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Breakdown of scaling in the 1D spin-1/2 Heisenberg ferromagnet

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The problem of the critical behavior of the spin-1/2 Heisenberg ferromagnetic chain has challenged many research workers since 1964. We discuss the critical exponents α and γ recently determined by Schlottmann and by Takahashi and Yamada in the context of previously known $T_c = 0$ critical properties of the 1D $s = 1/2$ XXZ model and the classical Heisenberg model, and we comment on the manifest breakdown of scaling in the $s = 1/2$ Heisenberg ferromagnet.

The critical behavior of the one-dimensional (1D) $s = 1/2$ Heisenberg ferromagnet (HB FM) at $T = 0$ has been a problem of interest for more than 20 years. A variety of numerical and approximate analytic approaches have yielded a considerable diversity of values for some of the $T_c = 0$ critical exponents. In Table I we list the nature of these approaches and the resulting exponent values in chronological order.[1-8] Very recently, Schlottmann,[6] and Takahashi and Yamada[7] have solved numerically the coupled integral equations of the Bethe-ansatz formalism by different and independent approaches. The fact that both calculations agree and predict the exponent values $\alpha = -1/2$ for the specific heat and $\gamma = 2$ for the susceptibility is reasonable evidence that these are the correct values. The purpose of this communication is to discuss these interesting results in the broader context of $T_c = 0$ critical behavior of quantum spin systems.[9] We wish to relate these new findings to the known $T_c = 0$ critical properties of other 1D spin models such as the $s = 1/2$ Heisenberg antiferromagnet (HB AFM), the more general $s = 1/2$ XXZ model, and the classical Heisenberg model. We continue a recent discussion focusing on the scaling behavior at the critical point of the $s = 1/2$ HB FM[4-6] by pointing out that this system does not only violate hyperscaling but scaling itself.[9] Finally, we make some observations on the relative accuracy of various numerical and approximate analytic approaches designed to solve this problem.

The scaling and hyperscaling hypotheses for a continuous phase transition imply that the six critical exponents α (specific heat), β (order parameter), γ (susceptibility), δ (symmetry-breaking field), η (correlation function), and ν (correlation length) are expressible in terms of only two scaling powers a_T and a_H as listed in Table II. Only the relations for η and ν, which are based on the (more stringent) hyperscaling hypothesis, involve the dimensionality D of the system. For $T_c = 0$ critical points, the temperature-like scaling variable is the absolute temperature T, giving rise to confluent singularities in the specific heat and the susceptibility for $T \to 0$.[10] The modified dependence on the two scaling powers a_T and a_H of the exponents α and γ is given at the bottom of Table II.

It is most illuminating to discuss the validity of these scaling relations for the 1D classical ($s = \infty$) and quantum $s = 1/2$ HB FM ($J > 0$) and HB AFM ($J < 0$),

$$H = -J \sum_{l=1}^{N} \mathbf{S}_l \cdot \mathbf{S}_{l+1} , \tag{1}$$

as well as for the more general $s = 1/2$ XXZ model,

$$H = -J \sum_{l=1}^{N} (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z) ,$$
$$-1 \leqslant \Delta \leqslant 1 , \tag{2}$$

in the light of the new results mentioned above. In the classical limit, the free energy and the two-spin equal-time correlation function are the same for the HB FM and the HB AFM except for a trivial change in sign. Therefore, the $T_c = 0$ critical properties are identical in the two cases even though the spectra of low-energy modes, specifically the linear spin-wave modes, are totally different: we have $\omega_k \propto k^2$ for the HB FM and $\omega_k \propto k$ for the HB AFM.

The following five critical exponent values can be inferred directly from the exact solution[11] of the classical Heisenberg chain:

$$(\alpha = -1), \quad \gamma = 2, \quad \delta = \infty, \quad \eta = 1, \quad \nu = 1 . \tag{3}$$

Here the value $\delta = \infty$ reflects the discontinuity in the $T = 0$ magnetization isotherm and $\eta = 1$ the lack of decay in the correlation function due to the fully ordered ground state. The value $\alpha = -1$ in parentheses is realized in the 1D n-vector model for all $n > 1$ except for $n = 3$, which is the classical Heisenberg model. Due to an anomaly, the standard linear cusp ($\alpha = -1$) in the specific heat is replaced by an exponential cusp ($\alpha = -\infty$) in this particular case.[10] Hence, if we disregard the anomalous behavior of the specific heat, the exponent values (3) satisfy the scaling relations of Table II for $a_T = a_H = 1$. If the low-temperature specific heat of the classical Heisenberg chain were dominated by the spin-wave modes, the corresponding critical exponent would be $\alpha = -1/2$ for the HB FM and $\alpha = -1$ for the HB AFM. It is then interesting to note that the values $\alpha = -1/2$ and $\alpha = -1$ are, in fact, realized in the quantum spin-1/2 version of the Heisenberg chain in accordance

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TABLE I. Values of the critical exponents α and γ resulting from various calculations.

Reference	Method	α	γ
Bonner and Fisher (1964)	Finite chain extrapolations	$-1/2$	~ 1.8
Baker, Rushbrooke, and Gilbert (1964)	High Temp. Series	$\cdots$	1.67 ± 0.07
Kondo and Yamaji (1972)	Two-time Green's functions	$-1/2$	2
Cullen and Landau (1983)	Suzuki-Trotter mapping	$\cdots$	~ 1.32
Lyklema (1983)	Monte Carlo	-0.3 ± 0.1	1.75 ± 0.02
Schlottman (1985)	Numerical	-0.49 ± 0.02	2.00 ± 0.02
Schlottman (1986)	Bethe ansatz	$-1/2$	2 + log. corr.
Takahashi and Yamada (1985, 1986)	Numerical Bethe ansatz	$-1/2$	2
Marcu, Müller, & Schmatzer (1985)	Monte Carlo	-0.261 ± 0.013	1.552 ± 0.008

with the $\omega_k \propto k^2$ and $\omega_k \propto k$ behavior of the lowest-lying excitations of the HB FM and HB AFM, respectively. Thus in the quantum case, the energy level distribution, which dominates the nature of the specific-heat curve, is sensitive to the dynamical properties of the model and therefore different at the FM and AFM ends of the spectrum. In contrast, the classical energy density depends only on the structure of the energy surfaces in phase space but not on the symplectic structure which governs classical spin dynamics. In the case of the Heisenberg model,[12] the energy density is the same for $J>0$ (HB FM) and $J<0$ (HB AFM), but no such symmetry exists for individual phase-space trajectories.

Let us have a closer look at the $s=1/2$ HB AFM. There exist exact results for the specific-heat exponent[13,14] and the correlation function exponent[15,16]: $\alpha=-1$, $\eta=2$. If scaling and hyperscaling hold, these exponents already determine the two scaling powers as $a_T=1$, $a_H=1/2$. The complete list of exponents can then be inferred from Table II:

$$\alpha=-1, \quad \gamma=1, \quad \delta=1, \quad \eta=2, \quad \nu=1\,. \tag{4}$$

However, the exponents γ, δ, and ν are still awaiting verification by direct determination.

The specific-heat exponent value $\alpha=-1$ is, in fact, known to be realized even for the more general $s=1/2$ *XXZ* model (2) throughout the regime $-1\leqslant\Delta<1$, which corresponds to a line of critical points with algebraically decaying correlation functions. Along this line, the correlation function exponent is known to vary continuously with the anisotropy parameter Δ.[15,16] Under the assumption that scaling and hyperscaling hold, one can infer from these exact results the following values for the two scaling powers and the five critical exponents[17]:

$$a_T=1, \quad a_H=1/2+\mu/2\pi \quad \text{with } \cos\mu=-\Delta\,, \tag{5a}$$

$$\begin{aligned}&\alpha=-1, \quad \gamma=1+\mu/\pi\,,\\ &\delta=(1/2+\mu/2\pi)/(1/2-\mu/2\pi)\,,\\ &\eta=2-\mu/\pi, \quad \nu=1\,.\end{aligned} \tag{5b}$$

In the limit $\Delta=-1$, which is equivalent to the HB AFM, the values (4) are recovered. At $\Delta=0$, which represents the *XY* model, we have

$$\alpha=-1, \quad \gamma=3/2, \quad \delta=3, \quad \eta=3/2, \quad \nu=1\,. \tag{6}$$

For this special case, the exponents γ and ν have been inferred from direct studies of correlation functions,[18,19] and the value $\delta=3$ was confirmed by the analysis of $T=0$ magnetization isotherms of finite chains.[20] In all other cases, the scaling predictions are still awaiting independent verification.

Now we turn to the $s=1/2$ HB FM ($\Delta=1$). It is the only case in the parameter range $-1\leqslant\Delta\leqslant1$ which is characterized by the property that both the quantum $s=1/2$ version and the classical $s=\infty$ version have the same type of ground state, a state with saturated long-range order. In all other cases, quantum fluctuations destroy the long-range order present in the classical version. Hence we obtain the same exponent values $\eta=1$ and $\delta=\infty$ for the $s=1/2$ HB FM as for its classical counterpart [see Eq. (3)]. Both results are consistent with the value $a_H=1$ for the magnetic scaling power. However, the newly found exponent values[6,7] $\alpha=-1/2$ and $\gamma=2$ are mutually exclusive within the scaling picture for given $a_H=1$.

Concerning the violation of the scaling hypothesis it can be argued[6,9] that the specific heat ($\alpha=-1/2$) is again anomalous, as in the classical case ($\alpha=-\infty$), and that the remaining exponents are the same as in the classical case thus causing no further problem.

Alternatively, the violation may signify a previously unanticipated complexity in the critical behavior of quantum spin chains. A good test would be a reliable calculation of the exponent ν directly from the temperature-dependent correlation functions.[22]

In any case, the $s=1/2$ HB FM has a most unusual critical point. The violation of scaling is perhaps attributable to the fact that some aspects of the transition have first-order

TABLE II. Dependence on the two scaling powers a_T (thermal) and a_H (magnetic) of the six most common critical exponents as implied by the scaling and hyperscaling hypotheses. Also given are the exponents α and γ for $T_c=0$ critical points, which have a modified dependence on the scaling powers. The other four exponents remain the same.

$\alpha=(2a_T-1)/a_T$ $\gamma=(2a_H-1)/a_T$	$\beta=(1-a_H)/a_T$ $\delta=a_H/(1-a_H)$	Scaling hypothesis
$\eta=2+D(1-2a_H)$	$\nu=1/Da_T$	Hyperscaling hypothesis
Modifications for $T_c=0$ critical points		
$\alpha=-1/a_T$	$\gamma=(2a_H+a_T-1)/a_T$	

character. The ground state of the $s = 1/2$ XXZ model changes at the HB FM point ($\Delta = 1$) from a nondegenerate singlet state in the easy-plane regime to a ferromagnetic doublet in the easy-axis regime. At the transition point the ground state is infinitely degenerate on top of its quasi-degeneracy with gapless excitation continua. In the well-known mapping of the 1D $s = 1/2$ XXZ model ground state onto the 2D six-vertex model,[21] the point $\Delta = 1$ corresponds to the critical point where the KDP model undergoes a transition from a critical phase at $T > T_c$ ($\Delta < 1$) to a ferroelectrically ordered phase at $T < T_c$ ($\Delta > 1$). The KDP transition is unusual, combining the characteristic features of both a first-order transition and a Prokovskii-Talapov type transition. The $T \to 0$ critical behavior of the HB FM ($\Delta = 1$) also displays Prokovskii-Talapov features combined with characteristics of a first-order transition.[22]

The availability of new exact results such as the critical exponents α and γ for the 1D $s = 1/2$ HB FM allows us to assess the degree of accuracy of various approximate methods employed in attempts to determine these values. An important observation made by Schlottmann[6] is that the true asymptotic critical behavior only sets in at very low temperatures, lower than the temperature range in which previous numerical studies could be expected to produce reliable results.[23] We observe from Table I that computer simulations and Monte Carlo calculations[4,5,8] turned out to be rather unreliable. The early high-temperature series expansions[2] and finite-chain extrapolations[1] were considerably more successful. Finite-chain extrapolations even produced a reasonable value for the critical amplitude of the specific heat. This is illustrated by the following comparison of the leading terms in an expansion of the entropy function as inferred (i) by Schlottmann[6] and (ii) by Takahashi and Yamada[7] from the numerical analysis of the Bethe ansatz and (iii) by Bonner and Fisher[1] from finite-chain extrapolations:

$$\text{(i)}\quad S \sim 1.5(k_B T/J)^{1/2} + O(T^{3/2})\,; \tag{7a}$$

$$\text{(ii)}\quad S \sim 1.563(k_B T/J)^{1/2} + O(T)\,; \tag{7b}$$

$$\text{(iii)}\quad S \sim 1.2(k_B T/J)^{1/2} + \dots\,. \tag{7c}$$

Finally, we should comment that the apparent exact values obtained by Kondo and Yamaji[3] are clearly an artefact of their Green's function procedure, which treats spin-wave excitations self-consistently and therefore produces, essentially, the critical fluctuations of ferromagnetic spin waves in 1D.

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