



Quantum spin lattice models

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QUANTUM SPIN LATTICE MODELS: A COUPLED-CLUSTER TREATMENT

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1. INTRODUCTION

Infinite one-dimensional chains of quantum-mechanical spins interacting via localized (typically nearest-neighbour) interactions, and their obvious extensions to regular lattices in higher numbers of dimensions, have been objects of theoretical interest for a very long time. Indeed, the exact energy eigenstates of the one-dimensional spin-half chain interacting via the isotropic Heisenberg interaction between neighbouring sites, were exactly solved in principle by Bethe¹ some sixty years ago. Since then the Bethe-ansatz type of solution has been discovered to be applicable to, and fundamental to, a much wider class of integrable Hamiltonian models. This latter feature undoubtedly explains by itself much of the continuing interest in these spin lattice models. Another reason is that, intriguingly, the exact method of Bethe seems to be surprisingly impervious to being extended to deal with similar models in a higher number of dimensions.

Furthermore, the form of the solution for the wavefunction, although exact, is so difficult to use in practice that even now various properties of the systems solvable by Bethe-ansatz techniques are not themselves exactly known. Such properties include the precise details of the long-range order in the system, which could be found from an exact knowledge of the asymptotic behaviour of the correlation functions at large distances.

In view of the enduring theoretical interest in the quantum spin chain and lattice models it is perhaps surprising that the various fundamental microscopic techniques of quantum many-body theory have scarcely been applied to them up to the present time. Indeed, quite apart from the above reasons, there are many features of the discrete spin lattice models that make them very attractive and challenging candidates for study by microscopic quantum many-body techniques. In the first place, most of the models are themselves analytically and conceptually simple, while being highly nontrivial to solve exactly. Indeed they contain some of the mathematically most intractable models. Nevertheless, they provide the many-body theorist with a nice mixture of exact results against which techniques and approximations can be judged and measured, and simply stated yet unsolved problems of fundamental interest. In fact, within a single class of model lattice problems one can often find an interesting combination of both integrable and nonintegrable systems.

An important feature of the discrete quantum spin lattice models,

especially in low dimensions, is that their behaviour is in many respects quite different, and often counter-intuitive, from that of their classical counterparts. Indeed, in this respect they are among the most quantum-mechanical of all many-body systems. In particular, they display interesting phase transitions and other unexpected behaviour as a function, for example, of the coupling parameters in the Hamiltonian, the dimensionality of the system, the value of the total spin quantum number of the individual spins, and the strength of the coupling to external magnetic fields, none of which is easily intuited by classical arguments. Of further interest to the theorist is that the various model systems may easily be studied in different numbers of spatial dimensions and on different geometrical lattices, for example, within the same formalism. Furthermore, these discrete lattice models are often also studied as proxies for various nonlinear quantum field theories of great theoretical interest, to which they correspond in either the continuum limit or some quasiclassical limit in which the spin quantum number $s \rightarrow \infty$, for example.

Finally, we note that discrete spin lattice problems are also of considerable experimental interest. Apart from such obvious candidates as the solid crystalline phases of ^3He , several lower-dimensional systems are also believed to be experimentally realizable. An example of a quasi-one-dimensional system is the material CsNiCl_3 which is believed to be an antiferromagnetic chain in which the magnetic nickel ions form chains with a strong $\text{Ni}^{++}-\text{Cl}-\text{Ni}^{++}$ superexchange coupling. Similarly, two-dimensional lattice systems are widely believed to provide a good model for the high-temperature superconductivity exhibited by the recently discovered ceramic oxide materials, in which the layered CuO_2 planes are thought to be an important aspect of the phenomenon.

For all of the above reasons it is our intention here to explore the applicability of the coupled cluster method (CCM) to quantum spin lattice models, since this method has now become firmly established as providing one of the most powerful and most accurate of all microscopic formulations of quantum many-body theory. It has been widely applied to many different types of physical systems, although not yet to spin lattice models,² with the exception of some pioneering work of Roger and Hetherington,² which was specifically directed to the problem of the ground state of solid ^3He .

A fundamental reason for the wide success of the CCM emanates from its parametrization of the exact many-body ground-state wavefunction as an exponential operator, $\exp(S)$, acting on some suitable noninteracting or model state. In this way the resulting perturbation or cluster expansion contains only linked terms. Coester and Kümmel³ have shown how the linked cluster operator S can be used as the generator of a similarity transformation for the exact ground-state problem. They thereby originated what has since become known as the CCM. A rather general and pedagogical discussion of the method has been given recently,⁴ and other more technical reviews have also described the CCM within the context of various specific fields of application.⁵⁻⁸

The range of numerically very accurate CCM applications has been wide. It includes problems in nuclear physics,^{5,8} both for finite nuclei and infinite nuclear matter;⁹ atomic and molecular systems in quantum chemistry;^{7,10-12} and the homogeneous electron liquid.^{6,13,14} More recently, the CCM has also been successfully applied to two systems not normally associated with traditional many-body physics, namely the quantum anharmonic oscillator,¹⁵⁻¹⁷ and the ϕ^4 relativistic quantum field theory.¹⁸

The particular spin lattice models^{2,4} under consideration here are first briefly reviewed in Sec. 2, where we also discuss some of the exact results that are known. One of the key features of the CCM is that it is a

biorthogonal (rather than an orthogonal) formulation of the quantum many-body problem, in which the corresponding bra and ket states are hence not maintained as being manifestly hermitian conjugate to each other. Accordingly, we first describe in Sec. 3 the coupled cluster (CC) parametrization of the ground ket energy eigenstate, with particular emphasis initially on the one-dimensional (1-d) spin-half ($s = \frac{1}{2}$) XXZ model. Although the ket state suffices to calculate the ground-state energy of the system via the Schrödinger equation, other properties require a knowledge of the respective bra state also. Its corresponding CC parametrization is discussed in Sec. 4.

In Secs. 3 and 4 we describe several intuitively appealing new CC approximation schemes which are especially tailored to the spin lattice models. After having demonstrated their usefulness for calculations of the ground-state energy in Sec. 3, we turn in Sec. 5 to the much more demanding calculation of the correlation function and the corresponding order parameter which determines the presence or absence of long-range (antiferromagnetic) order. In view of the rather successful outcomes of these calculations, we turn in Sec. 6 to their generalization to the corresponding two-dimensional (2-d) model on a square lattice, for which almost no exact results are known. Finally, our results are summarized and discussed in Sec. 7.

2. BRIEF REVIEW AND EXACT RESULTS

We are concerned with the general problem of N quantum-mechanical spins $\vec{s}_i \equiv \{s_i^a; a \equiv x, y, z\}$ on the sites $\{i\}$ of a given regular lattice in d dimensions. The spins obey the usual $SU(2)$ angular momentum algebra,

$$[s_j^a, s_k^b] = i\delta_{jk} \epsilon_{abc} s_k^c, \quad (1)$$

in terms of the usual three-dimensional antisymmetric unit tensor ϵ_{abc} , and where the summation convention is employed. The spin quantum number s may take any of the usual integral or half-integral values,

$$\vec{s}_k^2 = s(s+1); \quad s = 1/2, 1, 3/2, \dots \quad (2)$$

We shall mostly be interested in the infinite lattice limit where $N \rightarrow \infty$, and where periodic boundary conditions are used.

In the present paper we concentrate on the so-called XXZ model with nearest-neighbour interactions between the localized spins described by the (anisotropic) Hamiltonian,

$$H = \sum_{\langle ij \rangle} (s_i^x s_j^x + s_i^y s_j^y + \Delta s_i^z s_j^z), \quad (3a)$$

and where the notation $\langle ij \rangle$ refers to nearest-neighbour pairs. For example, in 1-d Eq. (3a) takes the explicit form,

$$H = \sum_{i=1}^N (s_i^x s_{i+1}^x + s_i^y s_{i+1}^y + \Delta s_i^z s_{i+1}^z), \quad (3b)$$

and with the periodic boundary condition that site $(i = N+r)$ is identical to site $(i = r)$. The Hamiltonian of Eq. (3b) is antiferromagnetic for $\Delta > -1$ and ferromagnetic for $\Delta \leq -1$. We note that Eqs. (3a,b) contain as three particular special cases the Ising model ($\Delta \rightarrow \infty$), the (isotropic) Heisenberg model ($\Delta = 1$), and the isotropic planar XY model ($\Delta = 0$). We also observe that the general XXZ Hamiltonian of Eq. (3a) commutes with the z -component of

the total spin operator, \vec{S}_T ,

$$\vec{S}_T \equiv \sum_i \vec{S}_i, \quad (4)$$

and hence the energy eigenstates are therefore simultaneous eigenstates of the z-component of total spin, S_T^z .

For the spin-half ($s = \frac{1}{2}$) 1-d Heisenberg ($\Delta = 1$) chain, the exact eigenstates were formally obtained by Bethe¹ in 1931 for arbitrary N . The difficulty of actually using these wavefunctions is perhaps first demonstrated by the fact that it was not until seven years later that Hulthén¹⁹ found the antiferromagnetic ground-state energy for the infinite ($N \rightarrow \infty$) chain, using an integral equation approach. Secondly, the continuing doubt about the nature of the long-range order even when the exact wavefunction had long been known in principle, and the fact that the Bethe-ansatz technique is inapplicable to the $d > 1$ case, led Anderson²⁰ and, independently, Kubo²¹ to introduce the approximate spin-wave theory to describe these systems. In 1958, Orbach²² generalized the method of Bethe to deal with the anisotropic ($\Delta \neq 1$) case considered here.

Moving beyond the ground state, the low-lying excited states of the $s = \frac{1}{2}$ Heisenberg model in 1-d were first investigated by des Cloiseaux and Pearson in 1962,²³ using a generalization of the earlier Hulthén approach. Later work of Yang and Yang²⁴ was also of importance for the XXZ model in this connection. A detailed description of the (so-called antiferromagnetic spin wave) excitations of the anisotropic $s = \frac{1}{2}$ Hamiltonian of Eq. (3b) was given by des Cloiseaux and Gaudin²⁵ in 1966. Nevertheless, it was not until 1981 that Faddeev and Takhtajan²⁶ cleared up the confusion that had existed until then concerning the precise nature of the Bethe-ansatz spin-wave excited eigenstates.

In particular, they established, specifically for the Heisenberg antiferromagnet, that the actual spin of a spin wave in the 1-d $s = \frac{1}{2}$ chain is equal to one half rather than the triplet ($s = 1$) or singlet ($s = 0$) values that had been assumed previously. They further showed that all physical states have integral values of spin and contain an even number of spin waves. The spin wave excitation is itself a kink rather than an ordinary "particle". In this way they also made contact between the eigenstates found by Bethe-ansatz techniques and those found by the application to this Heisenberg model²⁷ of the then very recently invented quantum inverse scattering method of Faddeev²⁸ and his coworkers. We note in passing that the quantum inverse scattering method (QISM) (or quantum spectral transform method) rejuvenates and makes much more transparent the depth and power of the conventional Bethe-ansatz technique. By contrast to the original coordinate-space formulation of the Bethe ansatz, the QISM essentially algebraizes the technique. It thereby allows the energy eigenvalues, and other integrals of the motion in more general cases, to be evaluated directly, without passing through the complicated intermediate stage of explicitly evaluating the corresponding eigenfunctions in their coordinate-space representation.

Out of the work discussed above, the following exact results have emerged for the $s = \frac{1}{2}$ linear XXZ chain. For values $\Delta \leq -1$, namely the ferromagnetic ($S_T^z = \pm \frac{1}{2}N$) regime, the exact ground-state (g.s.) energy is

$$E_g/N = \frac{1}{4}\Delta; \quad \Delta \leq -1. \quad (5)$$

There is a first-order phase transition to a 'critical' antiferromagnetic

phase at $\Delta = -1$. We note that whereas the perfectly aligned ferromagnetic state with all spins oriented along the z-axis is an *exact* eigenstate of both the quantum-mechanical Hamiltonian of Eq. (3b) and its classical counterpart, the corresponding perfectly ordered alternating Néel state $|\uparrow\downarrow\uparrow\downarrow\dots\rangle$, which is the classical antiferromagnetic ground state, is *not* an eigenstate of the quantum-mechanical Hamiltonian except in the Ising ($\Delta \rightarrow \infty$) limit.

On the antiferromagnetic side of the transition ($\Delta > -1$) the quantum-mechanical system has an Ising-like doubly-degenerate ground state only for $\Delta > 1$. This state has $s_T^z = 0$, and an energy given by the exact expression,

$$\frac{E}{N} = \frac{1}{4} \cosh \gamma - \frac{1}{2} \sinh \gamma \left[1 + 4 \sum_{m=1}^{\infty} (e^{2m\gamma} + 1)^{-1} \right]; \quad 1 < \Delta \equiv \cosh \gamma. \quad (6)$$

It is not difficult to show from Eq. (6) that in the Heisenberg and Ising limits the g.s. energy is given respectively as,

$$\frac{E}{N} = \frac{1}{4} - \ln 2; \quad \Delta = 1, \quad (7a)$$

$$\frac{E}{N} \xrightarrow{\Delta \rightarrow \infty} -\frac{1}{4} \left(\Delta + \frac{1}{\Delta} \right). \quad (7b)$$

At $\Delta = 1$ the system undergoes a second-order phase transition to a singlet ($s_T = 0$) nondegenerate ground state. This phase persists down to the ferromagnetic transition (i.e., for $-1 < \Delta < 1$). The g.s. energy of this phase is given by the exact expression,

$$\frac{E}{N} = \frac{1}{4} \cos \theta - \frac{1}{2} \sin^2 \theta \int_{-\infty}^{\infty} \frac{d\omega}{\cosh(\pi\omega) [\cosh(2\theta\omega) - \cos \theta]}; \quad |\Delta| < 1, \quad (8)$$

$$0 \leq \theta \equiv \cos^{-1} \Delta \leq \pi.$$

The g.s. energy of Eq. (8) is continuous at $\Delta = 1$ with that of Eq. (6). It can also be specifically evaluated for the planar XY model,

$$\frac{E}{N} = -\frac{1}{\pi}; \quad \Delta = 0. \quad (9)$$

The above two antiferromagnetic phases of the 1-d $s = \frac{1}{2}$ XXZ chain differ principally in their long-range order properties. These are conveniently summarized in terms of the spin-spin correlation function g_n defined by the relation,

$$g_n \equiv \langle \sigma_i^z \sigma_{i+n}^z \rangle, \quad (10)$$

in terms of the usual Pauli spin matrices, $\vec{\sigma} = \frac{1}{2} \vec{\sigma}$, and where the translational invariance implied by the periodic boundary condition assures the independence of g_n on the site position i and its dependence only on the relative spacing n of the two spins. The order parameter μ associated with the transition is then defined as

$$\mu \equiv \lim_{n \rightarrow \infty} |g_n|. \quad (11)$$

The Ising-like phase ($\Delta > 1$) is characterized by the presence of long-range order, $\mu > 0$, and by correlations which approach this limiting nonzero value exponentially. By contrast, the order parameter μ is zero in the range $|\Delta| < 1$, but this (otherwise disordered) phase is 'critical' in the usual sense of having correlations which decay algebraically (i.e., with power-law behaviour) to zero. In summary, the correlation function has the behaviour,

$$g_n \xrightarrow{n \rightarrow \infty} \begin{cases} (-1)^n (\mu + A\ell^{-n}) & ; \quad \Delta > 1 \\ (-1)^n Bn^{-\beta} & ; \quad -1 < \Delta < 1 \\ 1 & ; \quad \Delta < -1, \end{cases} \quad (12)$$

where the constants μ , A , B and ℓ , and the exponent $\beta > 0$, all depend on Δ . In particular, the order parameter has the limiting behaviour,

$$\mu \rightarrow \begin{cases} 1; & \Delta \rightarrow \infty \\ 0; & \Delta \rightarrow 1. \end{cases} \quad (13)$$

The two antiferromagnetic phases also differ qualitatively with respect to their excitation spectra. The excited states are usually given in terms of a dispersion law $\varepsilon(k)$ for the excitation energy, with respect to a momentum k lying in the first Brillouin zone, $-\pi \leq k \leq \pi$, although Faddeev and Takhtajan²⁶ have indicated that the fundamental excitation spectrum is actually that of a single $s_T = \frac{1}{2}$ kink with momentum $0 \leq k \leq \pi$. In the Ising-like phase ($\Delta > 1$) this single kink has exact excitation energy given by the relation,

$$\varepsilon(k) = \frac{K_1}{\pi} \sinh \gamma (1 - k_1^2 \cos^2 k)^{\frac{1}{2}}; \quad 1 < \Delta \equiv \cos \gamma, \quad (14)$$

where the parameter k_1 is given in terms of the complete elliptic integrals K_1 and K'_1 ,

$$K_1 = \int_0^{\frac{1}{2}\pi} d\theta (1 - k_1^2 \sin^2 \theta)^{-\frac{1}{2}}; \quad K'_1 = \int_0^{\frac{1}{2}\pi} d\theta [1 - (1 - k_1^2) \sin^2 \theta]^{-\frac{1}{2}}, \quad (15)$$

by the relation,

$$\frac{K'_1}{K_1} = \frac{\gamma}{\pi}. \quad (16)$$

The spectrum of Eq. (14) clearly shows the presence of a nonzero gap between the ground and first excited state at the zone boundary, $k = \pi$. By contrast, the critical phase displays a gapless excitation spectrum, $\varepsilon(k=\pi) = 0$, whose exact form is given as,

$$\varepsilon(k) = \frac{\pi}{2\theta} \sin \theta \sin k; \quad 0 \leq \theta \equiv \cos^{-1} \Delta \leq \pi, \quad 0 \leq k \leq \pi. \quad (17)$$

Finally, we note that the observed $s_T^z = \pm 1$ excitations are actually formed from two kink solutions of the form of Eq. (14) or Eq. (17). They have energy $E(k)$ given by the additive relation,

$$E(k) = \varepsilon(q) + \varepsilon(k-q), \quad (18)$$

and thus form a *continuum* (with respect to the parameter q) for a given value

of (total) momentum k . The lower boundary of this continuum gives the "antiferromagnetic spin waves" of Refs. [23,25].

If we now extend the discussion away from the 1-d Hamiltonian of Eq. (3b) for $s = \frac{1}{2}$ systems, either to higher dimensionality ($d > 1$) or to spins $s > \frac{1}{2}$, the situation changes dramatically. In the first place, if we consider the same $s = \frac{1}{2}$ XXZ Hamiltonian but for lattices in two or more dimensions, almost no exact results are known. In particular, the Bethe-ansatz technique of solution which was so useful in 1-d has never been successfully extended to provide exact solutions for the case $d > 1$.

Similarly, the Hamiltonian of Eq. (3a) or Eq. (3b) is not integrable for the case $s = 1$, even in 1-d, and exact results are not known. Nevertheless, there has been enormous interest in the last few years in the quantum spin chains with $s = 1$ and with various interactions between the spins, after the remarkable conjecture of Haldane²⁹ in 1983 concerning the isotropic Heisenberg model ($\Delta = 1$) for this case. Despite the fact that no exact results existed for XXZ-model chains with $s > \frac{1}{2}$, the prevailing opinion prior to the work of Haldane was that the $s = \frac{1}{2}$ phase diagram discussed above was probably also valid for arbitrary spins. This belief was supported by the analysis within the framework of the spin-wave approximation. Furthermore, as we have seen above, the transition between the two $s = \frac{1}{2}$ antiferromagnetic phases occurs at $\Delta = 1$, precisely where the symmetry of the Hamiltonian of Eq. (3b) changes. A naive (and ultimately spurious) extension of the universality principle which seemed to underlie this $s = \frac{1}{2}$ transition to higher spins, then indicated that the $s > \frac{1}{2}$ situation would in all likelihood be similar.

It thus came as a considerable surprise when Haldane conjectured²⁹ that a fundamental qualitative difference exists between the integer-spin and the half-odd-integer Heisenberg chains. Based on a mapping of the Hamiltonian of Eq. (3b) to the nonlinear σ -model, he predicted the existence of a new disordered ($\mu = 0$) ground state, in which the correlations decay exponentially to zero at large distances and for which there is a gap in the excitation spectrum, $\epsilon(k=\pi) \neq 0$. More specifically, it was postulated for the integral-spin XXZ chains in 1-d that the antiferromagnetically ordered Ising-like phase which exists at large anisotropy ($\Delta \gg 1$) would disappear as Δ was reduced to some critical value $\Delta_c > 1$. For $\Delta'_c < \Delta < \Delta_c$ a new nondegenerate disordered phase (the Haldane phase) was proposed, with a gap in the excitation spectrum and exponentially decaying correlations. Finally, for some range of values $\Delta < \Delta'_c$ (< 1) a gapless critical XY-like phase (with algebraically decaying correlations) may also appear, similar to the corresponding $s = \frac{1}{2}$ phase for $|\Delta| < 1$.

Although the initial controversy that greeted Haldane's conjecture is still not completely settled, most developments since then have lent support to it. For example, Lieb, Schultz and Mattis³⁰ had much earlier given a rigorous proof of zero gap in the excitation spectrum of the $s = \frac{1}{2}$ Heisenberg chain in 1-d. This proof has since been extended³¹ to arbitrary half-odd-integral values of s after Haldane's conjecture, but was also shown to fail for integral s . The conjecture has also been strongly supported by several Monte Carlo and exact diagonalizations of finite spin-one chains,³² and even by experimental results on such quasi-one-dimensional compounds as CsNiCl_3 mentioned in Sec. I. A recent review of the status of the Haldane gap has been given by Affleck.³³

Finally, we note that in view of the nonintegrability of the 1-d XXZ model, or indeed of the pure $\Delta = 1$ Heisenberg model, for the $s = 1$ case, other classes of $s = 1$ model Hamiltonians have also been studied. Of particular interest for present purposes is the class which comprises an arbitrary admixture of isotropic Heisenberg and biquadratic exchange, with Hamiltonian

given by

$$H = \sum_{i=1}^N \left[\cos\omega (\vec{s}_i \cdot \vec{s}_{i+1}) + \sin\omega (\vec{s}_i \cdot \vec{s}_{i+1})^2 \right] ; \quad s = 1 , \quad (19)$$

which contains the pure Heisenberg model considered by Haldane²⁹ as the special case $\omega = 0$ (point H in Fig. 1). Although it is known that that region $\pi/2 < \omega < 5\pi/4$ is ferromagnetic, the rest of what is almost certainly a rich and interesting phase diagram is certainly not known for this 1-d Hamiltonian. Nevertheless, tantalizing glimpses are provided by some known exact results since, remarkably enough, it contains some integrable models as special cases. Some of these have been indicated in Fig. 1.

For example, the case $\omega = \pi/4$ (point L in Fig. 1) corresponds to the integrable Schrödinger permutation model studied by Lai and Sutherland;³⁴ and the case $\omega = -\pi/4$ (point T in Fig. 1), which corresponds to³⁵ the

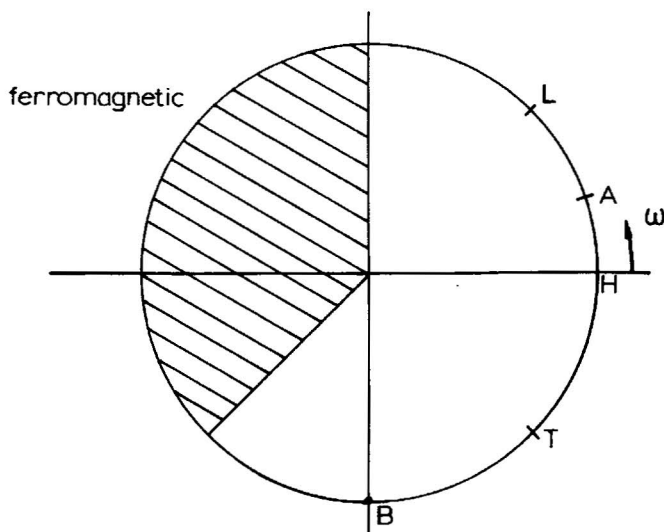


Fig. 1. A schematic indication of some of the known results for the ground-state phase diagram of the spin-1 quantum spin chain with Hamiltonian of Eq. (19), containing an arbitrary admixture of Heisenberg and biquadratic exchange. The labelled points refer to specific models discussed in the text.

Takhtajan-Babujian model is also solvable by Bethe-ansatz techniques, and can be shown to have zero gap. The exact ground state for the special case $\omega = \tan^{-1}(1/3)$ (point A in Fig. 1) was also solved by Affleck *et al.*,³⁶ who showed it to have a nonzero gap in the energy spectrum. Unlike the previous Bethe-ansatz ground-state solutions, this latter model has an exact ground state which can be written down simply in terms of 'valence bonds'. Finally, we note that the antiferromagnetic pure biquadratic $s = 1$ model, corresponding to the case $\omega = -\frac{1}{2}\pi$ (point B in Fig. 1), is also partially integrable.³⁷ In particular, its exact g.s. energy and excitation spectrum have been found by an exact mapping onto a special case of the $s = \frac{1}{2}$ XXZ-model Hamiltonian in 1-d.

In concluding this brief review, we hope that the above discussion has convinced the uninitiated reader that the discrete quantum spin chains in 1-d and lattices in $d > 1$ are systems which exhibit complex and interesting quantum-mechanical behaviour. We believe that they are prime candidates for study by the many-body techniques which have proven so successful for other condensed matter systems. In the remainder of this paper we describe the application to them of the coupled cluster method (CCM). We focus here wholly on the $s = \frac{1}{2}$ system since they have most exact results available for comparison. We therefore first study the 1-d XXZ-model Hamiltonian of Eq. (3b), and after demonstrating that the technique is capable of giving interesting results, we extend the calculations to the corresponding square lattice in 2-d, where almost no exact results are known. We intend in future work to extend the method further to deal with the $s = 1$ chains described by the Hamiltonian of Eq. (19) and other similar models.

3. CC TREATMENT OF THE GROUND KET STATE

For the spin- $\frac{1}{2}$ systems to which we henceforth restrict ourselves, it is convenient to introduce the Pauli spin matrices $\vec{\sigma}_k \equiv 2\vec{s}_k$ on each site k of the chain. Furthermore, we introduce the usual raising and lowering operators, albeit with a nonstandard normalization factor,

$$\sigma_k^{\pm} \equiv \frac{1}{2}(\sigma_k^x \pm i\sigma_k^y) . \quad (20)$$

The commutator relations equivalent to those in Eq. (1) are

$$[\sigma_k^-, \sigma_\ell^+] = -\sigma_k^z \delta_{k\ell} , \quad [\sigma_k^z, \sigma_\ell^{\pm}] = \pm 2\sigma_k^{\pm} \delta_{k\ell} . \quad (21)$$

In common with many other quantum-mechanical calculations, an essential feature of the CC approach is that the many-body correlations are referred to some model state, $|\Phi\rangle$. This is often chosen to be the ground state that the system would otherwise attain when the interactions or some part of them are turned off. In the CCM, the model state $|\Phi\rangle$ may be chosen rather generally. The one essential property for the standard formulation of CC theory is that $|\Phi\rangle$ is a *cyclic vector*. We thus assume that the algebra of all operators in the full many-body Hilbert space \mathcal{H} is spanned by the two subalgebras of creation and destruction operators defined with respect to the model state $|\Phi\rangle$. We assume further that these two subalgebras and the state $|\Phi\rangle$ are cyclic in the sense that all of the ket states in \mathcal{H} can be constructed as linear combinations of the states reached by operating on $|\Phi\rangle$ with the elements of the creation-operator subalgebra; and similarly for the bra states with respect to the state $\langle\Phi|$ and the elements of the destruction-operator subalgebra.

For purposes of the present paper we work wholly with the *Néel state* as our model state $|\Phi\rangle$, namely the exact ground state for the Ising antiferromagnet ($\Delta \rightarrow \infty$). For the 1-d spin- $\frac{1}{2}$ chain to which we initially restrict ourselves, this is the state $| - + - + - \dots \rangle$ in which half of the spins, say on the odd sites $i = 2n-1$ are in the down state $| - \rangle$ with respect to the z -axis as quantization axis, and the remaining spins, say on the even sites $i = 2n$, are in the up state $| + \rangle$,

$$\sigma^z |\pm\rangle = \pm |\pm\rangle, \quad \sigma^{\pm} |\mp\rangle = |\pm\rangle, \quad \sigma^{\pm} |\pm\rangle = 0 . \quad (22)$$

It is very convenient² for future notational purposes to carry out a rotation of the spins on all the even sites only by an angle π about the x -axis, so that the Néel state in this rotated (or Néel) basis has the

representation,

$$|\Phi\rangle = |-\ -\ -\ -\ \dots\rangle ; \quad \text{Néel basis} . \quad (23)$$

More generally, on even sites only we make the transformation,

$$\sigma_{2n}^- \rightarrow \sigma_{2n}^+, \quad \sigma_{2n}^+ \rightarrow \sigma_{2n}^-, \quad \sigma_{2n}^z \rightarrow -\sigma_{2n}^z ; \quad n = 1, 2, \dots . \quad (24)$$

In this basis the $s = \frac{1}{2}$ XXZ-model Hamiltonian of Eq. (3b) becomes,

$$H = -\frac{1}{4} \sum_{i=1}^N \left[\Delta \sigma_i^z \sigma_{i+1}^z + 2 \left(\sigma_i^+ \sigma_{i+1}^+ + \sigma_i^- \sigma_{i+1}^- \right) \right] , \quad (25)$$

and the operators $\{\sigma_i^+\}$ and $\{\sigma_i^-\}$ now represent, for *all* values of *i*, creation and destruction operators respectively with reference to the Néel model state. Henceforth, all of our calculations and definitions are given in terms of operators in this Néel basis in which, for example, the z-component of total spin from Eq. (4) is now given for a system of an even number, $N = 2M$, of spins as,

$$S_T^z = \frac{1}{2} \sum_{n=1}^M \sigma_{2n-1}^z - \frac{1}{2} \sum_{n=1}^M \sigma_{2n}^z . \quad (26)$$

We now introduce the usual CC parametrization for the exact N-spin ground ket state $|\Psi\rangle$, namely,

$$|\Psi\rangle = e^S |\Phi\rangle , \quad (27)$$

in terms of a cluster correlation operator *S* which may be expressed wholly in terms of creation operators. Thus, the *m*-body partition S_m of the cluster operator *S*,

$$S = \sum_{m=1}^N S_m , \quad (28)$$

has the following general form for the $s = \frac{1}{2}$ case in 1-d which we consider first,

$$S_m = \sum_{i=1}^N \sum_{r_1 < r_2 < \dots < r_{m-1}} S_{r_1 r_2 \dots r_{m-1}}^{(m)} \sigma_i^+ \sigma_{i+r_1}^+ \sigma_{i+r_2}^+ \dots \sigma_{i+r_{m-1}}^+ . \quad (29)$$

We note that the *m*-body coefficients $\left\{ S_{r_1 r_2 \dots r_{m-1}}^{(m)} \right\}$ in Eq. (30) are

independent of the site index *i* due to the translational invariance implied by the periodic boundary condition. Furthermore, in view of the fact that $[S_T^z, H] = 0$ for the XXZ Hamiltonian under consideration, we henceforth restrict ourselves only to states with quantum number $s_T^z = 0$, as is the case for the model Néel state $|\Phi\rangle$. This immediately restricts the sum in Eq. (28) to run only over even values of *m*, and it also puts further restrictions on the coefficients $\left\{ S_{r_1 \dots r_{m-1}}^{(m)} \right\}$, implied by the fact that we only consider

configurations in Eq. (29) in which as many spins on even sites as on odd sites are reversed (with respect to the model Néel state).

Although the above CC parametrization is exact, in practical applications we shall need to truncate the total possible number of cluster configurations in Eq. (29), in order to have tractable calculational schemes. Several such truncation schemes immediately suggest themselves. In the first place we consider the well-known so-called SUB n scheme in which in Eq. (28) we retain only those partitions of the cluster operators with $m \leq n$ and set to zero the remaining cluster operators S_m with $m > n$. This scheme has been widely applied in various areas of condensed matter theory (and see, e.g., Refs. 11-18), and has been found to be very accurate indeed (for other than hard-core repulsion interaction potentials) for many purposes. In the present case, the SUB2 approximation, for example, amounts to replacing Eqs. (28) and (29) by,

$$\begin{aligned}
 S_{\text{SUB2}} &= \sum_{i=1}^N \sum_{m=1}^M b_{2m-1} \sigma_i^+ \sigma_{i+2m-1}^+ ; \quad M = \text{integer part of } (N+2)/4 \\
 &\equiv \sum_{i=1}^N \sum_r^{\circ} b_r \sigma_i^+ \sigma_{i+r}^+ ,
 \end{aligned}
 \tag{30}$$

where the notation \sum° indicates a summation over the positive odd integers. The full SUB2 calculation thus involves a determination of the parameters $\{b_r; r = 1,3,5,\dots\}$ as $N \rightarrow \infty$. A further truncated SUB2- n subapproximation scheme involves keeping only the set of coefficients $\{b_r; r = 1,3,5,\dots,n-1\}$ with n even, by truncating the sum over m in Eq. (30) at the value $\frac{1}{2}n$.

The SUB n approximation scheme is by no means the only truncation hierarchy that we can envisage. The analysis of Faddeev and his coworkers²⁶⁻²⁸ in terms of *kinks* suggests that rather than counting the total number n of "wrong" spins (defined, as always, with respect to the Néel model state $|\Phi\rangle$) as in the SUB n scheme, we might concentrate attention instead on the total number of "kinks". Such ideas lead us naturally to the so-called PSUB n scheme in which at the given n^{th} level of approximation we keep only those configurations with no more than n "*plaquettes*". Each plaquette (or "domain") is defined to be a contiguous chain of wrong spins (of arbitrary length), which is terminated at each end by a "kink" (or "domain wall") which delimits it from any other plaquette present. Thus, by definition, each plaquette is separated from every other plaquette on the chain by at least one intervening "correct" spin (i.e., one unaltered from its Néel-state configuration). In the PSUB1 scheme, for example, the cluster operator is approximated as

$$\begin{aligned}
 S_{\text{PSUB1}} &= \sum_{i=1}^N \sum_{m=1}^{N/2} g_{2m} \sigma_i^+ \sigma_{i+1}^+ \sigma_{i+2}^+ \dots \sigma_{i+2m-1}^+ \\
 &\equiv \sum_{i=1}^N \sum_p^{\text{e}} g_p \sigma_i^+ \sigma_{i+1}^+ \sigma_{i+2}^+ \dots \sigma_{i+p-1}^+ ,
 \end{aligned}
 \tag{31}$$

where the notation \sum^{e} now indicates a summation over the positive even integers. A further truncated PSUB1- n subapproximation scheme involves keeping only the single plaquettes up to length n , where n is even, i.e., only those coefficients $\{g_p; p = 2,4,6,\dots,n\}$.

Finally, considerations of the importance of the localized nature of the interactions and/or the excitations lead to the so-called LSUB- n scheme, in which at the n^{th} level we keep only those configurations in Eq. (29) in which

spins are reversed (in all possible combinations compatible with $s_T^z = 0$) only over a "locale" of up to size n , where n now labels an even number of adjacent sites. It is clear that the LSUB-2 approximation in 1-d is hence identical to both the SUB2-2 and PSUB1-2 approximations. The LSUB-4 and LSUB-6 approximations on the other hand contain all $s_T^z = 0$ configurations for the cluster correlation operator S involving up to four and six adjacent sites respectively, namely,

$$S_{\text{LSUB-4}} = \sum_{i=1}^N \left(b_1 \sigma_i^+ \sigma_{i+1}^+ + b_3 \sigma_i^+ \sigma_{i+3}^+ + g_4 \sigma_i^+ \sigma_{i+1}^+ \sigma_{i+2}^+ \sigma_{i+3}^+ \right), \quad (32)$$

$$\begin{aligned} S_{\text{LSUB-6}} = S_{\text{LSUB-4}} + \sum_{i=1}^N \left(b_5 \sigma_i^+ \sigma_{i+5}^+ + f_{12} \sigma_i^+ \sigma_{i+3}^+ \sigma_{i+4}^+ \sigma_{i+5}^+ + f_{14} \sigma_i^+ \sigma_{i+2}^+ \sigma_{i+3}^+ \sigma_{i+5}^+ \right. \\ \left. + f_{23} \sigma_i^+ \sigma_{i+1}^+ \sigma_{i+4}^+ \sigma_{i+5}^+ + f_{34} \sigma_i^+ \sigma_{i+1}^+ \sigma_{i+2}^+ \sigma_{i+5}^+ \right. \\ \left. + g_6 \sigma_i^+ \sigma_{i+1}^+ \sigma_{i+2}^+ \sigma_{i+3}^+ \sigma_{i+4}^+ \sigma_{i+5}^+ \right). \quad (33) \end{aligned}$$

The interested reader might be amused to consider other approximation schemes, but we restrict ourselves here to the three schemes outlined above.

Regardless of the particular approximation scheme used, the actual CC methodology is now the same. We follow what is by now completely standard practice. Thus the g.s. Schrödinger equation, $H|\Psi\rangle = E_g|\Psi\rangle$, is first written in the form,

$$\hat{H}|\Phi\rangle = E_g|\Phi\rangle, \quad (34)$$

where for an arbitrary operator A we define the similarity transform \hat{A} as,

$$\hat{A} \equiv e^{-S} A e^S. \quad (35)$$

Secondly, the transformed equation (34) is then projected with the model bra state $\langle\Phi|$ and with the bra-state hermitian adjoints of each of the configurations contained in the particular approximation for the cluster operator S . In this way we obtain the relation,

$$E_g = -\frac{1}{4}N(\Delta + 2b_1), \quad (36)$$

for the g.s. energy, where $b_1 \equiv s_1^{(2)}$ as above, and a set of coupled nonlinear algebraic equations for the various cluster configuration coefficients. The actual evaluation of these equations is completely straightforward, if somewhat tedious in practice. If we write the XXZ Hamiltonian of Eq. (25) in the form $H = H[\{\sigma_i^+\}, \{\sigma_i^z\}, \{\sigma_i^-\}]$, it is clear that its corresponding transform is $\hat{H} = H[\{\hat{\sigma}_i^+\}, \{\hat{\sigma}_i^z\}, \{\hat{\sigma}_i^-\}]$. Furthermore, the comparable similarity-transformed basic spin operators may be evaluated for arbitrary cluster operator S of the form of Eqs. (28)-(29) as,

$$\begin{aligned} \hat{\sigma}_i^+ &= \sigma_i^+, & \hat{\sigma}_i^z &= \sigma_i^z + [\sigma_i^z, S], \\ \hat{\sigma}_i^- &= \sigma_i^- + [\sigma_i^-, S] + \frac{1}{2}[[\sigma_i^-, S], S]. \end{aligned} \quad (37)$$

Equation (37) demonstrates that the actual equations that need to be solved in any of our CC approximation schemes are of the form of coupled multinomial equations of at most fourth order.

For example, the full SUB2 equations may be readily evaluated to give,

$$2\Delta b_1 - 1 + 5b_1^2 - 2 \sum_{n=1}^{\infty} b_{2n-1} (b_{2n-1} + b_{2n+1}) = 0, \quad (38a)$$

$$2\Delta b_{2m-1} + 4b_1 b_{2m-1} - \frac{1}{2} \sum_{n=1}^{\infty} b_{2n-1} (b_{|2m-2n-1|} + b_{|2m-2n+1|} + b_{2m+2n-1} + b_{2m+2n-3}) = 0; \quad m \geq 2. \quad (38b)$$

The lowest subapproximation, SUB2-2, gives immediately from Eq. (38a),

$$3b_1^2 + 2\Delta b_1 - 1 = 0; \quad \text{SUB2-2}, \quad (39)$$

and hence, from Eq. (36), the corresponding estimate for the g.s. energy,

$$\frac{E_g}{N} = \frac{\Delta}{12} \left[1 + 2 \operatorname{sgn}(\Delta) \left(1 + \frac{3}{\Delta^2} \right)^{\frac{1}{2}} \right]; \quad \text{SUB2-2}, \quad (40)$$

Equation (40) has the exact asymptotic form for large Δ given by Eq. (7b). Interestingly, it is also exact at the transition point ($\Delta = -1$) to ferromagnetism, where $\frac{E_g}{N} = -\frac{1}{4}$. For the Heisenberg ($\Delta = 1$) and XY-planar ($\Delta = 0$) cases, the SUB2-2 results are $\frac{E_g}{N} = -5/12 \approx -0.417$ and $-\sqrt{3}/6 \approx -0.289$ respectively, which may be compared with the corresponding exact results from Eqs. (7a) and (9) of -0.443 and -0.318 , to the same number of significant figures.

The SUB2-n subapproximations to $\frac{E_g}{N}$ may also be evaluated for higher values of n , and what is most encouraging to find is how extremely rapidly convergent these estimates are with increasing n , at least for $\Delta \gtrsim 0$. Furthermore, and perhaps even more interesting, is the fact that the full SUB2 equations (38a,b) can also be solved exactly by Fourier transform techniques. We obtain the explicit solution,

$$b_{2m-1} = \frac{\kappa}{8\pi} \int_{-\pi}^{\pi} dx \left[1 - \left\{ 1 - k^2 \cos^2\left(\frac{1}{2}x\right) \right\}^{\frac{1}{2}} \right] \frac{\cos\left[\left(m - \frac{1}{2}\right)x\right]}{\cos\left(\frac{1}{2}x\right)}; \quad m \geq 1, \quad (41)$$

$$\kappa \equiv 4(\Delta + 2b_1), \quad k^2 \equiv \frac{(1 + 2\Delta b_1 + 2b_1^2)}{(\Delta + 2b_1)^2}.$$

By putting $m = 1$ in Eq. (41) we obtain a self-consistent equation for the coefficient b_1 . In this way we obtain, for example, the exact asymptotic limit of Eq. (7b), and the value $\frac{E_g}{N} \approx -0.419$ for the Heisenberg ($\Delta = 1$) chain. More importantly, we also find that the self-consistent equation for b_1 has a (real) solution only for values $\Delta \geq \Delta_c^{\text{SUB2}} \approx 0.37275$, and hence that there exists no SUB2 solution for smaller values of Δ . The estimates for $\frac{E_g}{N}$ as a function of Δ are compared in Fig. 2 with the exact value. The terminating point of the SUB2 solution is indicated by the point marked T.

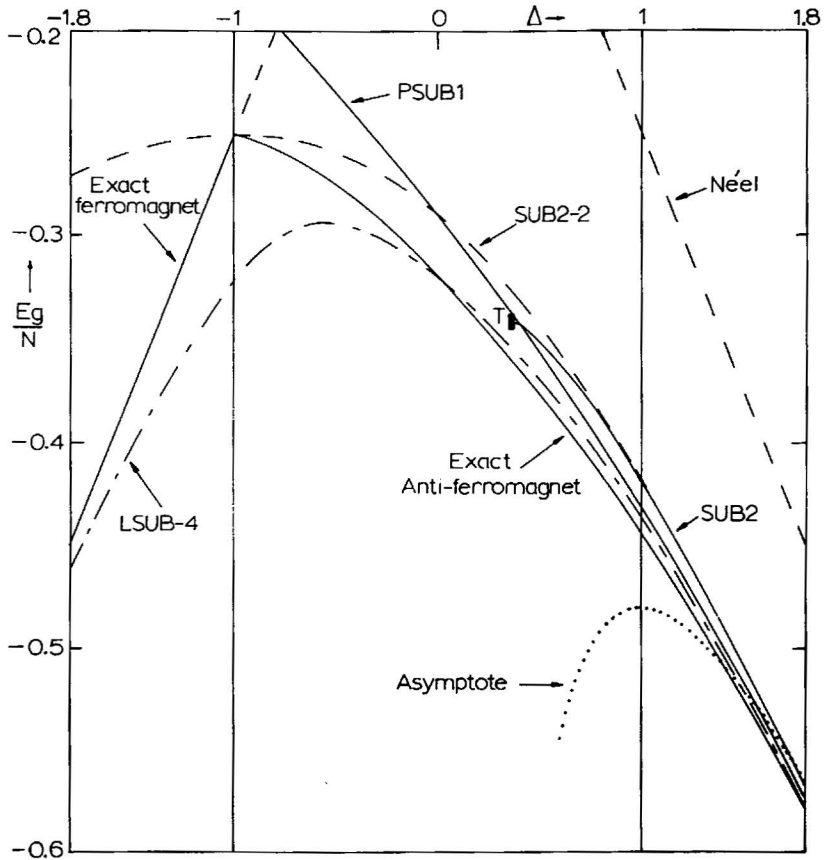


Fig. 2. The ground-state energy per spin, E_g/N , as a function of the anisotropy parameter Δ for the spin- $\frac{1}{2}$ quantum spin chain with XXZ-model Hamiltonian of Eq. (3b). The curves labelled SUB2-2, SUB2, PSUB1 and LSUB-4 are the results of the present work using various CC truncation schemes discussed in the text. The terminating point (at $\Delta = \Delta_c^{\text{SUB2}} \approx 0.3728$) of the SUB2 approximation is indicated by the point marked T. The exact results in the ferromagnetic ($\Delta < -1$) and antiferromagnetic ($\Delta > -1$) regimes are also shown, together with the exact $\Delta \rightarrow \infty$ asymptotic form of the latter, $E_g/N \rightarrow -\frac{1}{4}(\Delta + \Delta^{-1})$. The Néel result, $E_g/N = -\frac{1}{4}\Delta$, for the perfect classical antiferromagnet is also indicated.

The absence of a solution for $\Delta < \Delta_c^{\text{SUB2}}$ is a clear signal of a phase transition in the physical system, although without further evidence it is impossible to rule out that the SUB2 approximation simply breaks down for nonphysical reasons in this regime. However, even at this juncture, where we only have a knowledge of the ground ket state, there is further evidence that strengthens our belief that the terminating point of the SUB2 solution is indeed approximating the actual phase transition at $\Delta = 1$ from the ordered antiferromagnetic phase ($\Delta > 1$) to the critical phase ($\Delta < 1$). Thus, closer analysis of the two-reversal coefficients $\{b_n\}$ from Eq. (41) shows the asymptotic behaviour,

$$b_{2m-1} \xrightarrow{m \rightarrow \infty} \begin{cases} \alpha \xi^{-2m}; & \Delta > \Delta_c^{\text{SUB2}} \\ \gamma m^{-2}; & \Delta = \Delta_c^{\text{SUB2}} \end{cases}, \quad (42)$$

where α and ξ are functions only of Δ , and γ is a constant. This changeover from exponential to algebraic decay is clearly reminiscent of the comparable behaviour of the exact correlation function g_n at the exact transition point $\Delta = 1$, as given by Eq. (12). We return to a discussion of the SUB2 approximation for g_n in Sec. 5, after we have considered the corresponding approximation to the ground bra state in Sec. 4.

We turn our attention next to the PSUB1 approximation of Eq. (31), where the equations for the coefficients $\{g_n\}$ can be evaluated as,

$$-\frac{1}{2} + \Delta g_2 + \frac{3}{2}g_2^2 - g_4 = 0, \quad (43a)$$

$$\Delta g_{2m} - \Delta \sum_{n=1}^{m-1} g_{2n} g_{2m-2n} - g_{2m+2} + 2mg_2 g_{2m} + (1 - \delta_{m2}) \sum_{n=2}^{m-1} g_{2n} g_{2m+2-2n} = 0; \quad m \geq 2. \quad (43b)$$

The corresponding g.s. energy is again given by Eq. (36), with $b_1 \equiv g_2$. Although we have not sought an exact solution to this set of equations (for the infinite chain, $N \rightarrow \infty$), they may again readily be solved numerically for any PSUB1- n subapproximation. As shown in Table 1, this sequence of subapproximations is also rapidly convergent with increasing n , for all values of Δ . The numerical results for E_g/N are also shown in Fig. 2, where we clearly observe the superior accuracy of the PSUB1 approximation over the SUB2 approximation for essentially all values $\Delta > \Delta_c^{\text{SUB2}}$ with which comparison can be made. Nevertheless, for smaller values of Δ , the PSUB1 approximation both shows no sign of terminating and becomes increasingly inaccurate.

Finally, we turn our attention to the LSUB-4 approximation of Eq. (32), for which the equations for the cluster coefficients can be evaluated as,

$$1 - 2\Delta b_1 - 3b_1^2 + 2b_1 b_3 + 2b_3^2 + 2g_4 = 0, \quad b_1^2 - 4\Delta b_3 - 4b_1 b_3 + g_4 = 0, \quad (44)$$

$$\Delta(b_1^2 + 2b_1 b_3) - g_4(\Delta + 4b_1 + b_3) - 2b_1 b_3^2 = 0.$$

Although the LSUB-4 approximation contains only three coefficients, it would appear to include the most important configurations of both the previous SUB2

Table 1. The g.s. energy per spin, E_g/N , for the infinite ($N \rightarrow \infty$) 1-d spin- $\frac{1}{2}$ XXZ-model chain for various values of the anisotropy parameter Δ , and calculated in various PSUBI-n subapproximations. Also shown are the corresponding exact values.

Δ	E_g/N					
	PSUBI-2	PSUBI-4	PSUBI-6	PSUBI-8	PSUBI-10	Exact
5.0	-1.29858	-1.29944	-1.29947	-1.29947	-1.29947	-1.29950
2.0	-0.60762	-0.61436	-0.61509	-0.61517	-0.61517	-0.61722
1.0	-0.41667	-0.42966	-0.43099	-0.43111	-0.43111	-0.44315
0.0	-0.28867	-0.28867	-0.28867	-0.28867	-0.28867	-0.31831
-1.0	-0.25000	-0.16491	-0.17599	-0.17525	-0.17529	-0.25000

and PSUB-1 approximations for the exact cluster operator S , in view of the rapid convergence of the subapproximation sequences in both cases. It is therefore perhaps to be expected, at least for values of $\Delta \gtrsim 0$, that it is our most accurate approximation. This is borne out in Fig. 2, and some typical results are shown in Table 2.

In view of the very small number of independent cluster configurations contained at the LSUB-4 level, nor is it perhaps surprising that this approximation shows no sign of a terminating point or of any other signal of the phase transition at $\Delta = 1$. On the other hand, what is much more unexpected is the fact that the approximation seems also to track the exact g.s. energy quite well across the sharp first-order transition into the ferromagnetic regime ($\Delta \leq -1$), as can clearly be observed from Fig. 2. At the moment, however, we have no clear understanding of whether this is a real physical effect or a mathematical coincidence.

4. CC TREATMENT OF THE GROUND BRA STATE

For reasons that have been well described both in an earlier volume in this series³⁸ and elsewhere,³⁹ the CCM provides a biorthogonal rather than an orthogonal parametrization of the many-body wavefunctions. Thus, the respective bra and ket eigenstates are not kept as the manifestly hermitian conjugates of each other. Rather, the corresponding bra ground state $\langle \tilde{\Psi} |$ to $|\Psi\rangle$, where $\langle \tilde{\Psi} | H = E_g \langle \tilde{\Psi} |$, is parametrized in the normal CC scheme as,

$$\langle \tilde{\Psi} | = \langle \Phi | \tilde{S} e^{-S}, \quad (45)$$

where \tilde{S} is a new correlation operator. It is decomposed entirely in terms of destruction operators $\{\sigma_i^-\}$, in complete analogy to the way that the ket-state operator S was decomposed in Eqs. (28) - (29) in terms of creation operators,

$$\tilde{S} = 1 + \sum_{m=1}^N \tilde{S}_m, \quad (46a)$$

$$\tilde{S}_m = \sum_{i=1}^N \sum_{r_1 < r_2 < \dots < r_{m-1}} \tilde{S}_{r_1 r_2 \dots r_{m-1}}^{(m)} \sigma_{i+r_1}^- \sigma_{i+r_1+1}^- \sigma_{i+r_1+2}^- \dots \sigma_{i+r_{m-1}}^-. \quad (46b)$$

We note that the particular value of the constant term in Eq. (46a) implies the manifest normalization $\langle \tilde{\Psi} | \Psi \rangle = 1$ ($= \langle \Phi | \Psi \rangle$). Thus, the g.s. expectation value of an arbitrary operator A can be expressed as,

Table 2. A comparison of the LSUB-4 approximation and exact results for the g.s. energy per spin, E_g/N , for the infinite ($N \rightarrow \infty$) 1-d spin- $\frac{1}{2}$ XXZ-model chain for various values of the anisotropy parameter Δ .

Δ	E_g/N	
	LSUB-4	Exact
5.0	-1.29947	-1.29950
2.0	-0.61552	-0.61722
1.0	-0.43627	-0.44315
0.0	-0.31934	-0.31831
-1.0	-0.32110	-0.25000
-2.0	-0.50482	-0.50000

$$\bar{A} \equiv \langle \tilde{\Psi} | A | \Psi \rangle = \langle \Phi | \tilde{S} e^{-S} A e^S | \Phi \rangle = \langle \Phi | \tilde{S} \hat{A} | \Phi \rangle. \quad (47)$$

It is also clear that although the exact operators S and \tilde{S} must preserve the hermiticity relation, $\langle \tilde{\Psi} | = (|\Psi\rangle)^\dagger / \langle \Psi | \Psi \rangle$, subsequent approximation schemes usually will not.

In practical implementations of the CCM, the cluster operator \tilde{S} is truncated in exactly the same way as for the operator S . Thus, a given CC approximation scheme keeps only a selected subset of creation configurations from the expansion for S in Eqs. (28)-(29), the operator strings for which we denote generically as $\{C_I^+\}$; and precisely the same subset of their hermitian-conjugate destruction counterparts $\{C_I^-\}$ for the operator \tilde{S} . It is then not difficult to show³⁹ that the bra and ket g.s. Schrödinger equations are completely equivalent to the requirement that the expectation value, $\bar{H} = \langle \Phi | \tilde{S} e^{-S} H e^S | \Phi \rangle$, of the Hamiltonian should be stationary with respect to each of the coefficients of the set of configurations in S and \tilde{S} .

As a concrete example, the SUB2-approximation counterpart to Eq. (30) for the operator \tilde{S} is,

$$\tilde{S}_{\text{SUB2}} = 1 + \sum_{i=1}^N \sum_{m=1}^M \tilde{b}_{2m-1} \sigma_i^- \sigma_{i+2m-1}^-; \quad M = \text{integer part of } (N+2)/4. \quad (48)$$

In SUB2 approximation the g.s. energy expectation value \bar{H} is now a functional of both sets of amplitudes $\{b_{2m-1}\}$ and $\{\tilde{b}_{2m-1}\}$. The stationarity of \bar{H} with respect to \tilde{b}_{2m-1} gives the equations,

$$\langle \Phi | \sum_{i=1}^N \sigma_i^- \sigma_{i+2m-1}^- e^{-S} H e^S | \Phi \rangle = 0; \quad m \geq 1, \quad (49)$$

which lead precisely to the earlier coupled set of nonlinear equations (38a,b) which determine the coefficients $\{b_{2m-1}\}$. Similarly, the stationarity of \bar{H} with respect to b_{2m-1} gives the equations,

$$\langle \Phi | \tilde{S} e^{-S} \left[H, \sum_{i=1}^N \sigma_i^+ \sigma_{i+2m-1}^+ \right] e^S | \Phi \rangle = 0; \quad m \geq 1. \quad (50)$$

Equations (50) have the form of a coupled set of linear equations for the

coefficients $\{\tilde{b}_{2m-1}\}$, in terms of the coefficients $\{b_{2m-1}\}$, which are assumed known.

It is worth pointing out that the g.s. energy calculated by the above procedure, in *any* particular approximation scheme, is identical to that obtained from just the ket state a_S in Sec. 3, since the value of \bar{H} at the stationary point is just $E_g = \langle \Phi | e^{-S} | \Phi \rangle$ due to the stationarity conditions with respect to the bra-state amplitudes. We also remind the reader that although the g.s. energy has now been derived from a variational principle, the corresponding estimate from an arbitrary truncation scheme will *not* in general provide an upper bound to the exact result due to the lack of manifest hermiticity.

We illustrate the above procedure only for the SUB2 approximation. Explicit evaluation of Eq. (50) in this case leads to the counterparts for the bra-state coefficients to Eqs. (38a,b) for the SUB2 ket-state coefficients,

$$\begin{aligned} \delta_{m1} + 2(\delta_{m1} - 2)(\Delta + 2b_1)\tilde{b}_{2m-1} - 8\delta_{m1} \sum_{n=1}^{\infty} \tilde{b}_{2n-1} b_{2n-1} \\ + 2 \sum_{n=1}^{\infty} \tilde{b}_{2n-1} \left(b_{|2m-2n-1|} + b_{|2m-2n+1|} + b_{2m+2n-1} + b_{2m+2n-3} \right) = 0 ; m \geq 1 . \end{aligned} \quad (51)$$

In the first place these equations may be solved in any SUB2-n subapproximation. For example, Eq. (39) together with Eq. (51) restricted to keeping only the terms involving b_1 and \tilde{b}_1 , yield the explicit SUB2-2 solutions,

$$b_1 = \frac{1}{3}[(\Delta^2 + 3)^{\frac{1}{2}} - \Delta] , \quad \tilde{b}_1 = \frac{1}{2}(\Delta^2 + 3)^{-\frac{1}{2}} ; \quad \text{SUB2-2} . \quad (52)$$

Alternatively, Eqs. (51) can again be solved exactly by Fourier transform techniques, to give the explicit SUB2 solution,

$$\tilde{b}_{2m-1} = \frac{D}{\kappa} \frac{1}{2\pi} \int_{-\pi}^{\pi} dx \left[1 - k^2 \cos^2\left(\frac{1}{2}x\right) \right]^{-\frac{1}{2}} \cos\left(\frac{1}{2}x\right) \cos\left[(m-\frac{1}{2})x\right] ; \quad m \geq 1 , \quad (53)$$

where the constants k and κ are as given in Eq. (41), and D is given by,

$$D^{-1} = \frac{1}{2\pi} \int_{-\pi}^{\pi} dx \left[1 - k^2 \cos^2\left(\frac{1}{2}x\right) \right]^{-\frac{1}{2}} \left[1 - \frac{1}{2} \cos^2\left(\frac{1}{2}x\right) \right] - \frac{1}{2} . \quad (54)$$

It is again of interest to examine the asymptotic behaviour of the coefficients \tilde{b}_{2m-1} . We find,

$$\tilde{b}_{2m-1} \xrightarrow{m \rightarrow \infty} \begin{cases} a\lambda^{-2m} ; & \Delta > \Delta_c^{\text{SUB2}} \\ \Gamma & ; \quad \Delta = \Delta_c^{\text{SUB2}} \end{cases} , \quad (55)$$

where a and λ are functions only of Δ , and Γ is a constant.

5. CORRELATION FUNCTION AND ORDER PARAMETER

Having obtained an approximate description of the bra and ket ground states via any of the previously described CC truncation schemes, it is now

straightforward to calculate arbitrary g.s. expectation values. For present purposes one of the most interesting properties is the spin-spin correlation function g_n defined in Eq. (10), and the associated order parameter of Eq. (11). We recall that in the Néel basis in which all of our CC calculations have been performed, the perfect Néel antiferromagnet described by the model state $|\Phi\rangle$ itself (i.e., with $S \rightarrow 0$, $\tilde{S} \rightarrow 1$) has a constant unit correlation function, $g_n \rightarrow 1$, and exhibits perfect long-range order. In the original non-rotated basis this corresponds to $g_n \rightarrow (-1)^n$, as given by the Ising limit ($\Delta \rightarrow \infty$) of Eqs. (12)-(13).

In view of the interesting terminating point exhibited by the SUB2 truncation scheme, we henceforth concentrate our attention on this approximation. By inserting the parametrizations of Eqs. (30) and (48) into Eq. (10), we readily find that the SUB2 approximation for g_n is given by,

$$g_n = 1 - 8(1 - \delta_{no}) \sum_{m=1}^{\infty} \tilde{b}_{2m-1} b_{2m-1} + 4\tilde{b}_n b_n ; \quad \text{SUB2} , \quad (56)$$

We recall that the SUB2 coefficients $\{b_n\}$ and $\{\tilde{b}_n\}$ are defined (in the $s_T^z = 0$ subspace in which we are working) only for odd values of n . Hence, Eq. (56) demonstrates a peculiarity of the SUB2 approximation, namely that it gives a g_n which is constant (and equal to μ) for *all* even values of n ,

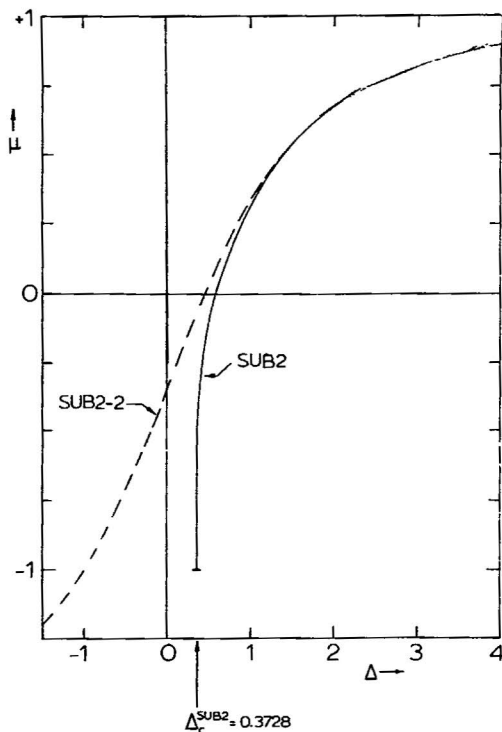


Fig. 3. The order parameter μ as a function of the anisotropy parameter Δ for the spin- $\frac{1}{2}$ quantum spin chain with XXZ-model Hamiltonian of Eq. (3b), as calculated in the CC approximation SUB2 and its subapproximation SUB2-2.

$$g_{2\ell} = \mu, \quad \ell \geq 1; \quad \text{SUB2}$$

$$= 1 - 8 \sum_{m=1}^{\infty} \tilde{b}_{2m-1} b_{2m-1}. \quad (57a)$$

On the other hand, for odd values of n , Eqs. (42) and (55) give the result,

$$g_{2\ell-1} = \mu + 4\tilde{b}_{2\ell-1} b_{2\ell-1}, \quad \ell \geq 1; \quad \text{SUB2}$$

$$\xrightarrow{\ell \rightarrow \infty} \begin{cases} \mu + A L^{-2\ell}; & \Delta > \Delta_c^{\text{SUB2}} \\ \mu_c + \delta \ell^{-2}; & \Delta = \Delta_c^{\text{SUB2}} \end{cases}, \quad (57b)$$

where the constants μ , A and L depend on Δ , and where μ_c and δ are constants. This behaviour, above and at the terminating point $\Delta = \Delta_c^{\text{SUB2}}$, may be compared with the exact behaviour (in the non-rotated basis) in Eqs. (12) and (13) on either side of the phase transition at $\Delta = 1$.

The order parameter μ itself may also be calculated explicitly in SUB2 approximation from Eqs. (41) and (53)-(54). We find the result,

$$\mu = \frac{1 - \frac{1}{\pi} \int_0^{\pi} dx \cos^2(\frac{1}{2}x) \left[1 - k^2 \cos^2(\frac{1}{2}x) \right]^{-\frac{1}{2}}}{\frac{1}{\pi} \int_0^{\pi} dx \left[1 + \sin^2(\frac{1}{2}x) \right] \left[1 - k^2 \cos^2(\frac{1}{2}x) \right]^{-\frac{1}{2}} - 1}; \quad \text{SUB2}. \quad (58)$$

The behaviour of this SUB2 approximation for the order parameter is shown in Fig. 3. We observe that μ actually takes unphysical values ($\mu < 0$) for values of Δ less than ≈ 0.616 , and approaches the limiting value $\mu_c = -1$ as $\Delta \rightarrow \Delta_c^{\text{SUB2}} \approx 0.373$, rather than the physically expected $\mu \rightarrow 0$ as $\Delta \rightarrow 1$. We note that the occurrence of these unphysical values is basically due to the non-hermitian nature of the approximated expectation value, i.e., that the bra and ket g.s. wavefunctions are not hermitian-adjoint to each other. Nevertheless, the crossover from exponential to algebraic decay at the terminating point precisely imitates the exact behaviour at the actual $\Delta = 1$ transition. We also show in Fig. 3 the comparable SUB2-2 result,

$$\mu = \frac{1}{3} \left[4\Delta(\Delta^2 + 3)^{-\frac{1}{2}} - 1 \right]; \quad \text{SUB2-2}, \quad (59)$$

which can be obtained by restricting the sum in Eq. (57a) to the $m = 1$ term only, and by using Eq. (52).

6. EXTENSION TO THE 2-d SQUARE LATTICE

Finally, we turn our attention to the extension to lattices in higher dimensions of the same spin- $\frac{1}{2}$ XXZ-model Hamiltonian of Eq. (3a). The recent discovery of high-temperature superconductors has greatly renewed interest in this area. Thus, Anderson⁴⁰ has suggested that the $s = \frac{1}{2}$ Heisenberg ($\Delta = 1$) Hamiltonian on a square lattice might provide an appropriate model for the interactions between the electrons in the singly occupied $d_{x^2-y^2}$ orbitals on

the copper atoms in these layered materials. As we have already discussed in Sec. 2, very few exact results are known for the Hamiltonian of Eq. (3a) in

dimensionality greater than one. However, it is now widely believed, on the basis of numerical work using both exact diagonalizations on small clusters and Monte Carlo calculations of various kinds (see, e.g., Ref. [41] and references cited therein), that the spin- $\frac{1}{2}$ Heisenberg model on the square lattice shows a staggered magnetization of approximately 60% of the corresponding classical value.

Nevertheless, to the best of our knowledge, no rigorous proof concerning long-range order for the 2-d square-lattice Heisenberg model has ever been given, although it is known that this model is disordered at *any* nonzero temperature.⁴² The strongest results of which we are aware are the recent proofs,⁴³ based on various sum rules and bounds on correlation functions, that the $s = \frac{1}{2}$ XXZ model in 2-d does have long-range order for $\Delta > 1.78$. (We note, however, that this proof certainly does not preclude the existence of long-range order for smaller values of Δ .) Finally, it is also known³⁰ that the ground state of a discrete spin- $\frac{1}{2}$ system is nondegenerate (and hence $s_{\uparrow} = 0$) in *any* number of dimensions and for *any* lattice which may be decomposed into two equivalent sublattices with antiferromagnetic (ferromagnetic) Heisenberg interactions between spins on different (the same) sublattices. In this context we remark only that the singlet nature of the ground state does not, of course, exclude the possibility of long-range order.

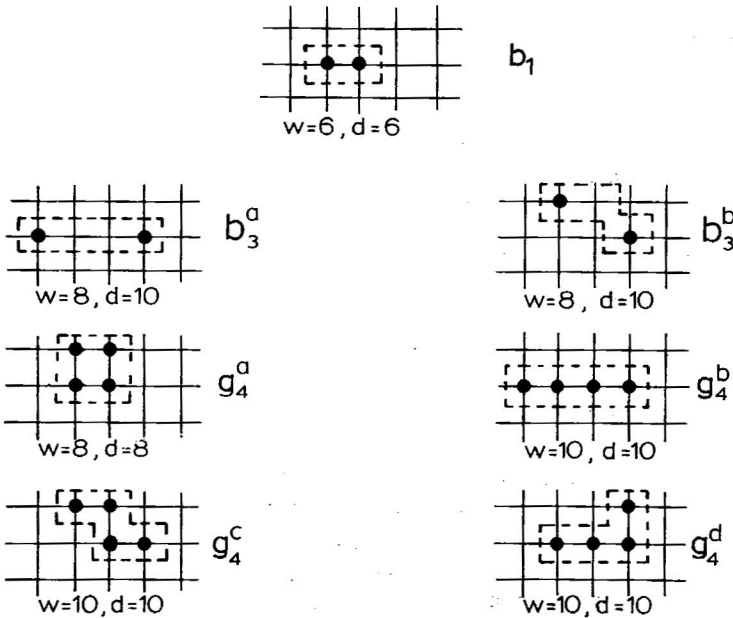


Fig. 4. A graphical illustration of the seven "wrong spin" configurations (with respect to the model antiferromagnetic Néel state) retained in the full LSUB-4 CC approximation scheme, for a spin- $\frac{1}{2}$ quantum spin system on the 2-d square lattice. The amplitude of each configuration contained in the correlation operator S associated with the ground ket state is as indicated to the right of each diagram. The corresponding parameters w and d for each configuration are described in the text.

In principle, the extension of the CC techniques outlined in earlier Sections to lattices of higher dimensionality is completely straightforward. The only point that we wish to discuss concerns the approximation schemes to be employed. In practice, this amounts to deciding which particular "configurations" to keep in the expansions of the cluster operators S and \tilde{S} , where each such configuration is defined in terms of a particular combination of "wrong" spins with respect to the model ($s_T^z = 0$) Néel state, just as in the 1-d case. For example, the analogues for the 2-d square lattice of the three LSUB-4 configurations defined explicitly in 1-d in Eq. (32) are the seven configurations denoted graphically in Fig. 4 in an obvious notation. These are defined to be those $s_T^z = 0$ configurations with up to four wrong spins over any four contiguous sites on the lattice.

Although we cannot expect that the same configurations will be important for all values of Δ , there are at least two physically appealing concepts which we might intuit to play an important role, at least in the regime where the quantum fluctuations have not destroyed the classical long-range order present in the Néel state. The first of these is simply the number, w , of "wrong bonds". In a classical picture the breaking of each bond in the antiferromagnetic regime costs energy, and hence configurations with larger values of w are expected to be weighted less. Secondly, an extension of the seemingly important concepts in 1-d of locale size and the number of kinks present, leads us to consider the length, d , of the "domain boundary" of a given configuration. This is defined to be the number of lattice bonds crossed by a shortest-path circuit (indicated in Fig. 4 by dashed lines) which encloses all of the wrong spins. The weights w and d for each of the LSUB-4 configurations are indicated in Fig. 4.

Some of the results for the g.s. energy displayed in Fig. 5 certainly seem to bear out the relevance of the above two criteria for estimating the relative importance of the various configurations (namely, that those with lowest values of w and d are more heavily represented in the g.s. ket wavefunction), at least for values of $\Delta \gtrsim 0.2$. For example, the two curves labelled LSUB-4' and LSUB-4" are two different subapproximations to the full LSUB-4 approximation, each of which includes only a subset of the seven configurations shown in Fig. 4. Both subapproximations contain the single SUB2-2 \equiv LSUB-2 configuration ($w=6, d=6$) denoted by its amplitude b_1 . On the one hand, the LSUB-4' subapproximation then also includes the single extra configuration of next highest importance by the above criteria, namely the ($w=8, d=8$) square configuration denoted by the amplitude g_4^a . On the other hand, the LSUB-4" approximation includes the three linear configurations denoted by the amplitudes b_1 ($w=6, d=6$), b_3^a ($w=8, d=10$), and g_4^b ($w=10, d=10$).

For the 2-d square lattice, the full SUB2 approximation (which includes all possible $s_T^z = 0$ configurations of two wrong spins) can again be solved by Fourier transform techniques. The corresponding SUB2 results for the g.s. energy are also shown in Fig. 5, where we observe that this approximation again has a terminating point (labelled T), at $\Delta = \Delta_c^{\text{SUB2}} \approx 0.795$, similar to that in the 1-d case. We note that the LSUB-4' subapproximation similarly terminates (at the point labelled T') for the 2-d lattice, so that there is no real solution in this case for $\Delta < -1.370$.

The actual numerical results for the g.s. energy per spin, E_g/N , for the spin- $\frac{1}{2}$ isotropic Heisenberg model ($\Delta = 1$) on the spin lattice, in various CC approximation schemes, are as follows: -0.648 (SUB2-2); -0.652 (SUB2); -0.650 (LSUB-4"); -0.653 (LSUB-4'); and -0.664 (full LSUB-4). These results may be compared both with the corresponding approximation of -0.658 from spin-wave

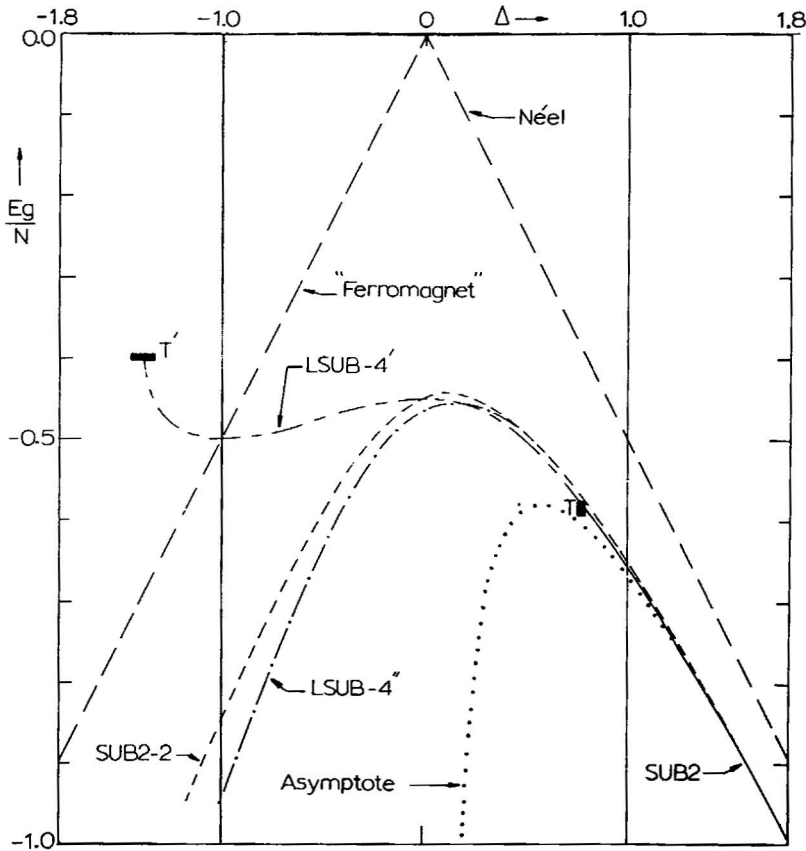


Fig. 5. The ground-state energy per spin, E_g/N , as a function of the anisotropy parameter Δ for the spin- $\frac{1}{2}$ quantum spin system on the 2-d square lattice interacting via the XXZ-model Hamiltonian of Eq. (3a). The dashed lines labelled "ferromagnetic" and Néel are the classical ferromagnetic and antiferromagnetic results, $E_g/N = \pm \frac{1}{2}\Delta$; and the dotted curve indicates the exact $\Delta \rightarrow \infty$ asymptotic form, $E_g/N \rightarrow -\frac{1}{2}\Delta - \frac{1}{6}\Delta^{-1}$. The remaining curves, labelled SUB2-2, SUB2, LSUB-4' and LSUB-4" are the results of the present work using the various CC truncation schemes discussed in the text. The terminating points of the SUB2 and LSUB-4' curves, at $\Delta \approx 0.795$ and $\Delta \approx -1.370$ respectively, are indicated by the corresponding points T and T'.

theory,²⁰ and with what is currently the best available result, namely $E/N = -0.6692 \pm 0.0002$, from two independent calculations using the Green function Monte Carlo method.^{41,44} It is clear that once again the various CC approximations both converge extremely rapidly for values of $\Delta \gtrsim 1$, and give good agreement with the very accurate results from large-scale stochastic simulations.

7. DISCUSSION

We have demonstrated that the CCM can be adapted for use with discrete quantum spin systems interacting via nearest-neighbour interactions of the XXZ-model type, both for the 1-d chain and the 2-d square lattice, at least for the spin-half case. Various practical truncation schemes have been explored, some of which are similar to those used in other continuous extended condensed-matter systems, and some of which are quite unique to these discrete lattice models. A few of these were also considered by Roger and Hetherington² who calculated the g.s. energies in 1-d and 2-d for the case $\Delta = 1$. The method has now not only been shown to be accurate for the g.s. energy, but also to be capable of giving valuable information on the correlation function and order parameter, and hence on the physically most interesting, and theoretically most difficult, questions of long-range order and phase transitions. Furthermore, various of the approximation hierarchies for incorporating the many-body quantum correlations allow us to make close contact with other physical concepts or theoretical devices that have proven to be valuable aids in describing these systems. Thus, we have already discussed the relationship of the PSUBn scheme to the description in terms of kinks due to Faddeev and his collaborators. It should also be clear to the reader that the SUB2 approximation, has much in common with the *resonating valence bond* description of the g.s. wavefunction proposed by Anderson.⁴⁵

In view of the demonstrated success of the CC methods described here, we believe that it is of interest to pursue these applications further. In this regard, at least five distinct extensions come immediately to mind. In the first place, the extension to spin-one systems interacting via the same XXZ-model Hamiltonians as discussed here and also the bilinear-biquadratic Hamiltonians of Eq. (19), are of obvious interest, particularly in view of our earlier discussion concerning Haldane's conjecture. Secondly, we intend to use the same methodology to explore such other similar models of current interest as the t-J model and the Hubbard model. A third obvious extension will be to explore the dependence of our results on the choice of model state. While it is clear that an exact CC calculation of the properties of the bra and ket ground states is independent of the model state, the same truncation scheme used with different model states can certainly lead to different approximate results. In this regard it is of special interest to try to tailor the choice of model state to a give phase, and indeed to approach a particular phase transition from descriptions based on different model states.

Fourthly, we note that the present discussion has concentrated wholly on g.s. wavefunctions and g.s. properties. It will certainly also be of interest to apply to all of the previous systems the excited-state version of the CCM due to Emrich.⁴⁶ We should thereby, for example, be able to discuss the presence or absence of a gap in the excitation spectrum. Of particular interest in this context will be the behaviour of the excitation spectrum as $\Delta \rightarrow \Delta_c^{\text{SUB2}}$ in the SUB2 approximation. Finally, whereas the entire discussion up until now has focussed entirely on the application of the so-called normal coupled cluster method, we also intend to apply the related, but potentially more powerful, version of CC theory -- namely, the extended coupled cluster method.^{38,39}

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