DOMAIN WALLS IN THE SPIN-$S$ QUANTUM ISING CHAIN

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Domain walls in the spin-$S$ quantum Ising chain at zero temperature are considered. Quantum effects prevent the walls from being sharp and delocalize the exact eigenstates. The absence of a characteristic length of the domain walls is reflected in the finite-size scaling of the spectrum of the Hamiltonian.

1 Introduction

Recently, there has been a growing interest in the study of interfaces with nontrivial geometry. Such interfaces may arise for example in domain walls in random magnets, fluid invasion in porous media, spreading on heterogeneous surfaces, biological membranes and vesicles or epitaxial growth. When do quantum effects play a significant role in such problems? For static properties in non-random systems such as an spin-$S$ antiferromagnet with nearest neighbor exchange interaction $J$, the following regimes exist. Near the critical temperature $T_N \sim J S^2$, thermal fluctuations dominate. In the ordered phase, for temperatures $T_c/S \ll T \ll T_c$, quantum effects due to the finiteness of $S$ are unimportant. For $T < T_c/S$, however, one is in the quantum regime, where the quantum statistics of spin waves and their interactions lead to dependences on $S$ and $T$ not present in the classical ($S \to \infty$) limit.

Useful insight to the problem may be gained by considering a simple 1D quantum system. We shall consider the domain walls at zero temperature of the following extension of the spin-$S$ Ising quantum chain

$$\mathcal{H} = -\frac{H}{2S} \sum_{n=1}^{L} S_x(n) - \frac{J}{2S^2} \sum_{n=0}^{L} S_z(n)S_z(n+1) - \frac{\epsilon J}{2S^2} \sum_{n=1}^{L-1} S_y(n)S_y(n+1)$$ (1)

where $S_{x,y,z}(n)$ is a quantum spin-$S$ operator at site $n$, $H$ is the transverse field, $\epsilon$ describes the anisotropy in the spin space, $J$ is the exchange coupling and $L$ is the number of sites. We shall work with the boundary conditions

$$S_z(0) = -S_z(L+1) = S$$ (2)

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Table 1: Ground state phase of the quantum Hamiltonian $H$. The phase boundaries are for spin $S = \frac{1}{2}$.

| phase | condition | $m(G(R))$                  |
|-------|-----------|----------------------------|
| D     | $\epsilon < h - 1$ | $0$ $R^{-1/2} \exp(-R/\xi)$ |
| F     | $h - 1 < \epsilon < h^2/4$ | $\neq 0$ $R^{-2} \exp(-R/\xi)$ |
| O     | $h^2/4 < \epsilon$ | $\neq 0$ $R^{-2} \exp(-2R/\xi) \Re(Be^{iKR})$ |

The study of finite values of $S$ rather than considering the classical limit $S \to \infty$ may be of interest, since several experimentally studied systems have a rather low value of $S$: $S = \frac{1}{2}$ in CsCoCl$_3$ and CHAB, $S = 1$ in CsNiF$_3$ and $S = \frac{5}{2}$ in TMMC. Profiles of various physical quantities have been investigated by several authors. Here we shall concentrate on the local magnetization profile

$$m(r) = S^{-1} \langle 0 | S_z(n) | 0 \rangle \quad , \quad r = n/(L + 1) \quad , \quad n = 0, 1, \ldots, L + 1 \quad (3)$$

where $| 0 \rangle$ is the ground state of $H$. In the sequel, we shall often use the notation $h = H/J$.

Depending on the parameters $h$ and $\epsilon$, there are three distinct ground state phases as indicated in table 1. Their properties are distinguished through the magnetization $m = \sum_r m(r)$ and the connected two-point function $G(R) = \langle S_z(R)S_z(0) \rangle - \langle S_z(R) \rangle \langle S_z(0) \rangle$. The correlation length $\xi$ and the wave vector $K$ are for $S = \frac{1}{2}$ known functions of $h$ and $\epsilon$. For higher spin $S > \frac{1}{2}$, the $F/O$ boundary is exactly known, while the $D/F$ boundary (which is in the Ising universality class) has to be found numerically. Besides studying the spin dependence of the profile eq. (3), we shall also ask how the profile changes between the two ordered phases $F$ and $O$.

Finally, the results presented here may have a bearing on certain nonequilibrium reaction-diffusion processes, when the master equation is rewritten in a Hamiltonian form. The resulting quantum Hamiltonians are almost identical to eq. (1) (at the O/F boundary) and surface fields model particle injection and extraction. Reactions of a single particle species are described by spin $\frac{1}{2}$, where the free fermion condition means that two particles react with infinite rate on encounter. That condition is apparently realised for the exciton kinetics in TMMC. Ground state order parameter profiles as considered here should be analogous to particle density profiles in the steady state.

In section 2, we review the results for the order parameter profile. In distinction to the classical case, quantum effects lead to the delocalization of the energy eigenstates and thus to wide profiles. In section 3, related spectral properties of $H$ will be described.
2 Order parameter profile for $S = 1/2, 1$ and $3/2$

We now display the results for the profile eq. (3). On finite lattices, the calculation of the profile from the lowest eigenstate of $\mathcal{H}$ through the Lanczos algorithm is completely standard. We begin with the profiles for the phase $F$, which is shown in Fig. 1 for $S = 1/2, 1$ and $3/2$. We observe the following. First, data for different lattice sizes (we used lattices up to $L = 16$) nicely collapse onto each other which implies that for the parameters considered the lattices are large enough to faithfully represent the $L \to \infty$ limit. Second, the profiles are quite wide and vary continuously with $r$. Third, the form of the profile is, at least for $S$ not too large, quite independent of the value of $S$. These differences grow larger when $h$ approaches the critical value (if $\epsilon = 0$, $h_c = 1$ for $S = 1/2$, $h_c \simeq 1.32587(1)$ for $S = 1$). Finally, the profile only depends weakly on $h$ for $h$ small enough.

Finding a quantum profile with a width $w \sim L$ of the order of the system size $L$ is in contrast with the sharp profiles of width $w \sim a$, the lattice constant, in the classical $S \to \infty$ limit. This result can be explained as follows. The boundary conditions eq. (4) require that at least one domain wall is present in the system. For $h = 0$ (and $\epsilon = 0$), the states of lowest energy of $\mathcal{H}$ are

$$|\uparrow\uparrow\cdots\uparrow\downarrow\rangle, \ldots, |\uparrow\cdots\uparrow\down\cdots\down\rangle, \ldots, |\down\down\cdots\down\rangle$$ (4)
for spin $S = \frac{1}{2}$ and for $L$ sites, there are $L + 1$ of these degenerate states. For $S = 1$ at $h = 0$ the $(L + 1) + L = 2L + 1$ states

\begin{align*}
|\uparrow\uparrow \cdots \uparrow\downarrow\rangle, \ldots, & \, |\uparrow\downarrow \cdots \downarrow\uparrow\rangle \\
|\uparrow\uparrow \cdots \uparrow0\downarrow\rangle, \ldots, & \, |\uparrow\downarrow \cdots \downarrow0\uparrow\rangle, \ldots, \, |\uparrow0\downarrow \cdots \downarrow\uparrow\rangle
\end{align*}

(5)

are degenerate. These states have a single sharp domain wall. Turning on $h$, the transverse field term acts like a hopping matrix between these states and the domain wall profile becomes broad as a result of the superposition of many sharp domain walls. Working in the subspace $\mathcal{M}$ of the states eqs. (4,5) with a single domain wall, the order parameter profile is found to be

$$m(r) = 1 - 2r + \frac{1}{\pi} \sin(2\pi r)$$

(6)

for both $S = \frac{1}{2}$ and $S = 1$. As can be seen from Fig. 1, for $h$ small enough eq. (6) is in excellent agreement with the data.

Indeed, for spin $S = \frac{1}{2}$, the correspondence between the domain walls and the lowest excitations can be made precise. Namely, for the quantum chain eq. (1) with open boundary conditions one can define the domain wall creation operators, with $a_n = \frac{1}{2} (S_x(n) + i S_y(n))$

$$D^+_n = \frac{1}{2} (c^+_n + c^+_{n+1}) + \frac{1}{2} (c^+_n - c_n) \, , \, c_n = \exp \left[ i \pi \sum_{\ell=1}^{n-1} a^+_\ell a_\ell \right] a_n$$

(7)

which satisfy the anticommutation relations $\{ D^+_n, D_m \} = \delta_{n,m}$, $\{ D^+_n, D^+_m \} = 0$. $D^+_n$ and $D_n$, respectively, create and annihilate a domain wall between the sites $n$ and $n + 1$. Then, for open boundary conditions rather than the ones specified in eq. (2) and for $S = \frac{1}{2}$, the quantum Hamiltonian becomes

$$\mathcal{H} = \sum_{n=1}^{L-1} D^+_n D_n + \frac{1}{\beta} \sum_{n=1}^{L-1} \left( D^+_n D_{n+1} + D^+_n D^+_{n-1} + \text{h.c.} \right)$$

$$-\frac{1}{2} H \sum_{n=1}^{L} \left( D^+_n D_n - D_{n-1} D^+_n + \text{h.c.} \right) - \frac{1}{2} J (L - 1)$$

(8)

where $D_L = D_0 = \frac{1}{2} (c_1^+ + c_1 + c_L^+ - c_L)$. The Hamiltonian thus describes domain wall transfer between nearest neighbor and next-nearest neighbor sites as well as domain wall pair creation and annihilation. This gives a nice interpretation to the well-known free fermion formulation. While in the F phase the next-to-nearest neighbor terms are unimportant, this is not so in the O phase.
Figure 2: Magnetization profile in the O phase for spin $S = \frac{1}{2}$ and $h = 0.01, \epsilon = 0.5$ for several values of the system size $L$.

Turning the profile in the O phase, different results are obtained from finite lattices for $L$ even and $L$ odd. For $L$ even, the lowest ground state remains non-degenerate and eq. (3) can be used. That is not so for $L$ odd, where there are for $h = 0$ and $\epsilon \neq 0$ two degenerate ground states $|0\rangle, |0'\rangle$ and these states remain close together even for $h \neq 0$. Then the order parameter profile is found from the eigenvalues $m_{\pm}(r)$ of the matrix

$$m_{\pm}(r) = S^{-1} \begin{pmatrix} \langle 0| S_z(n) |0\rangle & \langle 0'| S_z(n) |0\rangle \\ \langle 0| S_z(n) |0'\rangle & \langle 0'| S_z(n) |0'\rangle \end{pmatrix}, \quad r = n / (L + 1) \quad (9)$$

and $m_{+}(r)$ and $m_{-}(r) = -m_{+}(\frac{1}{2} - r)$ are related to each other through spatial reflection. One of these is shown in Fig. 2. We observe the following. First, finite-size effects are much larger than in the F phase. Second, $m(r)$ displays for $L$ finite step-like behavior and it looks as if the system were built from hard objects each occupying two lattice sites. When $h$ is increased, these composites soften until they melt at the O/F transition. Third, for $L$ odd, the reflection symmetry is lost. These results can be explained in the same way as before through the hopping of domain walls, as described by the Hamiltonian in the form eq. (8). Calculations become particularly simple for $h = 0$ and in the context of the subspace $M$ of the states eq. (4). We can then decompose
\[ M = M_e + M_o \] into the subspaces with an even and odd number of inverted spins, respectively. Then, the effective Hamiltonian decomposes into two which are identical to the one found in the treatment of the F phase, but for a redefined effective system size. We have \( L_{\text{eff}} = \frac{1}{2}(L+1) \) for \( L \) odd (twice) and \( L_{\text{eff}} = L/2 + 1 \) and \( L/2 \) for \( L \) even. It follows that in the \( L \to \infty \) limit the width of the terraces decreases and the order parameter profile goes toward a smooth and reflection symmetric limit. The phenomenon seen in Fig. 2 is thus a finite-size effect.

Finally, in the \( L \to \infty \) limit, we observe (for spin \( S = \frac{1}{2} \)) numerically a simple relation of the profiles \( m(r; h, \epsilon) \) between the F and the O phases, suggesting that

\[ m(r; h_{\text{eff}}(\epsilon), 0) \approx m(r; 0, \epsilon) \quad (10) \]

In the limit \( \epsilon \ll 1 \), the restriction to the subspace \( M \) is accurate and yields \( h_{\text{eff}}(\epsilon) = \epsilon \). For \( \epsilon \) finite, we find that phenomenologically \( h_{\text{eff}}(\epsilon) \approx \sqrt{\epsilon} \).

With increasing values of \( S \) the mechanism of quantum delocalization through hopping of the domain walls becomes less and less important as the classical limit is approached. Again, this is best understood within the subspace \( M \) of states with a single domain wall. The quantum hopping of a domain wall becomes analogous to a tunneling process, since there is at least in the semiclassical limit \( S \to \infty \) a finite energy barrier which prevents the free motion of the domain walls. This energy barrier vanishes for finite values of \( S \) in the thermodynamic limit. Starting from \( S = \frac{1}{2} \), the states can be such arranged that the hopping matrix elements between them become periodic functions, thus leading to a banded energy spectrum. The width of these bands decreases rapidly with \( S, W \sim H^{2-S} \). Finally, for \( S = \infty \), quasiclassical approximations become accurate and yield a sharp domain wall (for \( h \ll 1 \)) of the order of the lattice spacing.

The effects of temperature and of inhomogeneous transverse fields on the quantum profile have also been studied. The constant transverse field \( H \) is replaced by \( H(n) \) which takes the value \( +H \) in the left sector and \( -H \) in the right sector of the system. Then for \( S = \frac{1}{2} \) and \( \epsilon = 1 \), the profile \( e(n) = \langle 0 | S_x(n) | 0 \rangle \) can be calculated exactly. In distinction to the monotonous profiles of Figs. 3 and 4, \( e(n) \) is found to show oscillatory behavior in the O phase. For \( T \to 0 \), these oscillations are suppressed.

3 Nature of the spectrum

We have seen that at least qualitatively, the form of the profile \( m(r) \) can be understood in terms of the subspace \( M \) of the states with a single domain wall. While this approximation is \textit{a priori} applicable for \( h \ll 1 \), it is remarkable
that the clear separation of the states within $\mathcal{M}$ remains intact even for finite values of $h$. We can thus identify a subspace $\tilde{\mathcal{M}}$ of low-lying states (with $\mathcal{M} = \lim_{h \to 0} \tilde{\mathcal{M}}$) even though the states in $\tilde{\mathcal{M}}$ are no longer simply those states with a single domain wall. Indeed, we find that while the energy gaps of the states outside $\tilde{\mathcal{M}}$ are finite within the phases O and F, the states within $\tilde{\mathcal{M}}$ show a different behavior.

We begin with the F phase. Let $g(i) = E_i - E_0$ denote the $i^{th}$ gap. We then find the finite-size scaling $g(i) \sim L^{-\theta}$ with $\theta = 2$ for the $2SL + 1$ states within $\tilde{\mathcal{M}}$. Furthermore, the scaling amplitudes $a(i) = \lim_{L \to \infty} L^2 g(i)$ follow a simple pattern within $\tilde{\mathcal{M}}$. Namely $(i = 1, 2, 3 \ldots)$

$$r(i) = a(i)/a(1) = \frac{1}{3}i(i + 2) = \frac{1}{3}, \frac{8}{3}, 5, \frac{35}{3}, 16, \ldots$$  \hspace{1cm} (11)$$

We have checked these amplitude ratios within the entire F phase for both $S = 1/2$ and $S = 1$. This confirms the earlier observation that domain walls approach their asymptotic behavior algebraically.

For the O phase, the spectrum is different. We concentrate on $S = 1/2$ and $h = 0$. The basic structure of the levels is indicated in Fig. 3. For $L$ even, the states within $\tilde{\mathcal{M}}$ are grouped into doublets with a splitting of order $L^{-3}$ and the gaps between the doublets are of order $L^{-2}$. Thus the lowest gap scales with an exponent $\theta = 3$, while $\theta = 2$ for all other gaps. For $L$ odd, all levels are doubly degenerate with gaps between them of order $L^{-2}$ and $\theta = 2$ throughout. For the amplitudes, we find independently of the parity of $L$ the following pattern, consistent with the structure of eq. (11)

$$\rho(i) = a(i)/a(2) = 0, 1, 1, \frac{8}{3}, \frac{8}{3}, \frac{5}{3}, \ldots$$  \hspace{1cm} (12)$$

Eqs. (11,12) can be analytically reproduced by restricting to the space $\mathcal{M}$.
along the entire line $h = 0$. Qualitatively, the same structure persists through the entire O phase.

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