Out of equilibrium process in Ising quantum chains

T Platini and D Karevski

Laboratoire de Physique des Matériaux, UMR CNRS No. 7556, Université Henri Poincaré
(Nancy 1), B.P. 239,
F-54506 Vandœuvre lès Nancy cedex, France
E-mail: platini@lpm.u-nancy.fr, karevski@lpm.u-nancy.fr

Abstract. In this paper we present the results obtained concerning the relaxation behaviour of a non equilibrium Ising quantum chain. In particular, we have focused our attention into the transverse magnetization. The out-of-equilibriumness is generated by setting up an initial thermal inhomogeneity. We present two different initial conditions: a completely factorized state, where all the spins are thermalized independently and second a system-bath case, where half of the chain called the system is thermalized at a temperature \( T_s \) and the remaining half is at a temperature \( T_b \). In both cases, the magnetization profiles are calculated either analytically or numerically and show a scaling behaviour. It is also found that in the two-temperature case the magnetization relaxes in quantized steps in the strong transverse field region.

1. Introduction

Non-equilibrium dynamical behaviour of quantum spin chains has been studied first at the end of the sixties [2, 3, 4] and a renewed interest appeared in the last decade. In particular, more recently, the attention was put on the relaxation properties of homogeneous or disordered free fermionic chains initially prepared in nonequilibrium states [5, 6, 7, 8, 9, 12, 13, 14]. In this paper, we present the results obtained for the relaxation of the transverse magnetization in an Ising quantum spin chain initially prepared in a canonical factorised state:

\[
\rho(0) = \prod_j \rho_j, \quad \rho_j = \frac{1}{Z_j} e^{-\beta_j \mathcal{H}_j}
\]

where the density matrix \( \rho_j \) is a canonical state associated to \( j \)th part of the chain which is thermalized at a given temperature \( \beta_j^{-1} \). It means that the initial chain is split into non-interacting pieces, such that \( \mathcal{H}_0 = \sum_j \mathcal{H}_j \), each in contact with a specific heat bath. After the preparation has been performed, the various baths are removed so that one has a closed system distributed according to \( \rho(0) \). At time \( t = 0 \), the interactions \( \mathcal{H}_{j,j+1} \) between the different parts are putted in. The dynamics of the chain is then controled by the total Hamiltonian \( \mathcal{H} = \mathcal{H}_0 + \sum_j \mathcal{H}_{j,j+1} \). The influence of the interface interactions is crucial since it will governed the relaxation of the chain toward a new state. In this study our attention is putted on the relaxation behaviour of that initial interfaces generated by the initial thermal inhomogeneity. In particular, we present the transverse magnetization profiles obtained on two different situations. The first one is the case where all the spins are thermalized independently, that is we have

1 To whom correspondence should be addressed.
initially an assembly of non-interacting spins each put in contact with a specific thermal bath. The second case considered is a situation where the chain is split into two parts, one at low temperature called the "system", the other at high temperature called the "bath". So, in the system-bath case, we concentrate on the front dynamics generated by the interface between the system and the bath parts [12, 6, 13].

2. Dynamics and expectation values
The Hamiltonian of the Ising quantum chain is given by

\[ \mathcal{H} = -\frac{1}{2} \sum_{k=1}^{L-1} \sigma_k^x \sigma_{k+1}^x - \frac{h}{2} \sum_{k=1}^{L} \sigma_k^z \]  

where the \( \sigma \)s are the Pauli matrices and where \( h \) is the transverse field pointing in the \( z \)-direction. As it is well known, this Hamiltonian can be fermionized thanks to the Jordan-Wigner mapping [16], for example in terms of Clifford algebra \( \Gamma_1^n = \sigma_x^n \prod_{j=1}^{n-1} (-\sigma_j^z) \) and \( \Gamma_2^n = -\sigma_y^n \prod_{j=1}^{n-1} (-\sigma_j^z) \), followed by a canonical transformation [17, 12]. The dynamics of the lattice operators is easily solved and leads for the lattice Clifford operators to

\[ \Gamma_j^n(t) = \sum_{k,i} \langle \Gamma_i^k | \Gamma_j^n(t) \rangle \Gamma_i^k \]  

where the time-dependent contractions \( \langle \Gamma_i^k | \Gamma_j^n(t) \rangle \) are explicitly known in terms of the chain parameters. See [15] for more details.

The initial state we consider here is of the factorized form \( \rho(0) = \prod_j \rho_j \) with

\[ \rho_j = \frac{1}{Z_j} \exp(-\beta_j \mathcal{H}_j) \]  

where \( \beta_j \) is the inverse temperature of the subsystem \( \mathcal{H}_j \) which is a part of the full Hamiltonian \( \mathcal{H} \). \( Z_j \) is the corresponding partition function. The expectation value of an observable \( \mathcal{O} \) at time \( t \) is given by

\[ \langle \mathcal{O} \rangle(t) = \text{Tr} \{ \mathcal{O}(t) \prod_j \rho_j \} \]  

where \( \mathcal{O}(t) \) is the operator associated to the observable \( \mathcal{O} \) in the Heisenberg picture. To evaluate the expectation value \( \langle \mathcal{O} \rangle(t) \), one first has to express the operator \( \mathcal{O}(t) \) in terms of the elementary time-independent \( \Gamma^n_k \) Clifford operators. Then, one will have to evaluate expressions of the form

\[ \frac{1}{\Pi_j Z_j} \text{Tr} \{ \Gamma_{i_1}^{k_1} \cdots \Gamma_{i_n}^{k_n} e^{-\beta_j \mathcal{H}_j} \} \]

which can be calculated explicitly noticing that the Hamiltonians \( \mathcal{H}_j \) and can be expressed in terms of the lattice operators \( \Gamma_k \).

3. Transverse magnetization profiles
The transverse magnetization is very simply expressed in terms of the Clifford operators, since it is a local quantity. One has in the Heisenberg picture

\[ \sigma^z_n(t) = -i \Gamma_n^z(t) \Gamma_n^z(t) . \]

After some algebra, one obtains [15]

\[ \langle \sigma^z_n \rangle(t) = \sum_{k,k'} P_{n,n}^{k,k'}(t)(I)_{k,k'} , \]
with the time-dependent element
\[ P_{k,n',n}^{k,k'}(t) = \langle \Gamma_k^1 | \Gamma_n^1(t) \rangle \langle \Gamma_{n'}^2 | \Gamma_k^2(t) \rangle - \langle \Gamma_k^1 | \Gamma_{n'}^2(t) \rangle \langle \Gamma_n^2 | \Gamma_k^1(t) \rangle, \]
and the initial matrix
\[ I = \begin{pmatrix} I_1 & 0 & \ldots & 0 \\ 0 & I_2 & \ldots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & I_K \end{pmatrix} \]
where \( I_j \) is the initial matrix of the \( j \)-subsystem with entries \( (I_j)^{kk'} = \text{Tr} \{ i \Gamma_j^1 \Gamma_j^2 \rho_j \} \) where the \( \Gamma_j \)'s are associated to the hamiltonian \( H_j \).

### 3.1. Completely factorized initial state

In the completely factorized initial state \( \rho(0) = \rho^L_0 \) where all the spins are thermalized independently with local Hamiltonian \( H_n = -\frac{h}{2} \sigma^z_n \), the initial matrix \( I \) is diagonal: \( I_{k,k'} = \delta_{k,k'} \langle \sigma^z_k \rangle \). In the thermodynamical limit \( L \to \infty \), the contractions \( \langle \Gamma_k^1 | \Gamma_n^2(t) \rangle \) depend only on the difference \( n-k \) so that the transverse magnetization is given by a discrete convolution product
\[ \langle \sigma^z_n \rangle(t) = \sum_k F_k(n-k) \langle \sigma^z_k \rangle(0), \]
where the Green function \( F_k(n-k) = P_{n,n'}^{k,k'} \). At the critical point, \( h = 1 \), the basic contractions are expressed in terms of Bessel functions and one can show that [12, 1]
\[ F_k(p) = J_{2p}^2(2t) - J_{2p+1}(2t) J_{2p-1}(2t). \]

In the continuum limit, one can show that the Green function \( F_k(p) = \frac{1}{\pi} f(\frac{p}{t}) \) with the scaling function [12]
\[ f(u) = \frac{1}{\pi} \sqrt{1-u^2}, \quad |u| \leq 1 \]
and zero otherwise, which solves explicitly the completely factorized case. It is interesting to notice that the time behaviour of the transverse magnetization in this case is basically the same as in the situation when the starting initial state is a pure state of the form \( |\Psi\rangle = |\ldots \sigma_k \sigma_{k+1} \ldots \rangle \) where \( \sigma_k \) is the value of the z-component spin at site \( k \) [9, 12].

### 3.2. Two-temperature state

We turn now to the more complex case of where half of the chain is thermalized at inverse temperature \( \beta_s \) and the rest at inverse temperature \( \beta_b \). The transverse magnetization is given by the general formula (8) with an initial value matrix \( I \) which has non-diagonal terms, taking into account that within the system part, the spins are interacting with each other and consequently have non-vanishing correlations, the same being true for the bath-part of the chain. In order to avoid boundary terms, we will take the thermodynamical limit where, both system and bath sizes are sent to infinity. In the extreme case where \( T_s = 0 \) and \( T_b = \infty \), we arrive at a further simplification since in the initial \( I \) matrix, the bath initial matrix is vanishing. In figure 1 we show the rescaled transverse magnetization profile obtained numerically by exact diagonalisation of the Hamiltonians \( H_s, H_b \) and \( H \) at the critical field \( h = 1 \). We have the very simple expression:
\[ \langle \sigma^z_n \rangle(t) = m^{\text{sys}}_{\text{bulk}} \left[ \frac{1}{2} + f\left( \frac{n}{t} \right) \right] \]
Figure 1. Scaling function of the transverse magnetization obtained for times $t = 30, 60, 90, 120$ on chains of total size $L = 200$ at the critical field $h = 1$. The initial state is a two-temperature state with $T_s = 0$ and $T_b = \infty$. The deviation from the flat profile on the left is due to boundary effects and can be completely overcome in the thermodynamical limit.

where $m^z_{\text{sys}} = 2/\pi$ is the initial bulk magnetization of the system and where the scaling function $f(u)$ is given by

$$f(u) = \begin{cases} 
\frac{1}{2} & u \leq -1 \\
-\frac{1}{2}u & -1 < u < 1 \\
-\frac{3}{2} & u \geq 1
\end{cases}$$

One may notice that since the excitations travel with velocity $c(h = 1) = 1$, one expects effects only in the causal region $-1 < \ell/t < 1$ where $\ell$ is the distance from the initial interface. Outside the causal region, both system and bath parts are still equilibrated and nothing is changed since they are at equilibrium. The remarkable linearity of the profile is lost as soon as we have a departure from infinite and vanishing temperature. For finite temperature cases, the profile is rounded. In the off-critical region, $h > 1$, the transverse magnetization profile, in the case $T_s = 0$ and $T_b = \infty$, shows a feature that was already remarked in the XX-chain [18] context. Indeed, as one can see on figure 2 the magnetization relaxes in quantized steps. That is, if one concentrates near the front entering into the bath part (which has a vanishing magnetization, since it is at infinite temperature), one finds a staircase like structure with constant area steps. If one defines

$$m(\ell, t) \equiv \langle \sigma^z_\ell \rangle(t) - \langle \sigma^z_{\text{bath}} \rangle,$$

as it is clearly shown in figure 2, the magnetization deviation from the bath magnetization $\langle \sigma^z_{\text{bath}} \rangle = 0$ has a scaling behaviour of the form

$$m(\ell, t) = t^{-1/3}g\left(\frac{\ell - t}{t^{1/3}}\right)$$

where again $\ell$ measures the distance from the initial interface, that is the interface between the system and the bath. Numerically, as seen from figure (2), it seems that the envelope of the scaling function $g$ is a simple square-root, so that we have the conjecture

$$m(\ell, t) = At^{-1/3} \sqrt{\frac{t - \ell}{t^{1/3}}} \quad \ell < t,$$
Figure 2. Scaling of the transverse magnetization deviation $m(\ell, t)$ obtained for times $t = 80, 120, 160, 200$ at transverse field $h = 10$. One can see easily the quantized steps near the front dynamics. The full line is a guide for the eyes.

where $A$ is a function of the field strength $h$.

The scaling form (17) implies that since the width of the steps increases as $t^{1/3}$ and their height decreases as $t^{-1/3}$, the area of the steps is indeed constant during time. Each step carries a definite magnetic moment $\mu(h)$ depending on the field strength $h$. As $h$ is increased toward infinity, the magnetic moment carried by each step reaches the value one (found numerically), which is reminiscent of the fact that in this case, an up spin from the system initial state $|\Psi\rangle = |\uparrow \uparrow \ldots \uparrow\rangle$ (see the Hamiltonian (2)) is injected into the bath and carried by one step. This simple particle-like picture does not apply at the critical field value $h = 1$, since in this case, the initial system state is a critical one with long range correlations. We have seen numerically that the quantized steps picture is not present in the case $h < 1$.

4. Discussion

We have investigated the front propagation and scaling profiles of transverse magnetization inhomogeneities in the Ising quantum chain. The inhomogeneities were generated initially by local equilibration with several thermal baths at different temperatures. We have concentrated our study on two distinct configurations: the first one being the completely factorized case where all the spins were thermalized independently. The second one being the interface problem, where half of the chain is at a given temperature, the other half at another temperature. In both cases, in the asymptotic time regime the transverse magnetization exhibits a scaling form $t^{-1}M(n/t)$, where the scaling function $M$ depends on the initial temperatures and on the transverse field value $h$. An interesting feature of such relaxation problem is the scaling behaviour of the front itself. In particular, we have shown that in the large field situation, $h > 1$, the front has a staircase structure with scaling $t^{-1/3}g((\ell - t)/t^{1/3})$, meaning that the area of each step is conserved which implies a quantized relaxation of the magnetization, as already found in the XX-chain in Ref. [18].
Acknowledgments
The organizers of the stimulating AGEING AND THE GLASS TRANSITION summer school are gratefully acknowledged.

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