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Finite-length calculations of η and phase diagrams of quantum spin chains

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We present a novel means of calculating the exponent η for massless phases of quantum spin chains based on Luck's formula. Convergence is illustrated by comparison to exact results for spin $\frac{1}{2}$, and the method is used to estimate phase boundaries of the spin-1 chain with single-site and exchange anisotropy. Clear evidence is found in favor of a fluctuation-induced gap for the isotropic antiferromagnet. We elucidate the transition between two different planar phases at large negative D.

There is currently great interest and even controversy as to the nature of the ground state and excitations of one-dimensional quantum magnets. In particular, Haldane[1] has argued that for integral spin, but not half-integral, zero-point fluctuations are sufficiently strong in much of the phase close to the isotropic Heisenberg antiferromagnet not only to restore the spontaneously broken symmetry but, in addition, to generate a gap in the excitation spectrum. As the models for spin greater than $\frac{1}{2}$ do not satisfy conditions for integrability by the Bethe ansatz, one must look to numerical means of verifying these predictions, either by solving short chains exactly or by Monte Carlo simulation for slightly longer systems. While such an approach has provided suggestive evidence for Haldane's picture[2-4] this evidence is not compelling, essentially because of the limitation of the finite extent of the chains. It is important, therefore, to develop unambiguous means of determining phase boundaries which are less sensitive to such restrictions. It is with this aim that we present a novel method of calculating the critical exponent η in a critical phase of a one-dimensional quantum system. The significance of the exponent η is twofold: First, it is the single parameter that determines the analytic form of static and dynamic correlation functions for long wavelength and low frequencies, as calculated in the continuum limit for spin 1 by Timonen and Luther,[5] and, second, it defines the scaling dimension for the operators to which the phase becomes unstable.[6] Thus, calculation of η determines the mapping from the model defined on a lattice to the continuum limit in which correlation functions and stability are more easily understood.

In many cases, massless phases in one-dimensional systems can be described in the long-wavelength limit, by the Hamiltonian

$$H=\int dx[(1/2\rho)\pi^2(x)+c/2(\partial\phi/\partial x)^2] \quad . \tag{1}$$

Here ϕ is a Bose field, $\pi(x)$ is its conjugate momentum density, and ρ and c are effective-mass density and elastic constant, respectively. On a strip of finite width L and periodic boundary conditions, the correlation function of the operator $O(x,t)=\exp[i\phi(x,t)]$ is

$$\langle O(0,t)O(0,0)\rangle=\exp\left(-i\frac{2\pi\gamma vt}{L}\right)\left[1-\exp\left(-i\frac{2\pi vt}{L}\right)\right]^{-2\gamma} , \tag{2}$$

with $v=\sqrt{c/\rho}$, $\gamma=\frac{1}{4}\pi v\rho$. For $|vt|\ll L$ and in the thermodynamic limit $L\to\infty$, this decays as $|vt|^{-2\gamma}$, i.e., γ is the scaling dimension of O. On the other hand, for finite L the lowest Fourier component in Eq. (2) gives the energy gap ΔE between the ground state and the first excited state contributing to the correlation function. Consequently, one has

$$\gamma=L\Delta E/2\pi v \quad . \tag{3}$$

This is the analog of "Luck's relation"[7] for one-dimensional quantum systems. Contrary to isotropic classical two-dimensional systems, it involves not only the energy gap, but also the "sound velocity" v, which describes the inherent anisotropy between space and time. As expected, Eq. (3) is independent of an overall multiplicative factor in the Hamiltonian.

We note, following Cardy,[8] that Eqs. (2) and (3) can be obtained assuming conformal invariance of correlation functions, which is explicit for our Hamiltonian (1) but is believed to exist quite generally at critical points.

The sound velocity v can be evaluated from the energy difference ΔE_k between the ground state, which has wave number $k_0=0$, and the lowest excited state of wave number $k=2\pi/L$. This gives $v=L\Delta E_k/2\pi$, and

$$\gamma=\Delta E/\Delta E_k \quad . \tag{4}$$

We have used Eq. (4) to obtain numerical estimates of the scaling dimensions of various operators from finite-length calculations. As a test case we consider the spin-$\frac{1}{2}$ "XXZ" Hamiltonian

$$H=-\sum_r(S_r^xS_{r+1}^x+S_r^yS_{r+1}^y+J_zS_r^zS_{r+1}^z) \quad , \tag{5}$$

where r is the site index. For $|J_z|<1$, in the continuum limit this model is indeed described by a Hamiltonian of the form of Eq. (1) and, for $L=\infty$ $\langle S_0^xS_r^x\rangle\propto|r|^{-\eta}$, $\langle S_0^zS_r^z\rangle\propto|r|^{-2}+C(-1)^r r^{-\eta_z}$ with[9]

$$\eta=1/(\eta_z)=(1/\pi)\arccos(J_z) \quad . \tag{6}$$

We calculate η $(=2\gamma)$ numerically using the energy gap (ΔE) between the ground state (of magnetization $M=0$, $k_0=0$) and the lowest excited state with $M=1$, $k=0$, whereas for η_z the excited state has $M=0$, $k=\pi$. In all cases v is determined using the lowest excited state with $M=0$, $k=2\pi/L$. Results for $L=12$, $L=16$, and, for a few cases, $L=20$ are shown in Fig. 1. The general agreement between our numerical results for η and the exact values is good. The deviation in the vicinity of the isotropic ferromagnet point ($J_z=1$) is mainly due to the important curvature of the spin-wave dispersion curve in this region and the consequent inaccuracy of v. This problem can be avoided by fitting numerical values of $v(L)$ to the form $v(L)=v+a/L+b/L^2$, and using the extrapolated value of v in Eq. (3). This procedure leads to good agreement near the point $J_z=1$. Close to the isotropic antiferromagnet the calculated values of η apparently cannot follow the cusplike singularity of the exact curve when approached from the massless side, nor the jump to the constant value of 2 which the apparent value of η [twice the expression (4)], takes in the antiferromagnetic phase. Nevertheless, the discrepancies are not large at $J_z=-1$. We find $\eta=0.87$ instead of unity, and using $\eta=1$ as a criterion for the Kosterlitz-Thouless transition to the Néel state, the critical value of J_z would be -1.3 instead of -1. The agreement between exact and calculated values for η_z is not as good; however, the exact relation $\eta=1/\eta_z$ is obeyed over a large part of the parameter range. Note that for $J_z<-1$ the definition (4) will lead to zero for η_z, and thus $1/\eta_z$ must diverge. We finally remark that much longer lengths can be handled numerically using the Bethe ansatz equations. Integration of the Kosterlitz-Thouless flow equations would suggest that convergence to the asymptotic values is logarithmic at the critical coupling.[10]

We now turn to the anisotropic spin-1 chain with Hamiltonian

$$H=-\sum_r [S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + J_z S_r^z S_{r+1}^z - D(S_r)^2] \quad . \quad (7)$$

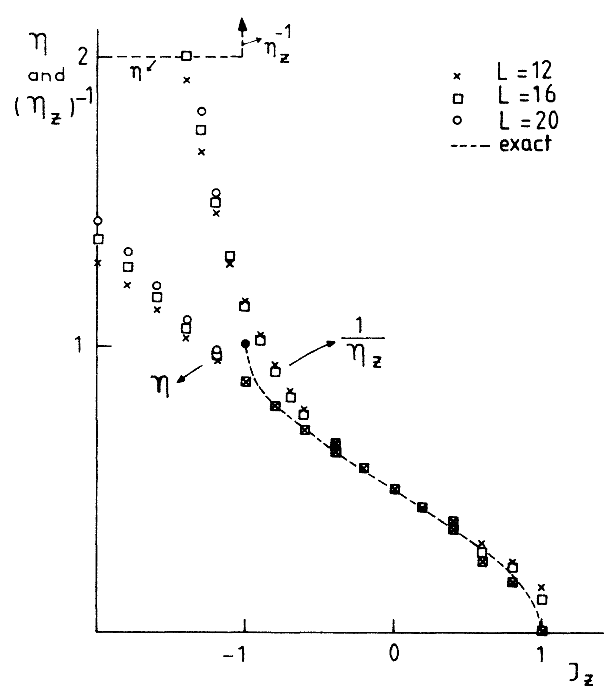

FIG. 1. Comparison of calculated values of η and $1/\eta_z$ to the exact values for $S=\frac{1}{2}$, for lengths $L=12$, 16, and 20. If for $J_z<-1$ we *define* η to be twice the expression (4), then $\eta=2$, $\eta_z=0$.

A continuum representation of this model has been given in Refs. 5 and 11 in terms of 2 scalar Bose fields ϕ_+ and ϕ_-. The dynamics of ϕ_+ is governed by the Hamiltonian

$$H^{(+)}=H_0+\alpha\int dx\, \cos\sqrt{8}\phi_+ \quad , \quad (8)$$

with H_0 given by Eq. (1), while $H^{(-)}$ is a continuum limit of the two-dimensional Ising model. The spin operators are

$$S^+(x) \propto \cos(\Theta_-/\sqrt{2})\exp(-i\Theta_+/\sqrt{2}) + (-1)^x \cos \times(\Theta_-/\sqrt{2}+\sqrt{2}\phi_-)\exp[-i(\Theta_+/\sqrt{2}+\sqrt{2}\phi_+)] \quad , \quad (9a)$$

$$S^z(x) \propto \frac{\partial\phi_+}{\partial x} + (-1)^x \cos(\sqrt{2}\phi_+)\cos(\sqrt{2}\phi_-) \quad , \quad (9b)$$

with $-(1/\pi)\partial\Theta_\pm/\partial x=\pi_\pm$. As a result of the separation of the Hamiltonian into (+) and (−) parts, spin-correlation functions are products of (+) and (−) components.

Specifically, for D or J_z not too negative, the Ising model ($H^{(-)}$) is in its disordered phase. Consequently, correlation functions involving only Θ_- (which is a disorder field) are constant at large distances, whereas ϕ_- correlations decay exponentially. A massless phase is then possible if the "cos" term in $H^{(+)}$ is irrelevant, and this implies $\eta \leq \frac{1}{4}$ in the massless phase, with $\eta=\frac{1}{4}$ at the boundary to a massive singlet phase.[6]

In Fig. 2 we show the length dependence of η, calculated as just described for $S=\frac{1}{2}$, for different values of J_z and D. For ferromagnetic coupling most of the length dependence comes from v. This can be eliminated using the extrapola-

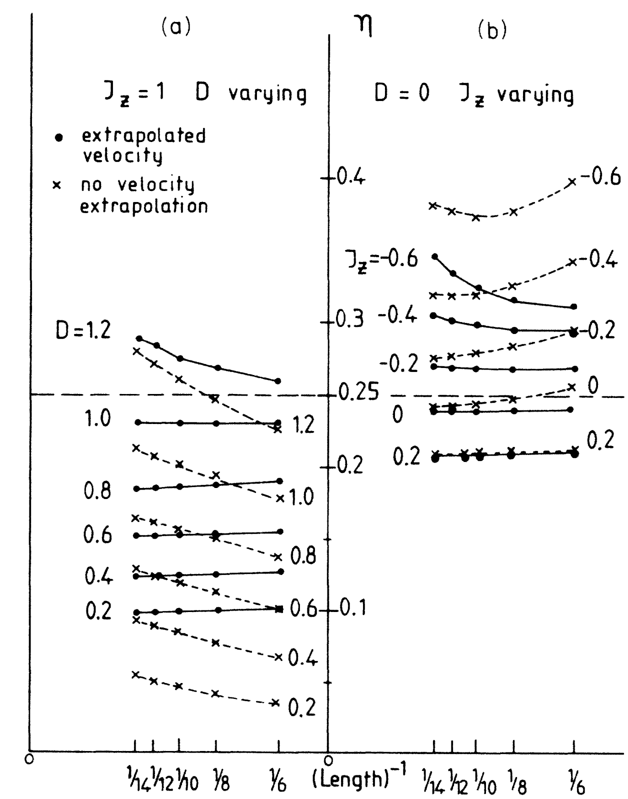

FIG. 2. Calculated values of η for $S=1$ for (a) $J_z=1$, D varying and (b) $D=0$, J_z varying. Crosses indicate values for gaps and velocities estimated from a single length; solid circles with the velocity extrapolated from $L=8$, 10, and 12.

tion procedure described above, and the resulting values of η are nearly length independent as long as $\eta < \frac{1}{4}$. On the other hand, if $\eta > \frac{1}{4}$ [$D = 1.2$ in Fig. 2(a)], no obvious convergence with increasing L is found. This behavior is clearly in agreement with a massless-singlet transition at $\eta = \frac{1}{4}$. The situation is somewhat less clear along the line $D = 0$ [Fig. 2(b)] and an increase of η with increasing length as for $D = 1.2$ in Fig. 2(a) is only obvious for $\eta > 0.30$. However, it is quite clear that the massless phase does not extend up to $J_z = -1$, in agreement with Haldane's prediction.[12] The crucial point, which we believe makes this statement more convincing than naive finite-size scaling, is that as well as asking whether gaps diminish more slowly than 1/length, which amounts, essentially, to looking for an apparent increase in the estimates of η (since the estimated velocity varies more slowly than the scaled gap), we have an absolute value, $\frac{1}{4}$, to compare it to. Thus, we may compare scaled gaps to absolute numerical values and not simply observe their "trends." This is the gain to be had by calculating velocities.[13] We note that an attempt[14] to implement Luck's formula that, incorrectly, did not include the velocity led to erroneous conclusions.

Using $\eta = \frac{1}{4}$ as the criterion for the massless phase, we find the phase boundary shown in Fig. 3. This boundary closely resembles that found by Botet and Jullien[2] using finite-size scaling, but we feel, for the reasons outlined, that the present results make it much more convincing. Also shown is a contour plot of $\eta(J_z, D)$ within the massless phase. From the weak length dependence displayed in Fig. 2 we expect our values of η to be accurate to within a few percent, with largest uncertainties close to the massless-singlet boundary. Note that $\eta = 0$ at the boundary of the ferromagnetic region (calculated by the crossing of the energies of the $M = 0$ and $M = L$ states) at $J_z = 1$, $D = 0$, but in general $\eta > 0$ along this line.

Defining an exponent η_2 by $\langle S_0^{+2} S_r^{-2} \rangle \sim |r|^{-\eta_2}$ from Eq. (9a) one expects $\eta_2 = 4\eta$. We have found numerically (using the $M = 2$ to $M = 0$ gap) that the relation is well obeyed. In contrast, and unlike the $S = \frac{1}{2}$ case within the massless region, we do not find convergent values of η_z, indicating that the alternating part of the $\langle S_0^z S_r^z \rangle$ correlation function decays exponentially, in agreement with Eq. (9b) and subsequent discussion.

Along a line in the $J_z - D$ plane, $D = -J_z$ in a continuum approximation, the operator driving the massless-singlet transition vanishes, so that the model remains critical. In finite scaling this line appears as a fingerlike protrusion from the massless phase, the width of which, however, decreases rapidly for longer lengths and seems to extrapolate to zero for $L \to \infty$. This line extrapolated from finite-size scaling with lengths 10 and 12 is shown in Fig. 3 together with calculated values of η. The line meets the singlet-antiferromagnetic transition at a multicritical point at $J_z = 3$, $D = 2.7$, where we find $\eta \approx 0.67$.

Up to now we have restricted our discussion to values

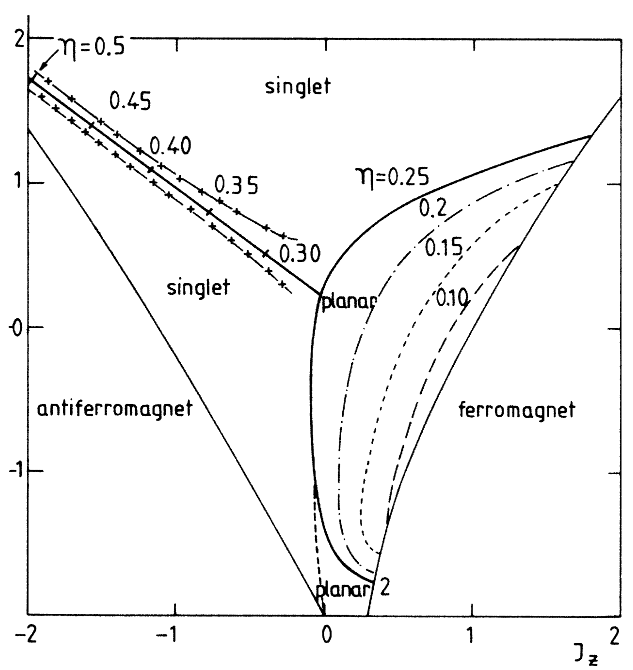

FIG. 3. Contours of η and the phase diagram for spin 1. The contours drawn are with gaps for length 12; the velocities extrapolated from $L = 8$, 10, and 12. The "finger" is shown for gap scaling for 10–12 as well as the line estimated for infinite L. The singlet to antiferromagnetic line is taken for scaling of the $k = \pi$ gap for lengths 10 and 12; the ferromagnetic boundary from crossing of the lowest eigenvalues of $M = L = 12$ and $M = 0$ subspaces. The "planar-2" phase is bounded on the left by the contour $\eta_2 = 1$; see Fig. 4 for further detail of $D < 0$.

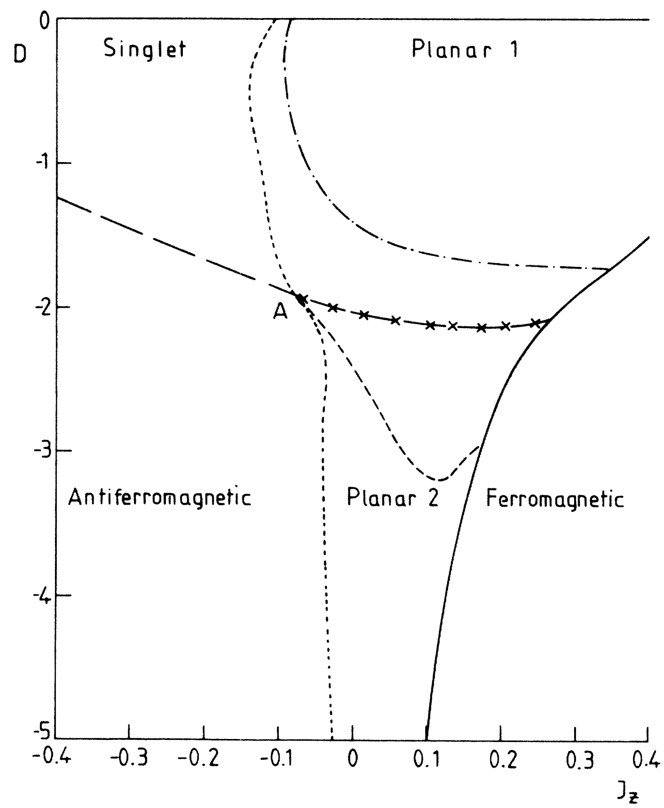

FIG. 4. The phase diagram for $-5 < D < 0$, $|J_z| \leq 0.4$. The contour $\eta = \frac{1}{4}$ is shown dash-dotted that of $\eta_2 = 1$ with short dashes. The long-dashed line satisfies $\eta_2 = 1/\eta_z$, the dash-crossed line scaling for the $M = 1$ to $M = 0$ gap ($L = 10$ and 12). We expect that the difference between the three lines separating planar-1 and -2 phases is a finite-size effect: They should collapse to a single line intersecting the $\eta_2 = 1$ contour at the multicritical point A.

$D > -1$. For large negative D the model can be transformed by perturbation expansion in $1/D$ into an effective spin-$\frac{1}{2}$ chain. The lowest excited states have $M=2$, not $M=1$ as above and a direct massless-antiferromagnetic transition where no intermediate singlet phase occurs. In Fig. 4 we show contours of $\eta=\frac{1}{4}$ and $\eta_2=1$ for $D<0$. For $D>-1.4$, $\eta_2\sim 4\eta$ as discussed above. However, below this value there appears a finite gap in the $M=1$ excitations so that formally $\eta=\infty$, whereas η_2 remains continuous and well defined. Moreover, below $D=-2.4$ we again find a well-defined value of η_z with $\eta_z=1/\eta_2$. This is precisely the behavior expected for the effective spin-$\frac{1}{2}$ model. In the thermodynamic limit we expect a sharp transition between the two types of massless phases ($\eta_2=4\eta$, $\eta_z^{-1}=0$ and $\eta=\infty$, $\eta_z=1/\eta_2$) and the boundary to join continuously the singlet-antiferromagnet transition. In this region the limitations of finite chains evidently preclude precise location of the boundaries: For infinite chains we would expect the three lines separating the planar-1 and planar-2 phases to coincide. In the continuum representation this transition occurs when the Ising sector ($H^{(-)}$) goes into the ordered phase. Then ϕ_- correlations are long ranged, whereas Θ_- correlations decay exponentially. As long as the $H^{(+)}$ sector remains massless, from Eqs. (9) one then expects power-law correlations of S^z and $(S^+)^2$, whereas S^+ correlations decay exponentially in agreement with our numerical results. Finally, if $H^{(+)}$ becomes massive, an antiferromagnetic state with long-range order is realized [cf. Eq. (9b)]. From this discussion, we expect the transition between the two massless phases to be Ising-like, similar to that found by Lee and Grinstein.[15] We remark that both the massless-antiferromagnet boundaries are characterized by $\eta_2=1$. In consequence, the boundary of the massless phases towards negative J_z may be assumed to be continuous through the multicritical point A of Fig. 4.

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[1] F. D. M. Haldane, Institute Laue Langevin Report No. SP81/95 (unpublished); Phys. Rev. Lett. **50**, 1153 (1983).
[2] R. Botet and R. Jullien, Phys. Rev. B **27**, 613 (1983).
[3] J. Solyom and T. Ziman, Phys. Rev. B **30**, 3980 (1984).
[4] J. B. Parkinson, J. C. Bonner, G. Muller, M. P. Nightingale, and H. W. J. Blote, J. Appl. Phys. **57**, 3319 (1985).
[5] J. Timonen and A. Luther, J. Phys. C **18**, 1439 (1985); see also A. Luther and D. J. Scalapino, Phys. Rev. B **16**, 1153 (1977).
[6] M. P. M. den Nijs, Phys. Rev. B **23**, 6111 (1981); J. L. Black and V. J. Emery, *ibid.* **23**, 429 (1981).
[7] J. M. Luck, J. Phys. A **15**, L169 (1982).
[8] J. Cardy, J. Phys. A **17**, L385 (1984).
[9] A. Luther and I. Peschel, Phys. Rev. B **12**, 3908 (1973).
[10] B. Horovitz, T. Bohr, J. M. Kosterlitz, and H. J. Schulz, Phys. Rev. B **28**, 6596 (1983).
[11] M. P. M. den Nijs, Physica A **111**, 213 (1982).
[12] M. P. Nightingale and H. W. J. Blote, Phys. Rev. B **33**, 659 (1986) have recently estimated the gap for the isotropic antiferromagnet by Monte Carlo methods for chains up to 32 sites long, with results in agreement with the present conclusion.
[13] K. A. Penson and M. Kolb, Phys. Rev. B **29**, 2854 (1984), for example, were restricted to making statements about the *ratios* of different exponents η by comparing ratios of scaled gaps.
[14] T. Schneider, U. Glaus, and E. P. Stoll, J. Appl. Phys. **55**, 2401 (1984).
[15] D. H. Lee and G. Grinstein, Phys. Rev. Lett. **55**, 541 (1985).