

Perturbation Expansions for Quantum Many-Body Systems

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A systematic method for developing high-order, zero-temperature perturbation expansions for quantum many-body systems is presented. The models discussed explicitly are spin models with a variety of interactions, in one and two dimensions. The wide applicability of the method is illustrated by expansions around Hamiltonians with ordered and disordered ground states, namely Ising and dimerized models. Computer implementation of this method is discussed in great detail. Some previously unpublished series are tabulated.

KEY WORDS: Quantum antiferromagnets; series expansions; many-body theory; low-dimensional magnetism.

1. INTRODUCTION

At zero temperature, quantum many-body systems can show very rich and complex behavior as parameters in the Hamiltonian are varied. Such $T=0$ phase transitions occur even in simple spin models which possess trivial classical ground states. Interest in the $T=0$ properties of various quantum spin system has grown tremendously in the past few years, due to several striking developments. Some theories of high-temperature superconductivity have focused attention on two-dimensional systems, particularly the square lattice, spin-1/2, Heisenberg antiferromagnet.⁽¹⁾ The venerable subject of antiferromagnetic Heisenberg spin chains was rein-

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vigorated by Haldane's conjecture⁽²⁾ that, at $T=0$, integer and half-integer spin chains should have dramatically different properties. Moreover, remarkable developments in two-dimensional field theory,⁽³⁾ in conjunction with the well-known correspondence between d -dimensional quantum systems at $T=0$ and $(d+1)$ -dimensional classical systems (see, e.g., ref. 4), has directed further attention to one-dimensional quantum spin models.⁽⁵⁾

A host of methods have been applied in studies of quantum spin systems. Several classes of "exactly solvable" models have been discovered.⁵ Exact (and quasiexact stochastic) calculations of the spectrum and eigenstates for finite systems, followed by extrapolation to the thermodynamic limit, have been carried out for many models in 1D,⁶ and for several 2D models as well (see, e.g., refs. 11). Also noteworthy are variational studies, particularly in 2D,⁽¹²⁾ mappings of 1D models to field theories (ref. 13, among many others), and real-space renormalization.⁽¹⁴⁾

In this paper, we describe a method for generating high-order perturbative (power series) expansions for many properties of a wide class of quantum spin systems. Such expansions, when analyzed by methods developed for the study of classical critical phenomena,⁽¹⁵⁾ lead to results which would be difficult to obtain by other means. Interpretation of the series is best treated in the context of specific problems, and is reserved for separate publications⁽¹⁶⁻²³⁾; however, many of the series are tabulated in the Appendix of this paper. Although we treat only spin models here, the technique readily generalizes to quantum lattice gases with either Fermi or Bose statistics.

Perturbative expansions for quantum spin systems have appeared sporadically in the literature of the past 30 years.⁷ Generally, a different technique was invented for each problem, and laborious calculations by hand led to short series for one or two properties. This is not to say that such work was without value. For example, Pfeuty and Elliott's studies of the transverse-field Ising model⁽²⁵⁾ motivated Suzuki's exact mapping between that model and the classical Ising model in one dimension higher.⁽²⁶⁾ The more recent work by Kadanoff and collaborators⁽²⁷⁾ also deserves mention. However, we feel that the potential of series expansions for revealing novel phase diagrams and critical behavior in quantum spin systems has not been fully exploited.

In contrast with previous work, our method permits expansions of qualitatively different character—both "ordered-state" and "disordered-

⁵ Models solvable by the Bethe-ansatz are discussed in refs. 6-8; other types of exactly solvable models are described in refs. 9.

⁶ Ref. 10 is one of the pioneering works in that field; a complete bibliography is beyond the scope of this paper.

⁷ Besides the other series work mentioned later, see also refs. 24.

state” expansions, as described below—to be treated within the same framework. Moreover, the technique is readily implemented on a computer in such a way that one can generate a host of different expansions without major modifications in the code. The method may be characterized as a connected cluster expansion, and indeed much of the formalism is identical to that of classical cluster expansions.⁽²⁸⁾ Naturally, there are also important differences between the classical and quantum cases. We defer further discussion of the technique itself to Section 2, and in the remainder of this section we focus, instead, on the specific applications where the technique has proven its worth.

The models we will consider in this paper consist of quantum spins (with $S = 1/2$ or 1) which sit on regular one- or two-dimensional bipartite lattices⁸ (linear chain, square, or honeycomb) and interact via nearest neighbor couplings. [Models with further neighbor couplings have also been studied; see Section 4.5. The most general coupling we have studied may be expressed as

$$\varepsilon_{ij}[(\mathbf{S}_i, \mathbf{S}_j)_A - \beta(\mathbf{S}_i, \mathbf{S}_j)_A^2] \quad (1.1)$$

where A governs *exchange anisotropy*, via

$$(\mathbf{S}_i, \mathbf{S}_j)_A = S_i^z S_j^z + A(S_i^x S_j^x + S_i^y S_j^y) \quad (1.2)$$

The coefficient ε_{ij} allows for *bond alternation* with respect to some fixed, nearest neighbor dimer configuration \mathcal{D} (i.e., a set of nearest neighbor pairs selected so that any spin lies in exactly one of the pairs), via

$$\varepsilon_{ij} = \begin{cases} 1 & \text{if } \{ij\} \in \mathcal{D} \\ \lambda & \text{otherwise} \end{cases} \quad (1.3)$$

The particular dimerizations we have employed are displayed in Fig. 1, namely, the unique nearest neighbor dimerization for chains, two dimerizations, which we denote as “columnar” and “staggered,” on the square lattice, and a “columnar” dimerization on the honeycomb lattice.

In this wide class of models, there are two distinct sets of Hamiltonians which are trivially solvable, and which may serve as “unperturbed Hamiltonians” about which one can expand.

(i) “Dimer models,” defined by $\lambda = 0$, consist of disconnected dimers. For sufficiently large β (e.g., greater than $-1/3$ for $S = A = 1$) and $A \neq 0$, each individual dimer possesses a unique ground state and a readily

⁸ Studies of models where the classical ground states are noncollinear, such as the triangular lattice antiferromagnet, require special attention and will not be discussed here. See ref. 20.

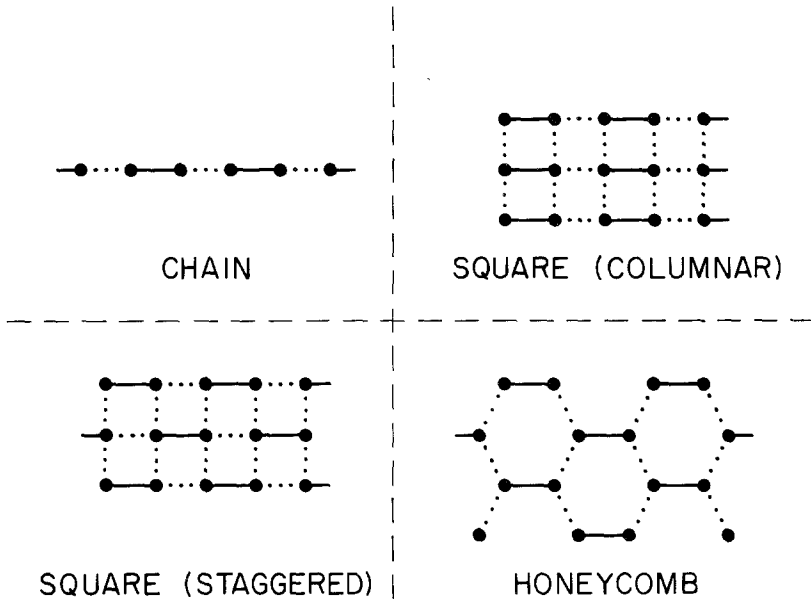


Fig. 1. Dimer configurations on the chain, square lattice, and honeycomb lattice, used to define "unperturbed" Hamiltonians.

calculable spectrum of $(2S + 1)^2 - 1$ excited states. The eigenstates of the entire system are simply characterized as products of the individual dimer states, and the corresponding eigenvalues are the sums of the dimer energies. We denote expansions in the variable λ about dimer models by "D-expansions."

(ii) "Ising models," defined by $\Delta = 0$, are completely classical, in that any state which is a product of local S^z eigenstates is itself an eigenstate. On bipartite lattices, for $\lambda > 0$ and $\beta > -1/S^2$, there are two ground states, namely, the "Néel states," in which all spins on one sublattice have $S^z = -S$ and all spins on the other have $S^z = S$. Expansions in Δ about Ising models will be referred to as "I-expansions."

Studies of zero-temperature properties of quantum spin systems by series expansions can be broadly classified into two types: disordered- and ordered-state expansions. The D-expansions lie in the former class. The defining characteristic of a disordered-state expansion is that the unperturbed Hamiltonian \mathcal{H}_0 has a unique ground state. Such expansions are, in many respects, analogous to classical high-temperature expansions. For example, continuous phase transitions are marked by the divergence of an appropriate susceptibility. For concreteness, consider the D-expansions

in the manifold of isotropic coupling ($\Delta = 1$), and write the Hamiltonian as $\mathcal{H} = \mathcal{H}_0 + \lambda \mathcal{H}_1$. The ground state of an isolated dimer is a spin singlet, and so is the ground state of \mathcal{H}_0 , since it is simply a product over singlets on dimerized neighbors. The part \mathcal{H}_1 then couples the dimers together; but since \mathcal{H}_1 is rotationally invariant in spin space, the ground state remains in the singlet subspace and has no staggered magnetization to *all* orders of perturbation theory. Nonetheless, the spontaneous development of antiferromagnetic (AF) order at some $\lambda_c > 0$ may be evident in expansions for various quantities for which series expansions may be generated; we describe these quantities in detail here.

(a) The “correlation sum,” or, more precisely, the AF, equal-time structure factor, is defined by

$$\mu_0 = \lim_{N \rightarrow \infty} N^{-1} \sum_{ij} \pi_{ij} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \lim_{N \rightarrow \infty} \sum_i \pi_{0i} \langle \mathbf{S}_0 \cdot \mathbf{S}_i \rangle \quad (1.4)$$

Here and below, angular brackets denote ground-state expectation values, and N is the number of spins in the system. The parity π_{ij} takes on value ± 1 , depending on whether or not spin i lies in the same sublattice as spin j . It is important to recognize that the expansions for μ_0 , and all other quantities described below, apply to the *infinite* system. Accordingly, the $N \rightarrow \infty$ limit will be implicit in the definitions which follow.

(b) The second moment of the correlation function is given by

$$\mu_2 = N^{-1} \sum_{ij} \pi_{ij} r_{ij}^2 \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \sum_i \pi_{0i} r_{0i}^2 \langle \mathbf{S}_0 \cdot \mathbf{S}_i \rangle \quad (1.5)$$

where r_{ij} is the Euclidean distance between spin i and spin j . An AF correlation length ξ may be defined by

$$\xi^2 = \mu_2 / \mu_0 \quad (1.6)$$

In doing so, one makes the tacit, and generally valid, assumption that $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ decays exponentially at large r_{ij} (modulo algebraic prefactors). One should note that a series for ξ^2 cannot be produced directly by our method, but can only be obtained by division of the series for the quantities employed in the definition.

(c) The ground-state energy

$$E_g = N^{-1} \langle \mathcal{H} \rangle \quad (1.7)$$

will certainly not diverge on approach to a critical point, but should, in general, exhibit a weak singularity there. As we shall see in Section 2, one

must necessarily generate the expansion for E_g in the course of calculating expansions for any other quantities, so ground-state energy series exist for every model we have studied, whether or not the series are useful.

(d) The AF susceptibility χ is defined in terms of the response to a symmetry-breaking staggered field H^\dagger via

$$\chi = - \left. \frac{\partial^2 E_g}{(\partial H^\dagger)^2} \right|_{H^\dagger=0} \quad (1.8)$$

At finite-temperature criticality, the divergences of χ and μ_0 are governed by the same exponent; indeed, for classical systems $\chi = \mu_0/T$, where T is the temperature. [Note that for $T > 0$, $\chi = -\partial^2 F/(\partial H^\dagger)^2$, where F is the free energy per site.] However, at $T=0$, χ and μ_0 are quite distinct, as can be seen by considering their relationships to the frequency-dependent AF structure factor $S(q_{AF}; \omega)$: the quantity μ_0 is proportional to $\int d\omega S(q_{AF}; \omega)$, while χ is proportional to $\int d\omega \omega^{-1} S(q_{AF}; \omega)$.⁹

For D-expansions with anisotropic exchange ($\Delta \neq 1$), it is proper and convenient to calculate anisotropic correlation moments rather than μ_0 and μ_2 ; discussion of that topic is reserved for Section 4.3.

In an *ordered-state* expansion, the unperturbed Hamiltonian possesses a finite number of degenerate ground states. Such expansions are analogous to classical low-temperature expansions. In particular, for I-expansions, \mathcal{H}_0 has two ground states related by a global $S^z \rightarrow -S^z$ spin-flip operation. As the perturbing, XY part of the Hamiltonian $\Delta \mathcal{H}_1$ is turned on, one looks for restoration of the symmetry of the Hamiltonian, that is, for the disappearance of order, by examining several quantities for which series may conveniently be generated by our method, and are defined below.

(a) The staggered magnetization along the z axis,

$$M^\dagger = N^{-1} \sum_i \pi_{0i} \langle S_i^z \rangle \quad (1.9)$$

should vanish on approach to the disordering transition at $\Delta_c > 0$. Of course, the angular brackets must now denote expectation values with respect to one of the two ground states; if averaged over both ground states, M^\dagger is identically zero for all Δ .

⁹ These standard formulae are used in the context of quantum spin chains by Hohenberg and Brinkman.⁽²⁹⁾

(b) The zz structure factor

$$\mu_0^{zz} = N^{-1} \sum_{ij} \pi_{ij} [\langle S_i^z S_j^z \rangle - \langle S_i^z \rangle \langle S_j^z \rangle] = \sum_i [\pi_{0i} \langle S_0^z S_i^z \rangle - \langle S_0^z \rangle^2] \quad (1.10)$$

should diverge as $\Delta \rightarrow \Delta_c$.

(c) The xy structure factor

$$\mu_0^{xy} = N^{-1} \sum_{ij} \pi_{ij} \langle S_i^x S_j^x + S_i^y S_j^y \rangle = \sum_i \pi_{0i} \langle S_0^x S_i^x + S_0^y S_i^y \rangle \quad (1.11)$$

will typically exhibit some singularity as $\Delta \rightarrow \Delta_c$. It need not diverge at criticality unless $\Delta_c = 1$, in which case naive correlation function scaling suggests that μ_0^{zz} and μ_0^{xy} should diverge with the same exponent. In one interesting case, namely the $S = 1/2$ Heisenberg-Ising chain,⁽¹⁸⁾ one can show that simple scaling does not hold, and that the two structure factors should diverge with distinct exponents which are, in fact, seen by means of series expansions.

(d) One can also consider the second moments of the xy and zz correlation functions, defined in the natural ways, and, as always, the ground-state energy series will be generated as a necessary precursor to any other calculations.

So far, the discussion has centered on what series *can be* calculated using the methods we have developed. Table I gives, in condensed form, a list of some series which *have been* constructed. For example, the first information it communicates is that I-expansions for E_g , M^\dagger , μ_0^{zz} , and μ_0^{xy} have been developed for the purely bilinear ($\beta = 0$), uniformly coupled ($\lambda = 1$), spin-half chain. The numbers in parentheses following each quantity denote the maximum order, in the appropriate variable, to which the series have been calculated for the quantity. Several of the quantities listed in the table have not yet been defined: μ_0^Δ , μ_2^Δ , and χ^{zz} appear in Section 4.3, while the “dimerization” D is discussed in Section 4.2. We should remark that the usage “ $\beta = 0$, Δ ” in Table I underneath “ $S = 1$, D-expansions” indicates not that we have computed two-variable series, in λ and Δ , nor that the coefficients of λ^n are known as functions $f_n(\Delta)$; but, rather, that for any *fixed* Δ we are able to generate the appropriate series in λ , and that we have done so for several Δ values.

As a final motivation for the series expansion method described in this paper, we display in Fig. 2 two sections of the phase diagram for the spin-1 chain.⁽¹⁷⁾ (Note that the diagram on the bottom is not identical to its counterpart in ref. 17: there was an error in the code for generating D-expansions for anisotropically-coupled $S = 1$ systems which was discovered long after ref. 15 appeared in print. For details, see ref. 23.) The

Table I. Series Generated Using the Method of This Work^a

$S = 1/2, \beta = 0$
I-expansions (in Δ), $\lambda = 1$
Linear chain
$E_g(22), M^\dagger(22), \mu_0^{zz}(22), \mu_0^{xy}(12)$
Square lattice
$E_g(10), M^\dagger(10), \mu_0^{zz}(10)$
D-expansions (in λ), $\Delta = 1$
Linear chain (the unique nearest neighbor dimerization)
$E_g(15), \mu_0(7), \mu_2(7), \chi(7)$
Square lattice (columnar dimerization)
$E_g(6), \mu_0(6), \mu_2(6), \chi(6)$
Square lattice (staggered dimerization)
$E_g(5), \mu_0(5), \mu_2(5), \chi(5)$
Honeycomb lattice (columnar dimerization)
$E_g(6), \mu_0(6), \mu_2(6), \chi(6)$
$S = 1$, Linear chain (the unique nearest neighbor dimerization)
I-expansions (in Δ)
$\lambda > 0, \beta > -1$ [resp. $\lambda = 1$]
$E_g(16[18]), M^\dagger(16[18]), \mu_0^{zz}(16)$
D-expansions (in λ)
$\beta = 0, \Delta > 0$
$E_g(11), \mu_0^A(5), \mu_2^A(5), \chi^{zz}(5)$
$\beta > -1/3, \Delta = 1$
$E_g(11), \mu_0^A(5), \mu_2^A(5), \chi^{zz}(5), D(10)$

^a The numbers in parentheses indicate the order to which the series have been evaluated, to date.

information used to construct the phase diagram comes entirely from analysis of I- and D-expansions, except for the knowledge that the point $\lambda = \Delta = \beta = 1$ is a multicritical (and, in fact, Bethe-ansatz-solvable) point. The series also allow one to estimate many critical exponents. When one considers the effort spent in performing finite-chain studies¹⁰ just to understand what happens along the line $\beta = 0, \lambda = 1$, with sometimes inconclusive and conflicting results, the power of the series expansion approach becomes yet more impressive.

The plan of the remainder of the paper is as follows: The next section

¹⁰ See in particular the exchange of opinions by refs. 31. Sogo and Uchinami⁽³²⁾ use a finite-temperature (and finite-size) quantum Monte Carlo method and deduce a $T=0$ phase diagram inconsistent with the Haldane conjecture (and which is almost certainly wrong—the effects of finite T are worse than they suppose). Zero-temperature finite-size studies of the gap at the isotropic point ($\Delta = 1$), such those of ref. 33, have convinced most observers that the structure of the phase diagram along the line $\lambda = 1, \beta = 0$ is as displayed in Fig. 2.

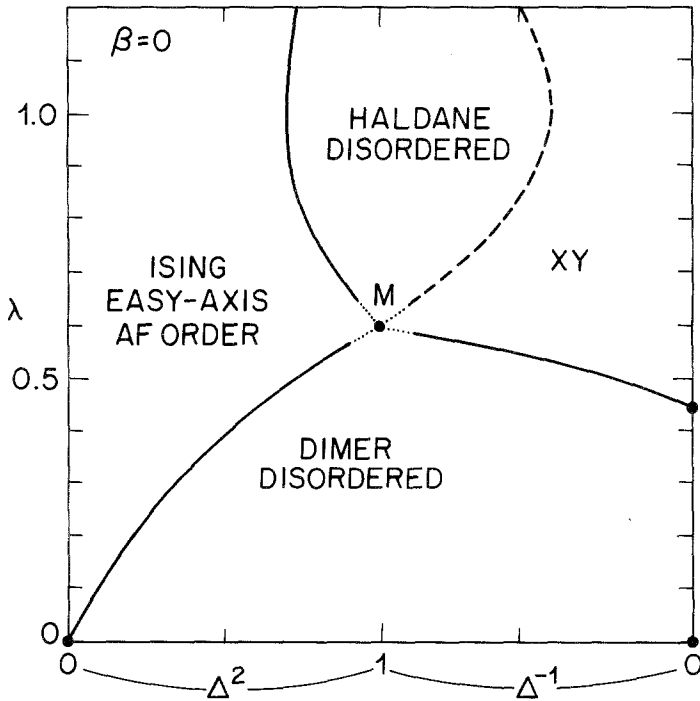
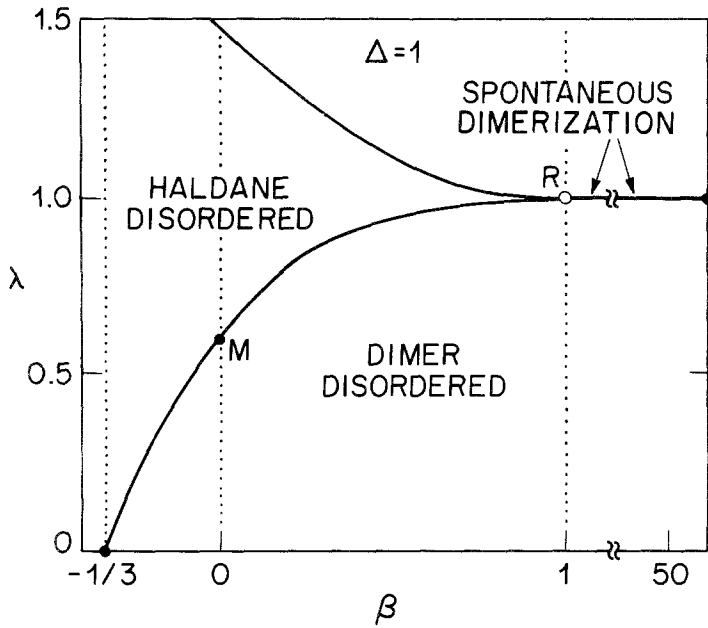


Fig. 2. Sections of the phase diagram for the $S=1$ chain, following Ref. 17. The point R ($\beta = \lambda = \Delta = 1$) is the integrable, Bethe-ansatz-solvable point. The point M is a multicritical point where the easy-axis-ordered "Ising" phase touches the manifold of Heisenberg symmetry, for $\beta=0$. All of the indicated phase boundaries are critical except for the line of "spontaneous dimerization," which is first-order.⁽³⁰⁾

lays out the general principles underlying all of the calculations. In particular, we show how much of the formalism of connected cluster expansions, which is well known in the context of high-temperature expansions for classical spin systems, applies equally well to coupling-constant expansions for quantum spin systems at $T=0$; however, the notion of connectedness requires reappraisal. We further show how the graphical “weights” can be accurately and efficiently computed, via a recursive implementation of Rayleigh–Schrödinger perturbation theory. In short, Section 2 provides a general scheme for constructing many $T=0$ quantum series expansions.

As one might expect, implementation of the general scheme is never entirely trivial, especially if one wishes to obtain high-order expansions (i.e., to the highest order possible using presently available computers). Thus, in Section 3 the most straightforward application of that scheme, to D-expansions for $S=1/2$ systems with $\beta=0$ and $\Delta=1$, is described at length. In Section 4 we discuss rather more briefly what is required to generate D-expansions for $S=1$ systems, and for general values of β and Δ . The special features of I-expansions are examined next, with particular attention to the nature of connected graphs in that case. The last part of Section 4 describes further expansions which have been generated by the method put forth in Section 2, and others which should be feasible, but which we have not yet attempted to carry out. Section 5 offers a conclusion, including a discussion of the relative merits of series expansion and standard finite-size diagonalization methods for studying quantum spin systems. The Appendix contains some of the series indicated in Table I, and gives references for those which appear elsewhere.

Readers primarily interested in *understanding* how the expansions central to refs. 16–23 (and other work in progress) are obtained may wish to stop after Section 2. The rest of the paper is written for those who might be interested in *doing* series expansions themselves, either to check our calculations or to gain insights into novel problems.

2. CLUSTER EXPANSIONS: GENERAL CONSIDERATIONS

We begin with a treatment of the basic principles of *cluster expansions* (more thorough discussions, in the context of expansions for classical models, may be found in ref. 28). It will be evident that the quantum mechanical nature of the systems we wish to study manifests itself mainly in the notion of connectedness and in the evaluation of the graphical *weights* (whose definition will follow). For classical systems, weights are usually trivial to evaluate, but for quantum systems at zero temperature it is not obvious how to compute the weights efficiently. Thus, we explicitly

derive a recursive implementation of Rayleigh–Schrödinger perturbation theory which is well suited to computer calculations.

Let us start by introducing some generic notation for the purposes of this section. Suppose that one is given an unperturbed Hamiltonian \mathcal{H}_0 and a perturbation \mathcal{H}_1 , and that the problem at hand is to study the zero-temperature characteristics of the one-parameter family of Hamiltonians given by

$$\mathcal{H} = \mathcal{H}_0 + \alpha \mathcal{H}_1 \tag{2.1}$$

In particular, one wants to obtain power series expansions, in the variable α , for various zero-temperature properties of \mathcal{H} . Denote by P such a generic *extensive* property (e.g., the total ground-state energy).

In the cases of interest to us, \mathcal{H}_1 (and \mathcal{H}_0 as well) is naturally expressed as a sum of various “local” terms. For example, all of the Hamiltonians discussed explicitly in Section 1 were of the form

$$\mathcal{H} = \sum_{\langle ij \rangle} h_{ij} \tag{2.2}$$

where $\langle ij \rangle$ ran over (some subset of all) nearest neighbor pairs and h_{ij} contained only the operators $S_i, S_i^z, S_j,$ and S_j^z . More generally, one might want to include in \mathcal{H} sums over nearest triples, etc. For any Hamiltonian with such character, it is both natural, and advantageous in the development of cluster expansions, to associate each term in \mathcal{H}_1 with an individual coefficient α_k . [Here k is a generic index which, for Hamiltonians of the form (2.2), would run over nearest neighbor pairs and could just as well be written ij .]

Now consider a formal multivariable expansion of P in powers of the α_k ,

$$P(\{\alpha_k\}) = \sum_{\{n_k\}} p\{n_k\} \prod_k \alpha_k^{n_k} \tag{2.3}$$

where each of the n_k runs over the nonnegative integers. As an extensive quantity, P will typically be proportional to N , the number of spins, and hence will be infinite in the thermodynamic limit. Similarly, $p_{\{0,0,\dots\}}$, which gives the value of P for \mathcal{H}_0 , will also be proportional to N . It will become clear as we proceed that any other $p_{\{n_k\}}$ can be obtained by considering only finite systems, and hence will remain finite in the thermodynamic limit. For convenience, and without loss of generality, we assume henceforth that P has been defined so that $p_{\{0,0,\dots\}} = 0$.

A *cluster expansion* comes about by a reorganization of the terms in the sum (2.3), so that it takes the form

$$P(\{\alpha_k\}) = \sum_C W_{[P]}(C) \tag{2.4}$$

where the sum now runs over all nonempty sets C of indices k , that is, over all clusters. The cluster “weight” $W_{[P]}(C)$ contains all terms in the expansion for P which have at least one power of α_k for all the k in that cluster and no powers of any other α_k . It is not hard to see that the regrouping of all the terms into weights is well defined and unique: the weight of a cluster is given in terms of various $P(\{\alpha_k\})$ by “subtraction of its subclusters.” To be precise, one can invert (2.4) to obtain

$$W_{[P]}(C) = P(C) - \sum_{C' \subset C} W_{[P]}(C') \quad (2.5)$$

where C' runs over all nonempty subclusters of C and $P(C)$ denotes the expansion (2.3) in which all α_k with $k \notin C$ are set to zero.

We invoked the multivariable expansion merely to find a formal definition for the weights. One is ultimately interested in setting all of the α_k equal to α . Once that is done, many clusters will give identical contributions to the expansions for any property P . Clearly, cluster related by the basic symmetries such as translations and various reflections will have the same contribution. We identify such a set of equivalent clusters by a graph G , and the number of such clusters per spin on the infinite lattice is called the lattice constant of the graph, $L(G)$. Thus we may express the property P for the infinite lattice as

$$P(\alpha)/N = \sum_G L(G) W_{[P]}(G) \quad (2.6)$$

where G runs over all graphs (or “distinct” clusters).

At first glance, Eq. (2.6), in conjunction with the definition (2.5), seems to be no more useful than the expression (2.3); however, a moment's reflection shows this not to be true. The essential feature of the weights is that if the cluster C contains s elements (i.e., indices of terms in \mathcal{H}_1), then by construction the coefficients of $\alpha^0, \alpha^1, \dots, \alpha^{s-1}$ in $W_{[P]}(C)$ are identically zero. (In some cases, such as I-expansions for E_g, M^\dagger , and μ_0^{zz} , one knows that higher powers of α also do not appear in the weights: see Section 4.4.) Thus, to obtain an expansion for P/N correct to order α^m , one needs only to identify and evaluate the weights of all graphs containing up to m elements. In general, this would still entail calculations for an infinite number of graphs. A crucial feature of many properties is that all “disconnected” graphs have weights which are identically zero, and only a finite number of “connected” graphs need to be considered at each order.

The exact meaning of “(dis)connected” depends on \mathcal{H}_0 and \mathcal{H}_1 . Every particular case must be given individual attention, and in Sections 3 and 4 the nature of connectedness is described for each type of expansion we have

generated. Here we define disconnectedness in a general context, and sketch the argument that disconnected graphs have zero weight.

A sufficient condition for a cluster C to have zero weight for a property P is the following: If C is the disjoint union of nonempty subclusters A and B , then

$$P(C) = P(A) + P(B) \Rightarrow W_{[P]}(C) = 0 \tag{2.7}$$

[The additivity of P implies that in the expansion (2.3) there can be no terms which include α_k for all $k \in C$, and hence $W_{[P]}(C) = 0$.]

Associated with any cluster C is a “cluster Hamiltonian” \mathcal{H}_C , consisting of the parts of \mathcal{H}_1 specified by C and also certain terms selected from \mathcal{H}_0 . To describe exactly which terms from \mathcal{H}_0 should be included in \mathcal{H}_C requires a brief digression. There are two main considerations. First of all, if the operator S_i^z (or S_i^x, S_i^y, \dots) is in one of those parts of \mathcal{H}_1 , then all terms in \mathcal{H}_0 containing S_i^z (etc.) must be included in \mathcal{H}_C as well. But there is an additional consideration. The unperturbed Hamiltonian partitions the infinite lattice of spins into basic units, so that an eigenstate of \mathcal{H}_0 is uniquely specified as a product of eigenstates of those units, for example, individual spins in the case of I-expansions, pairs of spins (dimers) for D-expansions, etc. In order to apply the weight-evaluation method to be described below, it is essential to include in \mathcal{H}_C sufficient terms from \mathcal{H}_0 that such units are kept intact.

Let us consider the nature of the vector space upon which \mathcal{H}_C acts. This space is clearly a product over spin spaces for some set of spins $\mathcal{S}(C)$. That set can contain, at most, all the spins for which the corresponding operators appear in \mathcal{H}_C . In a disordered-state expansion, all such spins are generally included in $\mathcal{S}(C)$, but in an ordered-state expansion that is not the case. Consider an I-expansion. The states of spins associated *only* with terms from \mathcal{H}_0 are unaffected by \mathcal{H}_C , and hence those spins should be excluded from $\mathcal{S}(C)$. Such spins may be appropriately termed “boundary” spins. Their states depend on the global eigenstate about which one chooses to expand, and they then influence the diagonal terms of \mathcal{H}_C just as would a fixed, position-dependent magnetic field on the boundary of the cluster. Furthermore, in evaluating cluster properties, such as the staggered magnetization, the boundary spins should not be included—it may be seen that such spins contribute only to zeroth order in perturbation theory.

$P(C)$ will typically be some functional of the ground state of \mathcal{H}_C . The properties for which we can generate series expansions will have no contribution from any cluster C for which the cluster Hamiltonian can be written as a sum of subcluster Hamiltonians acting on direct product spaces in the form

$$\mathcal{H}_C = \mathcal{H}_A \otimes I_B + I_A \otimes \mathcal{H}_B \tag{2.8}$$

where, as above, C is the disjoint union of nonempty A and B , and the I 's are appropriate identity operators. We take this as the basic notion of disconnectedness. Clearly, any cluster consisting of two well-separated pieces will satisfy this condition.

Since $\mathcal{H}_A \otimes I_B$ and $I_A \otimes \mathcal{H}_B$ commute, the ground-state energy will have a "connected graph expansion," that is, only connected graphs will have nonzero weights and thus need to be considered. Furthermore, the ground-state wavefunction for the disconnected cluster C can be written as

$$|\Psi_C\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle \quad (2.9)$$

We will now show that this is enough to guarantee connected graph expansions for various other quantities of interest.

The requirement (2.8) on disjoint clusters implies that $\mathcal{S}(C)$ is the disjoint union of $\mathcal{S}(A)$ and $\mathcal{S}(B)$. It then follows from (2.9) that for the sublattice magnetization, the relation

$$\sum_{i \in \mathcal{S}(C)} \pi_{0i} \langle \Psi_C | S_i^z | \Psi_C \rangle = \sum_{i \in \mathcal{S}(A)} \pi_{0i} \langle \Psi_A | S_i^z | \Psi_A \rangle + \sum_{i \in \mathcal{S}(B)} \pi_{0i} \langle \Psi_B | S_i^z | \Psi_B \rangle \quad (2.10)$$

holds, so that the disconnected cluster C has zero weight for M^\dagger .

A similar additivity property is easily demonstrated for the various correlation sums (and, indeed, for the individual correlation functions for any particular site-to-site distance). The terms in any of the correlation sums take the form $\mathcal{P}_{ij}(|\Psi_C\rangle)$, where \mathcal{P}_{ij} is a functional which depends only on the states of the spins on sites i and j . Additivity, and thence the existence of a connected cluster expansion, trivially follows if $\mathcal{P}_{ij}(|\Psi_C\rangle) = 0$ when $i \in \mathcal{S}(A)$ and $j \in \mathcal{S}(B)$. This requirement clearly holds for the correlation sums and moments defined in Section 1, but the case of μ_0^{zz} [see (1.10)] deserves special attention. It is essential that the functional

$$\mathcal{P}_{ij}(|\Psi_C\rangle) = \pi_{ij} [\langle \Psi_C | S_i^z S_j^z | \Psi_C \rangle - \langle \Psi_C | S_i^z | \Psi_C \rangle \langle \Psi_C | S_j^z | \Psi_C \rangle] \quad (2.11)$$

be used in constructing the series for μ_0^{zz} , rather than the apparently equivalent choice

$$\pi_{ij} \langle \Psi_C | S_i^z S_j^z | \Psi_C \rangle - (\langle \Psi_C | S_i^z | \Psi_C \rangle)^2 \quad (2.12)$$

because $|\langle S_i^z \rangle|$ is not site independent in a finite cluster (though it is in the infinite system) and hence the latter does not satisfy the condition on \mathcal{P}_{ij} mentioned above.

Quantities such as the AF susceptibility defined in (1.8) do not depend on the ground-state wave function, and so the above arguments do not

address whether they possess connected cluster expansions. However, it can be seen that if the staggered field Hamiltonian can be decomposed along the lines of (2.8) on disconnected clusters—which is easily checked—then the entire two-variable expansion of the ground-state energy in α and H^\dagger has a connected cluster expansion. Since χ amounts to the terms in that expansion which are second order in H^\dagger , it in turn will have a connected cluster expansion.

[It is sometimes possible to implicitly reorganize the perturbation expansion in a way that reduces the number of connected graphs for which weights need to be calculated. Let us revisit the original multinomial expansion (2.3), where an individual coefficient was associated with every term in the perturbing Hamiltonian. At that stage, one can partition the α_k into sets which are thereafter treated as a single unit: any cluster that contains one coupling from such a set must contain all the couplings in that set with the same strength. Subgraph subtraction, etc., works as before; the only difference is that the least possible power of α in $W_{[P]}(G)$ is no longer the number of terms of \mathcal{H}_1 in G , but rather the number of *sets* of terms of \mathcal{H}_1 in G . A demonstration of the usefulness of such “reorganized” expansions is given in Section 3, in the case of the D-expansion around the columnar dimerization of the square lattice Heisenberg model.

Yet another scheme for reorganizing the perturbation theory has proven useful for D-expansions with further neighbor interactions. (Let us restrict the following discussion to D-expansions, for simplicity.) Rather than defining clusters as sets of terms in \mathcal{H}_1 , one may define them as sets of terms in \mathcal{H}_0 . Associated with any such set of terms in \mathcal{H}_0 is a corresponding set of terms in \mathcal{H}_1 , which couple the dimers in \mathcal{H}_0 . A property $P(C)$ is then defined by setting to zero the α_k for all terms in \mathcal{H}_1 which are not so associated with the specified dimers of \mathcal{H}_0 . One can show that subgraph subtraction works as before, but that subgraphs should be defined in terms of subsets of the dimers (rather than of the interactions) and that for a cluster composed of m dimers, the weight $W_{[P]}(C)$ will generally vanish only up to order α^{m-2} . The details of the graph enumeration procedure must obviously be somewhat different from the method to be described in Section 3, but the modifications are straightforward and we will not discuss them further.]

Even after all the requisite graphs and their associated lattice constants have been identified for a given system, the process of generating the desired series expansions is far from complete. One must still calculate the weights $W_{[P]}(G)$ for each property P of interest and for each graph G ; to be more precise, one must calculate all of the $P(G)$ (with all the perturbing couplings α_k set equal to α) and then apply (2.5) to find the

weights. In the following paragraphs, we outline a procedure which, when implemented with care, can efficiently generate $P(G)$ series for the ground-state energy, some susceptibility-like quantities which we define below, and various ground-state expectation values.

Each graph G is associated with a finite-dimensional vector space [the product over the spin spaces for each spin in $\mathcal{S}(G)$] and a Hamiltonian restricted to that space (which we have called the cluster Hamiltonian). For notational convenience, we will drop further explicit references to G in the formulas, but the reader should keep in mind that every quantity such as \mathcal{H} , \mathcal{H}_1 , etc., depends on the graph under consideration. The cluster Hamiltonian has the form

$$\mathcal{H} = \mathcal{H}_0 + \alpha \mathcal{H}_1 + \beta \mathcal{H}_2 \quad (2.13)$$

where \mathcal{H}_0 and \mathcal{H}_1 are the restrictions of the full unperturbed and perturbing Hamiltonians to G ; the new term containing \mathcal{H}_2 is included so that a susceptibility may be defined by $\chi_\beta = -\partial^2 E / \partial \beta^2 |_{\beta=0}$. To proceed further, it is essential that, for any G , \mathcal{H}_0 should possess a unique ground state $|\Psi_0\rangle$.¹¹ If this condition is satisfied, then nondegenerate perturbation theory, as presented below, permits one to determine coefficients $e_{(i,j)}$ and vectors $\Psi_{(i,j)}$ in the expansions of the ground-state energy and unnormalized wave vector in the form

$$E = \sum e^{(i,j)} \alpha^i \beta^j \quad (2.14)$$

$$|\Psi_g\rangle = \sum |\Psi_{(i,j)}\rangle \alpha^i \beta^j \quad (2.15)$$

Once the expansion coefficients and vectors are known, it is formally straightforward to obtain series in α for the various $P(G)$:

$$E_g = \sum_i e_{(i,0)} \alpha^i \quad (2.16)$$

$$\chi_\beta = -2 \sum_i e_{(i,2)} \alpha^i \quad (2.17)$$

¹¹ If the *global* \mathcal{H}_0 has a unique ground state and a finite gap, this will generally hold. If, on the other hand, the global \mathcal{H}_0 has multiple ground states, then one of them must be chosen to expand about. The uniqueness of $|\Psi_0\rangle$ is enforced by the embedding of the graph G in the infinite system, which is chosen to be in some particular ground state. To be more concrete, consider an I-expansion. In that case, the choice of global ground state fixes the "boundary spins" of G (recall the discussion regarding the definition of the cluster Hamiltonian); these boundary spins provide a symmetry-breaking field which makes the ground state of G unique. Such a mechanism should hold generally: if the global \mathcal{H}_0 has multiple ground states, then in the representation in which \mathcal{H}_0 is diagonal, there ought to be boundary spins which affect (and are not acted on by) \mathcal{H}_G . If, however, the ground state of the global \mathcal{H}_0 is exponentially degenerate, then the field produced by the boundary spins is not generally sufficient to render the ground state of \mathcal{H}_G nondegenerate. The series expansion method described here cannot be applied in such cases.

and, for any operator \mathcal{O} ,

$$\langle \mathcal{O} \rangle = \langle \cdot | \cdot \rangle^{-1} \sum_{i,j} \langle \Psi_{(i,0)} | \mathcal{O} | \Psi_{(j,0)} \rangle \alpha^{i+j} \tag{2.18}$$

with

$$\langle \cdot | \cdot \rangle = \sum_{i,j} \langle \Psi_{(i,0)} | \Psi_{(j,0)} \rangle \alpha^{i+j} \tag{2.19}$$

We have found that a simple recursive formulation of Rayleigh–Schrödinger perturbation theory is ideal for computer calculations of the expansions (2.14) and (2.15). It is necessary to work in a basis $\{|k\rangle\}$ ($k = 0, \dots, M - 1$, M being the dimensionality of the relevant vector space) in which \mathcal{H}_0 is diagonal, with eigenvalues E_k . (In fact, our method is only useful in practice if \mathcal{H}_0 has some obvious representation in terms of “local” expectation values, for example, the spin representation for I-expansions.) In particular, set $|0\rangle = |\Psi_{(0,0)}\rangle$. Then, by inserting (2.14) and (2.15) into the Schrödinger equation

$$(\mathcal{H}_0 + \alpha \mathcal{H}_1 + \beta \mathcal{H}_2) |\Psi_g\rangle = E |\Psi_g\rangle \tag{2.20}$$

and collecting terms which multiply $\alpha^i \beta^j$, one obtains

$$\mathcal{H}_0 |\Psi_{(i,j)}\rangle + \mathcal{H}_1 |\Psi_{(i-1,j)}\rangle + \mathcal{H}_2 |\Psi_{(i,j-1)}\rangle = \sum_{i',j'=0}^{i,j} e_{(i',j')} |\Psi_{(i-i',j-j')}\rangle \tag{2.21}$$

where $|\Psi_{(i,j)}\rangle \equiv 0$ if i or j is less than 0. Before the desired recursion relations can be written, one must specify a “normalization convention,” that is, a set of values for $\langle 0 | \Psi_{(i,j)} \rangle$. Since $|\Psi_{(0,0)}\rangle$ is just the unperturbed ground state, we know $\langle 0 | \Psi_{(0,0)} \rangle = 1$, but all the other $\langle 0 | \Psi_{(i,j)} \rangle$ may be chosen arbitrarily: the choice will certainly affect the form of the states $|\Psi_{(i,j)}\rangle$, but will not affect either $e_{(i,j)}$ or $\langle \mathcal{O} \rangle$. A particularly convenient normalization convention is given by $\langle 0 | \Psi_{(i,j)} \rangle = 0$ for $(i, j) \neq (0, 0)$; with this choice, one immediately finds the recursion relations

$$e_{(i,j)} = \langle 0 | \mathcal{H}_1 | \Psi_{(i-1,j)} \rangle + \langle 0 | \mathcal{H}_2 | \Psi_{(i,j-1)} \rangle \tag{2.22}$$

and, for $k > 0$,

$$\begin{aligned} \langle k | \Psi_{(i,j)} \rangle = & \frac{1}{E_0 - E_k} \left(\langle k | \mathcal{H}_1 | \Psi_{(i-1,j)} \rangle + \langle k | \mathcal{H}_2 | \Psi_{(i,j-1)} \rangle \right. \\ & \left. - \sum' e_{(i',j')} \langle k | \Psi_{(i-i',j-j')} \rangle \right) \end{aligned} \tag{2.23}$$

where the primed sum runs over $i' = 0, \dots, i$ and $j' = 0, \dots, j$, excluding $(i', j') = (0, 0)$ and (i, j) .

This completes the formal “recipe” for generating coupling-constant

expansions for quantum spin systems at zero temperature. To recapitulate, one begins by identifying all the connected graphs and their lattice constants, which one must include in (2.6) in order to obtain expansions valid to some desired order. Then, for each graph, one must obtain an explicit representation for \mathcal{H}_0 , \mathcal{H}_1 , and \mathcal{H}_2 (if a susceptibility is to be calculated), so that the recursion relations (2.22) and (2.23) may be applied. The various properties of interest are then obtained following (2.16)–(2.19); one also needs the matrix elements, in the representation already chosen for the Hamiltonian, of every operator \mathcal{O} which may be needed to evaluate some property P . With the various $P(G)$ in hand, one then performs the subgraph subtraction (2.5) to obtain the weights $W_{[P]}(G)$. At this stage one should examine, for a graph containing m terms of \mathcal{H}_1 , the coefficients of terms up to α^{m-1} in the weights. As discussed following Eq. (2.6), those terms should identically equal zero; however, numerical roundoff errors will typically accumulate and leave them with some small value which serves to indicate the numerical accuracy of the series obtained. If those coefficients are not all nearly zero, one knows that something is wrong in the calculation: either a subgraph has been inadvertently omitted in (2.5), or, more likely, there is a coding error in the routines which calculate the $P(G)$. Finally, when the weights have been calculated for all the graphs, the last step is to evaluate the sums (2.6).

Let us conclude this section with an observation concerning the number-theoretic properties of the coefficients in these series expansions. It should be apparent from the recursion relations (2.22) and (2.23) that the energy eigenvalue series $e_{(i,j)}$ and the series for the matrix elements of the eigenfunctions $\langle k | \Psi_{(i,j)} \rangle$ arise entirely from rational arithmetic operations between matrix elements of \mathcal{H}_0 , \mathcal{H}_1 , and \mathcal{H}_2 . (The series for a property P associated with an operator \mathcal{O} requires further rational arithmetic operations involving the matrix elements of \mathcal{O} .) Hence, if all of these matrix elements are rational numbers, the resulting series must have rational terms as well. In fact, as will be seen in the following section, the requisite matrix elements are, indeed, rational for D-expansions in isotropically-coupled spin-half systems. In general, the matrix elements will not be rational, but they will in almost all cases be *algebraic*, that is, the solutions of finite-order polynomial equations with rational coefficients. For example, for isotropic D-expansions for $S > 1/2$, the matrix elements are, at worst, finite sums of rational multiples of square roots of integers. Arithmetic operations between algebraic numbers yield algebraic numbers, so, as a rule, series expansions in coupling constants for quantum spin systems yield algebraic (and in some circumstances, rational) coefficients. This fact has not proven relevant to the practical calculations of series, but it is an interesting point of principle.

3. DETAILS OF D-EXPANSIONS FOR $S = 1/2$

This section gives a detailed description of how D-expansions are carried out for systems with $S = 1/2$, $\beta = 0$, and $\Delta = 1$ on the lattices displayed in Fig. 1. We begin by characterizing the connected graphs and describing the method, which can be characterized as exhaustive enumeration on the lattice, which we used to identify all such graphs (up to the desired order). The next part of this section is concerned with the weight calculations. Particular attention is paid to the computational demands of high-order calculations. (For “more general” D-expansions, that is, for $S > 1/2$ spins with anisotropic and biquadratic interactions, the graph enumeration is unaffected. However, the weight calculations obviously require modifications, which are described in Section 4.) The final subsection describes some special features of the D-expansions in one dimension. [For several properties, such as the ground-state energy, it is possible to obtain expansions to higher order than for other properties, such as the spin-spin correlations, using exactly the same set of graphs. Thus, it has been possible to expand E_g for the $S = 1/2$ chain to $O(\lambda^{15})$ even though the moments of the structure factor are known only to $O(\lambda^7)$.]

3.1. Graph Enumeration

Graphs for D-expansions may be represented pictorially as points (denoting spins) connected by solid “bonds” (denoting interactions in \mathcal{H}_0) and wavy “links” (denoting interactions in \mathcal{H}_1). In one dimension, all the connected graphs may be trivially written down as is done in Fig. 3. For the various two-dimensional lattices, the number of graphs which contribute to the expansions at $O(\lambda^m)$ grows exponentially with m , and it is essential to implement systematic methods on a computer for generating the graphs in a form suitable for use by the weight-calculation programs.

For the three types of 2D lattices (plus dimer covering to represent \mathcal{H}_0) that have been studied, shown in Fig. 1, we list in Table II the number of additional connected graphs one has in each order. For the square

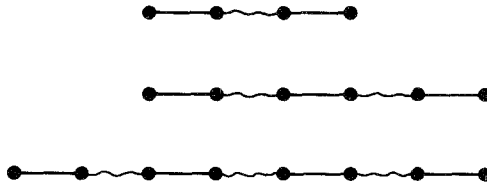


Fig. 3. Graphs for the simple D-expansion in one dimension with up to three links.

Table II. Number of Additional Graphs Needed in the Simple D-Expansions at Each Order for the Three Two-Dimensional Lattice/Dimerization Combinations Shown in Fig. 1

	Square (columnar)	Square (staggered)	Honeycomb
1	2	2	1
2	3	6	3
3	10	29	7
4	28	164	27
5	110	1094	99
6	433	—	427

lattice with *columnar* dimers, the two terms of \mathcal{H}_1 which connect a vertically-stacked pair of bonds are treated as a *single* link for the purpose of graph enumeration; recall the discussion in Section 2 about the “reorganization” of cluster expansions. Many more graphs would arise if that grouping of terms in \mathcal{H}_1 was not done. For example, the single graph in Fig. 4a stands in for the two distinct graphs in Fig. 4b which appear if the terms in \mathcal{H}_1 are not regrouped. Furthermore, as will become evident in Section 3.2, the weight calculations for the graph in Fig. 4a require no more effort than for either of the two graphs in Fig. 4b, so there is no reason whatsoever not to reorganize the perturbation theory in this way.

Figure 5 shows all the graphs for the honeycomb lattice with up to three links, along with their lattice constants. Note that many graphs with the same topology appear separately in this figure: at third order, three of the seven graphs share the topology of the linear chain, and thus give the same contribution to E_g , μ_0 , and χ . We insist, however, on enumerating all geometrically distinct graphs, so that μ_2 can be calculated. Moreover, any spin-spin correlation can then be obtained; such capability is essential for

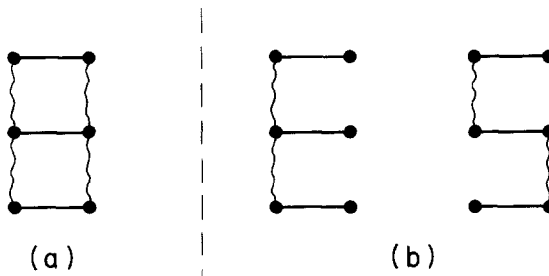


Fig. 4. Illustrative graphs for the D-expansion starting from the columnar dimer configuration on the square lattice; see text for discussion.

studies of frustrated systems where the character of the preferred ordering is not known *a priori*.

One *should* classify the geometrically distinct graphs by topology, calculate the full set of spin–spin correlations for a single graph from each topological equivalence class, and only as a final step use the geometric information to determine the contributions to μ_2 from each geometrically distinct graph. Such a procedure would undoubtedly reduce the computer time used in the weight calculations substantially compared to what we

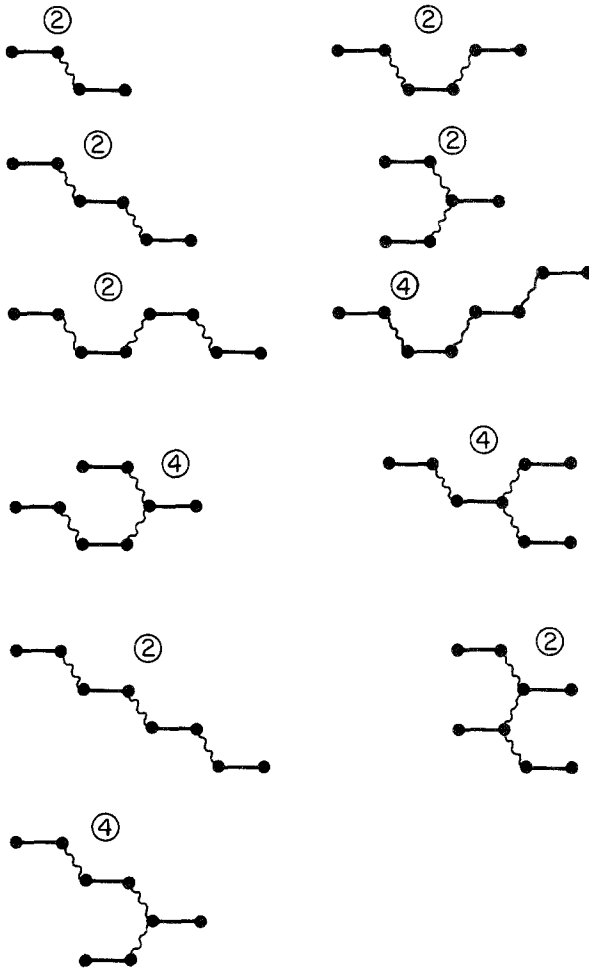


Fig. 5. Graphs with up to three links on the honeycomb lattice. The circled number next to each graph gives the number of translationally (but not otherwise geometrically) distinct forms of the graph, which is *twice* the lattice constant L use in Eq. (2.6).

did—which was to perform the weight calculation for every geometrically distinct graph. However, it seemed wise to do the first calculations without the additional complication of classifying graphs by topology—particularly since there are so few checks on the correctness of the graph enumeration, and the classification procedure is not so easy to program. Since the number of terms in the series which could be obtained by our “brute-force” approach using only modest computer time (on the order of 1 day on a Sun 3/50, of which only a few minutes was spent in graph enumeration) was often sufficient to obtain useful results, we eschewed the more sophisticated approach. However, the topological classification would probably be necessary if one wanted to obtain terms of higher order than have been calculated to date for these 2D models.

The method used to generate the connected graphs, namely, exhaustive enumeration on the lattice, is quite straightforward. Suppose one has identified all graphs with $N-1$ links. To find all those with N links, one takes each of the $(N-1)$ -link graphs in turn and attempts to graft a link [which will be accompanied by another bond, unless the link connects spins on two bonds already present in the $(N-1)$ -link graph] in every possible way onto every spin of the $(N-1)$ -link graph. Some of these attempts will be rejected because the graft overlaps a link already present. When the link *may* be legally attached to form an N -link graph, the graph is assigned an integer by a rule which yields the same number for all geometrically equivalent graphs, but different numbers for inequivalent graphs. This number is compared to the list of numbers assigned to all previously-generated N -link graphs. If it is already present on the list, the “new” graph is rejected. If not, the number is added to the list, and all the information about the graph needed for the weight program is the computed and written to a file. It is also easy to determine the connected subgraphs of the graph at this stage. [Recall that only connected subgraphs need to be accounted for in (2.5), since the disconnected ones have zero weight.] Each of the $2^N - 2$ proper subgraphs is given its integer representation, and only subgraphs for which the corresponding number can be found on the list of connected graphs are put on the list of connected subgraphs for the new N -link graph since the others, by construction, must be disconnected.

This telegraphic description of the enumeration method requires only a few additional remarks to constitute a complete recipe. First, the basic representation of graphs must be addressed. It is convenient to describe a graph by the coordinates of its links on a complementary lattice. (This is not the usual dual lattice, in which sites correspond to plaquettes of the original lattice.) To illustrate this, consider the honeycomb lattice with the dimer covering shown in Fig. 1, for which the complementary lattice is

sketched in Fig. 6. The complementary lattice is obtained by treating the links as the lattice sites (drawn as open circles) which are connected (by thin lines) if and only if the corresponding links share a spin or have spins on the same bond of the original lattice. The sites of the complementary lattice must then be imbedded in the Cartesian lattice with integer coordinates (this is entirely trivial for the lattice of Fig. 6, but less so in other cases), so that individual links may be denoted by ordered pairs of integers, and graphs by sets of such ordered pairs.

Second, one requires a “canonical representation” so that graphs which differ only by translations may be identified. We give here one of many possible definitions of a canonical representation, which is noteworthy only because it is what we have used in practice. If (x_i, y_i) denotes the coordinates of the links of a graph on the complementary lattice, then there is one link—call it the minimal link—which has the minimum x coordinate of all those links with the minimum y coordinate, that is, which is the leftmost of the lowest links. A graph is in canonical form if its minimal link is at some particular site on the complementary lattice, say $(x^{(0)}, y^{(0)})$. This is a correct procedure only if all links are identical up to lattice symmetries, as they are for the honeycomb lattice of Fig. 1. For both dimer configurations on the square lattice, however, there are two kinds of links, horizontal and vertical—call them types 0 and 1. A unique canonical representation can then be determined by the condition that the *minimal type 0* link must be at $(x^{(0)}, y^{(0)})$; if the graph consists of only type 1 links, the minimal link must be at some different site, say

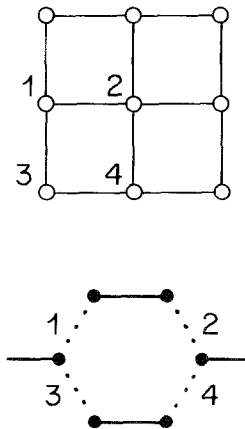


Fig. 6. (Bottom) The dimer-covered honeycomb lattice, and (top) its complement. The correspondence between the original and complementary lattices is shown explicitly by the labels.

$(x^{(1)}, y^{(1)}) = (x^{(0)}, y^{(0)} - 1)$. The imbedding of the complementary lattice will then be such that the types of links may be distinguished by the values of the coordinates modulo 2, for example.

Any cluster can now be given a numerical representation which is the same for all geometrically equivalent clusters but different for inequivalent clusters. First put the cluster in canonical form by an appropriate translation. Now suppose, as will always be the case, that all clusters in canonical form, with up to some fixed number of links, have x and y coordinates in the range 0 to $b - 1$. Assign each link (x_i, y_i) the number $d_i = x_i + by_i$. Sort the d_i in descending order and assign to the cluster the number $\bar{d} = \sum_{i=1}^{\# \text{links}} d_i b^{2(i-1)}$. The final numerical representation for the graph is obtained by calculating \bar{d} for all geometrically equivalent forms of the given cluster and taking the least of those \bar{d} as the numerical representation. (For the lattices of Fig. 1, geometrically equivalent clusters may be obtained by reflecting the given cluster about the x or y axis, and by inversion.) Finally, the lattice constant, up to an overall constant factor, is equal to the number of distinct \bar{d} values obtained for the various geometrically equivalent versions of the same graph.

This completes the discussion of graph enumeration for simple D-expansions; readers interested in the *full* details should write to the authors for copies of the computer programs. The same basic strategy of grafting links and assigning prospective graphs a unique integer can be (and has been) used for other, more challenging graph enumeration problems, as will be discussed in Section 4.4 for I-expansions.

3.2. Weight Calculations

The evaluation of weights for a given graph apparently entails a straightforward sequence of calculations. First there are the recursion relations (2.22) and (2.23); to obtain quantities such as μ_0 and μ_2 some expectation values must be evaluated using (2.18) and (2.19); finally, weights are determined by subgraph subtraction, Eq. (2.5). However, this list is not complete. Indeed, much of the computer time used in weight calculations is spent in putting the perturbing Hamiltonian \mathcal{H}_1 into matrix form, which we denote $[\mathcal{H}_1]$, suitable for the recursion relations. Even that cannot be done without first carrying out other calculations. In this subsection, the method we have used for calculating weights for the simple $S = 1/2$ D-expansions is described in detail.

Suppose the graph under consideration consists of n_D dimers coupled by some number n_1 of terms in \mathcal{H}_1 . The representation of the states of the system in which \mathcal{H}_0 is diagonal [which, as we pointed out earlier, *must* be used in order for the simple recursion relations (2.22) and (2.23) to hold]

is the “dimer representation,” in which each dimer is associated with one of the four eigenstates of a single dimer. The dimer eigenstates consist of one singlet and three triplet states; we denote them by 0 for the singlet and 1, 2, 3 for the triplet, with $S^z = 0, 1,$ and $-1,$ respectively. Every eigenstate of \mathcal{H}_0 may be written as a list of n_D integers $e_i,$ each in the range 0–3, or, alternatively, as a single integer

$$e = 1 + \sum_{i=1}^{n_D} e_i 4^{i-1} \quad (3.1)$$

in the range 1 to $2^{2n_D}.$ However, not all of these states are coupled to the unperturbed ground state by either \mathcal{H}_1 or \mathcal{H}_2 (if the latter represents a staggered magnetic field): both operators commute with the total S^z operator, and hence we may restrict the vector space to states with $S_{\text{tot}}^z = 0.$ There are

$$C(n_D) = \binom{2n_D}{n_D}$$

such states, which henceforth we refer to as the basis states.

The first step in the calculation is to find all eigenstates of \mathcal{H}_0 with $S_{\text{tot}}^z = 0$ and create two lookup tables. One table—actually, a two-dimensional array—puts each integer from 1 to $C(n_D)$ (which now serves to label the basis states) in correspondence with the representation of that state as a list of $e_i.$ The other table puts the integers from 1 to 2^{2n_D} [which index the full set of eigenstates of \mathcal{H}_0 though Eq. (3.1)] in correspondence with the label for the state in the basis if $S_{\text{tot}}^z = 0$ for the eigenstate, or with 0 otherwise.

Next, the unperturbed energy, that is, the expectation value of $\mathcal{H}_0,$ is calculated for each state in the basis. This is easy to do because one simply looks up the representation of the state as a list of $e_i;$ each value of e_i corresponds to some energy, namely $-3/4$ for $e_i = 0$ and $1/4$ for $e_i = 1, 2, 3,$ and these energies for the individual dimers are added to obtain the total unperturbed energy of the basis state.

Now one comes to the most challenging step, which is to calculate $[\mathcal{H}_1].$ It will become evident that $[\mathcal{H}_1]$ is a sparse matrix. Hence, it should be stored in a standard sparse-matrix format: rather than storing the entire $C(n_D) \times C(n_D)$ array $[\mathcal{H}_1]_{ij},$ two smaller arrays $[\mathcal{H}_1^{(\text{pt})}]$ and $[\mathcal{H}_1^{(\text{val})}]$ are used. For the former, the row index runs from 1 to $C(n_D)$ and the column index runs from 0 to $M,$ where M should be the maximum number of non-zero elements in any row. The elements of $[\mathcal{H}_1^{(\text{pt})}]$ are “pointers,” while the elements of the $C(n_D) \times M$ matrix $[\mathcal{H}_1^{(\text{val})}]$ are the actual (nonzero)

elements of $[\mathcal{H}_1]$; explicitly, this means that all nonzero elements of $[\mathcal{H}_1]$ are given by

$$[\mathcal{H}_1]_{i, [\mathcal{H}_1^{(pt)}]_j} = [\mathcal{H}_1^{(val)}]_{ij} \tag{3.2}$$

where i runs from 1 to $C(n_D)$ and j runs from 1 to $[\mathcal{H}_1^{(pt)}]_{i0} \leq M$.

The savings in memory is a factor of roughly $C(n_D)/2M$ compared to storing the matrix in the usual way. Furthermore, much computational effort is saved in matrix multiplication, which needs to be done at each step of the recursion formula, since only the nonzero elements of $[\mathcal{H}_1]$ will actually be used. To be precise, the multiplication of the vector V_i by $[\mathcal{H}_1]$ is performed as follows:

$$[\mathcal{H}_1]_{ij} V_j = \sum_{j=1}^{[\mathcal{H}_1^{(pt)}]_{i0}} [\mathcal{H}_1^{(val)}]_{ij} V_{[\mathcal{H}_1^{(pt)}]_j} \tag{3.3}$$

To see how $[\mathcal{H}_1]$ is calculated, consider just one of its terms, say $\mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)}$, where $\mathbf{S}_{(i)}$ corresponds to one of the spins on the i th dimer in the graph. Since each of these spins could be on either the right or left side of the dimer, there are four distinct terms of this form,¹² not all of which need appear in any particular \mathcal{H}_1 . It is clear that the matrix element of that operator between any two basis states written as (e_1, \dots, e_{n_D}) and (e'_1, \dots, e'_{n_D}) will be zero unless $e_j = e'_j$ for $3 \leq j \leq n_D$. Thus, the problem of constructing $[\mathcal{H}_1]_{ij}$ is reduced to repeated lookups in the four 16×16 matrices $\langle e_1, e_2 | \mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)} | e'_1, e'_2 \rangle$, all of which elements take on the value 0 or $\pm 1/4$. One of the matrices is displayed in Fig. 7; the others have zeros in the same positions, and differ only in some of the signs. No row of this matrix contains more than five nonzero elements, and thus an upper bound for the number of nonzero elements in any row of $[\mathcal{H}_1]$ is five times the number of terms in \mathcal{H}_1 . This shows that $[\mathcal{H}_1]$ is indeed extremely sparse.

The full calculation of $[\mathcal{H}_1]$ in sparse matrix form thus involves the following three nested loops: (1) A loop over the $C(n_D)$ rows of the matrix, i.e., over the basis states, which are converted to the dimer representation (e_1, \dots, e_{n_D}) by means of the lookup table constructed earlier. (2) A loop over the terms in \mathcal{H}_1 , i.e., over the links of the graph. (3) A loop over the 16 states (e'_1, \dots, e'_{n_D}) which could be coupled to (e_1, \dots, e_{n_D}) by the term in \mathcal{H}_1 . When a nonzero matrix element is found, it is placed in $[\mathcal{H}_1^{(val)}]$, and the corresponding $[\mathcal{H}_1^{(pt)}]$ is determined by looking up, in the other table constructed previously, the label for the basis state given the integer e' defined by Eq. (3.1).

¹² For the case of columnar dimers on the square lattice, there are only three such terms, since in our formulation of the perturbation theory for that case a “left-left” link is *always* accompanied by a “right-right” link, and vice versa.

(e_1, e_2)	(e'_1, e'_2)															
(0, 0)	•	•	•	•	•	-	•	•	•	•	•	•	•	•	•	•
(1, 0)	•	•	•	•	-	•	•	•	•	•	•	•	•	•	•	•
(2, 0)	•	•	•	•	•	•	-	•	-	+	•	•	•	•	•	•
(3, 0)	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
(0, 1)	•	-	•	•	•	•	•	•	•	•	•	•	•	•	•	•
(1, 1)	-	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
(2, 1)	•	•	-	•	•	•	•	•	•	-	+	•	•	•	•	•
(3, 1)	•	•	•	+	•	•	•	•	•	•	•	•	•	•	•	•
(0, 2)	•	•	-	•	•	•	-	•	•	•	+	•	•	•	•	•
(1, 2)	•	•	+	•	•	•	•	•	•	•	•	•	•	•	•	•
(2, 2)	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
(3, 2)	+	+	•	•	+	+	•	•	•	•	•	•	•	•	•	•
(0, 3)	•	•	•	-	•	•	•	•	•	•	•	•	•	•	•	•
(1, 3)	•	•	•	-	•	•	•	•	•	•	•	•	•	•	•	•
(2, 3)	+	-	•	•	-	+	•	•	•	•	•	•	•	•	•	•
(3, 3)	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•

Fig. 7. The matrix $\langle e'_1, e'_2 | \mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)} | e_1, e_2 \rangle$, where $\mathbf{S}_{(i)}$ represents the right spin for $i=1$ and the left spin for $i=2$. Dots stand for zeros, and \pm denotes $\pm 1/4$. Note that the dimer singlet state $e=0$ is taken to be $+(\uparrow\downarrow - \downarrow\uparrow)/\sqrt{2}$.

Before ending the discussion of $[\mathcal{H}_1]$, there is one detail worth mentioning. Since the lookup of matrix elements $\langle e_1, e_2 | \mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)} | e'_1, e'_2 \rangle$ takes place $C(n_D) \times (\text{number of terms in } \mathcal{H}_1) \times 16$ times, it is best to do it “in-line” and not as a subroutine call. This was discovered when doing early calculations for $S=1$ chains; a timing analysis showed that an embarrassingly large fraction of the total computational effort was devoted to *overhead* on the subroutine call which gave the matrix elements.

The matrix $[\mathcal{H}_2]$ is rather simpler to construct. Like $[\mathcal{H}_1]$, it is sparse and should be stored in an appropriate form. However, $[\mathcal{H}_2]$ does not couple dimers together, since its terms are $\pm S_k^z$, where k runs over the spins in the graph and the sign depends on the sublattice upon which the spin sits. If these terms are grouped into pairs corresponding to the dimers of \mathcal{H}_0 , then the terms within each pair are opposite in sign, and hence \mathcal{H}_2 conserves S^z on each dimer. The only nonzero matrix elements

$\langle e | S_1^z - S_2^z | e' \rangle$ are for $(e, e') = (1, 0)$ or $(0, 1)$: the staggered field turns the singlet into the $S^z = 0$ triplet state, up to a numerical factor, and vice versa, and it annihilates the other triplet states. Thus, the maximum number of nonzero elements in a row of $[\mathcal{H}_2]$ is n_D : it is yet more sparse than $[\mathcal{H}_1]$.

After \mathcal{H}_0 , \mathcal{H}_1 , and \mathcal{H}_2 have been put in the appropriate form, the recursion relations (2.22) and (2.23) may be applied to yield the energy and eigenvector series. With the vectors $|\Psi_{(i,0)}\rangle$ and the four 16×16 matrices $\langle e_1, e_2 | \mathbf{S}_{(2)} \cdot \mathbf{S}_{(2)} | e'_1, e'_2 \rangle$ in hand, the evaluation of matrix elements needed for calculating the series for μ_0 and μ_2 (or any desired spin-spin correlation function) can proceed directly.

Once all the series for the desired properties have been evaluated for a given graph, all that remains is subgraph subtraction (2.5) to obtain the weights, and, finally, the addition of the weights, multiplied by appropriate lattice constants, to give the series.

There are several checks on the calculation which can alert one to possible errors in the computer programs. As mentioned in Section 2, for any weight $W_{[p]}(G)$ one knows that the low-order terms (up to order λ^{p-1} , if G has p links) must be identically zero. This provides a fairly robust check that graphs have not been omitted, except perhaps in the highest order of the calculation, and that subtle errors, such as exceeding declared array dimensions, have not tainted the calculations. With double-precision arithmetic, we found that values which should have been identically zero were typically on the order of 10^{-13} or smaller. In addition, the results at lowest nontrivial order can be obtained by hand with modest effort; gross mistakes in the code can be detected in this way.

3.3. "Fortuitous Cancellations" for Chains

In the case of D-expansions for chains, one discovers that the weight for E_g for the graph containing p links vanishes not only to $O(\lambda^{p-1})$, but all the way to $O(\lambda^{2p-1})$. This empirical observation allows for an expansion of E_g to $O(\lambda^{2p+1})$ using only the graphs needed for the expansions to $O(\lambda^p)$ of μ_0, μ_2 , etc., and explains why, in Table I, the expansions for E_g in $S=1/2$ and 1 chains have been obtained to much higher order than those for other quantities. At present, there is no rigorous proof that this cancellation in the E_g weights holds for all p , although the calculations establish it as a numerical fact up to $p=7$ for $S=1/2$. It is also valid for $S=1$ chains with any value of the biquadratic coupling, where the calculations extend up to $p=5$ [except for $p=1$, for which the $O(\lambda)$ term is non-zero when $\beta \neq 0$]; presumably the cancellation holds for all S . For $S=1/2$, it also holds when *next-neighbor* interactions are included in \mathcal{H}_1 .

The dimerization, defined in Section 4.2, exhibits a cancellation in the

same cases as the energy, but only to order λ^{2p-2} . Hence the expansion may be calculated to $O(\lambda^{2p})$ using only the graphs with up to p links.

The susceptibility weight for $S=1/2$ chains exhibits no unexpected cancellations. However, the coefficient of λ^p in the weight for the p -link graph seems to be simply 2^{-p} . The reason for this is not known, but it has been exploited to obtain the expansion of χ to $O(\lambda^7)$ using only graphs with up to six links.

Although there is currently no general proof for the vanishing of terms to $O(\lambda^{2p}-1)$ for the energy weights in spin chains, there is a reasonable argument for it which can be made rigorous by an exhaustive analysis, at least for $S=1/2$ and small p . The argument goes as follows: In order to obtain a contribution to the energy weight at, say, $O(\lambda^n)$, one needs to find a term in $(\mathcal{H}_1)^n$ which has a nonzero expectation in the unperturbed ground state and which, in addition, contains *every* term in \mathcal{H}_1 as a factor at least once. We conjecture that any such terms in $(\mathcal{H}_1)^n$ will actually contain every term in \mathcal{H}_1 as a factor at least *twice*; the claim that the lowest-order nonzero term in the energy weight is at least of order λ^{2p} in a p -link graph follows directly.

Why is such a conjecture plausible? Consider the state of a dimer at one end of a chain. Its state can only be changed by the one term in \mathcal{H}_1 which connects it with the rest of the dimers in the chain. One sees from the matrix $\langle e_1, e_2 | \mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)} | e'_1, e'_2 \rangle$ in Fig. 7 that one application of the perturbation always takes a singlet state of the dimer into a triplet state; thus, the term of \mathcal{H}_1 which acts on the end dimer must appear at least twice, if it is to appear at all, in order to obtain a nonzero expectation value for a term in $(\mathcal{H}_1)^n$. Our conjecture is thus trivially established for $p=1, 2$, where every link is attached to a dimer at one end of the chain. For larger p , one can systematically examine all terms of $(\mathcal{H}_1)^n$ which could conceivably contribute to the energy weight. We do not have an inductive argument, which one might expect should exist.

For higher-spin chains the cancellation in energy weights may presumably be argued along similar lines. However, the cancellation in the dimerization for chains and the simple behavior of the leading term in the χ weights for $S=1/2$ chains remain entirely unaccounted for. We leave these as open problems. It might also be possible to find an elegant proof of the cancellation in energy weights, since the result seems to have a topological character, and appears to hold even for nonlinear graphs which do not contain loops.

4. OTHER MODELS

The calculational procedure laid out in the preceding section can be applied rather widely, with only relatively minor modifications in many cases. In the following subsections, the necessary modifications are discussed first for various D-expansions; specifically for $S = 1$ systems, and for models which include biquadratic and/or anisotropic interactions. In all of these cases, the graph enumeration problem is identical to that for the simple D-expansions of Section 3 and only the construction of the Hamiltonians needs to be addressed.

Next, the implementation of I-expansions is described. The required modifications are much more extensive than in the cases mentioned above; in particular, the character of the connected graphs for I-expansions is rather different from the character of those for D-expansions. Furthermore, because of a trivial local symmetry, many I-expansions turn out to be expansions in Δ^2 rather than Δ . For such quantities, the lowest order in the weight which has a nonzero coefficient can be determined by inspection; since most graphs contribute first in much higher order than one might naively expect, one can identify by hand the graphs with the most terms of \mathcal{H}_1 which need to be included in the calculation. The weight calculations for I-expansions also show a new feature: the number of basis vectors which must be kept turns out to be even less than the number of eigenstates of \mathcal{H}_0 with $S_{\text{tot}}^z = 0$.

The final subsection briefly mentions several further applications of the series expansion method. Some of them have been carried out, and are described in more detail elsewhere; others remain open for exploratory calculations.

4.1. Spin-1 Systems

The general scheme of the weight calculations for D-expansions in $S = 1$ systems is identical to that for $S = 1/2$ systems. Most of the required changes are obvious: the e_i of Section 3.2 now run from 0 to 8 rather than 0 to 3; the unperturbed energies for dimers are changed, etc. The few differences which deserve special mention are described below.

The most important difference between $S = 1$ and $S = 1/2$ systems, from the viewpoint of practical calculations, is in the number of states with which one must work in the weight calculations. The number of states in the $S_{\text{tot}}^z = 0$ basis for a graph with n_D dimers is given by

$$C_1(n_D) = \sum_{m=0}^{n_D} \frac{(2n_D)!}{[2(n_D - m)]! m! m!} \quad (4.1)$$

which, for $n_D = 1, \dots, 6$ equals 3, 19, 141, 1107, 8953, and 73789. These should be compared with the $C(n_D)$, which equal 2, 6, 20, 70, 252, and 924; clearly calculations for $S = 1$ systems require much more computer power than the analogous calculations for $S = 1/2$ systems. Indeed, for reasons of storage alone it proved necessary to use a supercomputer (IBM 3090 with extended addressing capability) to calculate weights for the linear graph with five links.

The matrices $\langle e_1, e_2 | \mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)} | e'_1, e'_2 \rangle$ used to construct $[\mathcal{H}_1]$ and evaluate spin-spin correlations must also be built anew for $S = 1$ systems. They are now 81×81 matrices, and they are difficult to write down without the aid of a computer. By hand, one can readily evaluate the matrix elements of $\mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)}$ in the *spin* representation,

$$[S \cdot S]^s = \langle S_{1,l}^z S_{1,r}^z S_{2,l}^z S_{2,r}^z | \mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)} | S_{1,l}^{z'} S_{1,r}^{z'} S_{2,l}^{z'} S_{2,r}^{z'} \rangle$$

(with l and r denoting left and right sites in a dimer). One can also write down the 9×9 orthonormal matrix $U_i = \langle S_{i,l}^z S_{i,r}^z | e_i \rangle$ which converts the state of a single dimer from the dimer to spin representation; its elements are the familiar Clebsch-Gordon coefficients for the addition of two spin-1 states. The 81×81 change-of-representation matrix for a pair of dimers $U_{12} = U_1 \otimes U_2$ may then be constructed by machine, and the $\langle e_1, e_2 | \mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)} | e'_1, e'_2 \rangle$ obtained by matrix multiplication as $U_{12}^T [S \cdot S]^s U_{12}$.

Finally, the staggered-field matrix elements $\langle e_1 | S_i^z - S_r^z | e'_1 \rangle$ used to construct \mathcal{H}_2 must be determined. This task can be done easily enough by hand.

4.2. Biquadratic Interactions

In performing series expansions for models with several different types of interactions, one often has some freedom in the allocation of terms between \mathcal{H}_0 and \mathcal{H}_1 . For the example at hand, if one wishes to study the $S = 1$ chains with

$$\mathcal{H} = \sum \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \beta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \tag{4.2}$$

by D-expansions, then either *all* the biquadratic terms could be put into \mathcal{H}_1 or the biquadratic terms associated with the dimers of \mathcal{H}_0 could be put into \mathcal{H}_0 (along with the appropriate $\mathbf{S} \cdot \mathbf{S}$ terms) and the remainder put into \mathcal{H}_1 . It is evident from Eq. (1.1) that we have chosen the latter alternative for our calculations. In the discussion below, only $S = 1$ systems will be considered, since for $S = 1/2$ there is no independent biquadratic term

[because $(\mathbf{S}_1 \cdot \mathbf{S}_2)^2 = 3/16 - \frac{1}{2}\mathbf{S}_1 \cdot \mathbf{S}_2$], and we have not done any calculations with $S > 1$.

The eigenvalues of \mathcal{H}_0 for a *single* dimer are $-2 - 4\beta$ for the singlet, $-1 - \beta$ for the triplet, and $1 - \beta$ for the quintuplet. Thus, when $\beta \leq -1/3$ the ground state of a single dimer is no longer nondegenerate and our method can no longer be applied. Note that if all the biquadratic terms were put into \mathcal{H}_1 , this problem would not arise for any value of β . Fortunately, the portion of the phase diagram with $\beta > -1/3$ is particularly interesting: recall Fig. 2.

In the construction of $[\mathcal{H}_1]$ only one new feature arises. The matrix elements $\langle e_1, e_2 | (\mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)})^2 | e'_1, e'_2 \rangle$ must be stored as an 81×81 matrix, as well as the $\mathbf{S}_{(1)} \cdot \mathbf{S}_{(2)}$ matrix.

For $S=1$ chains with biquadratic interactions, it turns out that “dimerization” is an interesting quantity to study. If we define

$$D = \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle - \langle \mathbf{S}_0 \cdot \mathbf{S}_1 \rangle \quad (4.3)$$

for the infinite chain, then $D=2$ for $\lambda=0$ if we take the dimers of \mathcal{H}_0 as having the even spins on their left sides. It is readily shown that D has a connected cluster expansion, using the usual connected graphs for D-expansions, if the property

$$\hat{D} = \sum (-)^{i+1} \langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle \quad (4.4)$$

is taken as its appropriate extensive version, to be calculated for each graph.

One might expect that as the *imposed* dimerization is removed, that is, $\lambda \rightarrow 1$, then D should approach 0. However, dimerization can be a *spontaneously* broken symmetry; that is what happens for $S=1$ chains with $\beta > 1$. Thus, with respect to D , the D-expansions are analogous to expansions about infinite magnetic field for classical Ising ferromagnets. In both cases, as the explicit symmetry-breaking term in \mathcal{H} is removed, one can look for a residual, spontaneous order. Furthermore, one knows that if $D > 0$ as $\lambda \rightarrow 1^-$, then by symmetry there is a first-order transition at $\lambda = 1$, since as $\lambda \rightarrow 1^+$ the ground state must have the opposite value of D .

4.3. Anisotropic Interactions

If anisotropic interactions

$$(\mathbf{S}_i, \mathbf{S}_j)_A = S_i^z S_j^z + \Delta(S_i^x S_j^x + S_i^y S_j^y) \quad (4.5)$$

are to be used, it is clear that the two-dimer matrix elements of $(\mathbf{S}_{(1)}, \mathbf{S}_{(2)})_A$ are needed. But, in addition, the *unperturbed* eigenstates depend on Δ ; the

ground state of \mathcal{H}_0 on a dimer is no longer a singlet (except when $\Delta = 1$), since that is not even an eigenstate of total spin. Fortunately, S_{tot}^z remains a good quantum number for all Δ , so the number of basis states involved in the weight calculations is the same as in the case of isotropic couplings.

A prerequisite for any weight calculation, then, is to calculate exact eigenvalues and eigenvectors (in the spin representation) for a single dimer subject to \mathcal{H}_0 . (It is worth noting that the ground state is nondegenerate for all $\Delta \neq 0$.) Using that spectral information, which is just the transformation matrix U of Section 4.1, the matrix $\langle e_1, e_2 | (\mathbf{S}_{(1)}, \mathbf{S}_{(2)})_\Delta | e'_1, e'_2 \rangle$ (with the e_i identifying true, Δ -dependent dimer eigenstates) may be readily calculated by the method described before. The important point is that $(\mathbf{S}_i, \mathbf{S}_j)_\Delta$ is no more difficult to express in the spin representation than $\mathbf{S}_i \cdot \mathbf{S}_j$.

Since the operator $(\mathbf{S}_i, \mathbf{S}_j)_\Delta$ is needed to create $[\mathcal{H}_1]$, it is natural to calculate the series expansions for moments of the anisotropic AF equal-time structure factor

$$\mu_k^A = \sum_i \langle (\mathbf{S}_0, \mathbf{S}_i)_\Delta \rangle r_{0i}^k \pi_{0i} \tag{4.6}$$

It is certainly possible to calculate the isotropic quantities μ_0, μ_2 as well. However, the only model for which D-expansions with anisotropic coupling have been calculated is the $S = 1$ chain without any biquadratic coupling. In that case only μ_0^A, μ_2^A , and χ^{zz} were calculated. (The last quantity describes the response of the ground-state energy to a staggered field along the z direction in spin space, and is exactly what was meant previously by χ —though in fact the response in an isotropically coupled system will not depend on the orientation of the field. In an anisotropically coupled system, the quantities $\chi^{xx} = \chi^{yy}$ are distinct from χ^{zz} , but cannot be easily calculated, since a staggered field along the x or y direction does not commute with S_{tot}^z .) It seemed that expansions for the other quantities would give no important additional information: see especially the discussion in ref. 15 pertaining to the D-expansions for $\Delta > 1$.

4.4. Ising Expansions

The *connected graphs* for I-expansions look rather different than those for D-expansions. Recall that all nearest-neighbor pairs of spins are coupled by terms of \mathcal{H}_0 . Thus, using points and solid and wavy lines to denote spins and terms of \mathcal{H}_0 and \mathcal{H}_1 , the *simplest* graph in 1D, which contains just one term of \mathcal{H}_1 , is shown in Fig. 8a. Two terms of \mathcal{H}_1 constitute a connected cluster if they share either a spin, as in Fig. 8b, or if a term of \mathcal{H}_0 joins them, as in Fig. 8c; it should be clear that in neither of these cases

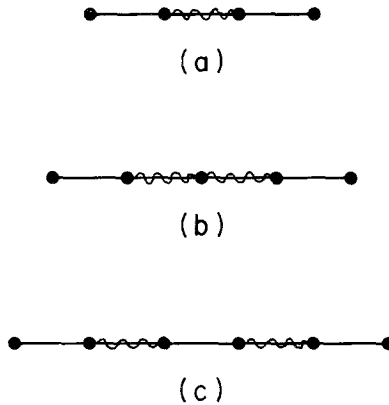


Fig. 8. Low-order graphs for the I-expansion in one dimension.

is a decomposition of the cluster Hamiltonian along the lines of (2.8) possible.

The number of connected graphs in 1D with m links is greater than 2^{m-2} , as can be seen by a quick argument: the $m-1$ gaps between the links can be of either length 0 or 1, which gives 2^{m-1} connected clusters. However, not all of these are geometrically distinct, since some may be related, in pairs, by inversion symmetry. Ignoring the possibility that a cluster may be mapped onto itself under inversion gives the lower bound of 2^{m-2} graphs. (The exact number is $2^{m-2} + 2^{\lfloor m/2 \rfloor - 1}$, with $\lfloor \cdot \rfloor$ denoting the greatest integer function.) Even in 1D the construction of connected graphs for I-expansions is not completely trivial. It is evident that the number of graphs grows much more rapidly with the number of links than for D-expansions; the difference is even more marked on the square lattice, where each link has, in effect, 22 possible “neighbors” to which it could be connected either directly or through a bond of \mathcal{H}_0 .

The number of connected graphs increases so rapidly with the number of links that one should immediately wonder how the I-expansions listed in Table I—expansions to order Δ^{10} on the square lattice, and to order Δ^{22} in 1D—could possibly be obtained. Indeed, it is only possible because for certain quantities, among them E_g , M^\dagger , and μ_0^{zz} , the lowest nonzero term in the weight for most m -link graphs appears not at $O(\Delta^m)$, but rather at $O(\Delta^{2m})$. Few m -link graphs contribute to those weights at $O(\Delta^m)$: on the square lattice, just one graph for $m=4$, none for $m=5$, one for $m=6$, and so on. In 1D, *all* m -link graphs contribute to those weights first at $O(\Delta^{2m})$.

To establish these claims, we begin with the full multinomial expansion (2.3). Each term in \mathcal{H}_1 should be thought of as carrying its own coef-

ficient Δ_{ij} . The aim now is to show that E_g , M^\dagger , and μ_0^{zz} are *even* functions of any Δ_{ij} which, roughly speaking, is not associated with a *closed loop of links*.

Consider the following local gauge transformation of the spin system: given a site i , rotate \mathbf{S}_i by π radians about the z axis, and, to compensate, change the signs of all the XY coupling J_{ij}^{xy} (equivalently, Δ_{ij}) affiliated with that site. This transformation leaves E_g , M^\dagger , and μ_0^{zz} unchanged, since it does not alter the z component of the spin; henceforth, these properties will be called *gauge-invariant*. Applying the transformation to all the spins on one sublattice of an infinite bipartite lattice reverses the signs of all the XY couplings. Thus, only even powers of Δ can appear in the I-expansions for gauge-invariant properties; the same is not true for μ_0^{xy} , for instance.

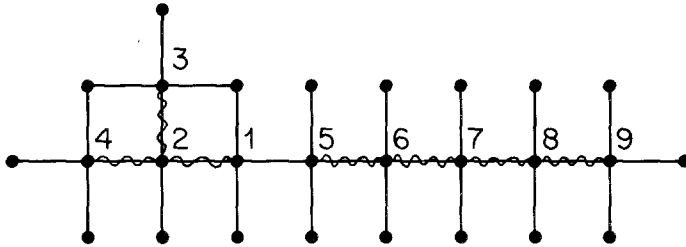
More information is gained by applying the transformation more selectively, to particular spins in a finite connected graph. Rather than deriving a general rule for determining the lowest-order nonzero term in the gauge-invariant weights, several illustrative examples will be worked through, and then a procedure for identifying all relevant graphs will be sketched.

Consider first the effect of applying the gauge transformation to a single spin in a graph, say, the spin labeled 1 in Fig. 9a. This changes the sign of only one term of \mathcal{H}_1 , namely, Δ_{12} ; hence, the gauge-invariant weights are even in Δ_{12} . By the same simple argument, the weights are also even in Δ_{23} , Δ_{24} , Δ_{56} , and Δ_{89} as well. To show that the weights are even in Δ_{67} (or Δ_{78}), the gauge transform can be applied to spins 6 and 5 (the first transformation sending Δ_{56} and Δ_{67} to their opposites, and the second sending Δ_{56} back to its original value), or, just as well, to spins 7, 8, and 9. In graph-theoretic terms, if one views the spins as vertices and the links—but not the terms of \mathcal{H}_0 —as edges, then the weights are even functions of any Δ_{ij} for which the corresponding edge is connected to any vertex of valence 1 through vertices of valence 2. In a 1D graph, *all* the links satisfy this criterion, and every m -link graph contributes first in order Δ^{2m} to gauge-invariant weights. In higher dimensions, the same is true for any graph consisting solely of *trees* of links.

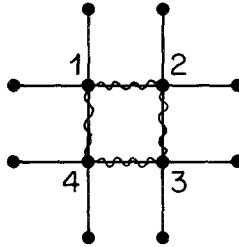
Graphs with *loops* of links require more effort to determine the lowest order to contribution to the gauge-invariant weights. For the graph in Fig. 9b, it is clear that the weights cannot be shown to be even in any particular Δ_{ij} by the strategy that succeeds for tree graphs. The lowest order term in its gauge-invariant weights is $O(\Delta^4)$, since no local gauge symmetry forbids the term $\Delta_{12}\Delta_{23}\Delta_{34}\Delta_{14}$.

However, it is not simply the case that *every* Δ_{ij} which is part of a closed loop can contribute in first order to the weights. A simple counterexample is provided by the 7-link graph in Fig. 9c. Although it

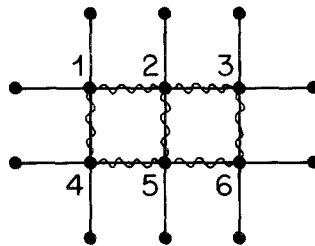
contains 7 links, it could not possibly contain an $O(\Delta^7)$ term in any gauge-invariant weight: those weights are even in Δ , since the signs of all the Δ_{ij} can be reversed by applying the gauge transform to spins 1, 3, and 5. Applying the transform to spin 5 alone reveals that the weights are even in the product $\Delta_{45}\Delta_{56}\Delta_{25}$; the same is true for the product $\Delta_{12}\Delta_{23}\Delta_{25}$. Therefore, the lowest order term in the gauge-invariant weights must be of the form $\Delta_{12}\Delta_{23}\Delta_{14}\Delta_{36}\Delta_{45}\Delta_{56}(\Delta_{25})^2 = O(\Delta^8)$.



(a)



(b)



(c)

Fig. 9. Illustrative graphs for the I-expansion on the square lattice. Labeled spins are referred to in the text.

The graphs on the square lattice contributing first to $O(\Delta^4)$ may now be quickly written down: they include only the six 2-link graphs in Fig. 10a, and the 4-link graph in Fig. 9b. The $O(\Delta^6)$ graphs are constructed by grafting one additional link onto each of the $O(\Delta^4)$ graphs, and there is also one 6-link graph, shown in Fig. 10b. At $O(\Delta^8)$, some of the graphs not obtained by grafting one link onto $O(\Delta^6)$ graphs are shown in Fig. 10c.¹³

¹³ There are two other graphs, not displayed, consisting of two four-link loops (as in Fig. 9b) connected by one and two bonds of \mathcal{H}_0 , respectively.

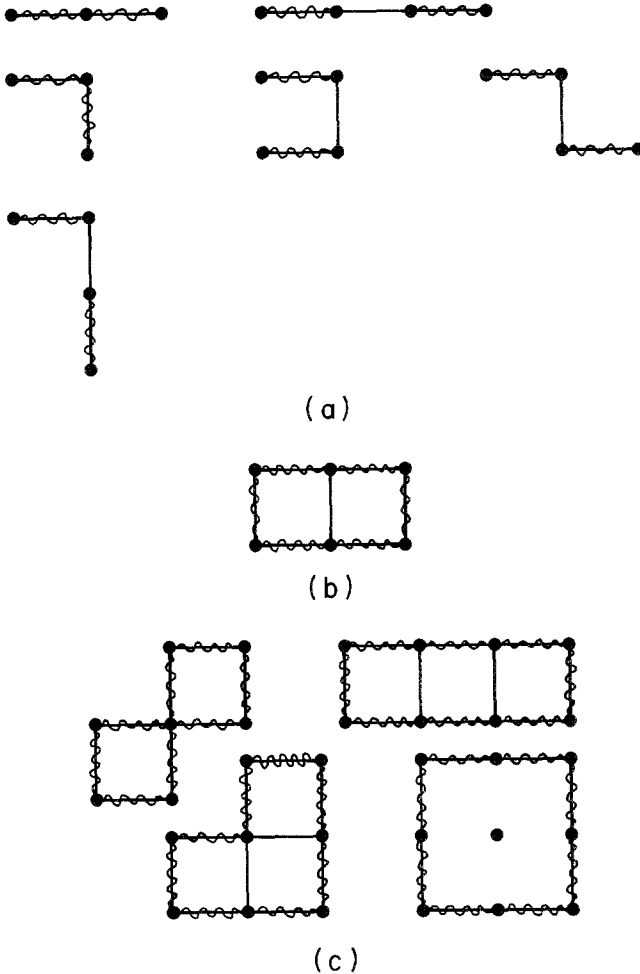


Fig. 10. Graphs for I-expansion on the square lattice; see text for explanation. For clarity, spins coupled to the rest of the graph only via \mathcal{H}_0 (“boundary” spins) are not drawn.

Notice that all of the graphs in Figs. 9b and 10bc which have m links and contribute to the gauge-invariant weights first at $O(\Delta^m)$ contain only vertices of valence 2 and 4; the converse is also true, since this graph-theoretic condition means that the local gauge symmetry does not prohibit the lowest-order term in the weights from containing each Δ_{ij} in the graph exactly once.

The general strategy for identifying graphs which contribute at some specified order should now be evident. It is a combination of exhaustive enumeration, to create graphs with $m + 1$ links contributing at order $\Delta^{2(p+1)}$ from those with m links contributing at order Δ^{2p} , plus unsystematic construction of any other graphs which contribute at order $\Delta^{2(p+1)}$. Although that unsystematic procedure risks missing graphs, there are sufficiently few which need to be found [at least to $O(\Delta^{10})$] that the risk has proven manageable. The alternative, a *complete* exhaustive enumeration of all $2(p + 1)$ -link graphs, is totally impractical; it would yield *many* more graphs, most of which would contribute nothing to the gauge-invariant weights up to the desired order.

The set of *basis states* which must be kept in the weight calculations for I-expansions is also different from the one used in D-expansions, that is, the $S_{\text{tot}}^z = 0$ subspace. The salient feature of I-expansions in this context is that spin-exchange occurs only across the *links* in a graph. Thus, for the graph in Fig. 11, there are only 8, rather than $\binom{6}{3} = 20$ states connected to the ground state by powers of \mathcal{H}_1 : not only is $S_{\text{tot}}^z = 0$ in each such state, but also $S_1^z + S_2^z = S_3^z + S_4^z = S_5^z + S_6^z = 0$. More generally, S^z is conserved within any subcluster of spins connected by links to each other, but only by bonds to other spins in the graph. It proved especially important to take advantage of these additional “conservation laws” in expansions in 1D, where the graphs contained up to 11 links (see Table I). For the 11-link graph in which none of the links shares a spin, the number of elements in the $S_{\text{tot}}^z = 0$ space is $\binom{22}{11} = 705,432$; but the actual number of basis states is only $2^{11} = 2048$.

4.5. Further Applications

There are several directions in which the work reported in this paper, and summarized in Table I, could be extended. Below, some ideas are listed, roughly in order of decreasing degree of development.

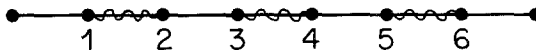


Fig. 11. An illustrative graph for the I-expansion. Labeled spins are referred to in the text.

One could try to calculate more *properties* of interest by means of the basic I- or D-expansions. In particular, from I-expansions Singh has recently obtained estimates of the transverse susceptibility and spin-wave stiffness^(19,20) and moments of the two-magnon Raman lineshape⁽²¹⁾ for the $S=1/2$ square-lattice Heisenberg antiferromagnet. These quantities are directly measurable; the calculations have aided in the interpretation of experimental data related to magnetic properties of La_2CuO_4 . Such calculations are possible because the 2D I-expansions are *convergent* all the way to the isotropic limit $\Delta=1$. It makes little sense to construct D-expansions for quantities of experimental interest in square-lattice Heisenberg antiferromagnets, since the series can only be reliably extrapolated up to the critical point $\lambda_c < 1$.

Using a dimer model as \mathcal{H}_0 , one could put *further-neighbor* (as well as nearest-neighbor) interactions into \mathcal{H}_1 . In one dimension, second-neighbor interactions can be treated using only the graphs which are present in the nearest-neighbor-only case, since second-neighbor spins lie on nearest-neighbor dimers. A few results for the 1D, $S=1/2$ case have been reported.⁽³⁴⁾ Antiferromagnetic second-neighbor interactions tend to frustrate the spin system, which responds by either *modulating* (i.e., tending to order in structures with period greater than 2, perhaps even incommensurately) or spontaneously *dimerizing*. Thus, to study these models properly one must calculate the dimerization D (just as for $S=1$ chains with biquadratic interactions) and the full set of spin-spin correlation functions.

On the square lattice, the influence of second (nearest-diagonal) and third (next-nearest axial) neighbor interactions is of special interest. Two theoretical approaches, namely expansions in $1/S$ (S , as usual, being the spin)^{(35),14} and $1/N$ [N , being the one in $SU(N)$, is ordinarily 2]⁽³⁷⁾ give quite different predictions for $S=1/2$ Heisenberg models. The former favors a nondegenerate, translationally invariant ground state, while the latter indicates a fourfold degenerate, columnar-dimerized ground state. An investigation of these models by D-expansions yields results more consistent with the latter.⁽²²⁾

Other Hamiltonians besides Ising and dimerized models could serve as the starting points for series expansions. The pure staggered field model $\sum_i \pi_{0i} S_i^z$ is a suitable \mathcal{H}_0 . An application which suggests itself is the study of the properties in the “Haldane phase” of $S=1$ chains, which cannot be reached from either Ising or dimerized models without encountering a phase boundary (recall Fig. 2), but should be accessible from the pure staggered field model by taking $\mathcal{H}_1 = -\mathcal{H}_0 + \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$. Some preliminary

¹⁴ Ref. 36 gives a variational calculation which gives similar results.

calculations have been performed,⁽³⁸⁾ but the series do not appear sufficiently well behaved to be competitive with direct finite-size diagonalization.

Another potential \mathcal{H}_0 , which is only suitable for integer-spin systems, is the pure single-spin anisotropy model $\sum_i (S_i^z)^2$. (If the spin were half-integer, then the ground state would be exponentially degenerate, with each S_i^z allowed to take on the values $\pm 1/2$ independently.) There have already been finite-size studies of the phase diagram for $S=1$ chains with single-spin anisotropy and anisotropic couplings⁽³⁹⁾; series calculations might provide a good check. No efforts have yet been made in this direction.

Finally, we note that the series method is not limited to the study of quantum spin systems. In principle, fermions or bosons could be treated, so long as they are restricted to sit on lattice sites and their interactions are short range. We have undertaken a preliminary investigation of the Hubbard model.⁽³⁸⁾ It is not yet clear whether series expansions will yield any useful results for such models, but, given the difficulty of studying highly correlated fermions, more effort along these lines may be worthwhile.

5. CONCLUSIONS

We have described a general scheme for generating various series expansions for quantum spin systems at $T=0$ and for several cases discussed the calculations in great detail. However, there are several matters which have been barely touched on, and which are addressed below: (1) Practical considerations, particularly the amount of computer time used in the calculations and the computer memory requirements, and (2) a comparison of series expansions with other numerical methods for studying similar problems.

Compared with other numerical methods for calculating spectra and ground-state properties, series expansions are *memory* intensive. (More to the point, our programs have large memory requirements: others may be able to do better.) Suppose one intends to calculate weights for a single graph, for which there are L states in the basis out of N altogether, up to m th order in \mathcal{H}_1 . Further suppose that the representation of each state, in terms of dimer or S_i^z eigenvalues, requires n integers, and that the maximum number of elements in a row of \mathcal{H} is M . One needs to store N integers for the first lookup table described in Section 3.2 and nL for the second; L real (floating-point) numbers for \mathcal{H}_0 ; $L(M+1)$ integers for $\mathcal{H}_1^{(\text{pt})}$ and LM reals for $\mathcal{H}_1^{(\text{val})}$. So far, this is no more storage than would be required for a finite-size calculation which failed to take advantage of symmetry considerations to block-diagonalize the Hamiltonian matrix—but

the lack of symmetries in typical cluster Hamiltonians compared with the symmetries of systems subject to periodic boundary conditions accounts for most of the extra storage required by the series method compared with finite-size diagonalization. There are also further requirements. It takes mL reals to hold the perturbation series of eigenvectors, and this is only for one weight calculation: if there are K graphs, then for each property of interest one must hold the weights for each graph as mK reals. If one wants to calculate all the spin-spin correlations, then the number of properties can be on the order of 100.

Since L and N grow exponentially with the order of calculation, storage requirements limit the number of terms which can be obtained even for one-dimensional systems. Using a machine with 1 gigabyte of memory, such as the IBM 3090 on which some of our calculations were run, it seems difficult to calculate weights in D-expansions for the 11-link $S = 1/2$ graph or the 7-link $S = 1$ graph.

Practical limits on CPU time have prevented us from attaining the highest order terms consistent with the memory requirements. The time required for the weight calculations for a single graph scales roughly with L (since that sets the number of lookups performed in calculating $[\mathcal{H}_1]$, and the number of multiplications in each matrix multiplication). The computation of weights in D-expansions for the 5-link $S = 1$ graph takes over 1 hour of IBM 3090 time, even after vectorizing the code. Thus, the 6-link $S = 1$ graph seems unfeasible for the present generation of computers; in any event, it is not clear that one or two more terms in the series would be worth the substantial additional effort. None of the conclusions we have drawn from series expansions would be qualitatively altered if the calculations had been done only to the order possible on a Sun 3/50: typically to only one order in λ (or two in Δ) less than the figures listed in Table I.

Regarding the relative merits of series expansions versus other numerical methods, especially exact diagonalization of small clusters, it is certainly *not* true that the series approach is superior to the others for all applications. Series cannot so easily be used to study finite-size corrections to the energy of a critical spin chain (to estimate its central charge⁽⁴⁰⁾). Series seem generally less well suited than finite-size calculations to determining spectra and dispersion relations, although further developments might change this. It is also clear that if the model of interest is not *close* to a trivial \mathcal{H}_0 —in that more than one continuous, or even one first-order, transition intervenes between \mathcal{H}_0 and $\mathcal{H}_0 + \mathcal{H}_1$ —then an informative series expansion will not be possible.

Nonetheless, it has been our experience that there are circumstances in which series expansions are an excellent tool, which can complement well the capabilities of alternate numerical methods. An example worthy of

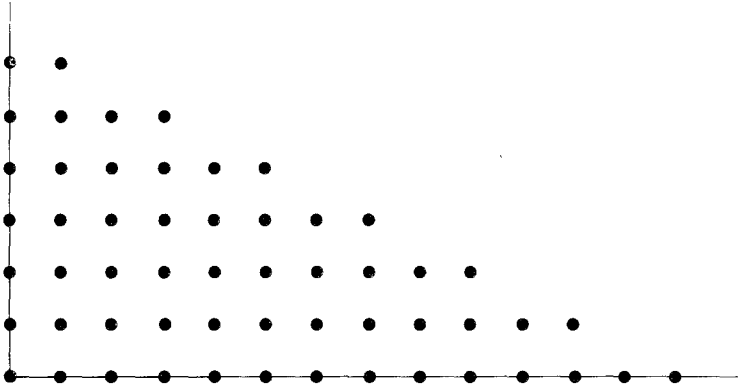


Fig. 12. The set of spins in the first quadrant which have a nonzero correlation with the spin at the origin, at order λ^6 , for the D-expansion about the columnar \mathcal{H}_0 .

special mention here is the study of quantum criticality in 2D, $S = 1/2$ antiferromagnets by means of D-expansions, where it seems unlikely that exact diagonalization will ever be competitive with series. Starting, for example, with the columnar-dimer \mathcal{H}_0 on the square lattice, series were obtained to $O(\lambda^6)$ in the remaining nearest-neighbor couplings. The set of correlations $\langle \mathbf{S}_0 \cdot \mathbf{S}_{\mathbf{R}} \rangle$ (folding all \mathbf{R} into the first quadrant, by symmetry) which have a nonzero term at $O(\lambda^6)$ or lower, and thus contribute to the μ_0 and μ_2 series in Table V, are shown in Fig. 12. In order to account for all of these correlations exactly in a finite-size calculation, one would need to work with a 28×14 spin system, while the present practical limit for exact diagonalization is 32 $S = 1/2$ spins.⁽⁴¹⁾ In essence, the cluster method for series expansions breaks the *big* problem indicated schematically in Fig. 12 into many smaller, more tractable problems; the increase in the number of problems, by a factor $\sim 2^{10}$ (the number of graphs), is more than made up in the reduction in the size of each, by a factor $\sim 2^{300}$ (taking “size” to mean the dimensionality of the relevant vector space).

We hope that by presenting our method for calculating series expansions in more detail than the typical reader might care to see, we have aided those few who might wish to do similar calculations themselves. To them, we add, good luck!

APPENDIX. TABULATED SERIES

Some series are presented here, in the order in which they are listed in Table I. The terms are exact, modulo roundoff conventions for the least significant figure displayed. The various properties (E_g , etc.) have already been defined; see especially Sections 1 and 4.

Table III. Coefficients of Δ^{2n} in the Ground-state Energy and Sublattice Magnetization Series, for the $S = 1/2$ I-Expansion in One Dimension

n	$4E_g$	$2M^+$
0	-1	1
1	-1	-1
2	0.25	-0.25
3	0	-0.0625
4	-0.015625	0.015625
5	-0.0078125	0.046875
6	-0.00195312	0.055664
7	0.00048828	0.053955
8	0.0010376	0.047791
9	0.00085449	0.040176
10	0.00051117	0.032555
11	0.00022316	0.025569

The numerical factors that accompany some of the properties in the table headings, for example, $8E_g$ for the $S = 1/2$ D-expansions, have sundry origins. To reduce the likelihood of typographical errors in the tables, the numbers given are those which come directly out of the weight calculation programs. The numerical factors then account for such things as overall

Table IV. Coefficients of λ^n in the Energy, Moments of the AF Correlation Function, and AF Susceptibility for the $S = 1/2$ D-Expansion in One Dimension

n	$800E_g$	$4\mu_0$	$4\mu_2$	χ
0	-300	6	3	1
1	0	3	13.5	1
2	-37.5	1.5	21.75	0.875
3	-9.375	0.875	27.687	0.8125
4	-2.5391	0.68880	32.605	0.77669
5	-1.4486	0.56472	36.926	0.74436
6	-0.94198	0.46579	40.819	0.71754
7	-0.57614	0.40089	44.387	0.69609
8	-0.39028			
9	-0.28877			
10	-0.21763			
11	-0.16740			
12	-0.13270			
13	-0.10748			
14	-0.088373			
15	-0.073682			

Table V. Coefficients of λ^n in the Energy, Moments of the AF Correlation Function, and AF Susceptibility for the $S = 1/2$ D-Expansions in Two Dimensions

n	Square (columnar)				Square (staggered)				Honeycomb			
	$8E_g$	$4\mu_0$	$4\mu_2$	χ	$8E_g$	$4\mu_0$	$4\mu_2$	χ	$8E_g$	$4\mu_0$	$4\mu_2$	χ
0	-3	6	3	1	-3	6	3	1	-3	6	3	1
1	0	9	22.5	3	0	9	28.5	3	0	6	21	2
2	-1.875	16.5	93.75	7.375	-1.125	18	123	8.625	-0.75	7.5	62.25	3.75
3	-0.84375	29.625	302.31	17.063	-0.84375	38.313	441.16	23.937	-0.1875	11	149.87	7.125
4	-0.33789	51.751	854.81	37.402	-0.75586	85.783	1451.0	65.171	-0.18359	16.747	334.33	13.171
5	0.24333	93.256	2225.5	79.690	-0.76383	198.34	4531.7	175.24	-0.12923	26.461	709.94	24.189
6	0.24172	168.77	5477.8	165.96	—	—	—	—	-0.11058	42.785	1460.1	44.109

Table VIII. Coefficients of λ^n for the Energy, Dimerization, Moments of the AF Structure Factor, and AF Susceptibility for D-Expansions of Isotropic $S = 1$ Chains with Biquadratic Interactions

n	$\beta = 1$					$\beta = 50$				
	$2E_g$	D	μ_0	μ_2	χ	$2E_g$	D	μ_0	μ_2	1000χ
0	-6	2	4	2	0.33333	-202	2	4	2	8.8300
1	-1.3333333	-0.5	2.	9	0.16667	-66.666667	-0.229581	0.91832	4.1324	2.0272
2	-0.4212963	-0.271123	1.13310	14.567	0.17411	-7.5234000	-0.238022	0.45764	4.3919	1.8480
3	-0.1177019	-0.153488	0.78414	18.776	0.17248	-2.9241467	-0.150893	0.23899	4.2679	1.5253
4	-0.0445983	-0.100913	0.61803	22.318	0.16937	-1.1063015	-0.085006	0.15277	4.0824	1.2672
5	-0.0226570	-0.069848	0.51510	25.436	0.16709	-0.4904475	-0.053929	0.11592	3.9145	1.0888
6	-0.0135836	-0.053203				-0.2828449	-0.040543			
7	-0.0091385	-0.043227				-0.1910365	-0.032816			
8	-0.0064956	-0.035896				-0.1351269	-0.026890			
9	-0.0047711	-0.030270				-0.0976497	-0.022236			
10	-0.0036219	-0.025985				-0.0727464	-0.018740			
11	-0.0028357					-0.0560639				

factors in the lattice constants: for the 1D D-expansions, each graph has a lattice constant of $1/2$, but instead $L(G)=1$ was used in the calculations. It is possible that the numerical factors could be in error. Fortunately, those factors are often either irrelevant in the analysis of critical properties or can be checked against known results. The zeroth-order terms are calculated by hand and carry the same warning and reassurance.

Most of the I-expansions for $S=1/2$ systems appear elsewhere in the literature. For the chain see Ref. 18, and for the square lattice see refs. 19 and 20. The only series not given in those papers are for the ground-state energy and staggered magnetization in one dimension; these are presented in Table III. Note that these series have been known exactly for some time,⁽⁴²⁾ and that the results from the numerical calculations agree with those values.

The D-expansions for the $S=1/2$ chain, which have been alluded to in ref. 16, are given in Table IV. The analogous expansions in two dimensions, for the three cases described by Fig. 1, are given in Table V. Some of these have already appeared in ref. 16, but all are displayed here for ease of comparison.

None of the expansions for $S=1$ chains have been published previously, though a report of their analysis has been given in ref. 17. Table VI presents I-expansions for selected values of λ at $\beta=0$. Table VII gives the D-expansions for $\beta=0$ with three values of Δ , corresponding to easy-axis, isotropic, and easy-plane couplings. Finally, Table VIII gives the D-expansions at $\Delta=1$ for $\beta=1$ and $\beta=50$. The expansions have been obtained for many more choices of β and λ (or β and Δ) than are presented in the tables: only a representative sample has been displayed, and the rest are available upon request.

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