Ordering and Criticality in Spin-1 Chains

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The $T=0$ behavior of the antiferromagnetic, nearest-neighbor, spin-1 chain is studied in a space of interactions which includes exchange anisotropy, bond alternation, and biquadratic exchange. We find that bond alternation can stabilize Néel order; that with sufficient biquadratic coupling the ground state may be spontaneously dimerized *and* simultaneously critical; and that there is a line of multicritical points where the Néel-ordered phase touches the manifold of isotropic coupling. Predictions of Affleck and Haldane regarding the criticality and ordering in these models are tested.

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The $T=0$ behavior of the antiferromagnetic, nearest-neighbor, spin-1 chain with the bilinear-biquadratic Hamiltonian

$$\mathcal{H}=\sum_i \epsilon(i)[(\mathbf{S}_i,\mathbf{S}_{i+1})_\Delta-\beta(\mathbf{S}_i,\mathbf{S}_{i+1})_\Delta^2], \quad (1)$$

where bond alternation is controlled by λ via

$$\epsilon(i)=\begin{cases}1, & \text{even } i,\\ \lambda, & \text{odd } i,\end{cases} \quad (2)$$

while exchange anisotropy is controlled by a parameter Δ via

$$(\mathbf{A},\mathbf{B})_\Delta=A^zB^z+\Delta(A^xB^x+A^yB^y), \quad (3)$$

has been the subject of several striking but largely untested predictions. Affleck[1] has suggested that any critical point of this model with $\Delta=1$ should lie in the universality class of the $k=2$ Wess-Zumino-Witten model, implying definite values for the critical exponents. The prediction for the exponent η has been verified for the Bethe-*Ansatz*-solvable model[2] $\lambda=\beta=\Delta=1$; none of the other exponents have been otherwise studied. No other concrete examples of such critical points have been examined, although Affleck[3] predicted that one should exist at $\lambda=\frac{1}{3}$, $\beta=0$, $\Delta=1$ (note, however, that the λ value should be exact only in the large-S limit). Later work by Affleck and Haldane[4] has cast doubt on the assumption of universality in the $\Delta=1$ manifold, but the situation is not at all clear.

Two types of spontaneous ordering have been the subject of much interest in these systems. The first is *antiferromagnetic* (AFM) ordering, which occurs for $\Delta<\Delta_c(\beta,\lambda)\leq 1$. Haldane[5] conjectured that, for isotropic exchange and no bond alternation, the AFM order should disappear at $\Delta_c<1$, and that the simple spin chain ($\beta=0$, $\lambda=\Delta=1$) should have a unique, disordered ground state and is an unexceptional point in a disordered phase which we denote the Haldane phase. The transition at Δ_c was argued to lie in the universality class of the 2D classical Ising model. Finite-size studies[6] have lent weight to these predictions, but the numerically estimated critical exponents at Δ_c are only in marginal agreement with Haldane's prediction.

The second type of ordering is *spontaneous dimerization.* Majumdar and Ghosh[7] found an exactly solvable spin-$\frac{1}{2}$ chain, which included next-neighbor interactions, and which had a spontaneously dimerized ground state. More recently, Affleck *et al.*[8] suggested, on the basis of a comparison between several simple trial states, that the ground state of the nearest-neighbor spin-1 model (1), for $\lambda=\Delta=1$ and $\beta>1$, may also be spontaneously dimerized.

We address these issues, and others, by means of high-order series expansions. Two classes of expansions have been generated, namely (i) "ordered-state" expansions in the variable Δ about $\Delta=0$ (Ising models), at fixed β and λ, and (ii) "disordered-state" expansions in the variable λ about $\lambda=0$ (dimerized models), at fixed β and Δ. The method by which the series were derived will be described elsewhere[9]; ratio techniques and differential approximants have been applied to analyze the resulting series.[10] Ordered-state expansions were carried out to up to order Δ^{18} for the ground-state energy per spin E_g, the sublattice magnetization $\tilde{M}=N^{-1}\sum_i(-1)^i\langle S_i^z\rangle$, and the zz AFM equal-time structure factor $\mu_0^{zz}=\sum_i[(-1)^i\langle S_0^zS_i^z\rangle-\tilde{M}^2]$. (Angular brackets denote ground-state expectation values.) Disordered-state expansions were calculated to up to order λ^5 for the anisotropic AFM equal-time structure factor and its second moment

$$\mu_0^\Delta=\sum_i(-1)^i\langle(S_0,S_i)_\Delta\rangle, \quad (4)$$

$$\mu_2^\Delta=\sum_i(-1)^i i^2\langle(S_0,S_i)_\Delta\rangle, \quad (5)$$

and the zz AFM susceptibility χ^{zz} (defined via the second derivative of E_g with respect to a staggered field applied along the z axis). The ratio $\mu_2^\Delta/\mu_0^\Delta$ defines ξ^2, the square of the ground-state AFM correlation length. For $\Delta=1$, we also calculated E_g to order λ^{11} and the "dimerization" $D=N^{-1}\sum_i(-1)^i\langle\mathbf{S}_i\cdot\mathbf{S}_{i+1}\rangle$ to order λ^{10}. Because of space limitations, we omit here all the series and details of their analyses: These will be presented else-

where.

Consider first the Hamiltonian (1) with pure bilinear coupling ($\beta=0$). The $T=0$ phase diagram in the λ,Δ plane suggested by our calculations is given in Fig. 1. As one increases Δ from 0 along trajectory a, that is, in the absence of bond alternation, AFM order is destroyed at point A before the coupling becomes isotropic. The estimated position of this critical point is $\Delta_c(\lambda=1,\beta=0)=0.841\pm0.002$, which is consistent with earlier estimates based on the diagonalization of finite chains.[6] The criticality at this point does, indeed, appear to be in the universality class of the classical 2D Ising model. We estimate that $\tilde{M}$ vanishes with an exponent $\beta=0.13\pm0.02$ (c.f. the 2D Ising value of $\frac{1}{8}$) and find that μ_0^{zz} diverges with an exponent $\gamma_s=0.73\pm0.05$ [c.f. the 2D Ising values $\eta=\frac{1}{4}$ and $\nu=1$, and the scaling relation[11] $\gamma_s=(1-\eta)\nu$].

It now applies some bond alternation and follows, say, trajectory b, the series quite unexpectedly shows that the stability of the Ising phase is *enhanced*, until λ reaches a value $\lambda_M=0.60\pm0.04$ at which Δ_c becomes 1. As λ is further decreased towards zero, $\Delta_c(\lambda,\beta=0)$ also falls to zero. The ordered-state series estimates of the critical exponents are consistent with classical 2D Ising criticality all along the line AMB, except possibly in the vicinity of the novel multicritical point M. Near this point, the $\tilde{M}$ series is extremely ill behaved, and the μ_0^{zz} series indicates $\gamma_s=0.95\pm0.20$, where the large uncertainty reflects our imprecise knowledge of λ_M.

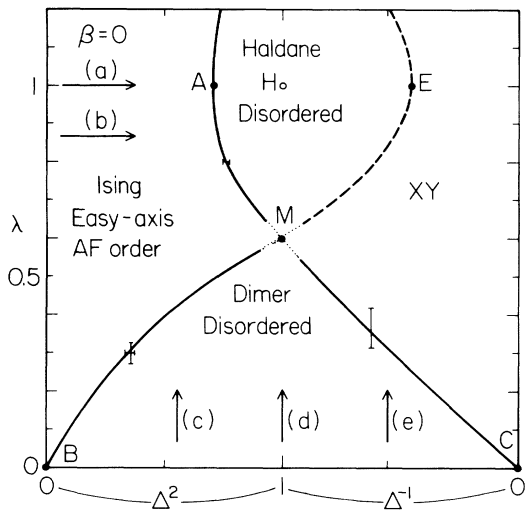

FIG. 1. Phase diagram in the λ,Δ plane for $\beta=0$; typical uncertainties in the phase boundaries are indicated by error bars. Note the broken horizontal scale. The point H indicates the simple isotropic spin chain. The point M is a novel multicritical point where all four phases meet and the Ising phase touches the manifold of isotropic coupling ($\Delta=1$); along trajectory d, M separates two disordered phases. The phase diagram is trivially symmetric under the replacement $\lambda\rightarrow\lambda^{-1}$.

The disordered-state expansions along trajectories such as c, d, and e also prove revealing. For $0<\Delta<1$, the estimated critical points $\lambda_c(\Delta,\beta=0)$ are consistent with the estimates from the ordered-state expansions. The series for χ^{zz}, μ_0^A, and μ_2^A all indicate divergences, as one expects since the transition is to an antiferromagnetically ordered state. Unfortunately, the series are too short to allow for reliable estimates of the exponents; if the critical λ values are biased to those indicated by the ordered-state expansions, then the resulting exponents are consistent with 2D Ising criticality within large uncertainties.

For $1<\Delta<\infty$, the χ^{zz} series becomes increasingly ill behaved as Δ increases, while the series for μ_0^A and μ_2^A remain well behaved. We take this as evidence that the incipient ordering along the critical line MC is XY-like. One might expect that there is a region of algebraic XY order, but the location of the presumed Haldane XY boundary EM is inaccessible to the present calculations.

The disordered-state expansions at $\Delta=1$ (trajectory d) directly probe the multicritical point M, where all four phases displayed in Fig. 1 meet. The quantities μ_0^A, μ_2^A, and χ^{zz} all diverge at M—where there is algebraic Néel order, even though the phases on both sides of the transition are disordered. Again, because λ_M is not precisely known, all exponent estimates suffer large uncertainties. For μ_0^A, μ_2^A, and χ^{zz}, the critical indices are, respectively, $\gamma_s=0.2\pm0.3$, $\gamma_s+2\nu=2.0\pm0.4$, and $\gamma=1.1\pm0.4$. Furthermore, we have calculated the crossover exponent ϕ at M by numerically differentiating the series with respect to Δ; we estimate[12] $\phi=1.1\pm0.3$.

Let us now examine what happens when a biquadratic term ($\beta\neq0$) is added to the interaction (see Fig. 2); we discuss only the disordered-state expansions for the isotropic case ($\Delta=1$). As β falls below zero, $\lambda_c(\beta)$, which

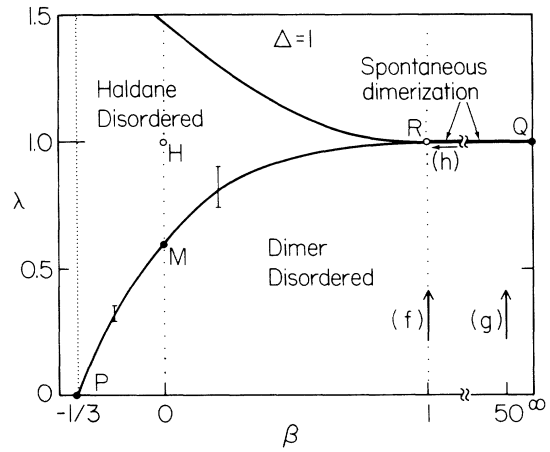

FIG. 2. Phase diagram in the λ,β plane for $\Delta=1$. Along QR, the system is both spontaneously dimerized and critical. For $\beta\leq-\frac{1}{3}$, our method of calculation cannot be implemented.

gives the position of the multicritical point analogous to M for each slice through the phase diagram at constant β, moves to $\lambda=0$ as β approaches $-\frac{1}{3}$. At $\beta=-\frac{1}{3}$ the singlet and triplet states of the dimers cross, so for all $\lambda=0$, $\Delta=1$, and $\beta\leq-\frac{1}{3}$ the ground state is exponentially degenerate and expansions cannot be performed by our methods.

As β increases from zero, $\lambda_c(\beta)$ also rises. Although the critical-point estimates are not precise, the smoothness of the extrapolations as functions of β strongly suggests that there is a line of multicritical points, of which M is an unexceptional member, coming out of the Bethe-*Ansatz*-solvable multicritical point R. Unfortunately, our estimates of the critical exponents along this line are not sufficiently precise to determine whether this line of multicritical points is in the same universality class as R, although they are consistent with the possibility.

At $\beta=1$ (trajectory f), we can use to our advantage the knowledge[2] that $\lambda_c=1$ to obtain reliable estimates for critical exponents for all of the quantities studied.[13] We find that the critical indices are $\gamma_s^{(R)}=0.15\pm0.15$, $\gamma_s^{(R)}+2\nu^{(R)}=1.56\pm0.05$, and $\gamma^{(R)}=0.9\pm0.1$. In addition, we define exponents for the energy and dimerization via $E_g-E_g^{(R)}\sim(1-\lambda)^{2-\alpha(R)}$ (plus possible analytic terms on the left-hand side) and $D\sim(1-\lambda)^{1/\delta_D^{(R)}}$; we estimate $2-\alpha^{(R)}=1.37\pm0.03$ and $1/\delta_D^{(R)}=0.34\pm0.02$. The field-theoretical calculations of Affleck predict[1] $\eta^{(R)}=\frac{1}{4}$, $\nu^{(R)}=\frac{8}{13}\approx0.615$, and[14] $1/\delta_D^{(R)}=\frac{5}{13}\approx0.385$. The exponent $\eta^{(R)}=\frac{1}{4}$ is in agreement with the Bethe-*Ansatz* solution. Taking that value for granted, and making standard scaling assumptions, we estimate $\nu^{(R)}=0.69\pm0.03$. Postulation of hyperscaling, namely $2-\alpha^{(R)}=2\nu^{(R)}$, gives $\nu^{(R)}=0.69\pm0.02$. Hence our results are consistent, within small uncertainties, with hyperscaling. Although our estimates of $\nu^{(R)}$ and $1/\delta_D^{(R)}$ appear inconsistent with Affleck's predictions, possible logarithmic corrections to the critical behavior[15] may have systematically shifted the exponents indicated by the series.

Consider next the results of the disordered-state expansions for $\beta>1$. We find unequivocally that the dimerization retains a *nonzero value* in the absence of an imposed bond alternation. For $\beta\gg1$, $D(\lambda=1)$ saturates at a value 0.75 ± 0.10, compared with the value of 2 at $\lambda=0$. Moreover, we find that as $\lambda\rightarrow1$ along a trajectory such as g, all the quantities μ_0^A, μ_2^A, χ^{zz}, E_g, and D are singular; thus the entire line $\lambda=\Delta=1$, $\beta>1$ constitutes a *critical phase*, in disagreement with the prediction of Affleck *et al.*[8] but in concurrence with the hints from finite-size studies of the energy gap.[16] For $\beta=50$, the exponents pertinent to AFM ordering are $\gamma_s=-0.15\pm0.20$, $\gamma_s+2\nu=0.75\pm0.05$, and $\gamma=0.25\pm0.05$. If one assumes that this dimerized critical phase is Lorentz invariant, then scaling implies $\nu=0.5\pm0.1$ and $\eta=1.5\pm0.3$—results markedly different from the values at R. The indices $1/\delta_D$ and $2-\alpha$, defined in the same way as their counterparts at R (except that a nonzero value for D at $\lambda=1$ must be allowed for), are estimated to be $1/\delta_D=0.5\pm0.2$ and $2-\alpha=1.5\pm0.2$. An important exponent which we are unable to estimate is β_D, which describes the vanishing of $D(\beta)$ along trajectory h.

Our findings regarding the criticality of the spontaneously dimerized phase are surprising on several grounds. First, since spontaneous dimerization is associated with broken discrete (reflection), rather than continuous, symmetry, one would not expect D to be singular on approach to the spontaneously dimerized phase along a trajectory such as g; however, the exponent $1/\delta_D$ is clearly less than unity. Second, hyperscaling, as manifested in the exponent relation $2-\alpha=2\nu$, appears to be violated by a significant amount: based on the estimates above, $2-\alpha-2\nu=0.5\pm0.3$. The scenario does seem to be similar to criticality below T_c in classical models with broken continuous symmetry, such as the Heisenberg model for $d>2$; perhaps the additional timelike direction of $T=0$ quantum systems somehow endows the apparently discrete symmetry with features of a continuous symmetry. Third, it is not obvious why the spin-spin correlations should become long ranged in the spontaneously dimerized phase. This behavior is, however, consistent with a picture for the λ,Δ phase diagram for $\beta>1$ like that in Fig. 1, but in which the Haldane phase has disappeared, leaving behind the single point $\lambda=\Delta=1$.

Another surprising result is the very existence of the phase boundary PR in Fig. 2, although it was anticipated by the field-theoretic arguments of Affleck and Haldane.[3] Since the spontaneous dimerization appears to be the order parameter for $\beta>1$, one expects bond alternation to play the role of an ordering field, which, according to standard dogma, should destroy any transitions for $\lambda\neq1$. However, there is no analog of the Yang-Lee circle theorem for this system, so such a phase diagram is not forbidden. A useful phenomenological analogy may be provided by the bicritical point in the classical Heisenberg model for $d>2$, with easy-plane and easy-axis anisotropy in that classical model playing the role of β ($\gtrless1$), and an applied field along an easy-plane direction playing the role of bond alternation.

To summarize, we have employed series expansions to investigate the $T=0$ phase diagram and criticality in the antiferromagnetic, spin-1, nearest-neighbor chain with exchange anisotropy, bond alternation, and biquadratic coupling. Many unexpected features of the phase diagram have been uncovered. We find that the disordered "Haldane" phase, which includes the simple spin-1 chain, cannot be reached by adiabatic continuation from the disordered "dimer" phase in the space of parameters studied here. (It is possible that the two phases are actually connected, but only if a staggered field is included in the Hamiltonian.[17]) In the absence of biquadratic coupling, and presumably for all $-1<\beta<1$, we have found

that bond alternation in sufficiently small amounts actually increases the stability of AFM Ising order. A spontaneously dimerized, critical phase was found to exist for $\beta > 1$. Still other questions related to the phase diagram remain to be explored. For example, what does the λ,Δ phase diagram look like for $\beta > 1$? One might also want to learn about the location of the Haldane-XY boundary.

Regarding the criticalities in this model, we have estimated a host of exponents, with special attention to those at the Bethe-*Ansatz*-solvable point R, and raised many questions. The criticality of the Haldane-Ising phase boundary is in excellent agreement with the results of the classical 2D Ising model. A remarkable result is the apparent critical behavior in the spontaneously dimerized phase. We hope the newly discovered phase boundaries, as well as the concrete estimates of exponents presented, will motivate further work in the field. Clearly, the nature of the interplay between the tendencies towards dimerization and antiferromagnetic ordering deserves further exploration.

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