Ground States of Low-Dimensional Quantum Antiferromagnets

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We have developed a general scheme for carrying out systematic perturbation expansions for ground-state properties of quantum lattice models. As an application, we study the onset of spontaneous Néel order in $S=\frac{1}{2}$ Heisenberg antiferromagnets by expanding around dimerized Hamiltonians. In one dimension (1D) we recover accurately the known exact results. On the square lattice we find novel critical points separating Néel ordered and disordered phases; the estimated critical exponents are consistent with those of the 3D classical Heisenberg model.

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The zero-temperature properties of quantum many-body systems and the location and character of ground-state instabilities (critical points) under changes of parameters in the Hamiltonian represent fundamental problems in condensed matter theory. Unlike classical statistical mechanics, where our understanding of critical phenomena and phase transitions is quite extensive, there have been few concrete developments in quantum criticality.[1] A notable exception is the case of one-dimensional systems.[2] Recent experimental[3] and theoretical[4] advances in high-temperature superconductivity have led to a resurgence of interest in some of these problems, in particular, to the question of long-range order in 2D Heisenberg antiferromagnets. We discuss here a general calculational scheme that addresses the topic of zero-temperature quantum criticality, and apply it to low-dimensional Heisenberg antiferromagnets. For 1D, we recover accurately the known exact results for alternating spin chains. In 2D we find that introducing bond alternation in the square lattice Heisenberg antiferromagnet leads to novel quantum critical points. These critical points, which separate Néel ordered and disordered phases, have critical exponents consistent with those of the 3D classical Heisenberg model, given proper interpretation of the 2D-3D correspondence.

The basic idea behind our work is that there are well defined phases in the parameter space of quantum Hamiltonians. Within a given phase the ground-state properties of one Hamiltonian can be accessed from that of another by adiabatic continuation, i.e., by following the evolution of the ground state under continuous variation in parameters. Adiabatic continuity of the ground state breaks down at phase boundaries, where singularities or crossings of energy levels occur. In order to implement this idea of adiabatic continuation in a concrete manner and investigate these quantum phase transitions, we shall borrow tools and techniques from classical critical phenomena, namely, series expansions and analysis.

We consider, specifically, spin-$\frac{1}{2}$ Heisenberg models on the linear chain and the square lattice with nearest-neighbor antiferromagnetic exchange J. Let us partition the infinite lattice into nearest-neighbor dimers and let H_0 be the part of the Hamiltonian containing the exchanges within dimers, while H_1 contains the remainder of the exchanges. We then consider the one-parameter family of models with Hamiltonian $H=H_0+\lambda H_1$. For $\lambda=0$ the spectrum of $H=H_0$ is trivial, the ground state is a product of singlets for each dimer and the energy gap to the lowest excited states is J. Turning on λ then couples the dimers; the full symmetries of the lattice are restored at $\lambda=1$. Note that we have chosen H_0 to be dimers primarily because this appears to be the simplest way to have a trivially diagonalizable system with a disordered ground state while maintaining rotational invariance in spin space. Our purpose is not primarily to study dimerized models *per se*, but rather to illustrate what are presumably more general properties of Heisenberg models.

We perform the adiabatic continuation *via* a high-order perturbation calculation in powers of λ, which is analyzed by means of standard series extrapolation methods developed for critical phenomena.[5] Since the ground state and the perturbation H_1 are both rotationally invariant in spin space, that symmetry cannot be broken in any order of the perturbation theory: One remains in the total-spin-zero subspace, with no sublattice magnetization. However, the symmetry can be spontaneously broken at some critical point, λ_c, where the perturbation expansion diverges. One cannot adiabatically continue past such a critical point to higher values of λ.[6] For the linear chain $\lambda_c=1$, while for the square lattice we find $0<\lambda_c<1$.

We obtain expansions in λ for the ground-state energy per site, E_0, the equal-time, antiferromagnetic (AF) structure factor, S_π (in 2D this is actually $S_{\pi,\pi}$), the correlation length, ξ, and the AF susceptibility, χ_π,

defined by

$$H\Psi_0 = NE_0\Psi_0 ,$$
$$S_\pi = \frac{1}{N}\sum_{i,j}\epsilon_{ij}\langle\Psi_0|\mathbf{S}_i\cdot\mathbf{S}_j|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle , \quad (1)$$
$$S_\pi\xi^2 = \frac{1}{N}\sum_{i,j}\epsilon_{ij}r_{ij}^2\langle\Psi_0|\mathbf{S}_i\cdot\mathbf{S}_j|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle ,$$
$$\chi_\pi = -\frac{\partial^2}{\partial(h^+)^2}E_0(h^+) ,$$

in the $N\rightarrow\infty$ limit, where N is the number of spins. Note that H, Ψ_0, E_0, S_π, χ_π, and ξ all implicitly depend on λ. Here h^+ is a staggered field, ϵ_{ij} is 1 if sites i and j lie on the same sublattice and -1 otherwise, while r_{ij} is the distance between i and j.

We have developed a general technique for carrying out systematic, high-order perturbation expansions for lattice-based quantum many-body systems. At $T=0$, these expansions require a perturbative diagonalization of infinite-dimensional matrices. Following the strategy of classical cluster methods,[7] we reduce the expansion for the infinite system to a sum of terms each of which involves only a finite cluster and hence a finite-dimensional Hilbert space. For a given cluster, one constructs the matrices for H_0 and H_1 in a basis in which H_0 is diagonal. Expressions for the ground-state energy and wave function are obtained through elementary recursion relations, and the wave function is then used to evaluate expansions for ground-state expectation values. The method is systematic enough that it can be carried out entirely on the computer. It is also general enough to study any quantum lattice model around a point where there is a gap in the spectrum[8] and the eigenstates are infinite direct products over states, each involving only a finite set of points in real or reciprocal space. Practical limitations are forced by considerations of computer storage and time. Recently, we have used these methods to generate expansions for the AF Heisenberg-Ising $S=\frac{1}{2}$ chain[9] to order $(J_{xy}/J_z)^{22}$ and a variety of expansions for the $S=1$ chain.[10] Application to Hubbard models is currently under consideration. Details of the method will be given elsewhere.

For the 1D linear chain there is only one type of nearest-neighbor dimerized configuration, and the problem reduces to the alternating spin chain.[11] The expansions have been developed to order λ^{15} for E_0 and to order λ^7 for S_π, ξ^2, and χ_π. Unbiased analysis of the energy series by inhomogeneous differential approximants[5] shows a critical point at $\lambda_c = 1.001 \pm 0.002$. Since the critical point is known to be exactly at $\lambda_c = 1$, a biased analysis helps in accurately determining various properties of the Heisenberg chain. We estimate the ground-state energy to be $E_0 = -0.443\,14 \pm 0.000\,01$ (the exact result being $\simeq -0.443\,147$). We estimate that S_π diverges with an exponent $\lambda_s = 0.05 \pm 0.15$, χ_π diverges with an exponent $\gamma = 0.79 \pm 0.05$, and ξ diverges with an exponent $\nu = 0.66 \pm 0.02$, which compare well with the conjectured exact answers of $O(\log)$, $\frac{2}{3}$ and $\frac{2}{3}$, respectively.[12] The details of the analysis will be presented elsewhere.[13]

For the square lattice there are infinitely many dimer configurations which can be used to specify H_0. A random dimerization would introduce quenched disorder into H, and so we consider only regular (periodic) dimerizations. One expects that the universal properties of the model, such as the topology of the phase diagram and the critical exponents, should not depend on the specific regular dimerization chosen. We have used two such dimer configurations as starting points for the expansions, namely, (A) and (B), shown in Fig. 1. Note that we have chosen (A) and (B) because they are the simplest cases, not because they have any particular physical significance (although they could be viewed as models of lattice distortions). The expansion coefficients, c_n, for E_0, S_π, χ_π, and ξ^2 are given in Table I; the expansions have been performed to orders 6 and 5, respectively. The energy series are ill behaved and are not used in the extrapolations reported here. The ratio of successive terms in the series for S_π, ξ^2, and χ_π are plotted versus $1/n$ in Fig. 2. These ratio plots[5,13] indicate critical points at $\lambda_c = 0.54 \pm 0.02$ for (A) and at $\lambda_c = 0.39 \pm 0.01$ for (B). [Note that (A) and (B) are distinct dimerizations and need not have the same λ_c.] The divergences of χ_π, S_π, and ξ^2 suggest strongly that the ground states are unstable towards Néel ordering beyond these points: Néel order for the uniform square lattice ($\lambda = 1$) has been found by many authors.[14-17]

Let us now consider the criticality at λ_c. Based on the symmetries of the problem at long wavelengths, Chakravarty, Halperin, and Nelson[17] have argued that criticality in the 2D quantum Heisenberg models at $T=0$ should lie in the universality class of the 3D classical Heisenberg model,[18] which has critical exponents for variation in temperature given by $\gamma = 1.40 \pm 0.02$ and $2\nu = 1.42 \pm 0.04$.[19] This correspondence implies that the critical point should be "Lorentz invariant"; i.e., the critical exponents for correlations in the spatial and temporal directions should be equal. Quite generally one can

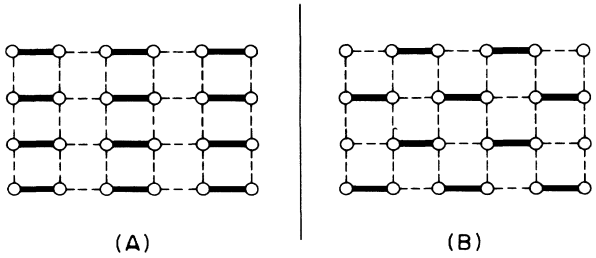

FIG. 1. Dimer configurations (A) and (B). The solid bonds represent the terms in H_0, while the dashed bonds represent the terms in H_1.

TABLE I. Expansion coefficients, c_n, for E_0, S_π, ξ^2, and χ_π as power series in λ, on the square lattice for dimer configurations (A) and (B).

	(A)				(B)			
n	$8E_0$	$4S_\pi$	ξ^2	χ_π	$8E_0$	$4S_\pi$	ξ^2	χ_π
0	−3	6	0.5	1	−3	6	0.5	1
1	0	9	3	3	0	9	4	3
2	−1.875	16.5	9.75	7.375	−1.125	18	13	8.625
3	−0.84375	29.625	25.042	17.063	−0.84375	38.313	38.833	23.937
4	−0.33789	51.751	58.969	37.402	−0.75586	85.783	111.90	65.171
5	0.24333	93.256	131.82	79.690	−0.76383	198.34	314.20	175.24
6	0.24172	168.77	284.65	165.96				

define a dynamic exponent z for the quantum problem by requiring that the gap, Δ, which gives the inverse correlation length in the time direction, vanish as $\Delta \sim \xi^{-z}$ as $\lambda \to \lambda_c$. Thus $z=1$ corresponds to Lorentz-invariant criticality.

We can estimate the exponents γ, ν, and γ_s in the present problem and obtain z through a simple scaling relation. The AF susceptibility, χ_π, is related to the frequency-dependent AF structure factor, $S_\pi(\omega)$, via[20] $\chi_\pi \sim \int d\omega S_\pi(\omega)/\omega$, while the equal-time structure factor $S_\pi \sim \int d\omega S_\pi(\omega)$. Thus by scaling one expects near criticality $S_\pi \sim \Delta \chi_\pi$; this yields the exponent relation $\gamma_s = \gamma - z\nu$. *D*log Padé analyses and ratio tests indicate that $2\nu = 1.7 \pm 0.3$, $\gamma_s = 0.8 \pm 0.2$, and $\gamma = 1.7 \pm 0.3$ for (A), and that $2\nu = 1.5 \pm 0.4$, $\gamma_s = 0.5 \pm 0.2$, and $\gamma = 1.3 \pm 0.3$ for (B). Furthermore, by scaling we get $z = 1.0 \pm 0.4$ for both (A) and (B). Thus, our results are consistent with a criticality that is Lorentz invariant, and furthermore, in the universality class of the 3D classical Heisenberg model (with λ playing the role of inverse temperature). For $\lambda > \lambda_c$ we thus expect long-range Néel order in the ground state.

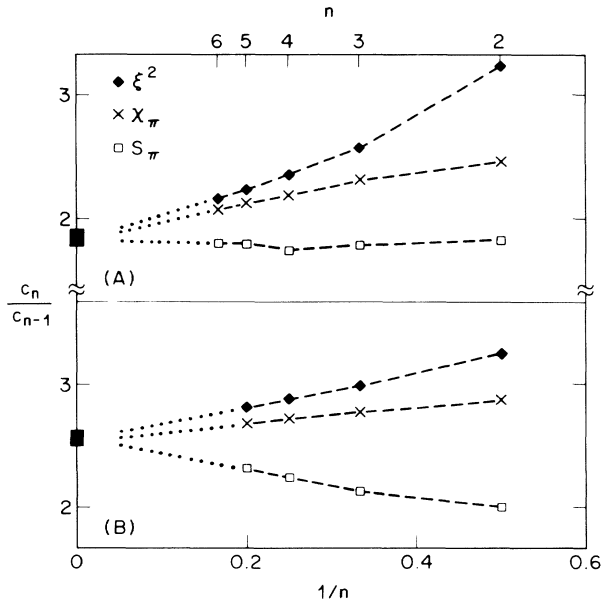

FIG. 2. Ratios of expansion coefficients for S_π, χ_π, and ξ^2 plotted vs $1/n$ for cases (A) and (B). The estimated values of $1/\lambda_c$ are indicated on the vertical axis.

Direct evidence for Néel ordering for $\lambda > \lambda_c$ can be obtained by expanding the sublattice magnetization $m^\dagger$ around the Ising limit ($J_{xy}=0$) for general values of λ, as is done for $\lambda = 1$ in Ref. 14. This gives

$$m^\dagger = \frac{1}{2} - \frac{J_{xy}^2}{36\lambda^2 J_z^2}\left(\frac{27\lambda^4+4\lambda^2+4\lambda+1}{4\lambda^2+4\lambda+1}\right) + O\left(\left[\frac{J_{xy}}{J_z}\right]^4\right). \quad (2)$$

Notice that to the displayed order, $m^\dagger$ is the same for cases (A) and (B)—the difference arises in the next order. The leading two terms give a reasonable estimate of $m^\dagger$ at $\lambda = 1$ and $J_{xy} = J_z$ if we remove the expected spin-wave singularity by changing to a new variable δ defined by[14] $[1-(J_{xy}/J_z)^2]^{1/2} = 1-\delta$. After the change of variable, one finds

$$m^\dagger = \frac{1}{2} - \frac{\delta}{18\lambda^2}\left(\frac{27\lambda^4+4\lambda^2+4\lambda+1}{4\lambda^2+4\lambda+1}\right) + O(\delta^2). \quad (3)$$

For $\lambda \to 0$, the coefficient of δ diverges; this is expected because disconnected Ising dimers are always disordered. We can estimate λ_c at $\delta = 1$ by setting $m^\dagger = 0$ in (3), which gives $\lambda_c \simeq 0.36$, a value not far from the critical points estimated earlier. This further strengthens the case that the observed critical points separate the Néel ordered and disordered phases.

To conclude, we have developed a general technique to carry out high-order perturbation expansions in quantum spin systems and applied it to the $S = \frac{1}{2}$ Heisenberg antiferromagnet on the linear chain and square lattice. The method accurately reproduces the ground-state properties of the alternating spin chain. For the square-lattice Heisenberg antiferromagnets we have found novel quantum critical points as a function of dimerization. These critical points appear Lorentz invariant, and their critical exponents are consistent with those of the 3D

classical Heisenberg model.

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[1]J. A. Hertz, Phys. Rev. B **14**, 1165 (1976); A. P. Young, J. Phys. C **8**, L309 (1975).

[2]E. H. Lieb and D. C. Mattis, *Mathematical Physics in One Dimension* (Academic, New York, 1966); J. C. Bonner, J. Appl. Phys. **61**, 3941 (1987).

[3]D. Vaknin *et al.*, Phys. Rev. Lett. **58**, 2802 (1987); G. Shirane *et al.*, Phys. Rev. Lett. **59**, 1613 (1987); J. M. Tranquada *et al.*, Phys. Rev. Lett. **60**, 156 (1988).

[4]T. M. Rice, Z. Phys. B **67**, 141 (1987), and references therein.

[5]For a general review of series analysis, see D. S. Gaunt and J. Guttman, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, London, 1974), Vol. 3. For differential approximants, see M. E. Fisher and H. Au-Yang, J. Phys. A **12**, 1677 (1979); D. L. Hunter and G. A. Baker, Jr., Phys. Rev. B **19**, 3808 (1979).

[6]An alternative possibility is that a different state becomes lower in energy for some λ; however, at the point of crossing it is orthogonal to the original one. This would be analogous to a first-order transition, and the adiabatically continued state (if it exists) would be metastable. A realization of this possibility could arise if one were to start from a dimer configuration and add *ferromagnetic* interactions, since a state of high spin could become lower in energy than the lowest-energy singlet state.

[7]For a discussion of cluster methods applied to classical systems, see, e.g., S. McKenzie, in *Phase Transitions Cargese,* edited by M. Levy, J. C. LeGuillou, and J. Zinn-Justin (Plenum, New York, 1980).

[8]Strictly speaking, one only requires a gap to any state that is connected to the ground state by a finite power of the perturbing Hamiltonian H_1.

[9]R. R. P. Singh, M. E. Fisher, and R. Shankar, Phys. Rev. B (to be published).

[10]R. R. P. Singh and M. P. Gelfand, Phys. Rev. Lett. **61**, 2133 (1988).

[11]For recent references, see, for example, G. Spronlen, B. Fourcade, and Y. Lépine, Phys. Rev. B **33**, 1886 (1986).

[12]See, for example, I. Affleck, D. Gepner, H. Shultz, and T. Ziman, to be published. The discrepancy in γ is presumably related to multiplicative logarithmic corrections.

[13]M. P. Gelfand, R. R. P. Singh, and D. A. Huse, to be published.

[14]D. A. Huse, Phys. Rev. B **37**, 2380 (1988).

[15]J. D. Reger and A. P. Young, Phys. Rev. B **37**, 5978 (1988).

[16]P. W. Anderson, Phys. Rev. **86**, 694 (1952); R. Kubo, Rev. Mod. Phys. **25**, 344 (1953).

[17]S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988).

[18]Note that Chakravarty, Halperin, and Nelson had in mind varying spin S as a parameter rather than the λ varied here.

[19]M. Ferer and A. Hamid-Aidinejad, Phys. Rev. B **34**, 6481 (1986), and references cited therein.

[20]See, e.g., P. C. Hohenberg and W. F. Brinkman, Phys. Rev. B **10**, 128 (1977).