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LETTER TO THE EDITOR

Quantum phase transitions in the J–J' Heisenberg and XY spin-$\frac{1}{2}$ antiferromagnets on a square lattice: finite-size scaling analysis

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Abstract
We investigate the critical parameters of an order–disorder quantum phase transition in the spin-$\frac{1}{2}$ J–J' Heisenberg and XY antiferromagnets on a square lattice. Based on the excitation gaps calculated by the exact diagonalization technique for systems up to 32 spins and finite-size scaling analysis we estimate the critical couplings and exponents of the correlation length for both models. Our analysis confirms the universal critical behaviour of these quantum phase transitions: they belong to 3D O(3) and 3D O(2) universality classes, respectively.

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The equivalence of the critical behaviour of D-dimensional quantum spin systems and $(D+1)$-dimensional classical spin systems is well recognized. This idea, combined with finite-size scaling was used previously many times to discuss the critical properties of infinite spin systems, see e.g., [1–3] for a review. However, these investigations were strongly limited with respect to the system size. Due to the recent advances in computer technology it is possible to treat bigger systems, e.g., up to 36 sites for spin $\frac{1}{2}$, and consequently to extract their critical properties using the finite-size scaling method [4, 5]. Our aim is to present in this Letter the results of such an investigation of critical parameters (coupling and exponents of correlation length) for the J–J' Heisenberg and XY spin-$\frac{1}{2}$ antiferromagnets on a square lattice.

The Hamiltonian of the model whose critical behaviour is examined is given by

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J' \sum_{\langle k,l \rangle} \vec{S}_k \cdot \vec{S}_l. \tag{1}$$

The first sum, denoted by $\langle i, j \rangle$, runs over pairs of nearest-neighbours on the square lattice connected by thin bonds (see figure 1), whereas the second one, denoted by $\langle k, l \rangle$—over

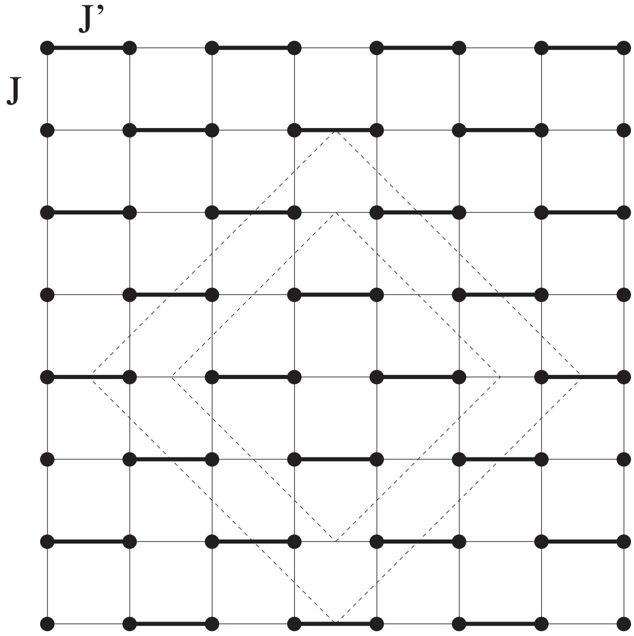

Figure 1. The J–J' model on square lattice. Finite systems of eight and 18 spins are marked by dashed lines.

nearest-neighbours connected by thick bonds. In the case of a Heisenberg spin system three Pauli matrices are included in the scalar product in equation (1), in the case of an *XY* system—only two are included. The model represents an antiferromagnet, i.e. both couplings are positive and additionally, $J' \geqslant J$. Clearly, what one can see here is the competition between long-range Néel order and the tendency for the formation of local singlets of two neighbouring spins, coupled via J'. In limiting cases this model reduces to the long-range ordered Heisenberg antiferromagnet on a square lattice for $J = J'$ on the one hand, and on the other to disjoint singlets (no staggered magnetization) for $J'/J \to \infty$. At some (J'/J) there exists a quantum phase transition between the gapless Neél phase and a gapped 'singlet' phase (quantum paramagnet). The properties of the J–J' Heisenberg model on the square lattice were first examined by series expansion (SE) [6] and more recently by the renormalized spin wave (RSW) approach [7], exact diagonalization (ED) and the coupled cluster method (CCM) [9] in order to observe the interplay between the local singlet formation tendency and the long-range Néel order. Although, in general, all those methods predict the existence of quantum phase transition, they differ drastically in the estimation of the critical coupling. Furthermore, there was only one attempt [6] to find critical exponents, however, the error in this estimation was rather large.

Let us now rewrite the Hamiltonian in such a form that the two above tendencies will be seen more clearly:

$$H = g\left(\sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j + \frac{1}{g^2}\sum_{\langle k,l\rangle} \vec{S}_k \cdot \vec{S}_l\right) \qquad 0 < g \leqslant 1. \tag{2}$$

Note that in equation (2) one has the same summation specification as in equation (1). The coupling constant g determines the relevant energy scale in the model under consideration and the term $1/g^2 = \lambda$ is analogous to an inverse temperature.

Table 1. Pseudo-critical points λ_c calculated for two Heisenberg systems of sizes given in the first column. The values of the gap Δ and its derivative Δ' at the pseudo-critical point λ_c are also listed. To find them 11 ED data points equally spaced around λ_c were fitted to the polynomial of fourth order in λ in the region of $\lambda_c \pm 0.005$. Five digits are exact.

System size	λ_c	Δ	Δ'
8	3.1166	4.144 95	1.523 50
18		2.763 30	1.710 55
8	2.9251	3.859 80	1.452 96
32		1.929 90	1.813 04
18	2.7648	2.204 67	1.446 63
32		1.653 50	1.625 65
Extrapolated	2.46(2)		

Table 2. Same as table 1, but for *XY* spin systems.

System size	λ_c	Δ	Δ'
8	4.9326	2.516 53	0.786 928
18		1.677 68	0.848 422
8	4.7705	2.390 28	0.770 058
32		1.195 14	0.942 901
18	4.6444	1.441 52	0.788 049
32		1.081 14	0.866 564
Extrapolated	4.56(2)		

In what follows the estimation of the critical value of g_c and critical exponent $1/\nu$ for the Heisenberg and *XY* Hamiltonians will be described. At the beginning one finds by the ED (Lanczos algorithm) the spin gap, defined as $\Delta = E_1 - E_0$ ($E_{0(1)}$ is the lowest energy in the $S^z = 0(1)$ sector) dependence versus $\lambda = 1/g^2$ for the Hamiltonian (2) on a square lattice for a sequence of finite systems. Note that all the systems, being elements of the sequence should be invariant under the same symmetry operations; in the opposite case it is not possible to find a proper scaling. In the system under examination one has only three such systems: with $N = 8$, 18 and 32 spins. Two of them are shown in figure 1, the third one has the same shape.

The spin gap, multiplied by the linear dimension of the system, $\Delta\sqrt{N}$, allows one to find the pseudo-critical points [3]: for the Heisenberg and *XY* systems one has three such points, collected in tables 1 (Heisenberg) and 2 (*XY*). Next one should extrapolate the sequence of pseudo-critical points to infinity. However, it is not possible here to employ any algorithm improving the convergence of the finite-lattice data sequence since the series is extremely short. Therefore we find it more accurate to use graphical methods to find the critical value of g. The sequences of pseudo-critical points for Heisenberg and *XY* system plotted versus $1/L^4$ are shown in figure 2. The estimate of $1/g_c^2 = 2.46(2)$ for the infinite Heisenberg system should be compared to the value 2.56 obtained by SE [6], to the value of 3.16 obtained by the CCM method, to the value of 2.45 from ED [9] and finally to the value of 5.0 [7] from the RSW approach. The extrapolated value of $1/g_c^2 = 4.56(2)$ for the *anisotropic XY* system is higher, as one should expect, than that for Heisenberg system since anisotropy acts against the singlet formation [8].

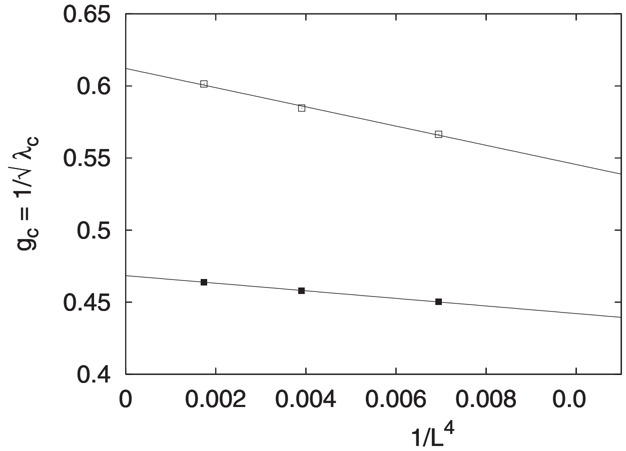

Figure 2. Extrapolation of the finite-system pseudo-critical points as a function of $1/L^4$. Open squares—Heisenberg model, filled squares—*XY* model.

The critical exponent for the correlation length, ν, may be estimated from the behaviour of the Callan–Symanzik β-function [1, 3, 10]:

$$\beta(\lambda)/g = \frac{\mathrm{d}}{\mathrm{d}g}\ln[g\Delta(\lambda)] \tag{3}$$

which, calculated for a finite system of linear size L in a pseudo-critical point, scales as

$$\beta(\lambda_c, L) \sim L^{-1/\nu}. \tag{4}$$

Usually, in order to see this scaling behaviour, one takes into account a sequence of $\beta(L_i)/\beta(L_{i-1})$ values calculated at the pseudo-critical points for some values of L_i, such that $L_i = L_{i-1} + 1$. Expanding

$$\beta(L_i)/\beta(L_{i-1}) \sim (1 + 1/L_i)^{-1/\nu} \sim 1 - \frac{1}{\nu}\frac{1}{L_i} + \cdots \tag{5}$$

one finds a linear behaviour of $(1 - \beta(L_i)/\beta(L_{i-1}))$ versus $1/L$ for all i. This is the 'linear' approximation. Note that the error is $\mathrm{O}(1/L^2)$. However, if one cannot find a sequence of finite systems fulfilling $L_i = L_{i-1} + 1$ (in our case $L_i = L_{i-1} + \sqrt{2}$) this approximation is rather crude because of the order of the error. This may be improved in the following way. First, let us note that in the following expansion, for small x

$$\ln\left(\frac{1+x}{1-x}\right) = 2x + \frac{2}{3}x^3 + \cdots \tag{6}$$

the term x^2 is absent and the error is $\mathrm{O}(x^3)$. Second, let us put

$$x = \frac{L_i - L_{i-1}}{L_i + L_{i-1}} \tag{7}$$

and expand

$$\ln[\beta(L_{i-1})/\beta(L_i)] \sim \frac{1}{\nu}\ln\left(\frac{1+x}{1-x}\right) \sim \frac{2}{\nu}\frac{(L_i - L_{i-1})}{(L_i + L_{i-1})} + \cdots. \tag{8}$$

Consequently one has a linear dependence of $\ln[\beta(L_i)/\beta(L_{i-1})]$ versus $1/L$:

$$\ln[\beta(L_{i-1})/\beta(L_i)] \sim \frac{\sqrt{2}}{\nu}\frac{1}{\bar{L}_i} + \cdots \tag{9}$$

Table 3. Values of critical exponent $1/\nu$ calculated for two pseudo-critical points for finite Heisenberg and *XY* spin systems and subsequently extrapolated to infinity. For comparison we also include values of the same exponents calculated by other authors.

System size	Heisenberg, O(3)	*XY*, O(2)
8–18	1.9841	1.6220
18–32	1.8323	1.6014
Extrapolated	1.44(4)	1.55(4)
	1.46(8) [11]	1.495(5) [13]
	1.418(6) [12]	1.49(1) [14]
		1.51(1) [15]

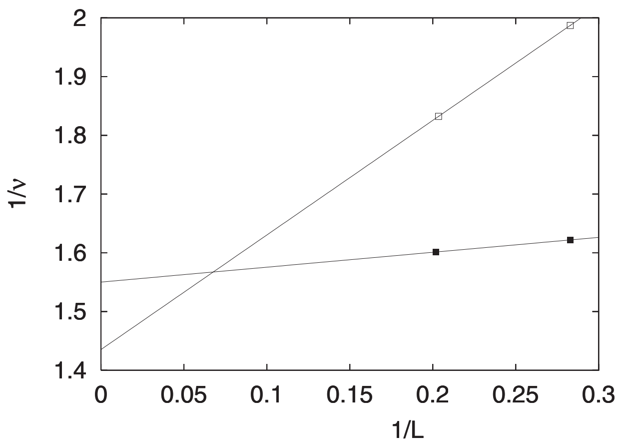

Figure 3. Extrapolation of the finite-system estimates of the $1/\nu$ exponent a function of $1/L$. Open squares—Heisenberg model, filled squares—*XY* model.

where $\bar{L}_i = (L_i + L_{i-1})/2$. The main advantage of this approach is a small finite size error, which in consequence enables one to examine smaller systems. However, there remains yet another problem. It is possible to consider scaling from two pseudo-critical points: (8–18) where $x = 1/5$ and (18–32)—where $x = 1/7$. For the third point the expansion (8) gives rather large finite size correction ($x = 1/3$) and this point has to be excluded. Thus, one can ask whether it is possible to find a scaling relation and to estimate critical exponent from two points only? The answer is yes, but the final error will be larger. Since the expansion (8) produces an error $O(x^3)$, it seems to be especially well suited to this purpose. To test this approach we have extrapolated the $1/\nu$ exponent from the data for the transverse Ising model on a square lattice [5] taking into account only two pseudo-critical points: (16–25) and (25–36). The estimate of $1/\nu = 1.586(7)$ obtained by simple linear extrapolation from these two points should be compared to the original one $1/\nu = 1.591(1)$ [5], extrapolated from four points.

The data collected in tables 1 and 2 enables one to calculate β-function from equation (3) and consequently $1/\nu$ from equation (9) for each pseudo-critical point of J–J' model; their values for the Heisenberg and *XY* Hamiltonians are listed in table 3 and the graphical extrapolation is shown in figure 3. The values of critical exponents for the same universality classes obtained by other authors are also displayed in table 3.

One should note that the error in the present approach is larger than in other finite-size scaling analysis, but as was mentioned this is a result of the small number of systems with required symmetry, see figure 1, and the error is still comparable with an error resulting from extensive Monte Carlo simulation [11, 12].

To conclude, we have presented the results of the investigation of the critical parameters for the quantum phase transitions in the spin-$\frac{1}{2}$ J–J' Heisenberg and XY antiferromagnets on a square lattice. The obtained values of the correlation length critical exponents strongly suggest that these transitions belong to the 3D O(3) and 3D O(2) universality classes, respectively.

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