\Psi_0^{g_0}\rangle$ of $H(g_0)$, and by the eigenvalues $E_{n\geq 0}^g$ and eigenvectors $|\Psi_n^g\rangle$ of the post-quench Hamiltonian $H(g)$. In particular, W_N is a stochastic variable with probability density [17, 18]

$$p(W_N) = \sum_{n\geq 0} |\langle \Psi_n^g|\Psi_0^{g_0}\rangle|^2 \delta(W_N - [E_n^g - E_0^{g_0}]), \quad (1)$$

where E_0^g indicates generically the extensive ground-state energy of $H(g)$. As p vanishes identically for W_N below $E_0^g - E_0^{g_0}$, we refer W_N to this threshold so that $W_N \geq 0$.

The probability $p(W_N)$ can be conveniently studied via its moment generating function

$$G(s) \equiv \langle \mathrm{e}^{-sW_N}\rangle, \quad (2)$$

which, for $N \to \infty$, exists in the complex half-plane containing $\mathrm{Re}\, s \geq 0$ (with possible zeros, see, e.g., Ref. [11]). For later purposes, we distinguish here a class A of systems in which W_N for large but finite N cannot exceed a certain extensive threshold Nw_M from the class B, encompassing most of the real systems, within which W_N can assume arbitrarily large values. Generically, in class A, $G(s)$ is defined for all $s \in \mathbb{R}$ with $G(s) \simeq \mathrm{e}^{-sNw_M}$ for $s \to -\infty$, whereas in class B, $G(s)$ is defined only for $s > -\bar{s} < 0$ with a generic singularity in its derivative at $-\bar{s}$. The quantum Ising chain in a transverse field and the free bosonic field belong to classes A and B, respectively.

The *quantum* to *classical* correspondence allows us to interpret the moment generating function $G(s)$ for $s > 0$ as the *partition function* of a *classical* system in a film geometry [9]. Indeed, Eq. (1) implies

$$G(s) = \langle \Psi_0^{g_0}|\mathrm{e}^{-s[H(g)-E_0^g]}|\Psi_0^{g_0}\rangle, \quad (3)$$

where $\langle \Psi_0^{g_0}|\mathrm{e}^{-sH(g)}|\Psi_0^{g_0}\rangle \equiv Z_{N\times s}$ is in fact such a partition function of the classical $d+1$-dimensional system with transfer matrix $\mathrm{e}^{-H(g)}$ corresponding to the *quantum* Hamiltonian $H(g)$, in a film geometry with transverse "surface" area N, "thickness" s and equal boundary conditions set by $|\Psi_0^{g_0}\rangle$. On the basis of $Z_{N\times s}$ one naturally defines the free energy $\mathcal{F}_{N\times s} \equiv -\ln Z_{N\times s}$ per k_BT, where T is the temperature of the corresponding classical system, which depends on the parameters of $H(g)$. In terms of the classical system, the variable s in Eq. (2) is the distance between the two confining surfaces which we assume to have a large transverse area N. Upon increasing s, the free energy density per unit area f decomposes in decreasing powers of s as [20]

$$f \equiv N^{-1}\mathcal{F}_{N\times s} \simeq sf_b + 2f_s + \text{corr.}, \quad (4)$$

where $f_b = \lim_{N,s\to\infty} \mathcal{F}_{N\times s}/(Ns)$ is the bulk free energy density and f_s is the surface free energy density, i.e., the energy cost for introducing separately each single boundary into the otherwise bulk system. The corrections "corr." in Eq. (4) vanish for $s \to \infty$. In order to separate the effects of confinement from the bulk behavior, one usually introduces the so-called *excess* free energy density per unit area $f_{ex} \equiv f - sf_b$, which plays a fundamental role in what follows and becomes independent of N in the limit of large N considered hereafter. In terms of the quantum system, one finds from Eqs. (3) and (4), that $f_b = E_0^g/N$, $f_s = -(\ln|\langle\Psi_0^{g_0}|\Psi_0^g\rangle|)/N$ [9] and therefore

$$G(s) = \mathrm{e}^{-Nf_{ex}(s)}. \quad (5)$$

For $s < 0$, f_{ex} is defined in terms of $G(s)$ by this equations and it lacks its thermodynamic interpretation.

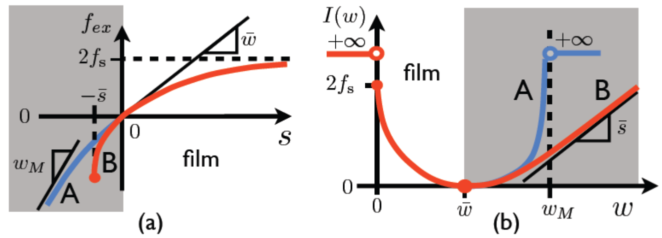

FIG. 1: (a) Sketch of the excess free energy density $f_{ex}(s)$ and (b) of the corresponding rate function $I(w)$ for classes A (blue) and B (red) discussed in the main text. The gray area highlights the range of variables for which f_{ex} does not have a thermodynamic interpretation.

Large deviations and universality – Equation (5) is crucial for understanding the emergence of universality in the large deviations statistics of the intensive work $w_N = W_N/N$. In fact, its distribution $p(w)$ for $N \to \infty$ can be determined by a saddle-point approximation of the inverse Laplace transform of $G(s)$, which actually provides a heuristic derivation of the Gärtner-Ellis theorem [14]. In particular, Eq. (5) implies that $p(w)$ has the form $\sim \exp[-NI(w)]$, where the *rate function* $I(w)$ is the Legendre-Fenchel transform of $f_{ex}(s)$ (and viceversa, under certain assumptions [14])

$$I(w) = -\inf_{s\in\mathbb{R}} \{sw - f_{ex}(s)\}, \quad (6)$$

in which the infimum is taken within the domain $\mathcal{D}$ of definition of $f_{ex}(s)$ and $G(s)$. Here we assume that $f'_{ex}(s)$ is continuous inside $\mathcal{D}$, i.e., that no first-order phase transitions occur in the system.

The generic features of $p(w)$ can now be inferred from Eqs. (5) and (6). First of all note that the excess free energy is such that $f_{ex}(0) = 0$ and $f'_{ex}(0) = \bar{w}$. Most importantly $f_{ex}(s)$ is a concave function of s [14] which approaches $2f_s$ for $s \to +\infty$. Figure 1 provides a sketch of $f_{ex}(s)$ and the corresponding $I(s)$ for the two classes A and B introduced above. The last two properties imply the existence of a threshold in $p(w)$: the infimum in Eq. (6) for $w < 0$ is $-\infty$ and consequently $p(w < 0) = 0$. The behavior of $I(w)$ close to the threshold $w \gtrsim 0$, instead, is determined by the one of $f_{ex}(s)$ for $s \to +\infty$

and in particular $I(0) = 2f_s > 0$, while the approach to it is determined by the corrections $f_{ex} - 2f_s$ in Eq. (4).

The universality of these finite-size corrections close to critical points [19] carries over into the large deviation statistics of $p(w)$ for $w \ll \bar{w}$. Indeed, if the post-quench Hamiltonian $H(g)$ is close to a quantum critical point the finite-size corrections $f_{ex} - 2f_s$ to the free energy density of the (near-critical) classical $d+1$-dimensional system, which are responsible for the so-called critical Casimir effect [19], take the universal scaling form $s^{-d}\Theta(s/\xi)$ for $s \gg a$, where $\xi \gg a$ is the correlation length and a some microscopic length scale. The scaling function Θ is *universal* in the sense of critical phenomena [19], as it depends only on the universality class of the classical critical point. In addition, due to the presence of the boundaries, Θ depends on their *surface universality class* [21] or, equivalently, on which among the few effective boundary (i.e., initial) states $\{|\Psi_i^*\rangle\}_i$, $|\Psi_0^{g_0}\rangle$ flows to as the critical point is approached. Once the scaling function Θ is known, the rate function is calculated via Eq. (6). In particular, if the post-quench Hamiltonian is critical, then $\xi = \infty$ and

$$I(w \lesssim \Delta) = 2f_s - \frac{d+1}{d}\Delta\left(\frac{w}{\Delta}\right)^{d/(d+1)} + \dots \qquad (7)$$

with $\Delta = d|\Theta(0)|$. While f_s and the possible corrections depend on the specific parameters of the initial state, the leading dependence of $I(w)$ on w is universal and non-analytic. In the case of finite but large ξ, $I(w)$ takes the scaling form $I(w) = 2f_s + \xi^{-d}\vartheta(w\xi^{d+1})$, where $\vartheta(y)$ is the Legendre-Fenchel transform of $x^{-d}\Theta(x)$ (and viceversa, see Eq. (6)). Note that ϑ is as universal as Θ and the latter can be inferred from the former. For $w \ll \xi^{-(d+1)}$, the approach to $2f_s$ is eventually controlled by $\Theta(x \gg 1) = \mathcal{C}x^a e^{-bx}$ where the universal constants a, b, and $\mathcal{C}$ depend, along with Θ, on the bulk and surface universality class of the transition, and they are known for a variety of universality classes [19] (e.g., $a = -1/2$, $b = 2$ for a quench of the quantum Ising chain within the same phase [9]). In this case, one finds $I(w \ll \xi^{-(d+1)}) \simeq 2f_s - (\xi/b)w \ln w^{-1}$ but with significant logarithmic corrections. Note that the universal edge singularities of the extensive work W_N discussed in Ref. [9] collapse onto the threshold when studied in terms of the intensive work w_N.

In order to illustrate the discussion above we focus on a free bosonic theory described by a Hamiltonian diagonalizable in independent momentum modes

$$H(m) = \int \frac{d^d k}{(2\pi)^d}\left(\frac{1}{2}\pi_k\pi_{-k} + \frac{1}{2}\omega_k^2\phi_k\phi_{-k}\right), \qquad (8)$$

where $[\phi_k, \pi_{k'}] = i\delta_{k,k'}$ and the integral runs over the first Brillouin zone $|k_i| < \pi$. We assume a relativistic dispersion relation $\omega_k(m) = \sqrt{k^2 + m^2}$ and consider quenches of the mass from m_0 to m [4, 15]. $H(m)$ captures the low-energy properties of a number of physical systems, including the ideal harmonic chain, interacting fermions and bosons in one dimension [23], and it models the relative phase fluctuations of split one-dimensional condensates [3]. $H(m)$ has a critical point at $m = 0$ and the corresponding classical theory is that of a Gaussian field φ in $d+1$ spatial dimensions and mass m. The quench is characterized by $\lambda_k \equiv [\omega_k(m_0) - \omega_k(m)]/[\omega_k(m_0) + \omega_k(m)]$ and from Eqs. (1), (2), and (5) one finds [15]

$$f_{ex}(s) = \frac{1}{2}\int \frac{d^d k}{(2\pi)^d} \ln\left[\frac{1 - \lambda_k^2 e^{-2\omega_k(m)s}}{1 - \lambda_k^2}\right], \qquad (9)$$

which is defined for $s > -\bar{s} = \sup_k(\ln|\lambda_k|)/\omega_k(m)$ and, as anticipated, belongs to class B. This f_{ex} can be decomposed as in Eq. (4) and upon approaching the critical point $m = 0$, i.e., for sufficiently large $\xi = m^{-1}$ and s, the correction $f_{ex}(s) - 2f_s$ takes the (m_0-independent) scaling form $s^{-d}\Theta_O(s/\xi)$ where $\Theta_O(x)$ is the scaling function of the critical Casimir effect for the classical field φ with boundaries belonging to the so-called *ordinary* surface universality class [21], corresponding to Dirichlet boundary conditions for φ. Θ_O can be read, e.g., in Eq. (6.6) of Ref. [22]. Accordingly, upon approaching the critical point, the ground state $|\Psi_0^{m_0}\rangle$ of $H(m_0)$ flows towards the fixed-point state $|\Psi_O^*\rangle$ corresponding to this surface universality class. However, as s decreases, $f_{ex}(s) - 2f_s$ calculated from Eq. (9) is no longer independent of m_0 and corrections to the critical Casimir term arise. These corrections are partly but effectively accounted for by changing $s \mapsto s + 2\ell_{\text{ext}}$ in the previous scaling form, where the so-called *extrapolation length* ℓ_{ext} [21] takes here the value m_0^{-1}. Effectively, the fixed-point Dirichlet boundary condition on φ is realized at surfaces located outside the film at a distance ℓ_{ext} from its boundaries, resulting in an effective film thickness $s + 2\ell_{\text{ext}}$ [4, 5, 21]. This correction is unnecessary for $s, \xi \gg \ell_{\text{ext}}$, while is increasingly important as ξ, s, or m_0 decrease. Figure 2 presents the rate function $I(w)$ (solid line) in $d = 1$ for a quench from a non-critical to the critical point. In panel (a) the vertical dashed line indicates the mean work $\bar{w}$. The dashed curve, instead, provides the quadratic approximation of $I(w)$ around $w = \bar{w}$, which describes the Gaussian distribution of the small fluctuations. While additional features of $I(w)$ are rationalized further below, panel (b) focuses on the region of small w, where universality is expected to emerge. The dash-dotted line corresponds to Eq. (7), with $\Theta_O(0) = -\Gamma(d)\zeta(d+1)/[(16\pi)^{d/2}\Gamma(d/2)]$ [22]. This universal behavior sets in rather close to the threshold. However, the agreement between $I(w)$ and Eq. (7) extends to a wider range by accounting for the correction due to ℓ_{ext} (dashed curve). The features displayed in Fig. 2 for $m = 0$ carries over to the case $m \ll m_0$, which requires the knowledge of the full scaling function $\Theta_O(x)$. For a fixed value of m, instead, the corrections to the scaling behavior due to ℓ_{ext} increase upon decreasing m_0 and eventually, after crossing the

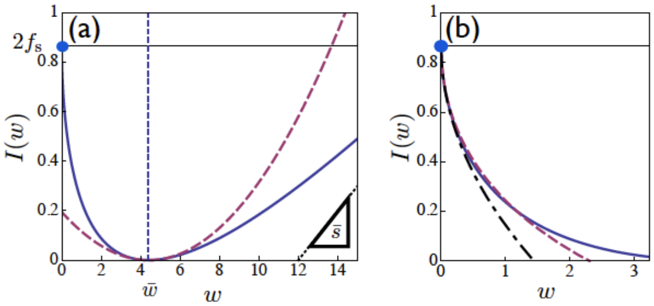

FIG. 2: Rate function $I(w)$ (solid line) of the work done on the lattice free bosonic theory in $d = 1$ and unit lattice spacing, for a quench from $m_0 = 20$ to the critical point. In panel (a) the dashed curve corresponds to the Gaussian distribution of small fluctuations around $\langle w\rangle = \bar{w}$. In panel (b), the dash-dotted curve is the prediction of Eq. (7) while the dashed curve accounts also for a non-vanishing $\ell_{\rm ext}$.

line $m = m_0$ of no quench, they lead to a change in the effective boundary state [5, 9] for $m_0 \to 0$.

Quantum regime and condensation – Let us now consider the case of large work $w \gg \bar{w}$. Upon increasing w further away from the threshold, the value $s^*(w)$ of s for which the infimum in Eq. (6) is attained — and which satisfies $f'_{ex}(s^*(w)) = w$ — decreases and so does the thickness of the corresponding film. The behavior of such a film is expected to become increasingly dominated by its microscopic details, with a generic lack of universality even close to the critical point. Correspondingly I decreases because $I'(w) = -s^*(w)$. For $w = \bar{w}$, $s^* = 0$ and $I(w = \bar{w})$ vanishes, while it grows again for $w > \bar{w}$, with $s^*(w) < 0$ (see Fig. 1). The rate function for $w > \bar{w}$ is thus determined by $f_{ex}(s)$ for $s < 0$ ("negative" film thickness), which lacks a thermodynamic interpretation because the quantum-to-classical correspondence does not hold in this case. The qualitative behavior of $I(w > \bar{w})$ depends crucially on the class the system belongs to. In Fig. 1 we report a sketch of (a) $f_{ex}(s)$ and (b) the associated rate function I corresponding to classes A and B discussed above and characterized by (A) a bound (e.g., the quantum Ising chain) or (B) an unbound spectrum (e.g., free bosonic theory). In particular, in case A, $I(w)$ diverges upon approaching w_M, with $I(w > w_M) = +\infty$ as required by the fact that $p(w)$ vanishes above the intensive threshold w_M. In case B, instead, $I(w \to \infty) \simeq \bar{s}w$ and therefore $p(w \gg \bar{w}) \sim \mathrm{e}^{-N\bar{s}w}$. This is seen in Fig. 2(a), though the asymptotic linear behavior for $w \gg 1$, with slope $\bar{s}$ (indicated by the dashed line) is actually approached only for rather large values of w. In general, $\bar{s}$ is system-specific and depends on the parameters of the quench.

Even though the emergence of universality is apparently limited to $w \ll \bar{w}$, systems belonging to class B might display unexpected universal properties in the fully quantum regime $w > \bar{w}$. Indeed, the statistics of the work done on the free bosonic theory in Eq. (8) displays, for $m_0 \to 0$, a behavior analogous to the Bose-Einstein condensation of the ideal gas in the grand canonical ensemble. This implies a transition in the large deviation statistics for $w > \bar{w}$ from exponential to algebraic. In fact, we note that the excess free energy $f_{ex}(s)$ in Eq. (9) has the same form as half the scaled cumulant generating function $\psi(s)$ of the fluctuations of the spatial density ρ_V of ideal Bose particles (of mass m_B) within a large region of volume V. At equilibrium in an ensemble with chemical potential $\mu \leq 0$ (in units of temperature β^{-1}) one finds $\psi(s) = \int \frac{\mathrm{d}^d k}{(2\pi)^d} \ln\left(\frac{1-\Lambda_k \mathrm{e}^{-s}}{1-\Lambda_k}\right)$, where $\Lambda_k = \mathrm{e}^{-\beta\varepsilon_k+\mu}$ with $\varepsilon_k = \hbar^2k^2/(2m_B)$ and the integral is over $\mathbb{R}^d$. Accordingly the plot of $\psi(s)$ has the form B in Fig. 1(a), with $\bar{s} = -\mu$. For the ideal Bose gas, the condensation occurs as $\mu \to \mu_c = 0$: the asymptotic slope $\bar{s} = -\mu$ of the rate function $I(\rho > \bar{\rho})$ vanishes together with the function itself (see Fig. 1(b)). The mean value $\bar{\rho} = \langle\rho\rangle = \psi'(0)$ above which this happens is the critical density for condensation $\rho_c = l^{-d}\zeta(d/2)$ [24], which is finite only for $d > d_c = 2$, where $l \equiv (2\pi\beta\hbar^2/m_B)^{1/2}$ is the thermal wavelength. I vanishes for $\rho > \rho_c$ because the probability $p(\rho)$ acquires an algebraic dependence on ρ — due to the contributions of fluctuations in single-particle states with small k — and indeed the momenta $\langle(\rho-\bar{\rho})^n\rangle$ with $n \geq d/2$ diverge as $\mu \to \mu_c$; e.g., $\langle(\Delta\rho)^2\rangle \propto (-\mu)^{-\alpha}$ where $\alpha = 2 - d/2$ for $d < 4$.

For the statistics of the work, m_0 plays a role similar to μ, although the occupation of the energy levels is determined by the non-thermal distribution generated by the quench and not by the Bose statistics. In fact, both m_0 and μ determine the k-dependence of $\lambda^2_{k\simeq 0}$ and $\Lambda_{k\simeq 0}$, respectively, on which the onset of the condensation depends. In the case of the intensive work, m_0 is the control parameter: for $m_0 \to 0$, $\langle w\rangle$ is finite for $d > d'_c = 1$ with a corresponding "critical value" $w_c(m)$. The emergence of $d'_c \neq d_c$ is due to the fact that the dependence of $\lambda^2_{k\simeq 0}$ on k crosses over from quadratic for $m_0 \neq 0$ to linear for $m_0 = 0$. Analogous crossover occurs in the condensation of an ideal Bose gas with relativistic dispersion [25]. The rate function $I(w)$ vanishes identically for $w > w_c$ and $p(w)$ acquires an algebraic dependence on w because of the slow asymptotic decay of the probability distribution of the work done on modes with small k, which are mildly confined in the initial state with $m_0 \to 0$. As a result, moments $\langle(w-\bar{w})^n\rangle$ with $n \geq d$ diverge in this limit with, e.g., $\langle(\Delta w)^2\rangle \propto \ln(m/m_0)$ in $d = 2$.

Conclusions – We discussed the qualitative features of the large deviation statistics of the work done during a quantum quench, highlighting the emergence of universality and, for bosonic systems, of a non-thermal condensation transition. Even though large fluctuations are exponentially rare as the system size increases, the value of the rate function $I(0)$ can be reduced by a suitable choice of the quench parameters, making them observable by a post-selection of experimental data.

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