Finite-size scaling and universality in the spin-1 quantum *XY* chain

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Abstract. The spin-1 XY chain in a transverse field is studied using finite-size scaling. The ground-state phase diagram displays a paramagnetic, an ordered ferromagnetic and an ordered oscillatory phase. The paramagnetic–ferromagnetic transition line belongs to the universality class of the 2D Ising model. Along this line, universality is confirmed for the finite-size scaling functions of several correlation lengths and for the conformal operator content.

In modern theories of (equilibrium) critical phenomena, the notions of scaling and universality play a central role. These notions are particularly useful when applied to finite systems using finite-size scaling techniques, see [1] for an extensive review. In this work, we study the effects of varying the spin quantum number on the thermodynamics of the well known XY quantum chain in a transverse field. For spin $\frac{1}{2}$, this model is exactly integrable in terms of free fermions and many of its properties are well studied, see [2, 3]. Besides being of interest in its own right (i.e. for the influence of the quantum effects on the order parameter profile [4]), this quantum Hamiltonian also arises from the master equation description of several *non-equilibrium* statistical systems, see [5]. Here we consider the spin-1 variant of this model, with the Hamiltonian

$$H = -\frac{1}{\zeta} \sum_{n=1}^{N} \left[h S_n^z + \frac{1+\eta}{2} S_n^x S_{n+1}^x + \frac{1-\eta}{2} S_n^y S_{n+1}^y \right] \tag{1}$$

where h is the transverse field, η measures the spin anisotropy, ζ is a normalization constant and N is the system size. We use periodic boundary conditions. Finally, the $S^{x,y,z}$ are spin-1 matrices

$$S^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad S^y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{2}$$

(Spin-1 Ising models were recently proposed to describe the adsorption of CO on graphite, see [6].) We are interested in the ground-state energy E_0, which plays the role of the equilibrium free energy (for reviews see [7, 8]) and in the correlation lengths ξ_i, related

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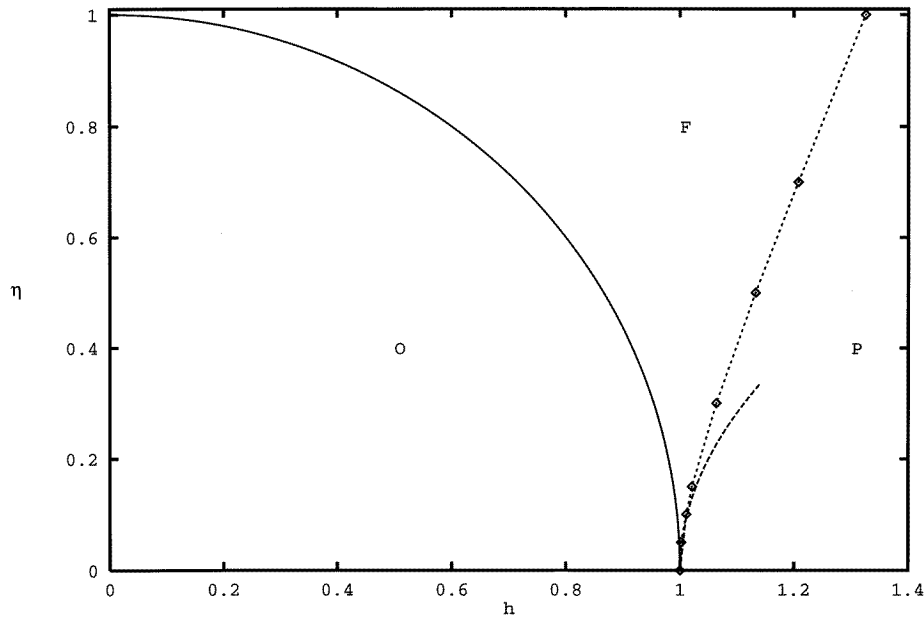
Figure 1. Ground-state phase diagram of the spin-1 XY model (1). P labels the disordered paramagnetic phase, F labels the ordered ferromagnetic phase and O labels the ordered oscillatory phase. The dotted curve gives the P/F transition which for $\eta \neq 0$ is in the 2D Ising universality class. The broken curve, given by $\eta = 2\sqrt{(h-1)/5}$, is the approximation to the P/F line as found from second-order perturbation theory around $\eta = 0$. The full curve represents the F/O transition as given by (5).

to the exponential decay of two-point correlation functions, given by the energy gaps $\xi_i^{-1} = E_i - E_0$. We calculate the low-lying spectrum of H for finite N (up to $N = 14$) using the Lanczos algorithm and then extrapolate towards $N \to \infty$, see [8] for details. The quantum Hamiltonian H commutes with the charge operator Q, the parity operator P and the translation operator T defined by

$$Q = \prod_{i=1}^{N} \left(2(S_i^z)^2 - 1\right) \qquad P S_n^{x,y,z} P^\dagger = S_{N+1-n}^{x,y,z} \qquad T S_n^{x,y,z} T^\dagger = S_{n+1}^{x,y,z}. \tag{3}$$

Eigenstates of H are thus characterized by the eigenvalues of Q, P and T, which serve to block-diagonalize H.

Our first task is to determine the phase diagram, shown in figure 1. We recognize three distinct phases. The first transition, between the paramagnetic phase P and the ferromagnetic phase F, is found from conventional finite-size scaling and will be shown below to be in the 2D Ising universality class. Close to a conventional critical point of second order, the following finite-size scaling form for the inverse correlation lengths is expected [9, 1]

$$\xi_i^{-1} = N^{-1} S_i \left(C N^y (h - h_c) \right) \tag{4}$$

where $h_c = h_c(\eta)$ is the critical point, $y = 2 - x_\epsilon$ a critical exponent, C is a non-universal metric factor and S_i is a *universal* scaling function. In particular, from 2D conformal invariance, it follows that $S_i(0) = 2\pi x_i$ [10], where x_i is a universal critical exponent. Now, the critical point h_c can be found from phenomenological renormalization [7]. The results, extrapolated to $N \to \infty$, are displayed in table 1. For $\eta = 1$ we find agreement with the earlier result [11] $h_c \simeq 1.3259$.

Table 1. Critical points $h_c(\eta)$ and conformal normalization $\zeta(\eta)$ for the spin-1 XY model along the Ising line. The numbers in brackets give the estimated uncertainty in the last digit.

η	0.05	0.1	0.15	0.3	0.5	0.7	1.0
h_c	1.002(1)	1.011(1)	1.0210(1)	1.0637(1)	1.1325(1)	1.2080(1)	1.32587(1)
ζ	—	0.170(1)	0.239(1)	0.4252(1)	0.6416(1)	0.8417(1)	1.12706(1)

Table 2. Extrapolated finite-size estimates for the critical point h_o and the exponent ν for the spin-1 XY model (1) as determined from the second ground-state level crossing $h_2(N)$ of (7).

η	0.1	0.3	0.5	0.7
h_o	0.9955(3)	0.9538(3)	0.8657(3)	0.7136(5)
ν	0.50(1)	0.48(2)	0.48(2)	0.47(3)

The second transition occurs between the ferromagnetic phase F and a new 'oscillatory' phase O. This transition is well known for the spin-$\frac{1}{2}$ case [2] and occurs along the line $h = h_o(\eta)$ where†

$$\eta^2 + h_o(\eta)^2 = 1 \,. \tag{5}$$

For spin $\frac{1}{2}$ it is known that while in the F phase the connected spin–spin correlation function $\langle S_R^x S_0^x \rangle_c$ decays monotonically with R, the oscillatory phase is characterized by a new wave vector K which modulates the spin–spin correlator [2]

$$\langle S_R^x S_0^x \rangle_c \sim R^{-2} \exp(-2R/\xi) \cos(KR) \,. \tag{6}$$

Furthermore, in the oscillatory phase there are level crossings in the ground-state energy which occur already for *finite* values of the number of sites N [12, 4]. It was shown in [12] that the location $h_k(N)$ of the kth level crossing satisfies a finite-size scaling law

$$h_o - h_k(N) \sim N^{-1/\nu} \tag{7}$$

where the exponent ν describes the scaling of the wave vector $K \sim (h_o - h)^\nu$ in the vicinity of the O/F transition line (for $h \leqslant h_o$). For spin $S = \frac{1}{2}$, it is known that $\nu = \frac{1}{2}$ [12].

We now ask whether a similar transition occurs for larger values of S. Indeed, it is known that for *arbitrary* spin S and periodic boundary conditions, the ground-state energy of H is doubly degenerate at $h = h_o(\eta)$ [13]. For spin $S = 1$, we have checked numerically that the first ground-state level crossing $h_1(N)$ always occurs at $h = h_o(\eta)$ for all finite N. In addition, the second crossing $h_2(N)$ converges towards $h_o(\eta)$, as apparent from the extrapolated data in table 2. The exponent found from equation (7) is consistent with $\nu \simeq \frac{1}{2}$, independently of η and in agreement with the exact result for spin $\frac{1}{2}$. This supports universality along the F/O transition line. In fact, having confirmed the same finite-size scaling behaviour of the level crossings in the ground-state energy for both spin $S = \frac{1}{2}$ and $S = 1$, we expect the features of the oscillatory phase known [2, 12] from $S = \frac{1}{2}$ to be present for $S = 1$ as well.

From now on, we concentrate on the P/F transition line. We expect this transition to be in the 2D Ising universality class, if $\eta \neq 0$. To see this, we compare the low-lying excitation spectrum of H with the prediction of conformal invariance [14, 8], following the

† Along this line H can also be obtained from the master equation of certain 1D stochastic systems [5].

steps outlined for the spin-$\frac{1}{2}$ case in [8, p 135]. Conformal field theory states that, after subtraction of a purely extensive term, H can be written in the form

$$H = \frac{2\pi}{N}(L_0 + \bar{L}_0) - \frac{\pi c}{6N} + \mathrm{o}\left(\frac{1}{N}\right) \tag{8}$$

where c is the central charge and L_0, $\bar{L}_0$ are generators of the Virasoro algebra which acts as a dynamical symmetry for H. As a consequence, eigenstates can be grouped into 'conformal towers', each represented by exactly one primary operator with conformal weights $(\Delta, \bar{\Delta})$. The scaling dimension of the corresponding eigenstate is $x = \Delta + \bar{\Delta}$. The scaled energies and momenta take the form

$$\mathcal{E}_{\Delta,\bar{\Delta}}(I, \bar{I}) \equiv \lim_{N\to\infty} \left(E_{\Delta,\bar{\Delta}}(I, \bar{I}) - E_0\right)\frac{N}{2\pi} = (\Delta + I) + (\bar{\Delta} + \bar{I}) \tag{9}$$

$$\mathcal{P}_{\Delta,\bar{\Delta}}(I, \bar{I}) \equiv \lim_{N\to\infty} P_{\Delta,\bar{\Delta}}(I, \bar{I})\frac{N}{2\pi} = (\Delta + I) - (\bar{\Delta} + \bar{I}) \tag{10}$$

with I, $\bar{I}$ integer. $E_{\Delta,\bar{\Delta}}$, $P_{\Delta,\bar{\Delta}}$, respectively, are the eigenvalues of H, $\mathrm{i}\ln T$ and E_0 is the ground-state energy. However, the application of these relations requires that the scaled energies $\mathcal{E}$ and momenta $\mathcal{P}$ are measured in the same units, thus fixing the normalization ζ of H accordingly. We find ζ by demanding that $\mathcal{E}_{0,0}(2, 0) = 2$ throughout [14]. The results for ζ are given in table 1.

Next, we determine the central charge. For $\eta = 1$, we find $c = 0.49999(1)$, close to the expected $c = \frac{1}{2}$ for the 2D Ising universality class. We did not compute c explicitly for other values of η, but expect c to be η-independent. In order to check the complete operator content, we give the extrapolated values of the scaled energies in the charge sectors $Q = 0$ and $Q = 1$ in tables 3 and 4. When comparing these spectra to the expected operator content of the 2D Ising model [14, 8], namely for the $Q = 0$ sector the conformal towers generated by the primary operators $(0, 0)$ and $(\frac{1}{2}, \frac{1}{2})$ (which correspond to the vacuum **1** and the energy density ϵ) and for the $Q = 1$ sector the conformal tower generated by $(\frac{1}{16}, \frac{1}{16})$ (which corresponds to the order parameter density σ), we find complete agreement. In particular, we read off the scaling dimensions $x_\sigma = \frac{1}{8}$ and $x_\epsilon = 1$ which determine the bulk critical exponents.

We now look at the finite-size scaling functions for the spin–spin and energy-energy correlation lengths $\xi_{\sigma,\epsilon}^{-1} = N^{-1}S_{\sigma,\epsilon}(C_{\sigma,\epsilon}z)$, see equation (4). From universality with $S = \frac{1}{2}$, we expect [3]

$$\frac{1}{2\pi}S_\sigma(C_\sigma z) = \frac{1}{8} + \frac{1}{4\pi}C_\sigma z + \frac{\ln 2}{4\pi^2}(C_\sigma z)^2 + \frac{1}{2}R_{1\frac{1}{2},0}\left(\frac{(C_\sigma z)^2}{4\pi^2}\right) - \frac{1}{8}R_{1\frac{1}{2},0}\left(\frac{(C_\sigma z)^2}{\pi^2}\right) \tag{11}$$

$$\frac{1}{2\pi}S_\epsilon(C_\epsilon z) = \sqrt{1 + \frac{(C_\epsilon z)^2}{\pi^2}} \tag{12}$$

where $z = N(h - h_c)$ is the finite-size scaling variable and $R_{1\frac{1}{2},0}(x)$ is a remnant function [15]. The spin-dependence should only enter into the metric factors C_σ and C_ϵ which are determined from S_σ and S_ϵ, respectively. In figure 2, we display the extrapolated finite-size data of $S_{\sigma,\epsilon}$ for $\eta = 0.7$ and find that they match nicely with the expected functional form. This confirms universality. Similar plots are obtained for other values of η. The results for the metric factors are collected in table 5. Our results are consistent with

$$C_\sigma(\eta) = C_\epsilon(\eta) = C(\eta). \tag{13}$$

It is interesting to compare these with the conformal normalization $\zeta(\eta)$ from table 1. Our data are roughly consistent with a linear relation $C^{-1}(\eta) = \alpha\zeta(\eta)$ with $\alpha \simeq 0.75$.

Table 3. Low-lying excitations for charge $Q = 0$ at the critical point. For each value of $\mathcal{E}$, the upper value corresponds to $\eta = 1$, the lower one to $\eta = 0.3$. A dash indicates that no level is present, a '?' indicates that the finite-size data did not converge. For $\mathcal{P} = 0$, all eigenstates shown have parity $P = +1$ and the lowest excitations with $P = -1$ occur for $\mathcal{E} \geqslant 6$.

$\mathcal{E}$	$\mathcal{P}$				
	0	1	2	3	4
5		?	5.03(3)	?	4.8(2)
		?	?	?	?
4	?	3.98	—	4.00(1)	3.95(3), 3.94(3)
	?	3.99(2)	—	3.9(1)	?
3	3.00(1)	—	3.000(1)	2.999(1)	—
	3.00(1)	—	3.001(1)	3.00(2)	—
2	—	2.00000(1)	2	—	—
	—	2.000(1)	2	—	—
1	1.00000(1)	—	—	—	—
	1.0002(2)	—	—	—	—
0	0	—	—	—	—
	0	—	—	—	—

Table 4. Low-lying excitations for charge $Q = 1$. For each value of $\mathcal{E}$, the upper value corresponds to $\eta = 1$, the lower one to $\eta = 0.3$.

$\mathcal{E}$	$\mathcal{P}$			
	0	1	2	3
$5\frac{1}{8}$	?	5.2(1), 5.18(2)	?	?
	?	?	?	?
$4\frac{1}{8}$	4.123(2)	—	4.128(2), 4.13(1)	—
	4.1(1)	—	4.13(1), ?	—
$3\frac{1}{8}$	—	3.124(1)	—	3.125(1), 3.124(1)
	—	3.12(1)	—	3.1(1), 3.1(1)
$2\frac{1}{8}$	2.1249(1)	—	2.1251(2)	—
	2.126(2)–2.121(2)			—
$1\frac{1}{8}$	—	1.12501(1)	—	—
	—	1.1249(1)	—	—
$\frac{1}{8}$	0.12499(1)	—	—	—
	0.1249(1)	—	—	—

Table 5. Non-universal metric coefficients C_ϵ, C_σ found from the scaling functions S_ϵ and S_σ, respectively.

η	0.3	0.5	0.7	1.0
C_ϵ	2.86(2)	2.01(2)	1.57(2)	1.21(2)
C_σ	2.86(2)	1.98(2)	1.57(2)	1.20(2)

A few comments are in order. Firstly, the observation (equation (13)) that the numerical value of the metric factor is independent of the physical quantity used for its determination is certainly in agreement with the scaling expectation (equation (4)) [1]. Similar results were recently reported for 2D percolation [16], where it was also checked that the metric factors
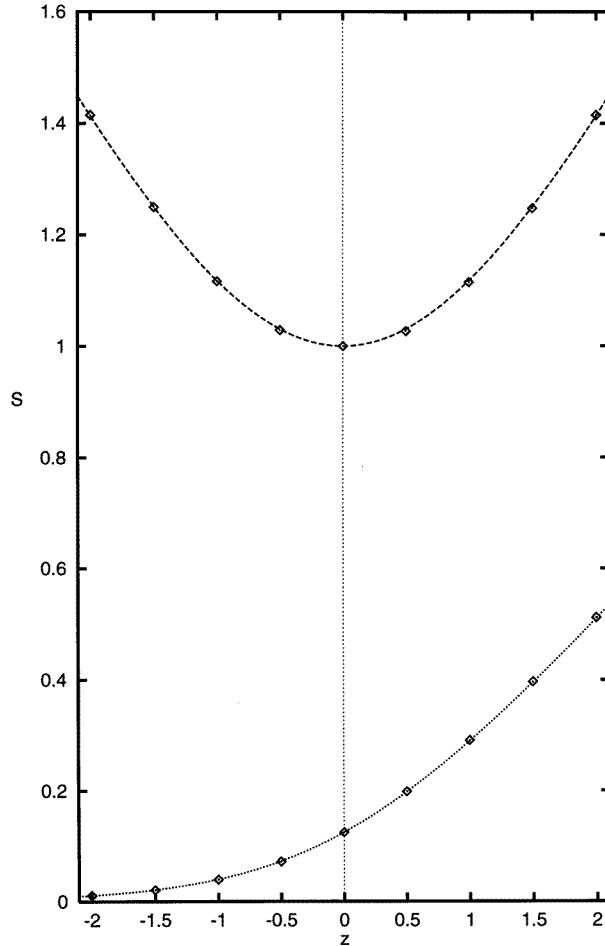
Figure 2. Finite-size scaling functions $S_\sigma(C_\sigma z)$ (lower curve) and $S_\epsilon(C_\epsilon z)$ (upper curve) as a function of the finite-size scaling variable $z = N(h - h_c)$ compared to the extrapolated finite-lattice estimates for $\eta = 0.7$ (points).

are independent of the boundary conditions. Secondly, our results confirm earlier work [17] on the universality of the finite-size scaling function S_σ in the 2D spin-1 Ising model. Thirdly, the observed linear relation between the conformal normalization ζ and the metric factor C can be understood in terms of conformal perturbation theory, see [14, 8]. In that framework, one would write for the non-critical quantum Hamiltonian $H = \frac{1}{\zeta}(H_c + g\phi)$, where H_c is the critical point quantum Hamiltonian, ϕ a perturbing relevant operator and g a non-universal coupling. In our case, $\phi = \epsilon$, the energy density and $g = h - h_c$. Since a given quantum Hamiltonian must in general be normalized to make conformal invariance applicable (see above), we note that only the finite-size scaling variable $N^{2-x_\phi}(h - h_c)/\zeta$ enters into a perturbative calculation of the energy spectrum. That is consistent with our finding $C \sim \zeta^{-1}$.

In conclusion, we have investigated the ground-state phase diagram of the spin-1 quantum XY chain in a transverse magnetic field. The structure of the phase diagram, obtained from finite-size scaling, is found to be very similar to the known spin-$\frac{1}{2}$ case. We

have explicitly confirmed the universality of the Ising line, with respect to the spin S as well as the spin anisotropy η, considering both the conformal operator content and the finite-size scaling functions of the first two correlation lengths.

Acknowledgments

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