Domain wall Dynamics of the Ising chain in a Transverse field

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We show that the dynamics of an Ising spin chain in a transverse field conserves the number of domains (strings of down spins in an up-spin background) at discrete times. This enables the determination of the eigenfunctions of the time-evolution operator, and the dynamics of initial states with domains. The transverse magnetization is shown to be identically zero in all sectors with a fixed number of domains. For an initial state with a single string of down spins, the local magnetization, the equal-time and double-time spin-spin correlation functions, are calculated analytically as functions of time and the initial string size. The domain size distribution function can be expressed as a simple integral involving Bessel functions.

The dynamics of the order parameter, and its correlation functions are related to experimental observables of interacting systems, related to the relaxation and transport processes. For systems with known low-temperature correlation functions, the dynamics can be extremely difficult to determine. For example, the determination of correlators for hard-core particles moving in one dimension has been done using the inverse scattering method. The one-dimensional Ising model in a transverse field has a complicated dynamics, and real-time correlation functions have been shown to have a simple structure near a quantum critical point.

In this paper, we study the zero-temperature dynamics of a one-dimensional transverse field Ising model. The dynamics does not conserve the spin here, and generates domain walls, which can propagate and fluctuate in size. The evolution of an initial state with one domain of down spins (a string of successive down spins in the background of up spins), involves creation of more domains and their complicated motion. We show that the number of domains is conserved at discrete times. As a direct consequence the transverse magnetization is identically zero for any state with a fixed number of domains. The calculation of the one-point and two-point correlators can be carried out using the domain eigenstates. In particular, the time evolution of initial states with exactly one string of down spins is presented.

Let us consider the Hamiltonian (on a ring of \(N\) sites)

\[
H \equiv H_z + H_x = -K \sum_i s_i^z s_{i+1}^z - \Delta \sum_i s_i^x + \frac{NK}{4} \tag{1}
\]

where \(s_i^z, s_i^x\) are the components of the spin-1/2 operator at site \(i\), \(K\) is the Ising interaction strength and \(\Delta\) is the magnetic field strength in x direction. A constant has been added for convenience, which we keep along with the Ising interaction term in \(H_z\). The above Hamiltonian can be diagonalized, and is extensively studied (see [3] for a recent review). Let us write the time evolution operator as (setting \(\hbar = 1\))

\[
U = e^{-itH_z} e^{-i\int_0^t \hat{H}_x(t') dt'} \equiv U_z \hat{U}_x \tag{2}
\]

where we have used the interaction representation, \(\hat{H}_x(t) = \exp (iH_x t) H_x \exp (-itH_x)\). The time-evolved operator \(\hat{s}_i^x(t)\) can be expressed in terms of \(s_i^x, s_{i+1}^x, s_{i-1}^x\), and we have

\[
\int_0^t \hat{s}_i^x(t') dt' = t(s_i^x(1 - \tilde{a}_i^2) + \sin \frac{Kt}{\tilde{a}_i^2} - s_i^y \tilde{a}_i^2 \sin \frac{Kt}{\tilde{a}_i^2})\]

where the operator \(\tilde{a}_i = (s_{i+1}^x + s_{i-1}^x)^2\). Now, let us consider discrete times \(t_n = n\tau\), where \(\tau = 2\pi/K\) (for \(K \sim 0.01eV, \tau \sim 10^{-13}\)). This simplifies the time evolution operator, which becomes \(U = \exp (itH_z) \exp (-itH_1)\),

\[
H_1 = \Delta \sum_i s_i^x \left( \frac{1}{2} - 2s_{i+1}^x s_{i+1}^x \right) \tag{3}
\]

For these discrete times, the evolution operator \(U_z\) has no role to play, it gives unity as an eigenvalue acting on any state with any number of down spins. The operator \(H_1\) can only act at sites with one up and one down spin on either side, in which case it will flip the spin. The polarized state, either all up or all down spins has no dynamics, as it is an eigenstate of \(H_1\) with eigenvalue zero. \(H_1\) operates on a state with a string of \(m\) down spins to generate states with either \(m+1\) or \(m-1\) down-spin strings. In time, the size of the string can change (from \(m = 1\), a lone down spin, to \(m = N-1\), a lone up spin) and the center of mass of the spring can move in either direction. Similarly the operator acting on a state with many strings of down spins, causes them to move and fluctuate in size, but the number of strings will remain the same.

Let us consider the subspace of one-string states, \(|l, m\rangle\) where \(m = 1, N-1\) denotes the length of the down-spin string starting from the site \(l = 1, N\). By arranging the basis states in the order \(|1, 1\rangle, .., |1, N-1\rangle, .., |N, 1\rangle, .., |N, N-1\rangle\), the Hamiltonian has a structure of \(N \times N\) tri-diagonal matrix with periodic boundary conditions. The diagonal positions are occupied by
a $N - 1 \times N - 1$ tri-diagonal matrix with open boundary conditions, and upper (lower) diagonal positions are occupied by a matrix with nonzero elements only on the lower (upper) diagonal positions. All the nonzero matrix elements are equal to $\Delta/2$. The eigenstates of the Hamiltonian $H_1$ can be easily constructed as

$$|k, q \rangle = A \sum_{l, m} e^{ik(2l+m)} \sin(qm)|l, m \rangle,$$

where $A$ is a normalization constant, and the two momenta $q = \pi l/N, l, N - 1$ and $p = \pi m/N, m = 1, N$ label the one-string eigenstates. The phase corresponds to the uniform motion of the center of mass of a string of $m$ down spins. The eigenvalue for this state is $\varepsilon(k,p) = 2\Delta \cos k \cos q$.

The eigenfunctions are the same as the two-magnon eigenfunctions of the XY model, or the two-fermion tight-binding eigenfunctions, labeled by two momenta $0 \leq q_1, q_2 \leq 2\pi, \psi_{ij} = A e^{ip(j+i)} \sin(q(j - i))$, using $i = l, j = l + m$ in the above, and the relative momentum $g = q_1 - q_2/2$, and the average momentum $p = q_1 + q_2/2$. In the two-magnon eigenfunction the labels $i, j$ stand for the two down spins, whereas here they stand for the first sites of the down-spin and up-spin domains in the domain eigenfunctions. Also, the range of $p$ here is $0 \leq p \leq 2\pi$, whereas for the domain eigenfunctions, we have $0 \leq k \leq \pi$. So the two ranges $0 \leq p \leq \pi$ and $\pi p \leq 2\pi$ of the two-fermion eigenfunctions map onto one range $0 \leq k \leq \pi$ of the domain eigenfunctions, and each value of $p$ corresponds to two eigenstates (in terms of the fermions, the two states are $\psi_{ij} = e^{p(l+j+1)} \sin(q(l-j))$ and similarly the raising operator has zero expectation value. Both the components of transverse magnetization vanish identically here. For the case of states with more number of strings, the argument is as follows. As the wave functions are 2n-fermion wave functions, a nonzero expectation value for $<s^-_i(t) =$ implies an off-diagonal long-ranged order, which is prohibited by an argument due to Yang[v], viz. the off-diagonal elements of a one-particle reduced density matrix cannot exhibit long range order. For a nonvanishing transverse magnetization, one has to construct superpositions of states drawn from different domain-number sectors. These states will be more meaningful for the low-temperature behaviour for $\Delta > K$.

Let us turn to the magnetization at a given site, and since $s^-_i$ is diagonal in this basis, we can express its expectation value as

$$\langle s^-_i(t) \rangle = \frac{1}{2} \left( \sum_{l=1}^{N} \sum_{i=1}^{N} \sum_{l=1}^{N} \sum_{i=1}^{N} |\phi_{lm}|^2 \right).$$

Let us denote $i = i_0 + r, j_0 = i_0 + r_0$, and choose $i_0 = N/2$ for convenience. Since $r = -a, r = r_0 - 1 + a$ are the argument of all the Bessel functions above is $x = 2\Delta t$. And $\phi_{ij} = \phi_{ij}$ for $j > i$, whereas $\phi_{ij} = \phi_{i+N+j}$ for $i > j$ (here the length of the down-spin string is $N - i + j$). Though the fermion wave function is the same for both cases, but for the domains it is quite different, $j < i$ configurations occur with negligibly small probabilities for a large $N$. The expectation values of operators at time $t$ reduce to sums over Bessel functions. Let us first consider the transverse magnetization, $<s^-_i(t) =$ would imply an off-diagonal long-ranged order which is prohibited by an argument due to Yang[v], viz. the off-diagonal elements of a one-particle reduced density matrix cannot exhibit long range order. For a nonvanishing transverse magnetization, one has to construct superpositions of states drawn from different domain-number sectors. These states will be more meaningful for the low-temperature behaviour for $\Delta > K$.

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equidistant locations from the string on either side of the string, those two sites will have the same magnetization for all times. Thus, it suffices to study $r > 0$. We have,

$$\langle s^z_i \rangle = \frac{1}{2}(f_1 f_2 - f^2)$$

(10)

where $f_1 = g(r)$, $f_2 = g(r - r_0)$, for $r \geq r_0$, $f_2 = -g(r_0 - r - 1)$, for $0 < r < r_0$, and the function $g(r) = \sum_{-r}^{r} J_n(x)$. It can be expressed as

$$g(r) = 1 - 2 \int_{-r}^{r} J_r(x_1) J_{r+1}(x_1) \, dx_1.$$  

(11)

The function $f(r, r_0) = 2 \sum_{r+1}^{\infty} J_n J_{n-r_0}$ can be written as

$$f(r, r_0) = \int_{0}^{\infty} \left( J_r J_{r+1-r_0} + J_{r+1} J_{r-r_0} \right) \, dx_1$$

$$= \frac{1}{r_0} \left( J_r J_{r+1-r_0} - J_{r+1} J_{r-r_0} \right) (r).$$

(12)

For a fixed value of $x$ as $r \to \infty$, $g \to 1$, $f \to 0$, which implies $\langle s^z_i \rangle \to 1/2$. This is because the domain wall will take $x \to r_0 + r$ time to reach the far away point. For fixed $r$, as $x \to \infty$, the two functions have the behaviour $g \to 0$, $f \to 2/\pi r_0$, for $r_0$ odd, and it is zero when $r_0$ is even. This implies all the spins within a size of $x$ from the initial position have an expectation value $-2/\pi^2 r_0^2$ for $r_0$ odd, whereas for even initial string sizes, the local magnetization fluctuates around a zero expectation value. The local magnetization is plotted as a function of the site index $r$, for various values of time in Fig.1, for an initial state with a string of 71 down spins.

The even-odd effect can be understood as follows. First we note that for $r_0$ odd (even), at later times odd (even) sizes are more probable than even (odd). Later we shall compute the size distribution function. The down-spin density is maximum at the center of the domain, and as we move away from the center the spin density drops. Most of the contribution for a negative magnetization should be coming from the probability of a site being a center of a domain. The center of mass of even-size domains cannot be a lattice site. Hence, for even $r_0$, the magnetization fluctuates around a zero mean. However, this even-odd discrepancy disappears for larger initial string sizes, viz. for $r_0 = 9$ the mean drops to $-0.002$ already. This is because as $r_0$ becomes larger, smaller-sized domain are less probable, as we shall see later. And large odd-size domain move slower, thus depleting the probability for a site to be a center of a domain.

Now we turn to the calculation of equal-time correlation functions. The off-diagonal correlation function is straightforwardly written as

$$\langle s^z_i(t) s^z_j(t) \rangle = \frac{1}{4} \left( F_1 F_2 - F^2 \right)$$

(14)

where $F_1 = g(r+s) - g(r)$ and $F = f(r, r_0) - f(r+s, r_0)$. The function $F_2$ has different dependencies in the three regimes, as, $F_2 = g(r-r_0+s) - g(r-r_0)$, for $r \geq r_0$, $F_2 = g(r_0 - r - 1) - g(r_0 - r - s - 1)$, for $r_0 < r < r_0$, $F_2 = g(r_0 - r - 1) + g(r + s - r_0)$, for $r < r_0$, $r + s \geq r_0$. For a fixed value of $x$, as the separation $s \to \infty$, these functions reduce as $F_1 \to f_1$, $F_2 \to f_2$, $F \to f$. And the two-point correlation function decouples, and becomes

$$\langle s^z_i s^z_{r+s} \rangle = \frac{1}{4} (F_1 F_2 - F^2).$$

(13)

Let us choose, $i = i_0 + r$, $j = i + s$, $j_0 = i_0 + r_0$, and $i_0 = N/2$ as before. Here there are three regimes, depending whether both $i$, $j$ are within the initial string, or both outside, or one of them is outside. The correlation function can be reexpressed as

$$\langle s^z_i(t) s^z_{r+s} \rangle = \frac{1}{4} (F_1 F_2 - F^2).$$

(14)

The double-time correlation functions are not very easy to evaluate. Let us define $C_{ij}(t_1, t_2) = \langle i(t_2) j(t_1) \rangle$. Setting $t_1 = 0, t_2 = t$, we have

$$C_{ij}(t, 0) = \langle s^z_i(t) \rangle \langle s^z_j(0) \rangle.$$ 

(15)

The operator $s^z_j$ can be taken out, as $| \phi_0 >$ is its eigenstate, and the rest is just $\langle s^z_i(t) \rangle$. But for an arbitrary $t_1 \neq 0$, the correlation function can be written as

$$C_{ij}(t_2, t_1) = \sum_{l,m,l' m'} (| \phi_{lm}(x_1) \rangle | \phi_{l'm'}(x_2) \rangle \langle s^z_i(t_2) | s^z_j(t_1) \rangle)$$

$$= \left( \sum_{l,m,l' m'} C_{ij}(t_2, t_1) \right) J_{l_1-l_2} J_{m_1-m_2} J_{l_1'-l_2'} J_{m_1'-m_2'}.$$

(16)

In the above, the argument of all the Bessel functions is the difference of time. The double-time correlation function is substantially more complicated, and a detailed analysis will be presented elsewhere.
We now turn to the domain-size distribution. The probability for a size $r$ to occur will depend on the initial domain size, and the time. We can write the probability as $\rho(r, r_0, x) = \sum |\phi_{ij}|^2 \delta_{j,i+r}$, which becomes, after replacing the delta function by a Fourier integral,

$$\rho = \frac{1}{\pi} \int_{-\pi}^{\pi} e^{i\phi r} [\cos(\phi r_0)h^2(0,x) - h^2(r_0, x)].$$  
(17)

We have defined another auxiliary function involving a sum over Bessel functions,

$$h(y, x) = \left| \sum_{k=-\infty}^{\infty} J_k(x)J_{k+y}(x)e^{ik\phi} \right| = J_y(2x|\sin\phi/2|),$$  
(18)

where we have used the summation rule for the Bessel functions in the last step. After a few more manipulations, we get

$$\rho = \frac{2}{\pi} \int_{0}^{1} \frac{dt}{\sqrt{1-t^2}} [J_{r+r_0}(2xt) - (-1)^r m J_{r-r_0}(2xt)]^2.$$  
(19)

In Fig. 3 we show the distribution function plotted against the domain size for a few values of $x$, for an initial state with one domain of down spins of size $r_0 = 10$. The probability is maximum for $r = r_0$, and as $x$ becomes very large all sizes are equally probable modulo an even-odd effect. The above distribution becomes simpler for the case of $r_0 = 1$ as

$$\rho(r, 1, x) = \frac{8r^2}{\pi x^2} \int_{0}^{\pi/2} J^2_r(2x\cos\phi).$$  
(20)

This distribution function can change substantially for initial states with more than one string of down spins. For a finite density $n$ of strings, the domain size $r$ is limited by the average domain spacing in the initial state. The probability is more for domain sizes $r < r_c \sim 1/n$.

In conclusion, we have explored the domain-wall dynamics for the Ising model in a transverse field in one dimension. The eigenstates of the time evolution operator are simple domain eigenstates for discrete times (multiples of $2\pi/K$). The transverse magnetization is identically zero in all sectors with different number of domains. Explicit calculations of the local magnetization and the spin-spin correlation functions are presented for initial states with one domain of down spins. Though the above analysis is valid for large $\Delta$ also, these domain states do not belong to the low-energy spectrum here. One can do a similar analysis with domain states using the eigenstates of $s_\square^z$ operators, which are more natural states for $\Delta > K$. Finally we would like to comment on the domains in two dimensions, where the situation is quite different. Firstly, the domains can have various shapes. Secondly, though at discrete times, the time evolution can be simplified analogously, however, the number of domains is not conserved. Another major difference is that the domain size is limited, and they do not move easily. For a domain of arbitrary shape at some time, the domain size at later times is limited by the size of the smallest rectangle into which the initial shape can be enclosed.

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[1] Quantum Inverse Scattering Method and Correlation functions, edited by V.E. Korepin et al. Cambridge University Press, Cambridge (1993)
[2] S. Sachdev and A.P. Young, Phys. Rev. Lett. 78, 2220 (1997)
[3] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. 16, 406 (1961).
[4] P. Pfeuty, Ann. Phys. 57, 79 (1970); B.M. McCoy et al., Phys. Rev. A4, 2331 (1971)
[5] Quantum Phase Transitions, by S. Sachdev, Cambridge University Press, Cambridge (1999).
[6] C. N. Yang, Rev. Mod. Phys. 34, 694 (1962).
[7] Table of Integrals, Series and Products by I. S. Gradshteyn and I. M. Rhyzhik, Academic Press, San Diego (1965).