Quantum relaxation after a quench in systems with boundaries

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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 quasi-stationary regime, which is followed by an exponentially fast reconstruction period. The non-thermal behavior observed at near-surface sites turns over to thermal behavior for bulk sites. Besides the standard time- and length-scales a non-standard time-scale is identified in the reconstruction period.

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 non-integrable 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 non-local 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 non-stationary, that means not time-translationally invariant, quantum relaxation following a quench: Preparing the quantum system in a non-eigenstate of its Hamiltonian, how is thermalization achieved during the time-evolution? How do correlations develop in time towards the stationary (i.e. time translationally 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 non-equilibrium 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 paper we will address these two issues: The non-stationary 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 paper 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 ($t \geq$

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

0). The Hamiltonian in Eq.(1) can be expressed in terms of free fermions[19], which is used in studies of its non-equilibrium properties[6, 16]. Very recently it has been shown[17] that the bulk transverse magnetization, σ_l^z, which is a local operator, has non-thermal behavior, whereas the bulk (longitudinal) magnetization, σ_l^x, which is a non-local operator, has effective thermal behavior. Here we concentrate on the latter quantity and study the time-dependence of its profile, namely the local spontaneous magnetization $m_l(t) = \lim_{b\to 0_+} {}_b\langle\Psi_0^{(0)}|\sigma_l^x(t)|\Psi_1^{(0)}\rangle_b$, where $|\Psi_0^{(0)}\rangle_b$ is the ground state of the initial Hamiltonian (1) in the presence of an external field b coupling to the total magnetization. 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] in which $m_l(t)$ is expressed in terms of a Pfaffian, which is evaluated as the square-root of the determinant of a $2l \times 2l$ antisymmetric matrix. For the surface site, $l = 1$, most of the calculations have been performed analytically, 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. Due to left-right symmetry we restricted ourselves to $l \leq L/2$. The results depend primarily on whether the system before and after the quench is in the ordered (**O**) or in the disordered (**D**) phase, see Fig.1 for different combinations of **O** and **D**. By means of these figures one can identify different time regimes, which can be interpreted in terms of quasi-particles, which are emitted at $t = 0$ at the two free surfaces and which travel with a constant speed, $v = v(h, h_0)$. They reach the reference point after

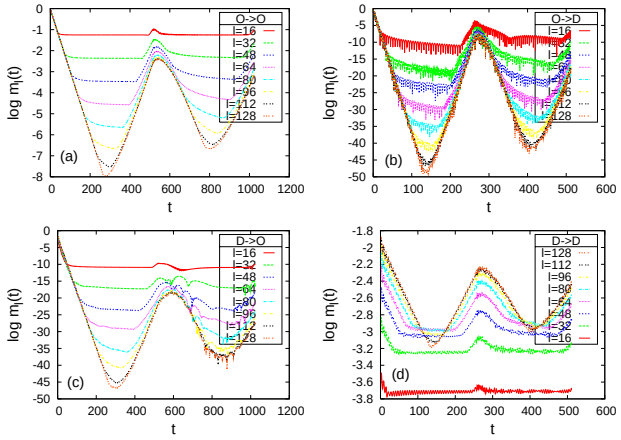

FIG. 1: (Color online) Relaxation of the local magnetization, $\log m_l(t)$, at different positions in a $L = 256$ chain after a quench with parameters: a) $h_0 = 0.0$ and $h = 0.5$ (**O** $\to$ **O**) b) $h_0 = 0.5$ and $h = 1.5$ (**O** $\to$ **D**) c) $h_0 = 1.5$ and $h = 0.5$ (**D** $\to$ **O**)d)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

time $t_l = l/v$ and $T - t_l$, respectively, and will cause interference afterwards. At time $T = L/v$ the two type of quasi-particles will be reflected and exchange their starting positions, leading to an approximate periodicity in the time-dependence. In the following we analyze the different regimes of the relaxation.

In the free relaxation regime: $t < t_l$ the surface emitted quasi-particles do not influence the behavior of the profile, which is position independent. The dominant decay of the magnetization is exponential:

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

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 quasi-stationary regime: $t_l < t < T - t_l$ there is an interference with one class of quasi-particles, which are emitted at the nearby surface and the relaxation in time is comparatively slow. This is illustrated in Fig.2 in which the magnetization profiles are shown at fixed times, $t < T/2$, for the same quenches as in Fig.1. For sufficiently large l the quasi-stationary magnetization has an exponential dependence, such that comparing its value at two sites, l_1 and l_2, we have

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

to which oscillating prefactors appear in the different domains of the quenches.

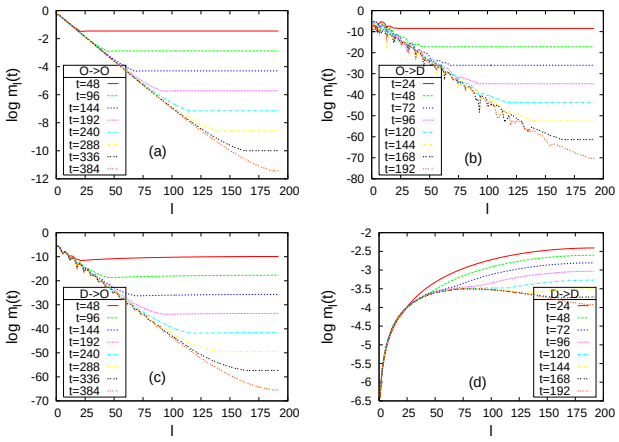

FIG. 2: (Color online) Nonequilibrium magnetization profiles, $\log m_l(t)$, at different times after a quench with parameters given in Fig.1 for $L = 384$. From the asymptotic values of the slopes one can measure the correlation length.

TABLE II: Correction to the quasi-stationary behavior for the surface magnetization in different domains of the quench.

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

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

$$\overline{m}_1 = \frac{(1-h^2)(1-h_0^2)^{1/2}}{1-hh_0}, \quad h_0, h < 1\,, \qquad (5)$$

and zero otherwise. Note that the nonequilibrium surface magnetization has different type of singularities for $h \to 1^-$ ($h_0 < 1$) and for $h_0 \to 1^-$ ($h < 1$) and that Eq.(5) involves the equilibrium result for $h = h_0$. We have analyzed the correction term, $\Delta(t, L) = m_1(t) - \overline{m}_1$, and its asymptotic behavior is summarized in Table II in the different domains of h and h_0. As a general observation these corrections are in power-law form, which signals that the relaxation of the surface magnetization has non-thermal behavior.

For $l > 1$ we observe that $\overline{m}_l$ is monotonously decreasing with l and thus $\overline{m}_l > 0$ for $h_0, h < 1$ and zero otherwise. The correction terms are identical to Table II so that a finite distance, l, the local magnetization has non-thermal behavior.

In the reconstruction regime: $T - t_l < t < T$ both classes of emitted quasi-particles contribute to the interference and the local magnetization has an increase which is exponentially fast in time:

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

In this period the magnetization is practically independent of the position. The rate of growth, $\tau'(h, h_0)$ depends on the conditions of the quench and it is found to be approximately proportional with $\tau(h, h_0)$. Their ratio is measured as $\tau/\tau' = 0.883 \pm 0.002$. It turned out to be useful to measure the cross-over time, $\tilde{t} = T/2$, which is defined as the crossing point of the two asymptotic regimes: $\overline{A}\exp(-\tilde{t}/\tau) = \overline{B}\exp(\tilde{t}/\tau')$, where $\overline{A}$ and $\overline{B}$ are averaged prefactors. During the cross-over time the quasi-particles 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 the two types of quasi-particles being reflected at he boundary reach sites repeatedly.

The time- and length scale, as defined in Eq.(3) and Eq.(4), respectively, as well as the characteristic quasi-particle 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 $\tau(h, h_0) \sim h^{-1}$. For $h_0 = 0$ the two singularities merge at $h = 0$: $\tau(h, h_0 = 0) \sim h^{-3}$. These results can be derived perturbatively.

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 $\tilde{\xi}(h) = \xi(h)h^2$. The two ratios $y^\tau(h)$ and $y^\xi(h)$, as shown in Fig.3a, 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 ($0 < h_0 <$

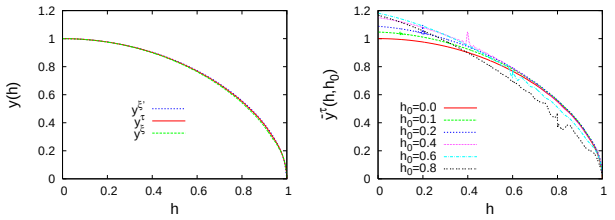

FIG. 3: (Color online) **Left:** The ratios $y^{\xi} = \Delta\tilde{\xi}(h)/\Delta\tilde{\xi}(0)$ and $y^{\tau} = \Delta\tilde{\tau}(h)/\Delta\tilde{\tau}(0)$ for a quench from $h_0 = 0$ as a function of h. The curve $y^{\xi'}$ derives from the exactly known form for $\xi(h)$, see text. **Right:** The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

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 $\overline{y}^{\tau}(h, h_0) = \Delta\tilde{\tau}(h, h_0)/\Delta\tilde{\tau}(0, 0)$ 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.3b 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 $\overline{y}^{\tau}(h, h_0) \approx y^{\tau}(h) = y^{\xi'}(h)$, 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 $T = T_{eff}$, $\tau_T(h, T)$, are identical. Using the analytic result at the critical point[22]: $\tau_T(h = 1, T) = 8/(\pi T)$ we arrive at $T_{eff}(h_0, h = 1) = 16(1 - h_0)/\pi^2$, 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 [23]: $\tau_T(h < 1, T) \approx (2/(\pi T))e^{\Delta/T}$, which for $|h - h_0| \ll 1$ leads to: $T_{eff} \approx -\Delta(h)/(2 \ln |h - h_0|)$.

To summarize we have identified different regimes in the non-equilibrium relaxation of the magnetization profiles of the quantum Ising chain with boundaries, which can be explained in terms of quasi-particles, being emitted at the surfaces during the quench. For sites at or near the surface non-thermal behavior is observed, manifested by a power-low relaxation form. For bulk sites a cross-over to thermal behavior is found, with exponentially decaying correlations, defining a relaxation time and a correlation length, which turn out to be identical in semi-infinite and in infinite systems and which obey presumably exact relations conjectured on the basis of the numerical data. Moreover, in a finite system an exponentially fast reconstruction of the local magnetization is observed, which involves a time-scale, τ' characterizing an approximately periodic dynamics.

Several results concerning observables that display thermal behavior in the bulk are expected to be valid also in other, even non-integrable spin chains: Absence of thermalization at the boundaries, identity of correlation time and length in infinite and semi-infinite systems and the presence of exponentially fast reconstruction in finite systems.

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