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LETTER TO THE EDITOR

Surface and bulk critical behaviour of the *XY* chain in a transverse field

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Abstract. The surface magnetization of the quantum *XY* chain in a transverse field is found for arbitrary nearest-neighbour interactions in closed form. This allows us to derive the bulk phase diagram in a simple way. The magnetic surface behaviour and the bulk correlation length are found exactly.

We consider the ferromagnetic anisotropic *XY* quantum chain in a transverse field with Hamiltonian [1]

$$\mathcal{H} = -\sum_{n=1}^{N} \left[h_n \sigma_n^z + J_n \frac{1 + \eta_n}{2} \sigma_n^x \sigma_{n+1}^x + J_n \frac{1 - \eta_n}{2} \sigma_n^y \sigma_{n+1}^y \right]. \tag{1}$$

The σ are the Pauli matrices, h_n is the local transverse field at site n and $|\eta_n| \leqslant 1$ is the local anisotropy between couplings in the x and y direction. When all the ηs are equal to unity one recovers the Ising quantum chain [2]. With a constant anisotropy factor, $\eta_n = \eta$, the phase diagram and bulk critical behaviour are known exactly [3]. Here we focus on the surface critical behaviour of the chain with free boundary conditions. To diagonalize the Hamiltonian, one has first to perform a Jordan–Wigner [4] transformation, introducing fermionic creation and annihilation operators c_n^+, c_n which satisfy the usual fermionic anticommutation rules. In terms of these new operators the Hamiltonian (1) is a quadratic form

$$\mathcal{H} = -\frac{1}{\zeta} \sum_{n,m=1}^{N} \left[c_n^+ A_{nm} c_m + \frac{1}{2} (c_n^+ B_{nm} c_m^+ - c_n B_{nm} c_m) \right] \tag{2}$$

where A is a symmetric matrix such that

$$A_{jk} = 2h_j \delta_{j,k} + J_{j-1} \delta_{j,k+1} + J_j \delta_{j,k-1} \tag{3}$$

and B is an antisymmetric matrix with elements

$$B_{jk} = -J_{j-1} \eta_{j-1} \delta_{j,k+1} + J_j \eta_j \delta_{j,k-1}. \tag{4}$$

The more efficient way to diagonalize the quadratic form (2) is to follow the procedure introduced by Lieb [5] which is valid for a general distribution of the coupling constants.

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To proceed, we introduce a new set of diagonal fermionic operators ε^+, ε which are a linear combination of the c^+ and c operators:

$$\varepsilon_q^+ = \sum_n \left[\phi_q(n) \frac{c_n^+ + c_n}{2} + \psi_q(n) \frac{c_n^+ - c_n}{2} \right] \tag{5}$$

where the $\phi_q(n)$ and $\psi_q(n)$ are real. The Hamiltonian (2) is diagonal:

$$\mathcal{H} = \sum_q \Lambda_q (\varepsilon_q^+ \varepsilon_q - \tfrac{1}{2}) \tag{6}$$

when the vectors $\Psi_q(\Phi_q)$ with components $\psi_q(n)(\phi_q(n))$ and the fermion excitation energies Λ_q satisfy the matrix relations

$$\begin{aligned} (A - B)\Psi_q &= \Lambda_q \Phi_q \\ (A + B)\Phi_q &= \Lambda_q \Psi_q. \end{aligned} \tag{7}$$

One may combine the previous matrix equations to deduce Λ_q^2 from the eigenvalue problem

$$(A - B)(A + B)\Phi_q = \Lambda_q^2 \Phi_q. \tag{8}$$

In order to solve the problem, one has to find the eigenvalues and eigenvectors of the excitation matrix $(A - B)(A + B)$. All the physical quantities, such as magnetization, energy density or correlation functions, can be expressed in terms of the eigenvectors Φ_q, Ψ_q and corresponding excitation energies Λ_q.

We now concentrate on the surface magnetic behaviour. The $x(y)$ component of the surface magnetization is obtained from the autocorrelation function $G_s^{x(y)}(\tau) = \langle \sigma_1^{x(y)}(0)\sigma_1^{x(y)}(\tau)\rangle$ in imaginary time τ where $\sigma_1^{x(y)}(\tau) = \mathrm{e}^{\tau\mathcal{H}}\sigma^{x(y)}\mathrm{e}^{-\tau\mathcal{H}}$. In the limit of large τ we have

$$\lim_{\tau \to \infty} G_s^{x(y)}(\tau) = [m_s^{x(y)}]^2. \tag{9}$$

Using the diagonal basis of $\mathcal{H}$, we obtain

$$m_s^{x(y)} = |\langle \sigma | \sigma_1^{x(y)} | 0\rangle| \tag{10}$$

where $|0\rangle$ is the ground state and $|\sigma\rangle = \varepsilon_1^+|0\rangle$ is the first excited state with one fermion. Noticing that $\sigma_1^x = c_1^+ + c_1$ and that $\sigma_1^y = \mathrm{i}(c_1 - c_1^+)$, and making use of (5), we obtain $m_s^x = \phi_1(1)$ and similarly $m_s^y = \psi_1(1)$.

Following Peschel [6], it is now possible to obtain a closed analytical formula for the $x(y)$ component of the surface magnetization. In the semi-infinite system ($N \to \infty$), in the ordered phase, the first gap $E_\sigma - E_0 = \Lambda_1$ vanishes due to spontaneous symmetry breaking. In this case, equation (7) simplifies to

$$\begin{aligned} (A - B)\Psi_1 &= 0 \\ (A + B)\Phi_1 &= 0. \end{aligned} \tag{11}$$

Noticing that changing η into $-\eta$ and m_s^x and m_s^y exchange, in the following we only concentrate on the x component of the surface magnetization.

To find the eigenvetor Φ_1 we can rewrite the matrix equation $(A + B)\Phi_1 = 0$ in the form

$$\begin{pmatrix} \phi_1(n + 1) \\ \phi_1(n) \end{pmatrix} = T_n \begin{pmatrix} \phi_1(n) \\ \phi_1(n - 1) \end{pmatrix} \tag{12}$$

where T_n is the 2×2 matrix

$$T_n = - \begin{pmatrix} \frac{2h_n}{J_n(1+\eta_n)} & \frac{1-\eta_{n-1}}{1-\eta_n} \\ -1 & 0 \end{pmatrix}. \tag{13}$$

Iterating equation (12) one arrives at

$$\begin{pmatrix} \phi_1(n+1) \\ \phi_1(n) \end{pmatrix} = (-1)^n \boldsymbol{T}_n \boldsymbol{T}_{n-1} \dots \boldsymbol{T}_2 \boldsymbol{T}_1 \begin{pmatrix} \phi_1(1) \\ 0 \end{pmatrix}. \tag{14}$$

The $(n+1)$th component of the eigenvector Φ_1 is then given by the expression

$$\phi_1(n+1) = (-1)^n \phi_1(1) \langle 1| \prod_{j=1}^{n} \boldsymbol{T}_j |1\rangle \tag{15}$$

where $\langle 1| \cdots |1\rangle$ stands for the 1, 1 component of the corresponding matrix. The normalization of the eigenvector, $\sum_n \phi_1^2(n) = 1$, leads to the surface magnetization:

$$m_s^x = \phi_1(1) = \left[1 + \sum_{n=1}^{\infty} \left| \langle 1| \prod_{j=1}^{n} \boldsymbol{T}_j |1\rangle \right|^2 \right]^{-1/2}. \tag{16}$$

For $\eta = 1$ we recover Peschel's formula [6] for the Ising model in a transverse field. This expression is valid for any distribution of the coupling constants of the chain provided that the first gap vanishes, i.e. in the ordered phase(s). The transition to the paramagnetic phase is characterized by a divergence of the sum in (16). Since for a one-dimensional quantum system with short-range interactions, the surface cannot order by itself, the surface transition is the signal of a transition in the bulk.

We consider in the following the homogeneous chain, $\eta_n = \eta$, $J_n = 1$ and $h_n = h \forall n$. In this case, all the $\boldsymbol{T}$ matrices are the same and it is easy to evaluate (16). The eigenvalues of $\boldsymbol{T}$ are

$$\lambda_{\pm} = \frac{1}{1+\eta} \left[h \pm \sqrt{h^2 + \eta^2 - 1} \right] \tag{17a}$$

for $h^2 + \eta^2 > 1$ and complex conjugates otherwise

$$\lambda_{\pm} = \frac{1}{1+\eta} \left[h \pm \mathrm{i}\sqrt{1 - h^2 - \eta^2} \right]. \tag{17b}$$

On the line $h^2 + \eta^2 = 1$ they become degenerate. First we note that the leading eigenvalue gives the behaviour of $\phi_1^2(n) \sim |\lambda_+|^{2n}$ which, for an ordered phase, implies that $|\lambda_+| < 1$, the first mode, is then localized near the suface. From equations (17a) and (17b) this corresponds to $h < h_c = 1$. When $h > 1$ a vanishing surface magnetization is obtained and the bulk is in the paramagnetic phase. The line $h = 1$ is the Ising transition line since for $\eta \neq 0$ it belongs to the Ising universality class. As can be expected from (17) and shown hereafter, the line $h^2 + \eta^2 = 1$ separates an ordinary ferromagnetic phase ($h^2 + \eta^2 > 1$) from an oscillatory one ($h^2 + \eta^2 < 1$). This line is known as the disorder line of the model. Finally, the line with vanishing anisotropy $\eta = 0$ corresponds to a continuous transition (with a diverging correlation length) and is called the anisotropic transition line, where the magnetization changes from the x to the y direction. In the ordered phase, the decay of the eigenstate Φ_1 gives the bulk correlation length, which is related to the leading eigenvalue λ_+ of the $\boldsymbol{T}$ matrix by

$$\phi_1^2(n) \sim |\lambda_+|^{2n} \sim \exp\left(-\frac{n}{\xi} \right) \tag{18}$$

so that

$$\xi = \frac{1}{2 \ln |\lambda_+|}. \tag{19}$$

Using (17), one obtains the correlation length in both the normal and oscillating phases [3]. In particular, one recovers the known result that the correlation length exponent $\nu = 1$ at both the Ising and anisotropic transitions.

Let us consider first the Ising transition line at a fixed anisotropy η. Then, close enough to the transition, we have $h^2 + \eta^2 > 1$. The eigenvalues $\lambda_\pm$ are real and it is easy to show that

$$\langle 1|T^n|1\rangle = \frac{\lambda_+^{n+1}}{\Delta\lambda}\left[1 - \left(\frac{\lambda_-}{\lambda_+}\right)^{n+1}\right] \tag{20}$$

where $\Delta\lambda = \lambda_+ - \lambda_-$. This expression reduces for large n to $\lambda_+^{n+1}/\Delta\lambda$. Using equation (16) we obtain the surface magnetization near the Ising transition:

$$m_s^x \simeq \left[\left(\frac{1+\eta}{2\eta}\right)^2 \lambda_+^4(1-\lambda_+^2)^{-1}\right]^{-1/2} \simeq \frac{2}{1+\eta}\sqrt{2\eta}(1-h)^{1/2}. \tag{21}$$

Thus the surface critical exponent is $\beta_s^I = \frac{1}{2}$ on the Ising transition line.

Close enough to the anisotropic transition line ($\eta = 0$), we are in the oscillatory phase. The complex conjugate eigenvalues $\lambda_\pm$ of equation (17b) can be parametrized as

$$\lambda_\pm = \rho\exp(\pm i\theta) \tag{22}$$

with

$$\rho = \sqrt{\frac{1-\eta}{1+\eta}} \qquad \theta = \arctan\left[\frac{\sqrt{1-h^2-\eta^2}}{h}\right]. \tag{23}$$

Using (14) a straightforward calculation shows that

$$\phi_1(n) = (-1)^n \frac{1+\eta}{\sqrt{1-\eta^2-h^2}}\left(\frac{\lambda_+^n - \lambda_-^n}{2}\right)\phi_1(1)$$

$$= (-1)^n\rho^n \frac{1+\eta}{h\tan\theta}\sin(n\theta)\phi_1(1). \tag{24}$$

We see from this expression the oscillatory nature of the phase with a wavelength given by θ^{-1} [3]. Close to the transition the normalization of the eigenvector leads to

$$m_s^x = 2\sqrt{1-h^2}\eta^{1/2} \qquad \beta_s^a = \frac{1}{2}. \tag{25}$$

Finally one can also consider the behaviour on the disorder line $h^2 + \eta^2 = 1$ separating the oscillatory phase from the normal one. On this line, the eigenvector is

$$\phi_1(n) = (-1)^n n\rho^{n-1}\phi_1(1) \tag{26}$$

with ρ defined in (23). Thus we obtain

$$m_s^x = \left[1 + \rho^{-2}\sum_{n=1}^{\infty} n^2\rho^{2n}\right]^{-1/2} = \left[1 + \frac{1+\rho^2}{(1-\rho^2)^3}\right]^{-1/2}. \tag{27}$$

Near the special point ($\eta = 0, h = 1$) we have simply $m_s^x \simeq 2\eta^{3/2}$ with a surface magnetic exponent equal to $\frac{3}{2}$. This special value is due to the merging of the two relevant fields of the model. We may note that this expression can be deduced from (21) or (25) using the constraint $h^2 + \eta^2 = 1$.

To summarize, we have determined the surface magnetic behaviour of the *XY* quantum chain using a very simple analysis. We have shown how to deduce the bulk phase diagram and the correlation length from the surface behaviour. This procedure may be of interest for other one-dimensional quantum systems where the surface behaviour is more tractable than the bulk one. Finally one may note that expression (16), cut off at some size L, may be used for finite-size scaling calculations with arbitrary couplings [7].

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