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LETTER TO THE EDITOR

Statistical mechanics of the 2D quantum XY model in a transverse field

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Abstract. The 2D quantum XY model is introduced and the phase diagram is obtained. The model shows a paramagnetic, an ordered ferromagnetic and an ordered 'oscillatory' phase. The line of phase transitions from the paramagnetic to the ferromagnetic phase is seen to be in the same universality class as the 3D Ising model. Along this line, critical exponents are $\nu = 0.629 \pm 0.002$ and $\beta = 0.324 \pm 0.009$.

In this letter we summarise the results of a study on the two-dimensional XY-model in a transverse field using finite size scaling. The Hamiltonian reads

$$H = -h \sum_n \sigma^z(n) - \sum_{(n,n')} \left\{ \frac{1}{2}(1 + \eta) \sigma^x(n) \sigma^x(n') + \frac{1}{2}(1 - \eta) \sigma^y(n) \sigma^y(n') \right\}, \quad (1)$$

where nearest-neighbour interactions are understood and σ^x , σ^y , σ^z are the Pauli matrices. Although the model is well known in one dimension (see e.g. Barouch and McCoy 1971), in two dimensions only the $\eta = 1$ case, which corresponds to the (2+1)D Ising model, has been studied (Marland 1981, Hamer 1983, Hamer and Irving 1984). For all values of η , H is taken as a quantum Hamiltonian with h as a temperature-like variable.

For $\eta \neq 0$, the global symmetry is Z_2 , thus H can be written as the direct sum of block matrices. The blocks are labelled by their charge 0 and 1, respectively, according to the eigenvalues of the operator

$$B = \frac{1}{2} \left[1 - \exp \left(i \pi \sum_n \sigma^z(n) \right) \right]. \quad (2)$$

Let $E_0(h)$ be the lowest eigenvalue of H in the charge sector 0 and $E_1(h)$ the lowest eigenvalue in the charge sector 1. Numerical calculations show that these are the two lowest eigenvalues of H . The energy gap is

$$m(h) = E_1(h) - E_0(h) \quad (3)$$

and the beta function reads (e.g. Hamer 1983)

$$\beta(h) = m(h) / [2hm'(h) - m(h)]. \quad (4)$$

The magnetisation is computed as follows (Yang 1952, Hamer 1982). Let $|0\rangle$, $|1\rangle$ be the eigenvectors corresponding to $E_0(h)$ and $E_1(h)$. Then the magnetisation is given by

$$M = \langle 0 | \mathcal{M} | 1 \rangle, \quad (5)$$

where the magnetisation operator per spin is (\mathcal{N} is the number of sites):

$$\mathcal{M} = \frac{1}{\mathcal{N}} \sum_n \sigma^x(n). \quad (6)$$

The following boundary conditions will be considered:

- (1) periodic boundary conditions in both charge sectors;
- (2) antiperiodic boundary conditions in the charge sector 0, and periodic boundary conditions in the charge sector 1.

For brevity, these boundary conditions will be referred to as 'periodic' (PP) and 'antiperiodic' (AP), respectively. For the (1+1)D case, the AP conditions give the exact energy gap for every lattice with at least two sites. Even if this does not hold true for more general models, the convergence of the estimates of the critical parameters is improved, as first shown for a Z_3 -spin-chain by Centen *et al* (1982).

The eigenvalues were obtained for square $N \times N$ lattices, with $N = 2, 3, 4, 5$.

We now consider the phase diagram shown in figure 1. One has a paramagnetic, an ordered ferromagnetic and an ordered 'oscillatory' phase. The critical line separating the paramagnetic and the ferromagnetic phases belongs to the 3D Ising universality class, if $\eta \neq 0$. The transition to the oscillatory phase is given for periodic boundary conditions by an N -independent zero of the energy gap which occurs at $h = h_z$, where h_z is given by

$$(h_z/2)^2 + \eta^2 = 1. \quad (7)$$

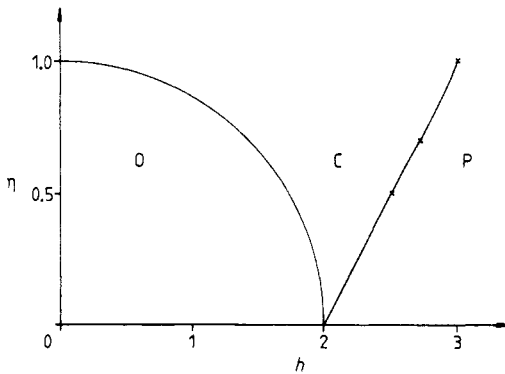


Figure 1. Phase diagram of the 2D quantum XY model. The phases are labelled as: P = paramagnetic; C = ferromagnetic (commensurate); O = oscillatory.

At the point $h = h_z$, the model displays a long-range antiferromagnetic ordering. This kind of effect has also been observed for a 1D quantum Heisenberg model (Kurmman *et al* 1982). For $h < h_z$, the energy gap shows an oscillating behaviour. Further investigations on the phases will be given in a later paper, (Henkel and Hoeger 1984).

From now on we concentrate on the Ising critical line. We shall determine the critical parameters using finite-size scaling theory (Fisher 1971).

Estimates (h_N) of the critical field $h_c(\eta)$ are obtained from both boundary conditions by solving

$$Nm_N(h_N) = (N-1)m_{N-1}(h_N). \quad (8)$$

The results are shown in table 1. Now the mean

$$\bar{h}_N = \frac{1}{2}(h_N^{PP} + h_N^{AP}) \tag{9}$$

is less dependent on N than h_N^{PP} or h_N^{AP} for $\eta = 1.0$ and $\eta = 0.7$. In these cases, the sequences \bar{h}_N is extrapolated with both the van den Broeck and Schwartz (1979) and the Lubkin (1952) algorithm. For $\eta = 0.5$ only the sequence h_N^{AP} is extrapolated. the mean of both algorithms is our estimate of $h_c(\eta)$. The results are:

$$\begin{aligned} h_c(1.0) &= 3.05 \pm 0.01, \\ h_c(0.7) &= 2.720 \pm 0.006, \\ h_c(0.5) &= 2.50 \pm 0.01, \end{aligned} \tag{10}$$

where the errors quoted in (10) are estimated from the fact that the sequence h_N decreases for periodic while increasing for 'antiperiodic' boundary conditions (this holds for $\eta = 1.0$ and 0.7 ; for $\eta = 0.5$ we expect the error to have the same order of magnitude as in the other cases).

Table 1. Finite-size estimates of the critical field $h_c(\eta)$ for periodic and 'antiperiodic' boundary conditions.

N	$\eta = 1.0$		$\eta = 0.7$		$\eta = 0.5$	
	PP	AP	PP	AP	PP	AP
2	3.841 10	4.800 00	3.926 37	4.431 75	3.963 33	4.230 30
3	3.164 56	2.999 79	2.711 80	2.715 68	2.409 90	2.503 06
4	3.084 05	3.022 97	2.732 45	2.709 74	2.492 49	2.502 25
5	3.060 95	3.036 05	2.726 31	2.713 59	2.501 98	2.500 87

Now we determine the critical exponent ν . In table 2 we give the slope of the energy gap evaluated at the fields h_N (see table 1). The value of ν can be estimated independently for each value of η , N and for each boundary condition from the finite-size behaviour of the beta function (4):

$$-\frac{1}{\nu_N(\varepsilon)} = \frac{\ln[\beta_N(h_N)/\beta_{N-1}(h_N)]}{\ln[(N + \varepsilon)/(N - 1 + \varepsilon)]} \tag{11}$$

where the parameter ε is introduced to check for stability. The stability region is bounded by those values of ε (denoted by ε_1 and ε_2 , respectively) at which the sequence

Table 2. Slope of the energy gap evaluated at the field h_{N_2} (see table 1) with $m = m(h - h_c)$.

N_1, N_2	$\eta = 1.0$		$\eta = 0.7$		$\eta = 0.5$	
	PP	AP	PP	AP	PP	AP
2, 3	1.7759	2.3399	1.7577	2.2223	1.7500	2.1427
	1.9597	2.7699	1.8551	2.6212	1.7318	2.4891
3, 4	1.9204	2.7552	1.8688	2.6253	1.8223	2.4897
	2.1370	3.1689	2.0520	3.0153	1.9607	2.8569
4, 5	2.1163	3.1509	2.0472	3.0092	1.9750	2.8532
	2.3325	3.5348	2.2434	3.3736	2.1462	3.1953

$1/\nu_N(\varepsilon)$ changes from monotonic (either increasing or decreasing) to oscillatory behaviour. We now take

$$1/\nu_N = \frac{1}{2}(1/\nu_N(\varepsilon_1) + 1/\nu_N(\varepsilon_2)) \quad (12)$$

to estimate $1/\nu$ with the accuracy

$$\Delta\left(\frac{1}{\nu_N}\right) = \frac{1}{2}|1/\nu_N(\varepsilon_1) - 1/\nu_N(\varepsilon_2)|. \quad (13)$$

These numbers are given in table 3 for $\eta = 1.0, 0.7$ and 0.5 and the different boundary conditions, together with the respective values for the ε 's.

The weighted mean of the data in table 3 gives for ν :

$$\nu = 0.629 \pm 0.002. \quad (14)$$

To improve convergence, the energy gap was taken as a function $m = m[(h - h_N)/h_N]$ for the AP1 case and $\eta = 0.7$ periodic boundary condition and in the form $m = m(h - h_N)$ for all the other cases.

Table 3. Finite-size estimates (equation (12)) for the exponent $1/\nu$. The numbers given in brackets at the bottom of each column are the respective values for ε_1 and ε_2 .

	N	PP	AP
$\eta = 1.0$	3	1.592 ± 0.002	1.60 ± 0.02
	4	1.592 ± 0.002	1.605 ± 0.015
	5	1.592 ± 0.002 (0.11/0.12)	1.604 ± 0.010 (-0.075/-0.020)
$\eta = 0.7$	3	1.57 ± 0.07	1.577 ± 0.007
	4	1.59 ± 0.05	1.575 ± 0.005
	5	1.58 ± 0.04 (-0.435/-0.25)	1.576 ± 0.004 (-0.07/-0.05)
$\eta = 0.5$	3	2.7 ± 1.0	1.61 ± 0.06
	4	2.8 ± 0.9	1.63 ± 0.04
	5	2.6 ± 0.8 (1.33/6.0)	1.62 ± 0.03 (0.01/0.205)

The magnetisation exponent β is determined by the same method. At the critical field $h_c(\eta)$ (equation (10)) the magnetisation was computed from (6) for periodic boundary conditions (see table 4). Going through the same kind of analysis, we obtain:

$$\beta = 0.324 \pm 0.009. \quad (15)$$

Table 4. Finite-size magnetisation at the critical field for periodic boundary conditions.

$N \backslash \eta$	1.0	0.7	0.5
1	1.0	1.0	1.0
2	0.7290	0.7063	0.6806
3	0.6036	0.5799	0.5531
4	0.5251	0.5030	0.4768
5	0.4699	0.4501	0.4223

The only estimates available in the literature are for the Ising model ($\eta = 1$) and periodic boundary conditions only (Hamer 1983, Hamer and Irving 1984), giving $\nu = 0.635 \pm 0.005$ and $\nu = 0.64$, respectively.

Our results compare well with the results available for the 3D Ising universality class (e.g. Le Gillou and Zinn-Justin 1980, Marland 1981, Pearson 1984, Pawley *et al* 1984).

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