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Finite-size scaling and integer-spin Heisenberg chains

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Finite-size scaling (phenomenological renormalization) techniques are trusted and widely applied in low-dimensional magnetism and, particularly, in lattice gauge field theory. Recently, investigations have begun which subject the theoretical basis to systematic and intensive scrutiny to determine the validity of finite-size scaling in a variety of situations. The 2D ANNNI model is an example of a situation where finite-size scaling methods encounter difficulty, related to the occurrence of a disorder line (one-dimensional line). A second example concerns the behavior of the spin-1/2 antiferromagnetic XXZ model where the $T=0$ critical behavior is exactly known and features an essential singularity at the isotropic Heisenberg point. Standard finite-size scaling techniques do not convincingly reproduce the exact phase behavior and this is attributable to the essential singularity. The point is relevant in connection with a finite-size scaling analysis of a spin-one antiferromagnetic XXZ model, which claims to support a conjecture by Haldane that the $T=0$ phase behavior of integer-spin Heisenberg chains is significantly different from that of half-integer-spin Heisenberg chains.

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INTRODUCTION

The numerical analysis of sequences of finite systems has been a powerful tool in the investigation of thermodynamic and critical properties of low dimensional systems in the thermodynamic limit.[1–3] The technique of finite-size scaling (also known as phenomenological renormalization)[4–6] has utilized concepts from scaling theory and renormalization group analysis to provide a systematic method for extracting quantitative values for critical properties in the limit $N\rightarrow\infty$. Hence the validity was established of extracting $N\rightarrow\infty$ information from finite systems, as assumed by the older, direct extrapolation methods. Finite systems, of course, do not display critical behavior, but temperature, ordering field, and finite-size deviations from criticality are all described by the same set of critical exponents. To obtain sequences of reasonable length for analysis, the method is essentially limited to 2D classical systems (where the properties of infinite strips of finite width are calculated by the transfer matrix technique) and 1D quantum systems (where finite chain calculations involve diagonalization of the Hamiltonian matrix). Finite-size scaling techniques are trusted and widely applied in low dimensional magnetism and related studies.[5,6]

A typical system close to its critical point is characterized by a temperature-like (nonordering) field and an ordering field, denoted by t and h, respectively. The critical point is given by $t=h=0$. For systems of finite size N, criticality implies a third condition, namely $1/N=0$. In fact, $1/N$ plays the role of a scaling field with exponent equal to unity. Scaling expressions may be formulated for the free energy $f=f(t,h,1/N)$ and the inverse correlation length $\kappa=\kappa(t,h,1/N)$, and the phenomenological renormalization approach yields values for the critical point and its exponents. Of specific interest here is the relation $\kappa(0,0,1/N)=\kappa_N\approx N^{-1}$, and hence the critical point is identified as the point where the curves $N\kappa_N$ intersect as a function of temperature (or any temperature-like parameter in general). For a 2D classical system and a lattice of $N\times\infty$ sites, κ_N may be obtained from the eigenvalues of the transfer matrix, $\lambda_0^{(N)}>|\lambda_1^{(N)}|\geqslant\ldots$:

$$\kappa_N=\ln|\lambda_0^{(N)}/\lambda_1^{(N)}|\,. \tag{1}$$

The free energy and inverse correlation length in 2D correspond to the ground-state energy and excitation energy gap, respectively, for quantum systems in 1D.

Recently, the bases of the finite-size scaling method have come under critical scrutiny,[8] which seems appropriate in view of the rapidly increasing number and areas of application(s). For example, finite-size scaling, like scaling theory generally, breaks down at sufficiently high dimensionality.[9] Here we focus on two situations in low D magnetism where the method has demonstrated potential for yielding misleading results. The first situation occurs in 2D Ising systems with competing interactions, and the second involves the essential singularity terminating a nonuniversal critical line. The suggestion follows that the finite-size scaling method should not be applied in routine fashion, but with caution when there is reason to suspect unusual critical behavior.

THE 2D ANNNI MODEL

The 2D ANNNI (axial next-nearest neighbor Ising) model is the 2D variant of a simple cubic 3D Ising model with competing interactions introduced to explain modulated magnetic phases observed experimentally in rare-earth systems. The 3D ANNNI model has n.n. ferromagnetic (FM) intraplane interactions (J_0); FM interactions (J_1) between n.n. planes, and *competing* antiferromagnetic (AFM) interactions (J_2) between n.n.n. planes. There is general consensus that the 3D ANNNI model shows a paramagnetic (PM) phase at high temperatures, a FM phase for values of the ratio of axial competing interactions $K=|J_2/J_1|<0.5$, and a modulated "antiphase" (2 spins up, 2 spins

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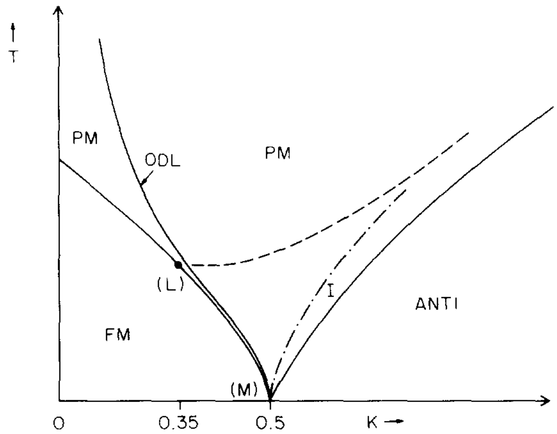

FIG. 1. Schematic phase diagram of the 2D ANNNI model as described in the text, including the pseudo Lifshitz point (L). Not mentioned in the text is an additional phase boundary line shown dash-dotted (for $K>0.5$) pertaining to an incommensurate phase (I) between PM and antiphase regions. The behavior of this line for large K is not yet well established.

down) for $K>0.5$. Between the three phase regions a multiplicity of modulated phases occurs, a large number of which converge at the "multiphase" point M, located at $T=0$, $K=0.5$. A second special point is a Lifshitz point where FM, PM, and modulated phase regions meet, located at $K\approx 0.27$. In the case of the 2D ANNNI model, where FM planes (J_0) are replaced by FM lines (J_0), the situation is less clear. Figure 1 is a sketch of the current status of the 2D phase diagram. The solid lines denote phase boundaries and other features whose existence is established by consensus. The 2D ANNNI model possesses a FM phase, an ordered antiphase, and a special point M at $K=0.5$. A body of early work including high-temperature series expansions,[10] Monte-Carlo simulation,[11] and perturbation series[12] indicated an additional phase region (shown by the dashed line in Fig. 1), believed to be modulated in analogy with the 3D ANNNI model, or incommensurate. A Lifshitz point (L) was indicated, located at $K\approx 0.35$. However, Peschel and Emery found an exact solution of the 2D problem along a special trajectory in $[T,K]$ space, which they called a "one-dimensional line" (ODL).[13] As an effect of competition in the axial interaction, the dimensionality of the problem is reduced by unity along the ODL, permitting an exact solution. Since $D=1$, the ODL is disordered (PM) for $T>0$, having a (multi-) critical singularity M at $T=0$.[14] Such phenomena were systematically investigated by Stephenson, who called them disorder lines, in a number of competing-interaction Ising models.[15] When FM and AFM interactions compete, the disorder line separates PM regions where the correlations show monotonic exponential decay and oscillatory exponential decay. Disorder lines appear to form a natural boundary which series, perturbation, and Monte Carlo techniques cannot reliably cross. The Peschel–Emery ODL, shown in Fig. 1, demonstrates conclusively that the early work predicting a Lifshitz point and associated intermediate phase is erroneous, since the system must be PM down to $T=0$ in the vicinity of the ODL. We note that, from Fig. 1, for $0.35\lesssim K<0.5$, the ODL runs very close to the FM phase boundary. The suggestion is that this feature is giving rise to the misleading results. This early work includes finite-size scaling studies on the 1D quantum analogue of the 2D ANNNI model.[12] For $0\leqslant K\lesssim 0.35$, the finite chain studies gave results for the FM phase boundary in good agreement with the perturbation series results. For $K>0.35$, however, the finite-size scaling approach initially ran into difficulty, since the first excited state was no longer a wave-vector $k=0$ state like the ground state. This feature meant that calculations on longer chains were required to obtain critical information in this K region, and led to the misleading suggestion that the k-sector variation indicated the presence of modulated phases for $K>0.35$, in agreement with the Monte Carlo and series methods. When the significance of the ODL was fully appreciated, finite-size scaling calculations were successfully extended using Roomany–Wyld β-function approximants.[16]

THE XXZ SPIN CHAIN

Recently, Haldane[17] has put forward an interesting conjecture that integer-spin XXZ antiferromagnetic chains show a very different kind of phase behavior at $T=0$ from half-integer-spin XXZ chains, which resemble the spin-1/2 case, the only case where an exact analytic solution is possible.[18] The Hamiltonian is given by

$$H=2|J|\sum_{i=1}^{N}\left[(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y)+\lambda S_i^zS_{i+1}^z\right]. \qquad (2)$$

In the case of spin-1/2, for $0\leqslant\lambda<1$ the system displays a gapless phase with continuously varying critical exponents (η, say) and long-range correlations which decay algebraically to zero (i.e., a Baxter-type nonuniversal line). An essential singularity occurs at the isotropic Heisenberg point, $\lambda=1$, terminating the nonuniversal line. For $\lambda>1$, the ground-state is twofold degenerate with long-range order, and the system displays an excitation energy gap. For integer-spin systems, Haldane predicts the occurrence of an intermediate phase, encompassing the Heisenberg point, $\lambda=1$. For $0\leqslant\lambda<\lambda_1$, a gapless, nonuniversal line is expected, terminating in an essential singularity at $\lambda=\lambda_1<1$. For $\lambda>\lambda_2$, where $\lambda_2>1$, the system has a gap and an ordered, degenerate ground state. The singularity at $\lambda=\lambda_2$ is expected to be of the transverse Ising model type. The new intermediate phase occurs for $\lambda_1<\lambda<\lambda_2$, and is characterized by an energy gap and a nondegenerate, nonordered ground state. Specifically, the isotropic Heisenberg point, $\lambda=1$, where the symmetry of the problem changes from easy-plane ($\lambda<1$) to easy-axis ($\lambda>1$) is not associated with any singular behavior.

Using finite-size scaling techniques and calculations on spin-1 XXZ chains of 2–12 spins, Botet and Jullien[19] have recently concluded that the $T=0$ phase behavior confirms the Haldane integer-spin conjecture. They find an essential singularity λ_1 located back at the XY limit and a singularity claimed to be of transverse Ising type at $\lambda_2\approx 1.18$, and conclude that the intermediate region $0<\lambda<1.18$ has a gap and a nonordered ground state. Our analysis, however, suggests that the numerical treatment of Botet–Jullien is less than conclusive and depends crucially on the reliability of finite-size scaling in the vicinity of (essential) singularities. We have repeated the Botet–Jullien analysis for the exactly solvable

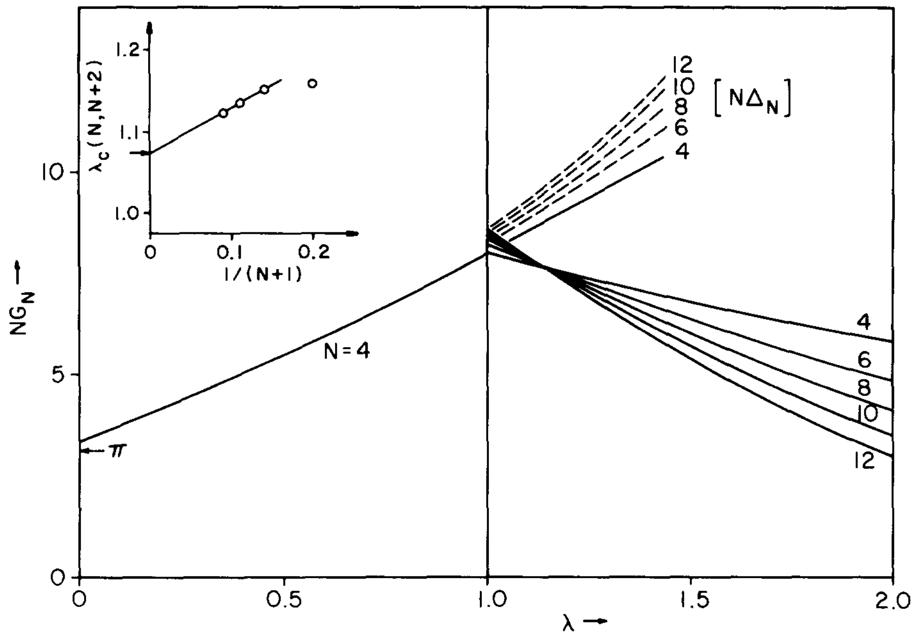

FIG. 2. Scaled gaps NG_N for $N = 4$, 6, 8, 10, and 12 for spin-1/2 XXZ chains plotted as solid curves as a function of λ, in analogy with Fig. 1 of Ref. 19. Data are available only for $\lambda > 1$ (except for NG_N for $N = 4$). The dashed curves for $N > 4$ denoted $N\Delta_N$ are $\lambda > 1$ continuations of scaled gaps for $\lambda < 1$. The NG_N successively cross at values of λ denoted $\lambda_c(N,N+2)$. The inset shows the crossing values λ_c plotted vs $(N+1)^{-1}$. They appear to extrapolate to a limiting $\lambda_c > 1$. For more details see Ref. 19.

spin-1/2 XXZ model, and a comparable plot to their Fig. 1 (of Ref. 19) is shown as Fig. 2. Here we have plotted the "scaled mass-gaps" NG_N as a function of anisotropy λ. The scaled gap is the excitation energy gap between ground state and first excited state multiplied by system size N. We have data for spin-1/2 systems with $N = 4$, 6, 8, 10, and 12 for $\lambda \geqslant 1$ only, but Solyom[20] has data for $N = 4$–12 for $0 \leqslant \lambda < 1$ also, and his independent results confirm our conclusions on the qualitative similarity of scaled-gap plots for spin-1/2 and spin-1 systems.[21] If the spin-1/2 data are interpreted according to the arguments of Botet–Jullien (BJ), they yield the same phase behavior found by BJ for spin-1, known rigorously to be incorrect for spin-1/2. The effect is attributable to the essential singularity at $\lambda = 1$. In fact, essential singularities (or, equivalently, the presence of logarithmic corrections) are well known to cause difficulty for approximate techniques. Misleading results are obtained unless due caution is exercised. The possibility should be considered that a strong singularity at the Heisenberg point for spin-1 may be giving rise to the phenomena interpreted by Botet–Jullien as supporting the Haldane conjecture.

There is only one significant difference between the behavior of the NG_N for spin-1/2 and spin-1. For finite systems up to 12 spins, the NG_N for spin-1/2 appear to be converging to a finite value at $\lambda = 1$, indicating a gapless phase in the thermodynamic limit, whereas for spin-1, the NG_N appear to be diverging, indicating the possibility of a gap. On the other hand, investigation shows that convergence with N is extremely slow in the vicinity of $\lambda = 1$ for spin-1/2, and longer chains of $\sim$25–30 spins are required to show the true, large N, asymptotic behavior.[21] Hence the question of whether spin-1 XXZ chains behave in accordance with the Haldane conjecture remains open, and further numerical studies are desirable.

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[1]J. C. Bonner and M. E. Fisher, Phys. Rev. **135**, A640 (1964).
[2]F. H. Ree and D. A. Chesnut, J. Chem. Phys. **45**, 3983 (1966).
[3]J. F. Nagle and J. C. Bonner, J. Phys. C **3**, 352 (1970).
[4]M. E. Fisher and M. N. Barber, Phys. Rev. Lett. **28**, 1516 (1972).
[5]H. W. J. Blöte and M. P. Nightingale, Physica **112A**, 405 (1982).
[6]M. P. Nightingale, Physica **83A**, 561 (1976); M. P. Nightingale, J. Appl. Phys. **53**, 7927 (1982).
[7]J. Kogut, Rev. Mod. Phys. **51**, 659 (1979).
[8]V. Privman and M. E. Fisher, J. Phys. A **16**, L295 (1983).
[9]E. Brézin, J. Phys. (Paris) **43**, 15 (1982).
[10]S. Redner (unpublished work) cited in Ref. 12.
[11]W. Selke and M. E. Fisher, Z. Phys. B **40**, 71 (1980).
[12]M. N. Barber and P. M. Duxbury, J. Phys. A **14**, L251 (1981).
[13]I. Peschel and V. J. Emery, Z. Phys. B **43**, 241 (1981).
[14]P. Ruján, J. Stat. Phys. **29**, 231 (1982).
[15]J. Stephenson, J. Math. Phys. **11**, 420 (1971). See also E. Barouch and B. McCoy, Phys. Rev. A **3**, 786 (1971) (XY model), and J. Kurmann, H. Thomas, and G. Müller, Physica **112A**, 235 (1982).
[16]P. M. Duxbury and M. N. Barber, J. Phys. A **15**, 3219 (1982). See also W. Selke, Z. Phys. B **43**, 335 (1981); W. Selke and J. M. Yeomans, Z. Phys. B **46**, 311 (1982); W. Selke, K. Binder, and W. Kinzel, Surf. Sci. **125**, 74 (1983).
[17]F. D. M. Haldane, Bull. Am. Phys. Soc. **27**, 181 (1982), and unpublished work.
[18]C. N. Yang and C. P. Yang, Phys. Rev. **147**, 303 (1966); **150**, 321, 327 (1966); **151**, 258 (1966).
[19]R. Botet and R. Jullien, Phys. Rev. B **27**, 613 (1983).
[20]J. Solyom (private communication and unpublished work).
[21]J. C. Bonner and G. Müller, Phys. Rev. B (to be published).