Dynamic scaling of fronts in the quantum *XX* chain

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The dynamics of the transverse magnetization in the zero-temperature *XX* chain is studied with emphasis on fronts emerging from steplike initial magnetization profiles. The fronts move with fixed velocity and display a staircase like internal structure whose dynamic scaling is explored both analytically and numerically. The front region is found to spread with time subdiffusively with the height and the width of the staircase steps scaling as $t^{-1/3}$ and $t^{1/3}$, respectively. The areas under the steps are independent of time; thus the magnetization relaxes in quantized "steps" of spin flips.

I. INTRODUCTION

Fronts often emerge in relaxation processes. Simple examples are the domain walls generated in phase-separation dynamics [1] but there is a long list of fronts (also called shocks, active zones, reaction zones, etc.) resulting from unstable dynamics in various physical, chemical, and biological systems [2,3]. Furthermore, fronts can also emerge due to the initial spatial separation of stable and unstable states [4].

Apart from being the instruments of relaxation, the importance of fronts is also due to their "catalytic" nature; namely, structures are built in them [5] and patterns often emerge in the wake of moving fronts [6]. Thus it is not surprising that much effort has been devoted to the description of their spatiotemporal structure [2,4].

In contrast to fronts in classical systems, not much is known about quantum fronts. The examples we are aware of are restricted to quantum spin chains: fronts or shocks have been seen in the *XX* model [7–9], in the transverse Ising chain [10,11], as well as in the Heisenberg model [12,13]. The detailed structures of the front regions, however, have not been elucidated even in these cases.

Having in mind the importance of the front dynamics, we set out to investigate the fronts emerging in the quantum *XX* chain. The transverse magnetization in this model is conserved and its relaxation is known to be governed by fronts provided an initial state with a spatial separation of distinct magnetizations ($\pm m_0$) is prepared [8]. The problem with such initial conditions is exactly solvable and thus we can follow the evolution of the spatiotemporal structure of the front in detail.

The main result of our calculations is that, in addition to the known [8] global scaling (finite front velocity and well defined magnetization profile in the $t \rightarrow \infty$ limit), there exists a dynamic scaling regime in the front, and the associated scaling function exposes a staircase structure in the magnetization profile. An important feature of the steps in the staircase is that, while their height decreases as $t^{-1/3}$ and their width increases as $t^{1/3}$, the areas under the steps are time-independent constants and, furthermore, the constants are the same for all the steps. The value of the constant (twice the magnetic moment of a spin) indicates that a step carries a

reversed spin with respect to the aligned initial state. These reversed spins move with the front velocity, keep their identity with respect to other reversed spins, and their spatial spread is subdiffusive. Thus the magnetization relaxes in well defined quantized "steps" (in space and in time). It should be noted that our results suggest that the quantum fronts and, in particular, the steps carrying a unit of spin flips, may be envisioned as ingredients in controlled transport of bitwise information in magnetic nanostructures.

We begin our calculations by presenting the *XX* model and describing the known results about the large-time dynamics of the fronts emerging from a steplike initial magnetization profile (Sec. II). Next, in (Sec. III), a scaling limit is investigated which reveals the details of magnetization profile in the front region. The physical meaning of the staircase shape of the profile is discussed in (Sec. IV), followed by a list of related problems that remain to be solved (Sec. V).

II. FRONTS IN THE *XX* MODEL: DYNAMICS AND GLOBAL SCALING

The system we investigate is the *XX* chain defined by the Hamiltonian

$$\hat{H} = -\sum_{j=-N+1}^{N-1} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y), \tag{1}$$

where the spins S_j^α ($\alpha = x, y, z$) are 1/2 times the Pauli matrices situated at the sites $[j = 0, \pm 1, \ldots, \pm(N-1), N]$ of a one-dimensional lattice. Free boundary conditions are used, and the thermodynamic limit $N \rightarrow \infty$ is assumed throughout the paper. The physical quantities are measured in their natural units: energy in $J\hbar^2$ where J is the nearest-neighbor coupling, magnetization in $\hbar$, length in units of the lattice constant a, and time in $1/J\hbar$.

Our principal aim is to investigate the time evolution of the (globally conserved) transverse magnetization

$$m(n,t) = \langle \varphi | S_n^z(t) | \varphi \rangle \tag{2}$$

emerging from an initial state $|\varphi\rangle$ with a steplike magnetization profile
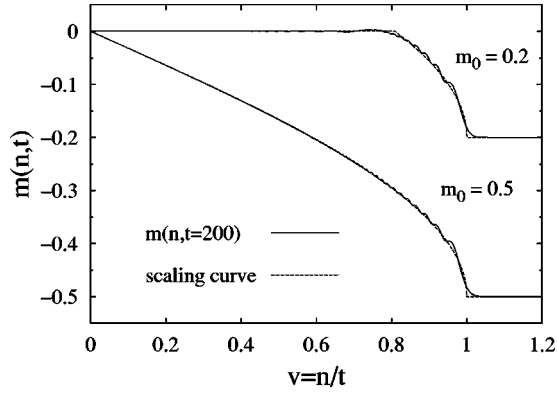
FIG. 1. Magnetization profiles emerging from steplike initial conditions [Eqs. (3) and (6)]. The large-time scaling limit is shown by dashed lines [Eq. (5) for $m_0=0.5$].

$$|\varphi\rangle = | \overset{-N+1}{\uparrow} \cdots \uparrow \overset{0}{\uparrow} \overset{1}{\downarrow} \downarrow \cdots \overset{N}{\downarrow}\rangle. \qquad (3)$$

Since the dynamics following from $\hat{H}$ can be described [14,15] in terms of local fermionic operators $(c_n, c_n^\dagger)$ whose Fourier transforms diagonalize $\hat{H}$, and since S_n^z can be expressed through the local fermionic operators as $S_n^z = c_n^\dagger c_n - 1/2$, the evaluation of $\langle\varphi|S_n^z(t)|\varphi\rangle$ is a relatively simple exercise. The calculations have been carried out in [8] with the result for $n \geq 1$ given through the Bessel functions of the first kind [16]

$$m(n,t) = -\frac{1}{2}J_0^2(t) - \sum_{l=1}^{n-1} J_l^2(t), \qquad (4)$$

while the expression for $n \leq 0$ is obtained from symmetry considerations $m(n,t) = -m(-n+1,t)$. The global scaling of $m(n,t)$ emerges in the $n \to +\infty$, $t \to +\infty$, and n/t=finite limit where $m(n,t)$ can be written in a scaling form $m(n,t) \to \Phi(n/t)$, and the scaling function $\Phi(v)$ is given [8] by
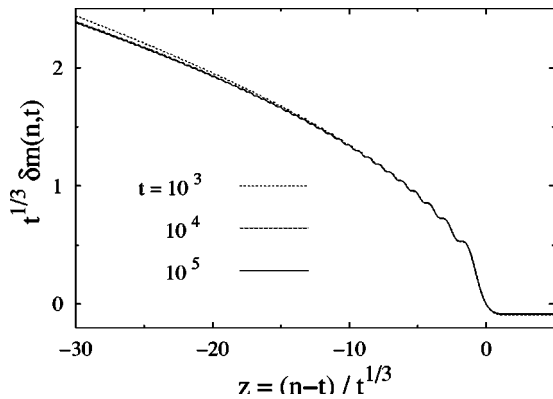

FIG. 2. Scaling in the front region. The magnetization measured from $m(t,t)$ is magnified as $t^{1/3}\delta m(n,t)$ while the distance from the front position is scaled as $z=(n-t)/t^{1/3}$. The analytically derived scaling limit [Eq. (11)] is indistinguishable from the $t=10^5$ curve in the z range plotted.

$$\Phi(v) = \begin{cases} -\pi^{-1}\arcsin(v) & \text{for } 0 \leq v \leq 1, \\ -1/2 & \text{for } v \geq 1. \end{cases} \qquad (5)$$

The $m_0=0.5$ curve in Fig. 1 shows $\Phi(v)$ together with the shape of $m(n,t)$ plotted against $v=n/t$ at finite time ($t=200$). As one can see, the magnetization displays a staircase structure near the edge of the front ($n/t \approx 1$). Our main concern will be the scaling properties (in both space and time) of this staircase structure.

For possible applications, it may be important that the front properties were tunable. Possibility for tuning can be seen by solving the problem for more general steplike initial states

$$\langle\varphi_{m_0}|S_n^z(0)|\varphi_{m_0}\rangle = \begin{cases} m_0 & \text{for } -N < n \leq 0, \\ -m_0 & \text{for } 1 \leq n \leq N, \end{cases} \qquad (6)$$

where $|\varphi_{m_0}\rangle$ is constructed by joining two half chains which are the ground states of the XX model at magnetizations $\pm m_0$. The expression to be analyzed for this case can be taken from Ref. [8], Eq. 12. It is more involved but its numerical evaluation does not pose difficulties. We shall not describe the numerical work but results for $m_0 \neq 0$ will be discussed and displayed (Figs. 1 and 3).

III. LOCAL SCALING IN THE FRONT

The present work on the dynamic scaling of the magnetization profile around the edge of the front ($n \approx t$) originates from our numerical studies of the deviation of the magnetization $\delta m(n,t) = m(n,t) - m(t,t)$ from its front value $m(t,t)$. As one can observe in Fig. 2, a well defined scaling function emerges in the limit $t \to \infty$ provided the magnetization and the region around $n \approx t$ are scaled by $t^{1/3}$ and $t^{-1/3}$, respectively.

An analytic understanding of the scaling seen in Fig. 2 can be developed by first using Eq. (4) to write $\delta m(n,t)$ as

$$\delta m(n,t) = \begin{cases} +\sum_{l=n}^{t-1} J_l^2(t) & \text{for } n < t, \\ 0 & \text{for } n = t, \\ -\sum_{l=t}^{n-1} J_l^2(t) & \text{for } n > t. \end{cases} \qquad (7)$$

Next, one can observe that, in what we call the scaling regime ($t \to \infty$, $n \to \infty$, and $|t-n| \approx t^{1/3}$), the sums above contain Bessel functions whose index (l) and argument (t) differ from each other at most by $|l-t| \sim \mathcal{O}(t^{1/3})$. This suggests the use of the following asymptotic expansion of Bessel function [16]:

$$J_n(n + zn^{1/3}) \approx 2^{1/3}n^{-1/3}\text{Ai}(-2^{1/3}z) + \mathcal{O}(,n^{-1}), \qquad (8)$$

where $\text{Ai}(z)$ is the Airy function. Indeed, in the scaling regime, the terms in the sums in Eq. (7) can be written as

$$J_l^2(t) \approx \frac{2^{2/3}}{l^{2/3}} \mathrm{Ai}^2\left(2^{1/3}\frac{l-t}{l^{1/3}}\right) \approx \frac{1}{t^{2/3}} F\left(\frac{l-t}{t^{1/3}}\right), \quad (9)$$

where $F(y) = 2^{2/3}\mathrm{Ai}^2(2^{1/3}y)$. Note that the last expression in Eq. (9) is obtained by replacing l by t in the factors $l^{1/3}$ and $l^{2/3}$, an approximation that is valid in the scaling regime.

The last step in deriving $\delta m(n,t)$ is the calculation of the sums in Eq. (7) using Eq. (9). In the scaling regime, the sums can be replaced by integrals and, introducing the variable $y = (l-t)/t^{1/3}$, both sums yield the same expression. As a consequence, we obtain a single scaling form for $n > t$ as well as for $n \le t$,

$$\delta m(n,t) = \frac{1}{t^{1/3}} G\left(\frac{n-t}{t^{1/3}}\right), \quad (10)$$

where the scaling function $G(z)$ is explicitly given by the following integral:

$$G(z) = -\int_0^z dy F(y) = -2^{2/3}\int_0^z dy\, \mathrm{Ai}^2(2^{1/3}y). \quad (11)$$

The scaling form (10) and the scaling function (11) are our central result. The staircase shape of the front follows from Eq. (11) while the scaling form (10) shows that the width of the steps increases as $w \sim t^{1/3}$ while their heights (measured from the $z \to \infty$ level) decrease as $h \sim t^{-1/3}$.

IV. QUANTIZED MAGNETIZATION TRANSPORT

An important feature of the scaling given by Eq. (10) is that since $w \times h \sim t^0$ the areas under the steps are constants. Thus a step carries a given amount of magnetic moment $\mu_s = w_s \times h_s$ where the subscript s denotes the sth step counted from the edge of the front. In principle, μ_s could depend on s but their numerical evaluation for the steps near the edge of the front ($1 \le s \le 8$) (see Table I) strongly suggests that $\mu_s = 1$ (the deviations from 1 can be attributed to the finiteness of the sums at finite t).

The $\mu_s = 1$ result can be derived for large-order ($s \gg 1$) steps. Indeed, as can be seen from Fig. 1, the height of the step can be estimated from the global scaling function $m(n,t) = -\pi^{-1}\arcsin(1-z/t^{2/3}) \approx -1/2 + \pi^{-1}\sqrt{2|z|}t^{-1/3}$, and thus $\delta m = h_s = \pi^{-1}\sqrt{2|z_s|}t^{-1/3}$, where z_s is the scaling variable at the sth step. Its value is found by finding the sth zero of $G'(z)$ which, in turn [see Eq. (11)], is obtained from the sth solution of the $\mathrm{Ai}(2^{1/3}z) = 0$ equation. The large-s asymptotic of the sth zero is given [16] by $|z_s| \approx (3\pi s)^{2/3}/2$, and thus

$$h_s = [3s/(\pi^2 t)]^{1/3}. \quad (12)$$

We need now to find the width of the sth step. Defining the borders of the steps as the consecutive inflection points on the staircase, one can see from Eq. (11) that the width of the step is given by the consecutive zeros of $\mathrm{Ai}'(2^{1/3}\tilde{z}_s) = 0$. The large-$s$ asymptotics of these zeros are known again [16] and we find $|\tilde{z}_{s+1} - \tilde{z}_s| \approx [\pi^2/(3s)]^{1/3}$. We should remember now that h_s was calculated for the original (unscaled) magnetization, and the width of the step must also be obtained in unscaled spatial coordinates. Consequently, we should scale $|\tilde{z}_{s+1} - \tilde{z}_s|$ by $t^{1/3}$, and thus

TABLE I. Magnetic moments carried by the steps (area below the steps in the magnetization profile) at finite times ($t = 10^3, 10^4, 10^5$). The borders of the steps were defined by the inflection points in the magnetization curve.

Step no. s	μ_s ($t=10^3$)	μ_s ($t=10^4$)	μ_s ($t=10^5$)
1	1.0183	1.0420	1.0379
2	0.9707	1.0154	1.0094
3	1.0371	1.0080	0.9934
4	0.9418	0.9710	1.0124
5	0.9022	0.9970	0.9986
6	0.9588	1.0070	0.9860
7	1.0123	0.9434	1.0128
8	0.9286	0.9866	1.0037

$$w_s = t^{1/3}|\tilde{z}_{s+1} - \tilde{z}_s| \approx [\pi^2 t/(3s)]^{1/3}. \quad (13)$$

Comparing Eqs. (12) and (13) we see that $h_s w_s = 1$, thus arriving at an important property of the staircase structure, namely, the steps of the staircase carry a unit of magnetization.

In order to see the relevance of the above result and to develop a picture about it, let us consider the magnetization flux in the front region. The total transverse magnetization $M^z = \sum_n S_n^z$ is conserved and so one can define the local magnetization flux $\hat{J}_n^z = S_n^y S_{n+1}^x - S_n^x S_{n+1}^y$, which is related to the local magnetization through the continuity equation. Thus, not surprisingly, one can derive a simple expression for the time evolution of the expectation value of $\hat{J}_n^z$ as well:

$$j(n,t) \equiv \langle\varphi|\hat{J}_n^z(t)|\varphi\rangle = \sum_{l=n}^{\infty} J_l(t)J_{l+1}(t). \quad (14)$$

The analysis of $\delta j(n,t) = j(n,t) - j(t,t)$ parallels that of $\delta m(n,t)$ and yields the same scaling structure in the front:

$$\delta j(n,t) = \frac{1}{t^{1/3}} G\left(\frac{n-t}{t^{1/3}}\right) = \delta m(n,t). \quad (15)$$

Adding $G(\infty)/t^{1/3}$ to both sides of the above equations, and taking into account that $j(n\to\infty,t) = 0$ and $m(n\to\infty,t) = -1/2$, and, furthermore, remembering that the front moves with velocity $v = 1$, we can write the above equations in a form that is easy to interpret:

$$j(n,t) = v\left[m(n,t) - \left(-\frac{1}{2}\right)\right]. \quad (16)$$

Since the sum of $[m(n,t) - (-1/2)]$ for an interval gives the number of up spins in that interval, the meaning of the unit area under the steps is as follows. The steps represent spatial intervals in which a single up spin is spread in the sea of down spins. These up spins behave like particles, they move with velocity $v = 1$, and provide the magnetization flux. Furthermore, they are localized in the sense that their spatial spread is subdiffusive ($\sim t^{1/3}$) [18]. The picture thus emerging is somewhat reminiscent of the hard-core boson descrip-
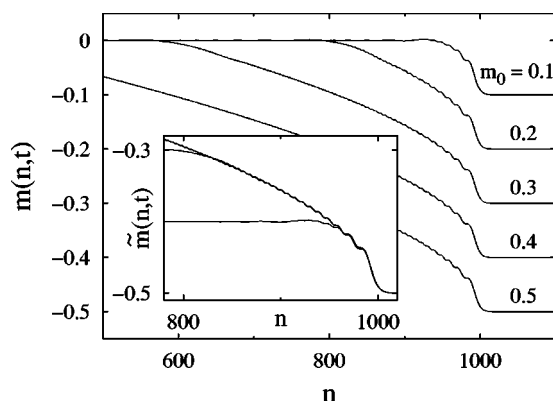
FIG. 3. Magnetization profiles at $t = 10^3$ for different initial values m_0 [Eq. (6)]. The inset with the curves shifted vertically down ($\tilde{m} = m - 0.5 + m_0$) demonstrates that the steps in the front region are independent of the value of m_0.

tion of the XX model near its critical external field [17].

From the point of view of possible applications, it is important that the staircase structure can be observed for other initial conditions as well. Using initial states $|\varphi_{m_0}\rangle$ with $\pm m_0$ steplike profile as described in Eq. (6), we found numerically that the staircase emerges again (see Fig. 3). Furthermore, the steps of the staircase were found to have the same size independently of the values of m_0 (see inset in Fig. 3). What is varied with m_0 is the number of steps $N(t, m_0)$ in the staircase.

We can estimate $N(t, m_0)$ by assuming (on the basis of numerical solutions) that scaling extends to the whole front region, up to the point where m reaches the steady state value of $m = 0$. Then $N(t, m_0)$ is found by locating the Nth step which has a width w_N such that a single spin flip changes the magnetization from $-m_0$ to 0. Since $m_0 w_N$ is the difference between the number of up and down spins in the Nth step, the above consideration gives the condition $-m_0 w_N + 1 = 0$. For large N, Eq. (13) gives the width w_N, and we obtain

$$N(t, m_0) \approx \pi^2 m_0^3 t / 3. \tag{17}$$

It should be noted that Eq. (13) is an excellent approximation also for step numbers of the order of unity, and so Eq. (17)

gives $N(t, m_0)$ for small N, as well. Indeed, e.g., Eq. (17) yields $N \approx 3$ for $t = 10^3$ and $m_0 = 0.1$ while the corresponding curve on Fig. 3 displays $N \approx 4$ steps.

An important feature of Eq. (17) is the strong dependence of the step number on the initial magnetization ($N \sim m_0^3$). This gives a sensitive control over how many steps arrive at a given point at a given time. Thus, in principle, one can imagine applications with the steps transferring bits of information in magnetic nanostructures.

V. FINAL REMARKS

The aim of the present study was to draw attention to the remarkable features of quantum fronts. In order to exploit these features in applications, answers would be required to a number of nontrivial questions. First, can fronts with properties found in the XX model be observed in other spin chains? In particular, are they present in nonintegrable systems? Second, how does the step structure change at small but finite temperatures? Finally, are the front properties robust enough to survive small perturbations arising from impurities? These are difficult problems but the available analytical and numerical techniques may be sufficient to tackle them.

In summary, our calculations exposed a dynamic scaling regime in the motion of fronts in the quantum XX model. The fronts display a staircase magnetization profile which has a simple interpretation in terms of single spin flips spread over the spatial extent of the steps. Whether these fronts have a direct application is an open question but their properties are intriguing enough to look for similar structures in more complex spin chains.

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