Quantum Relaxation after a Quench in Systems with Boundaries

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(Received 15 November 2010; revised manuscript received 15 December 2010; published 20 January 2011)

We study the time dependence of the magnetization profile, $m_l(t)$, of a large finite open quantum Ising chain after a quench. We observe a cyclic variation, in which starting with an exponentially decreasing period the local magnetization arrives to a quasistationary regime, which is followed by an exponentially fast reconstruction period. The nonthermal behavior observed at near-surface sites turns over to thermal behavior for bulk sites. In addition to the standard time and length scales a nonstandard time scale is identified in the reconstruction period.

DOI: 10.1103/PhysRevLett.106.035701 PACS numbers: 64.70.Tg, 05.70.Ln, 75.10.Pq, 75.40.Gb

Recent experimental progress in controlling ultracold atomic gases in optical lattices has opened new perspectives in the physics of quantum systems. In these measurements the coupling in an interacting system can be tuned very rapidly, commonly denoted as ''quench'', for instance by using the phenomenon of Feshbach resonance and the couplings to dissipative degrees of freedom (such as phonons and electrons) are very weak. As a consequence, one can study coherent time evolution of isolated quantum systems. Among the fascinating new experiments we mention the collapse and revival of Bose-Einstein condensates [1], quenches in a spinor condensate [2], realization of one-dimensional Bose systems [3], and measurements of their nonequilibrium relaxation [4].

Concerning the theoretical side of quantum quenches here the first investigations had been performed on quantum XY and quantum Ising spin chains [5–7] before the experimental work has been started. The new experimental results in this field have triggered intensive and systematic theoretical researches, which are performed on different systems, such as 1D Bose gases [8], Luttinger liquids [9], and others [10]. Besides studies on specific models there are also field-theoretical investigations, in which relation with boundary critical phenomena and conformal field theory are utilized [11,12].

One fundamental question of quantum quenches concerns the nature of the stationary state of this nonequilibrium quantum relaxation including the issue of thermalization and potential descriptions by Gibbs ensembles. For nonintegrable systems exact thermalization of stationary states was conjectured [13], however, the numerical results on specific systems are controversial [13–15]. On the other hand, integrable systems are sensitive to the initial states and their stationary states are thermal-like, being in a form of a generalized Gibbs ensemble [8].

Thermalization includes generically (i.e., away from critical points) an exponential decay of correlation functions in the stationary state on length and time scales that can be related to the correlation length and time of an equilibrium system at an effective temperature depending on the parameters of the quench [7,16,17]. Some quantum systems do not thermalize completely and display a different behavior for correlation functions of local and for nonlocal operators, such that the former do not exhibit effective thermal behavior [16]. An interesting issue not being addressed so far is the characterization of the nonstationary, that means not time-translation invariant, quantum relaxation following a quench: Preparing the quantum system in a noneigenstate of its Hamiltonian, how is thermalization achieved during the time-evolution? How do correlations develop in time towards the stationary (i.e., time-translation invariant) state, is there a time dependent correlation length, etc.?

Another important issue concerns quantum relaxation and potential thermalization in the presence of boundaries. Theoretical studies of nonequilibrium quantum relaxation have focused on bulk sites up to now, but all real systems have a finite extent and they are bounded by surfaces and the physical properties in the surface region are considerably different from those in the bulk [18]. Obviously an interesting question is whether the time and length scales characterizing the stationary relaxation in the bulk is altered in the vicinity of the boundary, and how thermalization is achieved there.

In this Letter we will address these two issues: The nonstationary quantum relaxation after a quench and the effect of boundaries. For this we focus on a computationally tractable model for a quantum spin chain and study the relaxation of profiles of observables in the early time steps as well as their behavior in the long-time limit. We also address the behavior in large, but finite systems and study the consequences of the recurrence theorem.

The system we consider in this Letter is the quantum Ising chain defined by the Hamiltonian

$$\mathcal{H} = -\sum_{l=1}^{L-1} \sigma_l^x \sigma_{l+1}^x - h \sum_{l=1}^{L} \sigma_l^z, \qquad (1)$$

in terms of the Pauli matrices $\sigma_l^{x,z}$ at site l. In the nonequilibrium process the strength of the transverse field is suddenly changed from h_0 $(t<0)$ to h $(t\geq 0)$. The Hamiltonian in Eq. (1) can be expressed in terms of free fermions [19], which is used in studies of its nonequilibrium properties [6,16]. The bulk transverse magnetization, σ_l^z, which is a local operator, has nonthermal behavior [5,11,17], whereas the bulk (longitudinal) magnetization, σ_l^x, which is a nonlocal operator, has effective thermal behavior [17]. Here we concentrate on the latter quantity and study the time dependence of its profile, $m_l(t) = \lim_{b\to 0_+ b}\langle\Psi_0^{(0)}|\sigma_l^x(t)|\Psi_0^{(0)}\rangle_b$, where $|\Psi_0^{(0)}\rangle_b$ is the ground state of the initial Hamiltonian (1) in the presence of an external longitudinal field b. According to [20] this can be written as the off-diagonal matrix element of the Hamiltonian (1):

$$m_l(t) = \langle\Psi_0^{(0)}|\sigma_l^x(t)|\Psi_1^{(0)}\rangle. \qquad (2)$$

Here, $|\Psi_1^{(0)}\rangle$ is the first excited state (which is the ground state of the sector with odd number of fermions) of the initial Hamiltonian $(t<0)$. In the ordered phase, $h_0 < h_c = 1$, where $m_l(t<0)>0$, $|\Psi_1^{(0)}\rangle$ is asymptotically degenerate with the ground state, $|\Psi_0^{(0)}\rangle$. For $h_0 \geq h_c$ the magnetization vanishes as $m_l(t<0)\sim L^{-x}$ with the system size for $t<0$. The decay exponent, x, is different at the critical point, $h=h_c$, and in the paramagnetic phase, $h>h_c$, as well in the bulk $(l/L = O(1))$ and at the boundary $(l/L\to 0)$; see Table I.

To calculate the magnetization profile in Eq. (2) we have used standard free-fermionic techniques [19,21]. For the surface site, $l=1$, most of the calculations are analytical, whereas for $l>1$ numerical calculations have been made for large finite systems up to $L=384$.

We have performed quenches for various pairs of transverse fields, h_0 and h and calculated the time dependence of the local magnetization at different sites, $l\leq L/2$. The results depend primarily on whether the system before and after the quench is in the ordered (**O**) or disordered (**D**) phase; see Fig. 1 for different combinations of **O** and **D**. One can identify different time regimes that can be interpreted in terms of quasiparticles, which are emitted at $t=0$, travel with a constant speed, $v = v(h, h_0)$, and are reflected at the boundaries.

As argued in Ref. [11] only those quasiparticles are quantum entangled that originate from nearby regions in space, others are incoherent. When the latter arrive at a reference point l they cause relaxation of local observables (such as magnetization). Here we extend this picture by noting that in a system with boundaries the same quasiparticle can reach the point l twice (or more) at different times after reflections. This induces quantum correlations in time signalized by the reconstruction of the value of the local observable. In the following we analyze the different regimes of the relaxation.

In the free relaxation regime $t<t_l = l/v$, only incoherent quasiparticles pass the reference point resulting in an exponential decay of the magnetization (cf. Fig. 1):

$$m_l(t)\equiv m(t)\approx A(t)\exp(-t/\tau), \qquad t<t_l, \qquad (3)$$

with an oscillating prefactor, $A(t)$. In the regime $h>h_c$ and $h_0<h_c$ we have $A(t)\sim\cos(at+b)$, thus $m(t)$ changes sign. On the other hand in the other parts of the phase diagram $m(t)$ is always positive, i.e. $A(t)\sim[\cos(at+b)+c]$, with $c>1$. The characteristic time scale, $\tau=\tau(h,h_0)$, is the relaxation or phase coherence time, which is extracted from the numerical data. The exponential form of the decay in Eq. (3) indicates thermalization, at least for bulk sites, which is in agreement with the similar decay of the autocorrelation function.

In the quasistationary regime $t_l<t<T-t_l$, $T=L/v$, two types of quasiparticles reach the reference point l: type 1 passed l only once at a time $t'<t$ and type 2 passed it twice at 2 times $t'<t''<t$, with a reflection at the nearby boundary between t' and t''. These two types interfere, resulting in a comparatively slow relaxation (cf. Fig. 1). Deep inside the ordered phase the quasiparticles can be identified with kinks moving with a speed $\pm v$ [22] and in the regime $t_l \ll t \ll T$ half of the quasiparticles reaching the site l are of type 1 (flipping the spin at l once) and half of them type 2 (flipping it twice), leading to a quasistationary relaxation.

The magnetization profiles for fixed times $t<T/2$ are shown in Fig. 2 for the same quenches as in Fig. 1. For

TABLE I. Decay exponent of the off-diagonal (longitudinal) magnetization in the initial (equilibrium) period.

	$h_0=h_c$	$h_0>h_c$
Bulk	1/8	1/2
Boundary	1/2	3/2

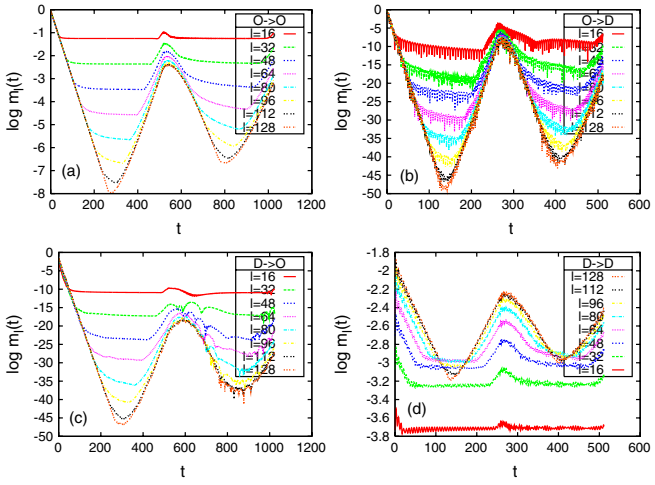

FIG. 1 (color online). Relaxation of the local magnetization, $\log m_l(t)$, at different positions in a $L=256$ chain after a quench with parameters: a) $h_0=0.0$ and $h=0.5$ (**O** → **O**) (b) $h_0=0.5$ and $h=1.5$ (**O** → **D**) (c) $h_0=1.5$ and $h=0.5$ (**D** → **O**) (d) $h_0=1.5$ and $h=2.0$ (**D** → **D**).

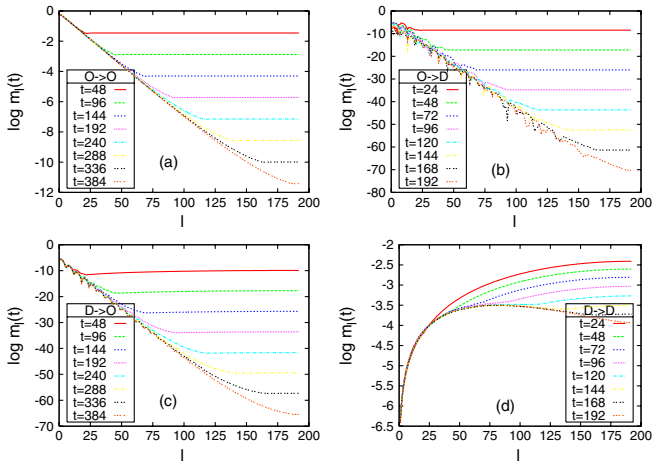

FIG. 2 (color online). Nonequilibrium magnetization profiles, $\log m_l(t)$, at different times after a quench with parameters given in Fig. 1 for $L = 384$. From the asymptotic values of the slopes one can measure the correlation length.

sufficiently large l the quasistationary magnetization has an exponential dependence, such that comparing its value at two sites, l_1 and l_2, we have

$$m_{l_1}(t_1)/m_{l_2}(t_2) \approx \exp[-(l_1 - l_2)/\xi], \tag{4}$$

with oscillating prefactors.

In the limits $L \to \infty$ and $t \to \infty$ one can define a quasistationary limiting value which will be denoted by, $\bar{m}_l$. For the surface site we have the exact result

$$\bar{m}_l = \frac{(1-h^2)(1-h_0^2)^{1/2}}{1-hh_0}, \qquad h_0, \qquad h < 1, \tag{5}$$

and zero otherwise. Note that the nonequilibrium surface magnetization has different type of singularities for $h \to 1^-$ ($h_0 < 1$) and for $h_0 \to 1^-$ ($h < 1$). We have analyzed the correction term, $\Delta(t, L) = m_1(t) - \bar{m}_1$, and its asymptotic behavior is summarized in Table II in the different domains of h and h_0. These corrections are in power-law form, which signals that the relaxation of the surface magnetization has nonthermal behavior.

For $l > 1$ we observe that $\bar{m}_l$ is monotonically decreasing with l and thus $\bar{m}_l > 0$ for $h_0, h < 1$ and zero otherwise. The correction terms are identical with those given in Table II so that a finite distance, l, the local magnetization has nonthermal behavior.

In the reconstruction regime: $T - t_l < t < T$ more and more quasiparticles of type 2 reach the reference point, which implies, within a kink-picture, that incoherent spin flips in the past are progressively reversed by quasiparticles returning to the site l after reflection. For monodisperse quasiparticles (velocity v) one would expect a T-periodicity and thus $m_l(t) = m_l(T - t)$, i.e., an exponential increase in t with a growth rate similar to the initial decay rate. Indeed, we find

$$m_l(t) \equiv m(t) \approx B(t)\exp(t/\tau'), \qquad T - t_l < t < T, \tag{6}$$

TABLE II. Correction to the quasistationary behavior for the surface magnetization in different domains of the quench.

	$h_0 < h_c$	$h_0 > h_c$
$h < h_0$	$t^{-1}\cos(at + b)$	$L^{-3/2}[\cos(at + b) + c]$, $c > 1$
$h > h_0$	$t^{-3/2}\cos(at + b)$	$t^{-1/2}[\cos(at + b) + cL^{-3/2}]$

which is practically position independent and where the growth rate of $\tau'(h, h_0)$ depends on the conditions of the quench, being approximately proportional to $\tau(h, h_0)$: $\tau/\tau' = 0.883 \pm 0.002$. It turned out to be useful to measure the crossover time, $\tilde{t} = T/2$, which is defined as the crossing point of the two asymptotic regimes: $\bar{A}\exp(-\tilde{t}/\tau) = \bar{B}\exp(\tilde{t}/\tau')$, where $\bar{A}$ and $\bar{B}$ are averaged prefactors. During the crossover time the quasiparticles travel a distance, $L/2$, thus their speed is given by $v(h, h_0) = L/2\tilde{t}$, which can be measured accurately. We have noticed, that for $h < 1$ the speed is proportional to h: $v(h, h_0) = ha(h, h_0)$, where $a(h, h_0)$ is practically independent of h_0 and has just a very week dependence on h close to $h = 1$. The typical values are in the range $a(h, h_0) \approx 0.86$–0.88. For $h \geq 1$ the speed is practically constant and has no h dependence.

Approximate periodicity with T starts for $t > T$, when quasiparticles start to be reflected a second time and the spin-configuration of the system becomes approximately equivalent to that at $t - T$.

The time and length scale, as defined in Eq. (3) and (4), respectively, as well as the characteristic quasiparticle speed $v(h, h_0) = \xi/\tau$, can be extracted with high numerical accuracy from our data for the magnetization profiles, typically with a precision of 3–4 digits. Complementary calculations of the autocorrelation function $G_l(t) = \langle\Psi_0^{(0)}|\sigma_l^x(t)\sigma_l^x(0)|\Psi_0^{(0)}\rangle$, and the equal-time correlation function, $C_t(r) = \langle\Psi_0^{(0)}|\sigma_{l+r}^x(t)\sigma_l^x(t)|\Psi_0^{(0)}\rangle$ show that they yield the same correlation time and length, but with less accuracy. Based on our results for the profiles we have conjectured possibly exact results about the relaxation time, as discussed below.

The relaxation time $\tau(h, h_0)$ is divergent at two points: (i) at the stationary point, $h = h_0$, where $\tau(h, h_0) \sim (h - h_0)^{-2}$ and (ii) for small h, where $\tau(h, h_0) \sim h^{-1}$, which can be derived perturbatively. For $h_0 = 0$ the two singularities merge at $h = 0$: $\tau(h, h_0 = 0) \sim h^{-3}$.

To obtain information about $\tau(h, h_0)$ away from the singularities we consider a quench from the fully ordered initial state ($h_0 = 0$) first. A quench into the disordered phase ($h \geq 1$) yield to high numerical accuracy $\tau(h \geq 1, h_0 = 0) = \pi/2$, i.e., independent of h. For a quench into the ordered phase ($h \leq 1$) we introduce $\tilde{\tau}(h, h_0 = 0) = h^3\tau(h, h_0 = 0)$ to get rid of the singularity at $h = 0$. In the limit $h \to 0$ we obtain $\tilde{\tau}(h = 0, h_0 = 0) = 3\pi/2$, and for $h > 0$ we consider the ratio: $y^\tau(h) = \Delta\tilde{\tau}(h)/\Delta\tilde{\tau}(0)$ with $\Delta\tilde{\tau}(h) = \tilde{\tau}(h) - \tilde{\tau}(1)$ and compare it with a similar expression for the correlation length $y^\xi(h) = \Delta\tilde{\xi}(h)/\Delta\tilde{\xi}(0)$ with $\Delta\tilde{\xi}(h) = \tilde{\xi}(h) - \tilde{\xi}(1)$, where

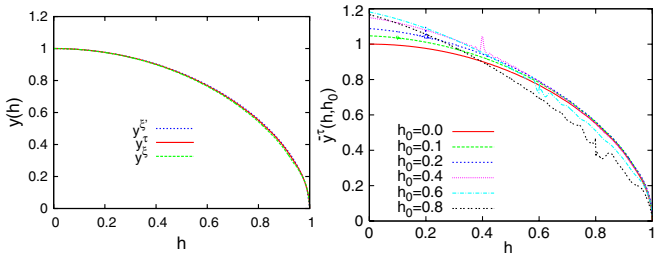

FIG. 3 (color online). Left: The ratios $y^{\xi} = \Delta\tilde{\xi}(h)/\Delta\tilde{\xi}(0)$ and $y^{\tau} = \Delta\tilde{\tau}(h)/\Delta\tilde{\tau}(0)$ for a quench from $h_0 = 0$ as a function of h. The curve $y^{\xi'}$ derives from the exactly known form for $\xi(h)$;see text. Right: The ratios $\bar{y}^{\tau}(h, h_0) = \Delta\tilde{\tau}(h, h_0)/\Delta\tilde{\tau}(0, 0) = \tau(h, h_0)$ $h(h - h_0)^2/\pi - (1 - h_0)^2/2$ for various h_0 as a function of h.

$\tilde{\xi}(h) = \xi(h)h^2$. The two ratios $y^{\tau}(h)$ and $y^{\xi}(h)$, as shown in Fig. 3(a), are almost indistinguishable. Since $\xi(h) = -1/\log((1 + \sqrt{1 - h^2})/2)$ is known exactly [7], the relaxation time for a quench from an ordered initial state ($h_0 = 0$) can therefore be estimated very accurately, if not exactly, by the relation $y^{\tau}(h) = y^{\xi}(h)$.

Starting from a partially ordered initial state ($0 < h_0 < 1$) we define $\tilde{\tau}(h, h_0) = h(h - h_0)^2\tau(h, h_0)$ and find to high numerical accuracy that the limiting value at $h = 1$ is given by: $\tilde{\tau}(h = 1, h_0) = \pi(1 - h_0)/2$. Away from $h = 1$ we study the ratio $\bar{y}^{\tau}(h, h_0) = \Delta\tilde{\tau}(h, h_0)/\Delta\tilde{\tau}(0, 0)$ with $\Delta\tilde{\tau}(h, h_0) = \tilde{\tau}(h, h_0) - \tilde{\tau}(1, h_0)$ which is identical to $y^{\tau}(h)$ for $h_0 = 0$ and which is plotted in Fig. 3(b) for different values of h_0. The curves for all values of h_0 are quite close to each other, and at $h = 1$ they all have a singularity, $\sim\sqrt{1 - h}$. Therefore one obtains a very good estimate for the relaxation time from $\tilde{\tau}(h, h_0)$ by $\bar{y}^{\tau}(h, h_0) \approx y^{\tau}(h) = y^{\xi'}(h)$, which is given in an analytical form (see above).

The thermal-like stationary state can be characterized by an effective temperature T_{eff} [16] which is defined through the condition, that the relaxation time in the stationary state after a quench, $\tau(h, h_0)$, and the equilibrium correlation time at temperature $T = T_{\text{eff}}$, $\tau_T(h, T)$, are identical. Using the analytic result at the critical point [23]: $\tau_T(h = 1, T) = 8/(\pi T)$ we arrive at $T_{\text{eff}}(h_0, h = 1) = 16(1 - h_0)/\pi^2$, which is compatible with the numerical data in Ref. [16]. In the ferromagnetic phase, $h < 1$, and in the limit $T \ll \Delta(h)$, $\Delta(h)$ being the gap, the relaxation time is given by [22]: $\tau_T(h < 1, T) \approx (2/(\pi T))e^{\Delta/T}$, which for $|h - h_0| \ll 1$ leads to: $T_{\text{eff}} \approx -\Delta(h)/(2\ln|h - h_0|)$.

To summarize we have identified different regimes in the nonequilibrium relaxation of the magnetization profiles of the quantum Ising chain with boundaries, which can be explained in terms of quasiparticles that are reflected at the surfaces. For sites at or near the surface nonthermal behavior is observed, manifested by a power-law relaxation form. For bulk sites a crossover to thermal behavior is found, with exponentially decaying correlations, defining a relaxation time and a correlation length that is identical in semi-infinite and in infinite systems and which obey presumably exact relations conjectured on the basis of the numerical data. In a finite system an exponentially fast reconstruction of the local magnetization is observed, involving a time-scale, τ', and characterizing an approximately periodic dynamics.

Several results for observables displaying thermal behavior in the bulk are expected to be valid also in other, even nonintegrable spin chains: Absence of thermalization at the boundaries, identity of correlation time and length in infinite and semi-infinite systems and an exponentially fast reconstruction in finite systems.

This work has been supported by the Hungarian National Research Fund under Grants No. OTKA K62588, No. K75324, and No. K77629 and by a German-Hungarian exchange program (DFG-MTA).

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