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Quantum relaxation and finite-size effects in the XY chain in a transverse field after global quenches

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Abstract – We consider global quenches in the quantum XY chain in a transverse field and study the nonequilibrium relaxation of the magnetization and the correlation function as well as the entanglement entropy in finite systems. For quenches in the ordered phase the exact results are well described by a semiclassical theory (SCT) in terms of ballistically moving quasi-particle pairs. For finite systems quasi-periodic behaviour of the dynamical evolution of the local order parameter and the correlation functions is predicted correctly including the period length, an exponential relaxation, a quasi-stationary regime and an exponential recurrence in one period. In the thermodynamic limit the SCT is exact for the entanglement entropy and its modified version following the method of Calabrese P. *et al.*, *J. Stat. Mech.* (2012) P07016, is exact for the magnetization and the correlation function, too. The stationary correlation function is shown to be described by a generalized Gibbs ensemble.

Introduction. – Recent progress of experimental work on ultracold atomic gases in optical lattices [1–10] allowed to study the unitary time evolution of quantum systems in a nonequilibrium situation, *i.e.*, after a so-called global quench. This is usually achieved by a sudden change of the parameters of the quantum system within a time scale that is much shorter than the characteristic time the system needs to relax into a stationary state. The basic questions in this context are i) the dynamical characteristics of the relaxation process and ii) the possible existence of a stationary state after long times. In three-dimensional systems fast relaxation into a thermal stationary state has been observed. In contrast to this, in quasi–one-dimensional systems the relaxation process has been found to be much slower and to lead to an unusual nonthermal stationary state [6]. This result has stimulated intensive theoretical work [11–31] to clarify the effect of integrability of the system on the relaxation process as well as on the nature of the stationary state. It is commonly expected that observables of nonintegrable systems effectively thermalize, which means that their stationary state is described by a thermal Gibbs ensemble. Numerical studies of different nonintegrable systems are in favour of this expectation [12–21]; however, some contradictory results indicate that the issue could be more complicated [22–24,30]. On the other hand, in integrable systems, due to the existence of integrals of motion, the stationary state is expected to be represented by a generalized Gibbs ensemble (GGE) [12], in which each mode corresponding to a conserved quantity is characterized by its own effective temperature. Results on integrable systems are mainly collected on free-fermion models, such as on the transverse Ising chain, for which several analytical and numerical results have been recently obtained [32–45]. Qualitative features of the relaxation process can be explained with a quasi-particle (QP) picture [13,46]: The quench changes the total energy of the system by an extensive amount, which creates QPs homogeneously in space, moving ballistically with a constant velocity. Due to the conservation of momentum, the QPs are created in pairs with opposite

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velocity and these QP pairs are quantum entangled. This QP picture has been used to explain the time evolution of the entanglement entropy [35,47] and has been made quantitative with a semiclassical (SC) theory to predict also the relaxation of the local magnetization and correlation function [39,41,48]. The basic idea of this SC theory is, that the QPs can be identified with kinks or domain walls in the spin chain that are created through the quench and then move uniformly via the action of the σ^z operator in the transverse field term on states in the σ^x representation. A priori there is no reason to expect a similar mechanism to be at work when the Ising symmetry is missing, as, for instance, in the XY model, in particular when the transverse field is absent. In this letter we will show that a quantitative description of the relaxation process with uniformly moving kink pairs is also applicable for finite and infinite XY chains. The main reason is that the $\sigma^y\sigma^y$ operator in the XY model has a similar effect on states in the σ^x representation as the σ^z operator in the TIC, namely creation and translation of kinks, in this case not by 1 but by 2 lattice spacings.

Therefore, we study in this letter the XY chain in a transverse field (denoted simply as XY chain). This model is integrable and has been studied in detail both in equilibrium [32,49] and out of equilibrium [32,35] after a global quench. Here we consider large finite chains and calculate the time dependence of the entanglement entropy, the local magnetization and the equal-time correlation function by free-fermion techniques [32,49]. These results are then compared with the prediction of our SC theory. We show that in the thermodynamic limit the SC theory provides exact results for the entanglement entropy. For the magnetization and for the equal-time correlation function the SC theory can be modified along the lines of ref. [41], so that it will become asymptotically exact [42,44], too.

Model and the free-fermion representation. – The XY chain is defined by the Hamiltonian

$$\mathcal{H} = -\frac{1}{2}\sum_l \left[\frac{1+\gamma}{2}\sigma_l^x\sigma_{l+1}^x + \frac{1-\gamma}{2}\sigma_l^y\sigma_{l+1}^y\right] - \frac{h}{2}\sum_l \sigma_l^z \quad (1)$$

in terms of the Pauli spin operators $\sigma_l^{x,y,z}$ at site l. Generally, we consider large open chains of length L. The parameters $0 \leqslant \gamma \leqslant 1$ and $h \geqslant 0$ denote the strength of the anisotropy and the transverse field, respectively. The special case $\gamma = 1$ represents the transverse Ising model, and for $h = 0$, $\gamma = 0$ the Hamiltonian reduces to the XX chain (see the equilibrium phase diagram in fig. 1).

We consider global quenches (at zero temperature), which suddenly change the parameters of the Hamiltonian from γ_0, h_0 for $t < 0$ to γ, h for $t > 0$. For $t < 0$ the system is assumed to be in equilibrium, *i.e.*, in the ground state of the Hamiltonian $\mathcal{H}$ with parameters γ_0 and h_0, which is denoted by $|\Phi_0\rangle$. After the quench, for $t > 0$, the state evolves coherently according to the new Hamiltonian as $|\Phi_0(t)\rangle = \exp(-\imath\mathcal{H}t)\,|\Phi_0\rangle$. Correspondingly the time evolution of an operator in the Heisenberg picture is $\sigma_l(t) = \exp(\imath\mathcal{H}t)\,\sigma_l\exp(-\imath\mathcal{H}t)$.

We calculate the equal-time correlation function $C_t^{xx}(l_1,l_2) = \langle\Phi_0\,|\sigma_{l_1}^x(t)\sigma_{l_2}^x(t)|\,\Phi_0\rangle$, which for large separations is given by $C_t^{xx}(l_1,l_2) = m_{l_1}(t)\,m_{l_2}(t)$, where $m_l(t)$ is the local magnetization. In the initial state in the thermodynamic limit one has $m_l(0) > 0$ ($m_l(0) = \mathcal{O}(1/L)$) for $h_0 < 1$ ($h_0 > 1$) and at $h_0 = 1$ there is a quantum critical line, which belongs to the (transverse) Ising universality class [50] for $\gamma > 0$, *i.e.*, $m_l(0) \sim L^{-1/8}$.

Using standard techniques [49], the Hamiltonian in eq. (1) is expressed in terms of fermion creation and annihilation operators $\eta_p^\dagger$ and η_p as

$$\mathcal{H} = \sum_p \varepsilon(p)\left(\eta_p^\dagger\eta_p - \frac{1}{2}\right), \quad (2)$$

where the sum runs over L quasi-momenta and the p values are determined by the boundary condition: $0 < p < \pi$ ($-\pi < p < \pi$) for free (periodic) chains. The energy of the modes is given by

$$\varepsilon(p) = \sqrt{\gamma^2\sin^2 p + (\cos p - h)^2} \quad (3)$$

and the Bogoliubov angle Θ_p diagonalizing the Hamiltonian is given by $\tan\Theta_p = \gamma\sin p/(\cos p - h)$. The correlation function is written as a Pfaffian, which is then evaluated through the determinant of an antisymmetric matrix. The local magnetization is calculated in the form of the off-diagonal matrix element [50] $m_l(t) = \langle\Phi_0\,|\sigma_l^x|\,\Phi_1\rangle$, where $|\Phi_1\rangle$ is the first excited state of the initial Hamiltonian.

The entanglement entropy between a block of l contiguous spins and the rest of the system is defined as $\mathcal{S}_l = \mathrm{Tr}_{i\leqslant l}[\rho_l\log\rho_l]$, where $\rho_l = \mathrm{Tr}_{i>l}|\Phi_0\rangle\langle\Phi_0|$ is the reduced density matrix, which evolves in time as $\rho_l(t) = \exp(\imath\mathcal{H}t)\rho_l\exp(-\imath\mathcal{H}t)$ For free-fermion models see the calculation in ref. [51].

The semiclassical theory. – As mentioned in the introduction, QPs are created after the quench at $t = 0$. For the XY chain these QPs are the free fermions described above. The wave packets formed by the free fermions move ballistically with a constant velocity $\pm v_p$, which is obtained in the SC theory as

$$v_p = \frac{\partial\varepsilon(p)}{\partial p} = \frac{\sin p\left[h - \left(1-\gamma^2\right)\cos p\right]}{\varepsilon(p)}. \quad (4)$$

The position of the QP pairs at times $t > 0$ can be easily calculated from their creation position and their velocity; in finite open chains the QPs are reflected at the boundaries.

We also need the creation probability $f_p = f_p(h_0,\gamma_0;h,\gamma)$ of the QP pair. Here we make use of the fact that in a homogeneous system the QPs are created uniformly in space and that f_p corresponds to the occupation probability of mode p in the initial state $|\Phi_0\rangle$, thus $f_p = \langle \Phi_0 | \eta_p^\dagger \eta_p | \Phi_0 \rangle$. For the XY model it is expressed through the difference $\Delta_p = \Theta_p - \Theta_p^0$ of the Bogoliubov angles as $f_p = \frac{1}{2}(1 - \cos\Delta_p)$ with

$$\cos\Delta_p = \frac{(\cos p - h_0)(\cos p - h) + \gamma\gamma_0 \sin^2 p}{\varepsilon(p)\,\varepsilon_0(p)}, \qquad (5)$$

where the index 0 refers to quantities before the quench. We note that in open chains f_p has a small position dependence near the boundaries, which to leading order can be neglected for long chains.

Each pair of entangled QPs (and only those) with one partner moving within the block and simultaneously the other in the rest of the system, contributes an amount given by the binary entropy $s_p = -(1-f_p)\ln(1-f_p) - f_p \ln f_p$ to the entanglement entropy. Summing up the contributions of all QP pairs, one obtains the value of the entanglement entropy at the given time.

In the σ^x representation the QPs represent kink-like excitations. As described first for thermal excitations in ref. [52] and generalized afterwards for quantum quenches in ref. [41], a QP passing site l changes the sign of the local magnetization operator σ_l^x. If in a finite system the same QP visits l several times, σ_l^x changes sign only if the number of visits is odd. Summing up the contributions of all QPs which have passed l before t, one obtains the local magnetization [41]

$$m_l(t) = m_l(0) \cdot \exp\left(-\frac{2}{\pi}\int_0^\pi \mathrm{d}p\, f_p(h_0,h)\, q_p(t,l)\right), \qquad (6)$$

where for $l \leqslant L/2$ and $t \leqslant T_p = L/v_p$,

$$q_p(t,l) = \begin{cases} v_p t, & \text{for } t \leqslant l/v_p, \\ l, & \text{for } l/v_p < t \leqslant (L-l)/v_p, \\ 1 - v_p t, & \text{for } (L-l)/v_p < t \leqslant T_p. \end{cases} \qquad (7)$$

For $t > T_p = L/v_p$ q_p is periodic: $q_p(t + nT_p, l) = q_p(t,l)$. Similarly the correlation function can be calculated [41]. For quenches deep in the ferromagnetic phase an excellent agreement between the SC theory and the exact results is obtained. For quenches close to the critical point the agreement is less good since here the kinks are not sharply localized and the domain walls have a finite extent of the order of the equilibrium correlation length. In the thermodynamic limit this effect can be taken into account by using an effective occupation probability [41]

$$f_p \to \tilde{f}_p = -\frac{1}{2}\ln|\cos\Delta_p| \;. \qquad (8)$$

Since $\cos\Delta_p = 1 - 2f_p$, one has $\tilde{f}_p = f_p + \mathcal{O}(f_p^2)$, implying $\tilde{f}_p = f_p$ for small QP density to first order. For large QP density, *i.e.*, for large quenches, the replacement (8) represents a phenomenological improvement of the SC theory and follows from an asymptotically exact evaluation of the correlation function by Calabrese, Essler and Fagotti for the transverse Ising chain [42,44]. As a matter of fact this evaluation works analogously for other free-fermion models, such as for the XY chain. In the following we use this modified SC theory also for finite chains in order to calculate the time evolution of the magnetization and the correlation function.

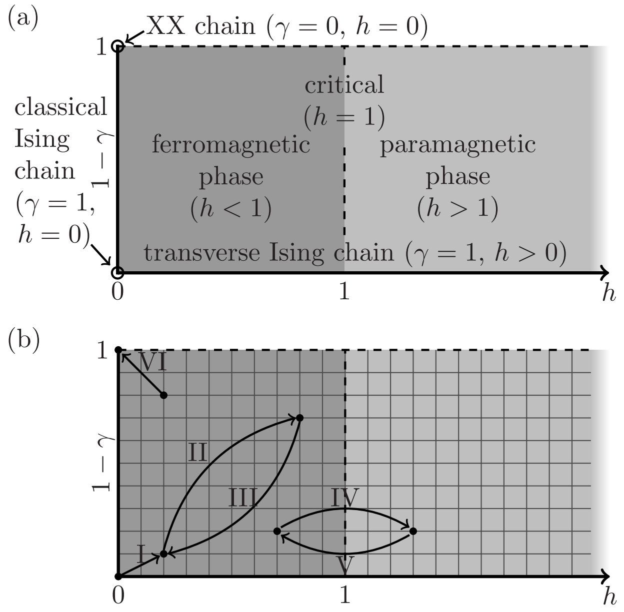

Fig. 1: (a) Equilibrium phase diagram of the XY model at $T = 0$, restricted to the anisotropy range $\gamma \in [0,1]$. For $h < 1$, $\gamma > 0$ the system is ferromagnetic (FM) indicated by a nonvanishing magnetization $m = \langle\sigma^x\rangle > 0$ in the limit $L \to \infty$, for $h > 1$ the system is paramagnetic ($m = 0$, PM). The transition at $h = 1$ between the FM and PM phase is of 2nd order and in the universality class of the transverse Ising model (TIM) ($\gamma = 0$). The point ($\gamma = 1$, $h = 0$) represents the classical Ising model, the point ($\gamma = 0$, $h = 0$) is the XX chain, and the critical point at $\gamma = 0$, $h = 1$ is in a universality class different from the TIM. (b) Sketch of the different quenches ($h_0, \gamma_0 \to h, \gamma$) considered in this letter.

Results. – We have performed quenches with six different pairs of parameters $(h_0, \gamma_0) \to (h, \gamma)$ as indicated in the phase diagram in fig. 1. Besides the relatively small quench in the ordered phase (I) we have performed larger quenches in the ordered phase (II and III) as well as quenches between the ordered and the disordered phase (IV and V) and a quench to the XX model (VI).

Entanglement entropy. The dynamical entanglement entropy calculated by the free-fermionic method for a finite chain of length $L = 256$ and for various sizes of the block, l, are shown in fig. 2 together with the predictions of the SC theory. We observe an excellent agreement for short times before the first maximum, where the first QP that have undergone a reflection at a boundary reach the middle of the chain. Small deviations are caused by these reflections and accumulate in the subsequent periods. In the SC calculation one should analyse the trajectory of the QP pairs which for free boundary conditions is summarized as follows. If the QP pair is created at site j, then for $t < T_p = L/v_p$ the pair contributes to the entropy within the interval $t_{p,1} < t < t_{p,2}$ with $t_{p,1} = |l - j|/v_p$ and

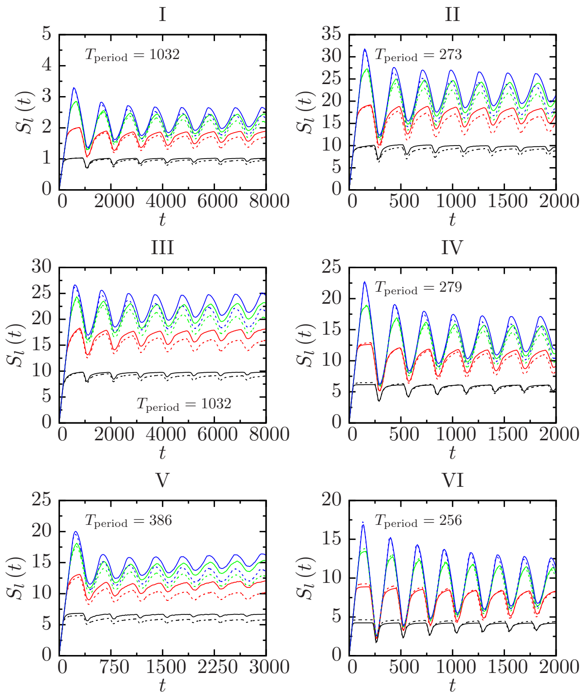

Fig. 2: (Colour on-line) Time evolution of the entanglement entropy of the block of the first l sites of the chain with free boundary conditions after the six quench protocols in fig. 1. Free-fermion (SC theory) results are indicated by full (broken) lines ($-: l=32$; $-: l=64$; $-: l=96$; $-: l=128$).

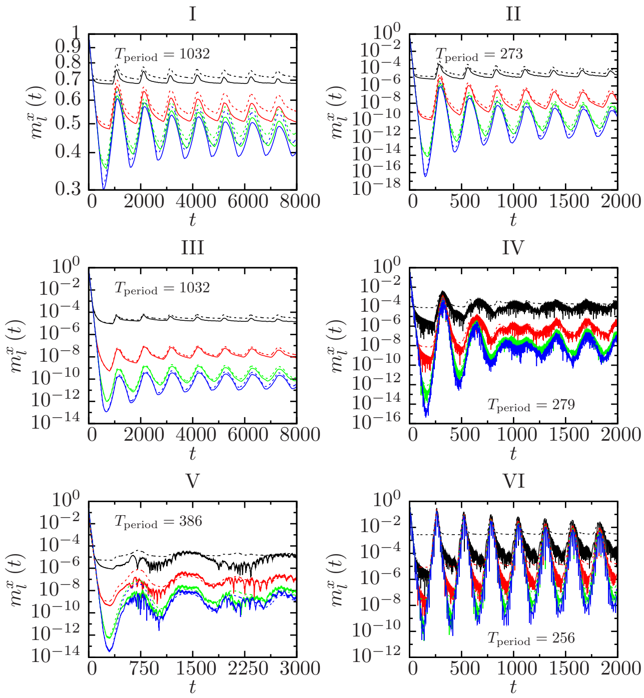

Fig. 3: (Colour on-line) Time evolution of the local magnetization $m_l(t)$ after the six quench protocols in fig. 1. Free-fermion (SC theory) results are indicated by full (broken) lines ($-: l=32$; $-: l=64$; $-: l=96$; $-: l=128$). Note that the y-axis is logarithmic such that straight curve segments represent either exponential relaxation (negative slope) or exponential reconstruction (positive slope).

$t_{p,2}=\min\left[(l+j)/v_p,(2L-(l+j))/v_p\right]$. For $T_p<t<2T_p$ this effective interval is $t_{p,3}<t<t_{p,4}$ with $t_{p,3}=2T_p-t_{p,2}$ and $t_{p,4}=2T_p-t_{p,1}$. For $t>2T_p$ the process is repeated with a period of $2T_p$.

As seen in fig. 2, the time evolution of the entropy starts linearly, reaching a l-dependent maximum. Afterwards there is a linear decrease and the process is repeated quasi-periodically as for the transverse Ising chain [53] with a period $T_{\rm period}=L/v_{\max}$, where $v_{\max}$ is the maximum group velocity $\max_p\{v_p\}$. In the $L\to\infty$ and $l\gg 1$ limits the SC theory predicts

$$S_l(t)=\begin{cases} t\dfrac{1}{2\pi}\displaystyle\int_0^\pi \mathrm{d}p\, v_p s_p, & t<l/v_{\max},\\[2ex] l\dfrac{1}{2\pi}\displaystyle\int_0^\pi \mathrm{d}p\, s_p, & t\gg l/v_{\max}, \end{cases} \tag{9}$$

which corresponds to the exact results [35].

Local magnetization. The local magnetization $m_l(t)$ calculated by the free-fermion method for finite open chains of length $L=256$ and at various positions are shown in fig. 3 together with the predictions of the modified SC theory for the six different quench protocols. If the quench is performed between two parameter points within the ordered phase, the modified SC theory represents an excellent description of the relaxation process, in particular for short times ($t<T_{\rm period}/2$). If the quench involves the disordered phase as well or the XX point, the agreement is less good. The origin of the deviations here is the same as for the entanglement entropy discussed above. However, the qualitative features of the time evolution of the magnetization is similar in all cases in fig. 3: For finite systems the SC theory correctly predicts quasi-periodic behaviour including the periodic time $T_{\rm period}$, an exponential relaxation, a quasi-stationary regime and an exponential recurrence in one period. These features have also been previously found for the the transverse Ising chain [39,41].

In the limit $L\to\infty$ in the modified SC theory we have

$$m_l(t)=m_l(0)\exp\left(-t\frac{2}{\pi}\int_0^\pi \mathrm{d}p\, v_p\tilde f_p\theta(l-v_pt)\right.$$
$$\left.-l\frac{2}{\pi}\int_0^\pi \mathrm{d}p\,\tilde f_p\theta(v_pt-l)\right) \tag{10}$$

which defines the quench-dependent relaxation time $\tau_{\rm mag}$ and the correlation length $\xi_{\rm mag}$ as

$$\tau_{\rm mag}^{-1}=\frac{2}{\pi}\int_0^\pi \mathrm{d}p\, v_p\tilde f_p,\qquad \xi_{\rm mag}^{-1}=\frac{2}{\pi}\int_0^\pi \mathrm{d}p\,\tilde f_p. \tag{11}$$

Correlation function. The space dependence of the equal-time correlation function, $C_t^{xx}(r)=C^{xx}\left(\frac{L-r+1}{2},t;\frac{L+r+1}{2},t\right)$, $r=1,3,\ldots,L-1$ between two sites symmetrically located between the boundaries of the system calculated by the free-fermion method for $L=256$ and for various times is shown in fig. 4 together with the predictions of the modified SC theory

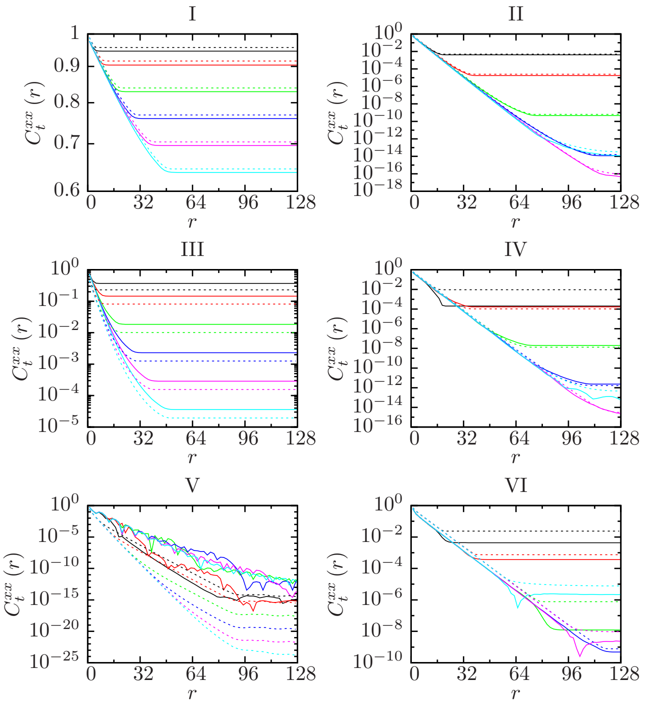

Fig. 4: (Colour on-line) Equal-time correlation function $C_t^{xx}(r)$ for fixed time t after the six quench protocols in fig. 1 as a function of the distance r. Free-fermion (SC theory) results are indicated by full (broken) lines (— : $t=10$; — : $t=20$; — : $t=40$; — : $t=60$; — : $t=80$; — : $t=100$).

for the same quenches as indicated in fig. 1. Also in this case, an excellent agreement is seen for short times before the stationary regime is observed. The agreement remains good for quenches between two parameter points in the FM phase. As for the magnetization, the agreement is less satisfactory if the quench involves also the disordered phase or the XX point. The origin of the deviations here is the same as for the entanglement entropy. In the $L\to\infty$ limit in the modified SC theory the correlation function is given by

$$C_t^{xx}(r) = C_0^{xx}(r)\exp\left(-t\frac{4}{\pi}\int_0^\pi \mathrm{d}p\, v_p\tilde{f}_p\theta(r-2v_pt) -l\frac{2}{\pi}\int_0^\pi \mathrm{d}p\,\tilde{f}_p\theta(2v_pt-r)\right), \tag{12}$$

which is analogous to the formula for the local magnetization in eq. (10). Note that the time τ_{corr} and the length scale ξ_{corr} of the correlation function is related to that of the magnetization as $\tau_{\mathrm{corr}}=\tau_{\mathrm{mag}}/2$ and $\xi_{\mathrm{corr}}=\xi_{\mathrm{mag}}$ as for the transverse Ising chain [41].

Discussion. – We have studied the nonequilibrium relaxation dynamics of the quantum XY chain after global quenches. In particular, we have considered the time evolution of the entanglement entropy as well as the relaxation of the magnetization and the equal-time correlation function in finite systems. The numerical results obtained with the free-fermion techniques were compared with the predictions of the SC theory. For the entanglement entropy an excellent agreement was found for all types of quenches and the SC results were shown to be exact in the $L\to\infty$ limit. For the magnetization and for the equal-time correlation function the SC theory provides a very good approximation if the quench is performed between two points deep within the ordered phase. For two points in the ordered phase closer to the critical line we showed that one can modify the SC theory by introducing an effective particle occupation number, see in eq. (8), which provides exact results in the thermodynamic limit. In a finite system new phenomena such as reconstruction of the magnetization and the correlation function occur, which is explained in terms of reflected QPs at the open boundaries of the chain or, for periodic boundary conditions, in terms of the recurrence of the QPs.

The XY chain after a sudden quench does not thermalize, since the QP occupation probability cannot be described by a Gibbs distribution, or, more concretely, there is no effective temperature T_{eff} depending on the quench parameters, for which $f_p\sim\exp(-\varepsilon_p/T_{\mathrm{eff}})$. Since all modes are conserved quantities, one rather expects that each mode has its own effective temperature $T_{\mathrm{eff}}(p)$, which can be identified as follows.

When one compares the correlation length $\xi_{\mathrm{corr}}=\xi_{\mathrm{mag}}$ in eq. (11) with the thermal correlation length ξ_T at a finite temperature T [32],

$$\xi_T^{-1} = -\frac{1}{\pi}\int_0^\pi \mathrm{d}p\,\ln\left|\tanh\frac{\varepsilon(p)}{2T}\right|, \tag{13}$$

one observes in both cases an average over all modes. One can formally obtain ξ_{corr} and ξ_{mag} from (13) by attributing a p-dependent effective temperature $T_{\mathrm{eff}}(p)$ to the contribution of the p-mode, *i.e.*, replacing the integrand in (13) by $\ln|\tanh(\varepsilon_p/2T_{\mathrm{eff}})|$. This then implies

$$\tilde{f}_p = -\frac{1}{2}\ln|1-2f_p| = -\frac{1}{2}\ln\left|\tanh\frac{\varepsilon(p)}{2T_{\mathrm{eff}}(p)}\right|, \tag{14}$$

which leads to the relation

$$\min(f_p,1-f_p) = \frac{1}{\exp\left(\frac{\varepsilon(p)}{T_{\mathrm{eff}}(p)}\right)+1}. \tag{15}$$

Here, on the right-hand side, there is the Fermi distribution function, thus the nonequilibrium occupation probability of the free-fermion mode f_p (or that of the corresponding hole: $1-f_p$) is equal to its equilibrium thermal occupation probability at $T_{\mathrm{eff}}(p)$. We note that the same relation holds for the transverse Ising chain [41] and it is expected to be valid for free-fermion models in general. This supports the conclusion that after a sudden quench the XY chain reaches a stationary state in which correlations are described by a generalized Gibbs ensemble.

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