Edge exponents in work statistics out of equilibrium and dynamical phase transitions from scattering theory in one-dimensional gapped systems

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I discuss the relationship between edge exponents in the statistics of work done, dynamical phase transitions, and the role of different kinds of excitations appearing when a nonequilibrium protocol is performed on a closed, gapped, one-dimensional system. I show that the edge exponent in the probability density function of the work is insensitive to the presence of interactions and can take only one of three values: $+1/2$, $-1/2$, and $-3/2$. It also turns out that there is an interesting interplay between spontaneous symmetry breaking or the presence of bound states and the exponents. For instantaneous global protocols, I find that the presence of the one-particle channel creates dynamical phase transitions in the time evolution.

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Out of equilibrium phenomena in quantum systems have been given a large amount of attention recently. The interest was largely spun by the advent of new experimental techniques in cold atoms and solid state quantum devices where coherence can be maintained for far longer times than previously [1], and therefore the unitary evolution after a quantum system is taken out of equilibrium has become an important and well studied concept. This has been renewing interest in some fundamental and long-standing questions in statistical mechanics, and at the same time bringing new ideas and phenomena into the spotlight. One such concept is that of dynamical phase transitions (DPTs), which refers to nonanalytical behavior detected in the Loschmidt echo (LE) [2] and affecting the time evolution of certain observables in a characteristic way [3]. For the important class of global, instantaneous, nonequilibrium protocols (dubbed as quantum quenches), this phenomenon can be understood in terms of the Fisher zeros of the partition function corresponding to singularities of the free energy: The LE in this case is equivalent to the partition function with imaginary temperature [2]. While DPTs have been the subject of a growing number of both analytical and numerical works, a clear physical mechanism accounting for them has yet to emerge [2–7].

Another interesting quantity is the work performed when taking the system out of equilibrium [8]. With the discovery of nonequilibrium fluctuation relations [9] this is interesting on its own right, but it is also intimately connected to the LE for certain important protocols [10]: In the case of quantum quenches, the LE and the probability density function (PDF) of the work done are related by Fourier transformations. Furthermore, it seems now that although the work itself is not an observable [10], due to being a positive operator valued measure, it can in principle be measured on an enlarged system [11]. One of the most striking features of the statistics of work is the robustness and universality of the edge singularity exponent in its PDF at the lower limit, corresponding to the opening of the first continuous channel of realizing the quench, i.e., the emission of two (quasi)particles with opposite momenta [4,12,13]. This robustness has already been demonstrated with respect to the details of the protocol [4].

In this paper, we will concentrate on the role of interactions, and we will determine the possible exponents emerging from the statistics of work in one-dimensional gapped systems. We will connect the different values to different kinds of quasiparticle contents. We establish that the crucial property is the existence or absence of one-particle excitations, which can appear, e.g., in the form of bound states or when the initial or the final system is spontaneous symmetry breaking. We also find that the exponent is extremely robust and, in fact, close to criticality, there are only three possible values (excluding fine tuning): $+1/2$, $-1/2$, and $-3/2$, independent of the relevant critical point and the symmetries of the system. Our results are also interesting with respect to DPTs: For global quenches we can predict the emergence of a transition by looking at the pre- and postquench particle contents.

In the following, we first discuss the possible edge singularity exponents through a scattering theoretical argument. We then study the case of spontaneous symmetry breaking on the example of the Ising model. Then we move on to discuss the sine-Gordon model, which provides a low-energy effective field theory description of many interesting condensed matter systems, e.g., one-dimensional magnets of the XYZ and XXZ types and Mott insulators [14]. Finally, the connection to the LE is studied.

Edge exponent from scattering theory. We apply quantum field theoretical scattering theory to extract the exponents. This approach is natural since the edge exponent is determined only by the low-energy part of the spectrum, and quantum field theory gives the universal low-energy effective description valid close to criticality.

Suppose we perform some finite T time nonequilibrium protocol on our system,

$$H[g(t_0)] = H_0 \rightsquigarrow H_1 = H[g(t_0 + T)], \tag{1}$$

beginning in, e.g., the ground state of an initial Hamiltonian H_0, which is allowed to evolve by a different, local Hamiltonian that may itself be explicitly time dependent through a coupling, e.g., the magnetic field $H[g(t)]$. At the end of the protocol we arrive in some state that can be expanded

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in terms of asymptotic states of the final Hamiltonian H_1. Asymptotic states form an eigenbasis of the fully interacting theory and have a perfectly good interpretation as collections of asymptotically free particles with mass and appropriate quantum numbers. (In most of the interesting physical cases such a basis exists.) We write the expansion as

$$|0\rangle^0 \rightsquigarrow |e\rangle = |0\rangle^1 + \sum_{\{a_n\}} \sum_{\{p_n\}} K^{\{a_n\}}_{\{p_n\}} |\{p_n\}\rangle^1_{\{a_n\}} + \cdots , \quad (2)$$

where the eigenstates contain the stable (quasi)particle excitations of species a_n and momentum p_n. Since we consider a nonadiabatic, finite-time process, the amplitudes $K^{\{a_n\}}_{\{p_n\}}$ in general will be nonzero, however, we note that for the multiparticle states to acquire an appreciable weight, the inverse time scale of the protocol should be much larger than the gap, $1/T \gg m$.

Now consider the PDF of the work done on the system during the protocol defined as

$$P(W) = \sum_{\text{eigenstates } |\Psi\rangle \text{ of } H_1} \delta(W - E_\Psi + E_{gs,0}) |\langle \Psi | e\rangle|^2, \quad (3)$$

signifying two projective energy measurements before and after the protocol and summing over all the possible transitions weighted by the respective overlaps. Supposing a translationally invariant initial state and time-evolving Hamiltonian, the one-particle part can only consist of zero-momentum particles responsible for Dirac deltas in the PDF, and the low-energy behavior of the continuum part is dictated by the two-particle creation amplitudes $\langle p_1 p_2 | e\rangle = K(p_1)\delta(p_1 + p_2)$ relative to the particles with lowest mass m (only states with zero total momenta are allowed because of translation invariance).

In Ref. [12], for an integrable quantum field theory in the quench limit, it was observed that if there are no particle multiplets, the continuum part starts as

$$P(W \gtrsim 2m) \sim |K(\sqrt{W^2 - 4m^2})|^2 (W - 2m)^{-1/2}, \quad (4)$$

where the density of states near the threshold was supposed to go as $\rho(E) \sim (E - 2m)^{-1/2}$. Here, we observe that Eq. (4) depends only on the relativistic dispersion $E(p) \equiv E_{|p,-p\rangle} = 2\sqrt{m^2 + p^2}$ and density of states and therefore generalizes to finite-time protocols on arbitrary interacting relativistic quantum field theories. Now we use the relation

$$K(p) = S(-2p)K(-p), \quad (5)$$

with $S(p)$ being the two-particle scattering amplitude. This can be verified by considering a state $|\Psi\rangle = \int_{-\infty}^{\infty} dp K(p)|p,-p\rangle$ and using the definition of the scattering amplitude $|p,-p\rangle = S(2p)|-p,p\rangle$ to obtain $|\Psi\rangle = \int_{-\infty}^{\infty} dp K(-p)S(-2p)|p,-p\rangle$, proving Eq. (5). Noting that in one dimension for any interacting theory the scattering amplitude has the superuniversal property $S(0) = -1$,[1] we see that the two-particle amplitude is odd near $p = 0$. The simplest choice realizing this would be $K(p \approx 0) \sim p$, giving $P(W \approx 2m) \sim (W - 2m)^{1/2}$, which was indeed observed when quenching inside a single phase in the Ising [4] and sinh-Gordon models [12]. However, one could also imagine $K(p \approx 0) \sim p^{-1}$, or in fact any odd power. Incidentally, the choice p^{-1} yields $P(W \approx 2m) \sim (W - 2m)^{-3/2}$, an edge behavior observed when quenching through the quantum critical point in the Ising model [4].

In this paper we argue that in one dimension and close to criticality (or when a relativistic dispersion is expected) the exponents $1/2$ and $-3/2$ are in fact the only natural ones in any interacting system. In the special case of free bosons with $S(0) = 1$, a third exponent is seen instead, $P(W \approx 2m) \sim (W - 2m)^{-1/2}$, which is confirmed by explicit calculation in Ref. [16].

We show that the only way for an extensive quench to be realized with a singular two-particle amplitude, e.g., $K(p \approx 0) \sim p^{-1}$, is in the presence of a zero-momentum one-particle excitation in the expansion (2). Vice versa, if there is a nonzero one-particle term in Eq. (2), the corresponding two-particle amplitude has a pole at $p = 0$. To see this correspondence, we note that extensivity of free energy is expected for translationally invariant initial states in thermodynamically large systems because the translation operator does not change throughout the protocol. The asymptotic expansion of the partition function calculated in the postprotocol system in finite volume L and inverse temperature R reads

$$Z = 1 + a_1 L e^{-mR} + \sum_I \frac{\varepsilon(p_I)}{L\varepsilon(p_I) + 2\delta'(2p_I)} |K(p_I)|^2 e^{-2R\varepsilon(p_I)} + \cdots , \quad (6)$$

where the fraction in the two-particle term accounts for the difference in the density of states in finite and infinite volumes (for details, see Ref. [17], where the equivalent boundary field theoretical problem was considered). $\varepsilon(p)$ is the one-particle energy at momentum p, $\delta(p)$ the phase shift, $S(p) = e^{i\delta(p)}$, and I labels the quantized finite-volume states. At the bottom of the spectrum the quantized momenta behave as $p_I \sim L^{-1}$, so both $\varepsilon(p)$ and $\delta'(p)$ are finite. As shown already in Ref. [17], if the two-particle amplitude has a first-order pole at $p = 0$, the only way for the free energy to be extensive $F = \log Z \sim L$ is in the presence of a nonzero one-particle contribution, and in fact the coefficient a_1 is related to the residue of the pole of $K(p)$ [17,18]. This is because the part of the two-particle contribution coming from the pole of $K(p)$ is superextensive of order L^2 and needs to be canceled exactly in $\log Z$.[2] One can also see that a more singular behavior of $K(p)$ at zero cannot be canceled by the one-particle contribution, therefore we can restrict $K(p)$ to be

$$K(p \approx 0) \sim p^{2k+1}, \quad k \geqslant -1. \quad (7)$$

[1]See Ref. [15] after Eq. (6.13) or consider the simple quantum mechanical problem of potential scattering, where it can be seen by elementary considerations that in the low-energy limit, i.e., when the potential can be approximated by a Dirac delta, the phase shift is always π corresponding to $S = -1$.

[2]It is interesting to note that the extensivity of the nonequilibrium protocol gives the same condition for $|e\rangle$ as the one obtained in boundary field theory for sensible boundary states from considerations involving the crossed channel [18,19].

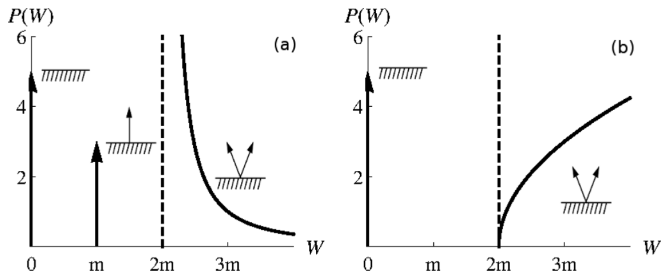

FIG. 1. Extensivity of the initial state and a local, translationally invariant, interacting Hamiltonian evolution requires a singular edge exponent of $-3/2$ in the PDF of the work done if the protocol can be realized by the emission of a single zero-momentum particle (a). In the absence of the one-particle realization the edge is nonsingular with an exponent of $+1/2$ (b).

Considering this last equation, we expect that, without a fine tuning in the parameters,[3] the two-particle amplitude is linear for small momenta unless there is a realization of the protocol with the emission of a single particle, in which case the amplitude will have a simple pole at $p = 0$ (see Fig. 1).

In the following, we discuss two scenarios leading to a one-particle contribution in the after-protocol state. In the first case, the system is spontaneous symmetry breaking (SSB) either before or after the protocol. The second, equally interesting case is when the model has a more complicated particle content, such as the sine-Gordon model, where bound state one-particle contributions can appear without crossing a critical point.

Spontaneous symmetry breaking. We take the simplest SSB system, the Ising model in a transverse field close to criticality, in the thermodynamic limit equivalent to free massive Majorana fermions. Depending on the sign of the mass, the system is either in the unbroken (disordered) $m > 0$ or the broken symmetry phase $m < 0$ (ordered). To determine the condition for the one-particle contribution to appear, we need to recall the Hilbert space structure of Majorana fermions.

The Hilbert space can be divided into two sectors, with two ground states, according to either adopting a periodic (Neveu-Schwartz, NS) or antiperiodic boundary condition (Ramond, R). The excitations are free fermions, and in finite volume the boundary conditions require that the zero-momentum excited states have even fermion numbers relative to the ground state. In the broken phase and in the thermodynamic limit, the energies of the two ground states become degenerate, and in fact the two infinite-volume ground states are the superpositions [20]

$$|\uparrow\rangle = \frac{1}{\sqrt{2}}(|\text{NS}\rangle + |\text{R}\rangle),$$
$$|\downarrow\rangle = \frac{1}{\sqrt{2}}(|\text{NS}\rangle - |\text{R}\rangle). \tag{8}$$

[3] Fine tuning is understood in the sense that for different exponents to appear, $K'(0) = 0$ would be required, however, the derivative $K'(p)$ has no simple physical meaning, and therefore this corresponds only to an accidental choice of protocol parameters.

The excitations over these states are kinks interpolating between the two vacua, i.e., moving domain walls. In the disordered, unbroken phase the R ground state acquires a mass relative to the NS ground state and becomes a one-particle state, so the zero-momentum R sector can be interpreted as a collection of states containing an odd number of particles. The vacuum is the NS vacuum and the excitations are fermions corresponding to spin waves. Now, the states from different sectors have no overlaps with each other because they have different topological properties, so if the initial state contains one sector, that sector will survive any protocol.

There is an important difference between arriving in the same or arriving in a different phase as the initial one. Let us first take the case of starting and ending the protocol in the disordered phase. In this case, the initial state is the NS vacuum and there is no overlap between NS and R states, so we have no one-particle contribution in the expansion (2). Contrary, if we start from one of the ordered ground states and arrive in the disordered phase, because of the presence of the R sector, initially we do expect a one-particle contribution. The remaining cases can be obtained by the Kramers-Wannier (KW) duality and using the fact that the work statistics has to be identical to that of the dual protocol (the operator corresponding to the work is invariant under the KW duality).

In summary, we obtained that when a protocol begins and ends in different phases, the amplitude $K(p)$ has a pole, while if no phase boundary is crossed, it remains linear. This is in fact the correct result as calculated in Refs. [4,21]. But contrary to the explicit calculations available (e.g., Refs. [4,12,16,21,22]), our considerations here depended only on the structure of the Hilbert spaces before and after the protocol, and therefore we expect them to generalize to other SSB situations, e.g., to protocols between phases of the three-state Potts or parafermionic models in the following way. For discrete symmetry breaking $G \to H \subset G$, we can partition the Hilbert space according to the representations of G/H in both the symmetric and broken phases, but, importantly, in the broken phase, the lowest lying states in all the sectors are degenerate and in infinite volume the physical vacua are linear combinations of these, while in the symmetric phase there is only one vacuum and the other sectors will contain one-particle states. Since local operators (relative to the Hamiltonian) have a zero matrix element between the different sectors, for a protocol starting in the broken phase and ending in the symmetric, we will in general have one-particle excitations in the expansion (2).

To conclude this section, we comment on the effect of finite volume on the Ising example. Consider the disordered-to-ordered quench when only the NS sector is involved. With a periodic boundary condition (PBC) there is no one-particle state in the broken phase in finite volume, however, in infinite volume such excitations do exist (see Fig. 2). On the other hand, the cases of large finite and infinite volumes should not be qualitatively different, and indeed an explicit calculation of the two-particle amplitude [4,21] shows an infrared pole in $K(p)$ independent of the volume. Careful examination of the calculation for the work PDF from the exact two-particle amplitude (available through techniques developed for the boundary thermodynamic Bethe ansatz [17,18,23]) shows that a finite-volume infrared regularization in the Ising model only allows for the appearance of the one-particle Dirac delta

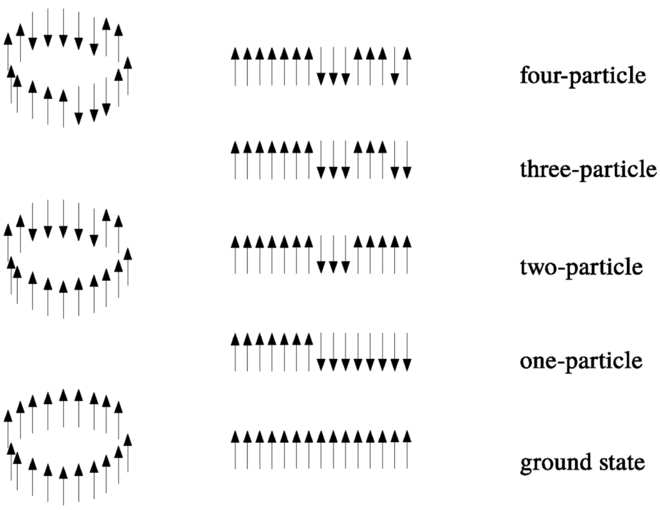

FIG. 2. Zero-momentum excitations in the finite- and infinite-volume Ising model in the ordered phase.

when the volume goes all the way to infinity, in accordance with the available excitations. These observations show that our thermodynamic argument connecting the one-particle contribution and the pole only works in infinite volume. Indeed, the finite-volume vacuum $|\mathrm{NS}\rangle$ for $m < 0$ does not satisfy clustering and therefore an extensive free energy is not expected at all.

Bound states. One-particle contributions in the expansion (2) can also arise in models with more complicated spectra: When the postprotocol Hamiltonian supports bound states, their appearance is not forbidden by translation and parity invariance (which was crucial in Refs. [24–26] to establish the structure of the after protocol state), and we expect that generally they appear in protocols performed on such models.

To support this idea, we made numerical calculations on the sine-Gordon model with PBCs in small volume using the truncated conformal space approach [27,28]. We found that, both when quenching between the repulsive (no bound states) and the attractive (bound states present) regimes and when quenching inside the attractive regime, there are finite one-particle contributions in the expansion (2) [29]. Our predictions seem to be supported by the numerical results of Ref. [5], where DPTs were observed without crossing a phase boundary for quenches in the XXZ model with staggered magnetic fields in the parameter regime, where the low-energy reduction is the sine-Gordon model.

Implications for the dynamics. We propose that for global quenches the remarkable universality of the edge exponent in the work PDF can be detected in the large time behavior of the LE, and based on whether or not a one-particle realization is allowed, one can predict if a DPT will be encountered during time evolution. LE is defined by $L(t) = |\mathcal{L}(t)|^2 = |\langle\Psi_0|e^{iH_0t}e^{-iH_1t}|\Psi_0\rangle|^2 = |\int_{-\infty}^{\infty} dW e^{-iWt}P(W)|^2$ and it is connected to the work PDF by a Fourier transform. To every new channel for increasing W corresponds an edge with some exponent α_{nj} (n being the number of particles emitted in the new channel and j labels the particle species), so the long-time behavior of the Loschmidt amplitude reads

$$\mathcal{L}(t) = 1 + \sum_j b_{1j} e^{im_j t} + \sum_j b_{2j} e^{2im_j t} t^{-1-\alpha_{2j}} + \text{higher particle terms}, \tag{9}$$

where the first term comes from the vacuum, the second from one-particle, and the third from two-particle contributions. Compared to the two-particle terms, the higher particle contributions are less singular, therefore these should be invisible in the long-time limit.

For the bosonic $\alpha = -1/2$, we get $L(t) - L(\infty) \sim t^{-1/2}$, and for the interacting $\alpha = 1/2$, $L(t) - L(\infty) \sim t^{-3/2}$. Interestingly, when there is a one-particle contribution to a given species j, we would get $L(t) - L(\infty) \sim t^{1/2}$, which is nonphysical and apparently signals that the low-energy degrees of freedom cannot capture the long-time behavior of the LE, and we expect nonanalytic behavior during the time evolution, or, by definition, a dynamical phase transition.

While this is an intriguing observation, we do not suggest a one-to-one correspondence between one-particle contributions in the expansion of the initial state and DPTs. In Ref. [6], it was found that in the XY model it is possible to have DPTs without a singular $K(p)$ two-particle amplitude. Instead, their results also show that whenever there is a singularity in the amplitude, there are also DPTs in the LE, supporting the physical relevance of the one-particle channel.

Conclusions. We proposed that the lowest edge exponents in the probability density function of the work done during a nonequilibrium protocol correspond to the realization of the protocol by emitting two particles and are extremely robust to perturbations in gapped one-dimensional systems. In fact, in the presence of interactions, there are only two possibilities depending on whether the protocol can also be realized by emitting only one particle or this is forbidden. We discussed two cases where such a one-particle process is allowed: when the protocol begins and ends in different phases of a SSB model and when there are bound states in the particle spectrum. We also proposed that if the one-particle realization is allowed, the time evolution of the Loschmidt echo shall exhibit a dynamical phase transition.

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