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Ground-State Energy of a Quantum Chain with Competing Interactions

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We show rigorously that the ground state of a quantum chain with competing ferromagnetic nearest and antiferromagnetic next nearest interactions undergoes a transition from ferromagnetic to helical type, in the isotropic case, for a certain value of the relevant ratio of coupling constants. Boundaries of the phase diagram are also determined in the anisotropic case. The stability of a special quantum state (corresponding to a classical modulated phase of $\varphi = \pi/3$) is analyzed by an extension of Holstein–Primakoff arguments, along a line of constant ratio of couplings, showing in particular a sequence of (instability) gaps. Finally, a natural adaptation of a variational wave function due to Huse and Elser is used to study several portions of the phase diagram, with very good agreement with previous theoretical results.

KEY WORDS: Quantum chain; competing interactions; ferromagnetic and helical ground state; spin waves; variational wave functions.

1. INTRODUCTION AND SUMMARY

Frustrated Heisenberg models have been a subject of great recent interest, as demonstrated by two reviews.[1,2] This is mostly due to the search for a two-dimensional model with a spin-liquid or resonating-valence-bond ground state, related to the possible magnetic origin of high-T_c superconductivity.[1] There is, however, a further general interest in nonclassical states, such as twisted or chiral states, again in two dimensions, but most work on the subject has been numerical,[2] except in one dimension, where some analytical results have been found. Among the latter is the

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antiferromagnetic Heisenberg model with competing next-nearest-neighbor interactions:

$$\mathscr{H} = \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + p \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+2} \tag{1}$$

where $p > 0$.

For $p = 1/2$ and the spin quantum number $S = 1/2$, Majumdar and Ghosh found the exact ground state in the form of a nearest-neighbor dimer state[3] and further anisotropic generalizations have been studied.[4,5] Affleck *et al.*[6] have found the first rigorous example of an $S = 1$ quantum chain with a resonating-valence-bond ground state, and in ref. 7 a (helical) ground state of a Heisenberg chain with Dzyaloshinski–Moriya (DM) interactions has been constructed by the Bethe Ansatz. This list is not exhaustive, refs. 8 and 9 may be referred to for further references.

In this paper we study a model related to (1):

$$\mathscr{H}_N = -\sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + p \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+2} \tag{2}$$

where $\mathbf{S}_i$ are spin-one-half operators,

$$\mathbf{S}_{N+i} = \mathbf{S}_i \tag{3}$$

and

$$p > 0 \tag{4}$$

Although (1) and (2) differ only by a change of sign in the nearest neighbor interaction, the ground-state properties of the two models are entirely different. Rather than of dimer type as in (1), the ground state of (2) is of helical type for $p > 1/4$, and ferromagnetic for $p \leqslant 1/4$, as will be rigorously shown in Section 2. The latter part had already been shown by Bader and Schilling[10] by a beautiful and very simple method.

Hence, in contrast to the ground state of the DM model of ref. 7, which is helical for all parameter values, (2) exhibits a ($T = 0$) "phase transition," in agreement with the classical model (ref. 11, or ref. 9, Chapter 3). This behavior is also similar to the ground state of the one-dimensional ANNNI chain, but there the transition is between the ferromagnetic and the (2, 2) state[12] and occurs at $p = 1/2$, not $p = 1/4$. One is therefore naturally led to a model which interpolates between the two:

$$\begin{aligned}\mathscr{H}_N(p, \Delta) = &-\sum_{i=1}^{N} \{\Delta(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + S_i^z S_{i+1}^z\} \\ &+ p \sum_{i=1}^{N} \{\Delta(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y) + S_i^z S_{i+2}^z\}\end{aligned} \tag{5}$$

with

$$0 \leqslant \Delta \leqslant 1 \tag{6}$$

and (4) again assumed to hold. $\mathscr{H}_N(p, 0)$ reduces to the one-dimensional ANNNI chain, and $\mathscr{H}_N(p, 1)$ is the isotropic model (2). This model may thus be viewed as a quantum analog of the ANNNI model (for another one, see ref. 9, Chapter 5).

Our main motivation in this paper is to investigate how quantum fluctuations alter the Ising or classical ground-state structures, for the simple model (5). Even in the Cayley tree, ANNNI models display an enormously rich phase diagram, with a multitude of modulated phases and multicritical points.[13] What happens to such modulated phases in quantum systems? This question does not seem to have been investigated in detail (see, however, ref. 14). In Section 3, we discuss the stability of a particular modulated phase along a special line of the phase diagram. The elementary excitations are studied in the usual approximation of keeping only quadratic terms in boson operators and starting from a (classical) ground state. Justification of this (Holtein–Primakoff) approximation is difficult even for large S in the pure ferromagnetic case,[15] but it is widely believed (and may be checked in some cases.[15]) to yield the correct results even for $S = 1/2$. Due to the competing interactions, however, a more sophisticated form of the Bogoliubov transformation is required, and is developed in Section 3. The final result shows forbidden zones (gaps) in the excitation spectrum for $\Delta \neq 1$. This is interpreted there in the light of the effect of quantum fluctuations on the modulated phases, and some conjectures are formulated.

Due to the next-nearest-neighbor interaction in (5), Bethe Ansatz methods are not applicable. In addition to the previously mentioned exact result for $\Delta = 1$, some other analytical results are given in Section 2. They lead to the following conjecture for $\Delta = 1$. Let us define the operator

$$S^z = \sum_{i=1}^{N} S_i^z \tag{7}$$

Clearly, $[S^z, \mathscr{H}_N(p, \Delta)] = 0$. Let $M \in [0, N/2]$ denote the eigenvalues of S^z. The conjecture is: for $p > p_0 = 1/4$ and $\Delta = 1$, the ground state lies—for N even—in the sector $M = 0$. For $p \leqslant p_0$ the ground state is ferromagnetic. Since further analytical results seem to be out of reach, we attempted to find a good variational wave function. This is accomplished in Section 4, where we propose a modification of the Ansatz used by Huse and Elser,[16] in order to accommodate for the angles corresponding to the helicoidal state or modulated phases. The boundary between the ferromagnetic and

modulated-phase region, as well as the boundary of the modulated phase corresponding to $\theta = \pi/3$, are found. The data agree very well with the existing exact results. The conclusion of Section 4 is that (properly modified) Huse–Elser wave functions are excellent even for models with competing interactions. Section 5 is a conclusion, where we also state some of the open problems.

2. RIGOROUS RESULTS

For $\mathscr{H}_N(p, \Delta)$ a variational upper bound for the ground-state energy E_N exists:

$$E_N \leqslant \min\{-\tfrac{1}{4}Np, \tfrac{1}{4}N(p-1)\} \tag{8}$$

The bound $E_N \leqslant N(p-1)/4$ is obtained by calculating the expectation value of $\mathscr{H}_N(p, \Delta)$ of any of the two degenerate ferromagnetic ground states $\Omega_{fN}^{(+)} = \otimes_{i=1}^{N} |+\rangle_i$ or $\Omega_{fN}^{(-)} = \otimes_{i=1}^{N} |-\rangle_i$, where $S_i^z |\pm\rangle_i = \pm \tfrac{1}{2} |\pm\rangle_i$, and $E_N \leqslant -Np/4$ results from the variational wave function $|2\rangle = |++--++--\cdots\rangle_N$ (or the translate of $|2\rangle$ by one lattice space), in an obvious notation. The terms in $\mathscr{H}_N(p, \Delta)$ involving the operators S_i^x and S_i^y yield zero in the expectation values on any of the above (Ising) wave functions. For $p \geqslant 1/2$, $-N/4 \leqslant N(p-1)/4$, which means that the wave function $|2\rangle$ has lower (Ising) energy.

The method of Bader and Schilling[10] is very simple and elegant. It was originally formulated in the context of the isotropic model (2), but we shall need it for the slightly more general Hamiltonian (5), so a brief review is in order. We write

$$\mathscr{H}_N(p, \Delta) = \sum_C \mathscr{H}^C(p, \Delta) \tag{9}$$

where $\sum_C$ denotes a sum over "cells" of the "cell Hamiltonians" $H^C(p, \Delta)$. For cells with three sites, for instance (the same used in ref. 10), and $C = C_0 = \{1, 2, 3\}$,

$$\begin{aligned}\mathscr{H}^C = &-\tfrac{1}{2}\{\Delta(S_1^x S_2^x + S_1^y S_2^y) + S_1^z S_2^z + \Delta(S_2^x S_3^x + S_2^y S_3^y) + S_2^z S_3^z\} \\ &+ p\{\Delta(S_1^x S_3^x + S_1^y S_3^y) + S_1^z S_3^z\}\end{aligned} \tag{10}$$

The sum (9) is over all (overlapping) cells with three sites, $C = \{1, 2, 3\}$, $\{2, 3, 4\}$, $\{3, 4, 5\}$, etc. Periodic boundary conditions are assumed for $\mathscr{H}_N(p, \Delta)$ (*not* for the individual cell Hamiltonians, which have free boundary conditions) and correction for multiple counting due to cell overlap [this accounts for the factor 1/2 in the p-independent terms of (10);

for next-nearest-neighbor interactions and cells of three sites, there is no multiple counting] guarantees together that the two terms, on the r.h.s. and l.h.s. of (10), are *equal*. By (10) one has the *lower* bound:

$$E_N \geqslant N E_0^{(C)} \tag{11}$$

where

$$E_0^{(C)} = \text{smallest eigenvalue of } \mathscr{H}^C(p, \Delta) \tag{12}$$

$E_0^{(C)}$ is, of course, independent of which cell C is considered. If

$$E_0^{(C)} \geqslant \frac{p-1}{4} \tag{13}$$

it follows from (11) that there exists a ferromagnetic ground state of $\mathscr{H}_N(p, \Delta)$, because $(p-1)/4$ is the ferromagnetic ground-state energy per spin, and $\Omega_{JN}^{(\pm)}$ is an eigenstate of $\mathscr{H}_N(p, \Delta)$.

We now compute $E_0^{(C)}$, given by (12). In contrast to (2), for which the total angular momentum S^2 commutes with $\mathscr{H}_N$, only S^z, given by (7), commutes with $\mathscr{H}_N(p, \Delta)$. By the symmetry of rotation by π about the x or y axis, we need only consider the subspace with $M \geqslant 0$. For the present case, $M = 3/2$ and $M = 1/2$. The $M = 3/2$ subspace is spanned by $|+++\rangle$, whose energy equals the ferromagnetic ground-state energy per spin $(p-1)/4$, and may thus be discarded. The $M = 1/2$ subspace is spanned by the vectors $|++-\rangle$, $\phi\,|+-+\rangle$, and $|-++\rangle$. The Hamiltonian matrix in this subspace is

$$\frac{1}{4}\begin{pmatrix} -p & -\Delta & 2p\Delta \\ -\Delta & 1+p & -\Delta \\ 2p\Delta & -\Delta & -p \end{pmatrix} \tag{14}$$

One eigenvalue is

$$E_0 = \tfrac{1}{4}(-p - 2p\Delta) \tag{15}$$

and the others are

$$E_\pm = \tfrac{1}{8}\{1 + 2p\Delta \pm [(1 + 2p - 2p\Delta)^2 + 8\Delta^2]^{1/2}\} \tag{16}$$

By (13), the ferromagnetic phase occurs in the region defined by the two inequalities

$$\frac{1}{4}(p-1) \leqslant E_0 \Rightarrow p \leqslant \frac{1}{2(1+\Delta)} \tag{17}$$

$$\frac{1}{4}(p-1) \leqslant E_- \Rightarrow p \leqslant \frac{1+\Delta}{2} \tag{18}$$

Somewhat surprisingly, this (presumably) rough bound yields the correct result $p_0 = 1/2$ for $\Delta = 0$ (Ising case).[12] It also yields $p_0 = 1/4$ for $\Delta = 1$ (isotropic case), which, of course, agrees with ref. 10. Is the real transition point for $\Delta = 1$ closer to the Ising value $p_0 = 1/2$ or to the classical value[11] $p_0 = 1/4$? One might expect the anisotropic quantum (Ising) limit to be closer, since we are treating the case of small spin, $S = 1/2$. For that purpose, a cell with *four* sites seems much more natural, because it accommodates a structure "of type" $|2\rangle$, i.e., $|2\rangle$ with quantum fluctuations. However, the bound obtained with four-site cells is worse than the one given by three-site cells; for $\Delta = 1$, for instance, we get $p_0 = 2/9 = 0.222\ldots$. We are going to show below that, for $\Delta = 1$, the ferromagnetic phase extends up to $p = 1/4$. Thus, the three-site cells yield the exact result! This result is, in our opinion, amazing. One would expect an improvement as the number of sites in a cell increases, because the lower bound becomes exact in the limit of cell size equal to N.

Proposition 2.1. There exists a saturated ferromagnetic ground state for $\mathscr{H}_N(p, 1)$ if and only if $p \leqslant p_0 = 1/4$.

Proof. We already know that the ground state is ferromagnetic for $p \leqslant 1/4$ by the previous (Bader–Schilling) result. Let

$$\mathscr{U}_N = \exp(A_N) \tag{19}$$

where

$$A_N = i\theta \sum_{l=1}^{N} l S_l^x \tag{20}$$

Then

$$\begin{aligned} \mathscr{U}_N^+ \mathscr{H}_N \mathscr{U}_N = &- \sum_{l=1}^{N} \{\cos\theta\, \mathbf{S}_l \cdot \mathbf{S}_{l+1} + (1+\cos\theta)\, S_l^x S_{l+1}^x + \sin\theta (\mathbf{S}_l \times \mathbf{S}_{l+1})^x\} \\ &+ p \sum_{l=1}^{N} \{\cos 2\theta\, \mathbf{S}_l \cdot \mathbf{S}_{l+2} + (1-\cos 2\theta)\, S_l^x S_{l+2}^x \\ &+ \sin 2\theta (\mathbf{S}_l \times \mathbf{S}_{l+2})^x + O(1) \end{aligned} \tag{21}$$

where $\times$ denotes vector product, and $O(1)$ denotes the effect of $\mathscr{U}_N^+(\cdot)\,\mathscr{U}_N$ on boundary terms, which therefore tend to zero upon division by N. By (21)

$$\langle \Omega_{fN}^{(\pm)}, \mathscr{U}_N^+ \mathscr{H}_N \mathscr{U}_N \Omega_{fN}^{(\pm)} \rangle = -\frac{N}{4}\cos\theta + \frac{pN}{4}\cos 2\theta + O(1) \tag{22}$$

where $\Omega_{fN}^{(\pm)}$ is any of the two degenerate ferromagnetic ground states as previously defined. Hence, the energy e_∞ of the normalized state $\mathcal{U}_N\Omega_{fN}^{(\pm)}$ in the thermodynamic limit is

$$e_\infty = \tfrac{1}{4}(-\cos\theta + p\cos 2\theta) \tag{23}$$

If $p > 1/4$, e_∞ assumes its minimum value $e_\infty^{\min}$ for $\theta = \arccos(1/4p)$ and

$$e_\infty^{\min} = \frac{1}{4}\left(-p - \frac{1}{8p}\right) < \frac{1}{4}(p-1) \tag{24}$$

This proves the proposition by the variational principle. ∎

Remark. We have not considered the possible nonunicity of ground state of the infinite system, hence the cautious statement of Proposition 2.1. A nonsaturated ferromagnetic ground state has not been ruled out for $p > 1/4$, but even in this case a "ground-state phase transition" occurs, because the ground-state energy per unit volume is, for $p > 1/4$, lower than that of the (saturated) ferromagnetic phase, which occurs for $p \leqslant 1/4$.

The physical meaning of $\mathcal{U}_N$ is clear: it rotates each spin around the x axis by the same angle θ relative to the previous one, and hence generates a "helical" configuration. Thus, one may conjecture that the ground state is of helical type for $p > 1/4$.

It is interesting to know whether this ground state belongs, for N even, to the $M = 0$ sector. Unfortunately, the Lieb–Mattis theorem[17] does not apply, so that a rigorous proof is missing. We therefore solved the $N = 4$ case with periodic boundary conditions exactly. This solution will also be important as a test of the Huse–Elser variational wave function in Section 4. The total spin S has in this case the possible values $S = 0, 1, 2$. The degeneracy d_s of the state $|S, S\rangle$ is given by[18]

$$d_s = (2S+1)\frac{4!}{(3+S)!\,(2-S)!} \tag{25}$$

For $S = 0$ this yields $d_0 = 2$. The two orthogonal, normalized states are

$$|00\rangle^1 = \frac{1}{2}\{|-+-+\rangle + |+-+-\rangle - |-++-\rangle - |+--+\rangle\} \tag{26}$$

$$|00\rangle^2 = \frac{1}{\sqrt{12}}\{|-+-+\rangle + |+-+-\rangle + |-++-\rangle + |+--+\rangle - 2|++--\rangle - 2|--++\rangle\} \tag{27}$$

which may readily be found by angular momentum techniques. The Hamiltonian matrix in this subspace is

$$\frac{1}{2}\begin{pmatrix} 3 & \sqrt{3}\,(2p+1) \\ \sqrt{3}\,(2p+1) & (-4p+1) \end{pmatrix} \tag{28}$$

whose lowest eigenvalue is $E_0^{(4)} = -3p$. For $p > 1/4$, $E_0^{(4)}$ is smaller than the ferromagnetic ground-state energy $E_F^{(4)} = (p-1)$. Thus, for $p > 1/4$, the ground state lies in the $M = 0$ subspace.

Section 4 provides further evidence that for $p > p_0$ and $\Delta = 1$ the ground state is in the $M = 0$ sector for N even. Assuming that this result is true we have (in the case without anisotropy):

Proposition 2.2. If $(\Omega_N, S^z\Omega_N) = 0$ for Ω_N a ground state, if $p > 1/4$, $\mathscr{H}_N(p, 1)$ is gapless in this region.

Proof. The proof follows Affleck and Lieb[19] and, indeed, was sketched by them also for situations such as occur in the present case. Let

$$A_N = i \sum_{l=1}^{N} l S_l^z \tag{29}$$

Then

$$[\mathscr{H}_N(p, 1), A_N] = \sum_l \{ -(\mathbf{S}_l \times \mathbf{S}_{l+1})^z + 2p(S_l \times S_{l+2})^z \} \tag{30}$$

and defining

$$\mathscr{U}_N = \exp(A_N) \tag{31}$$

we have

$$\mathscr{U}_N^+ \mathscr{H}_N(p, 1)\, \mathscr{U}_N - \mathscr{H}_N(p, \Delta) = B_N + C_N \tag{32}$$

where

$$B_N = (1 - \cos\theta) \sum_{l=1}^{N} (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y) + p(\cos 2\theta - 1) \sum_{l=1}^{N} (S_l^x S_{l+2}^x + S_l^y S_{l+2}^y) \tag{33}$$

and

$$C_N = -\sin\theta \sum_{l=1}^{N} (\mathbf{S}_l \times \mathbf{S}_{l+1})^z + p \sin 2\theta \sum_{l=1}^{N} (\mathbf{S}_l \times \mathbf{S}_{l+2})^z \tag{34}$$

Taking

$$\theta = \frac{2\pi}{N} \tag{35}$$

we have that the expectation value of B_N in a normalized state is $O(N^{-1})$. Writing $\sin 2\theta = 2 \sin \theta \, (\cos \theta - 1 + 1)$ in the second term of C_N, we see by (30) that the expectation value of C_N on a normalized state is the same as that of the operator

$$\sin \theta \, [\mathscr{H}_N(p, 1), A_N] \tag{36}$$

plus a term $O(N^{-2})$. The operator (36) has zero expectation value on any eigenstate of $\mathscr{H}_N(p, 1)$ (such as the ground state), and hence the proof proceeds as in ref. 19. ∎

Unfortunately, for the infinite system the best results[19] cannot distinguish the situation with unique ground state and no gap from the one with a degenerate ground state.

In the case of nonzero Ising anisotropy $0 < \Delta < 1$, the classical ground-state energy is given by the formula (61), below. It is conceivable [see (61)] that the corresponding phase diagram is very rich, with many commensurate phases and perhaps even a devil's staircase. In particular, for some (p, Δ) a possible helical phase with period of seven sites, whose Ising version would be (3up, 4down), might occur. Therefore, a nonzero ground-state magnetization cannot be excluded.

3. SPIN-WAVE THEORY

In this section we formulate a spin-wave theory appropriate for modulated structures.[20] To this end, we consider first the classical $(S \to \infty)$ limit of Hamiltonian (5). In this limit the operator $\mathbf{S}_l/S$ becomes a unit vector $\mathbf{s}_l$ and $\mathscr{H}/S^2$ becomes a classical Hamiltonian $\mathscr{H}_{cl}(\{\mathbf{s}_l\})$. As one varies the parameters p and Δ, the classical ground state is expected to display a multitude of modulated structures besides the ferromagnetic one. For a fixed value of the parameters we denote by $\{\mathbf{m}_l\}$ the set of values of $\{\mathbf{s}_l\}$ that gives a minimum of $\mathscr{H}_{cl}$.

Next we define a transformation on the Hamiltonian (5) such that the classical ground state will be the ferromagnetic state. Let us denote by $\mathbf{r}$ the unit vector parallel to the magnetization of the ferromagnetic state. If we

denote by $\mathbf{n}_l$ the unit vector parallel to $\mathbf{m}_l \times \mathbf{r}$ and by θ_l the angle between $\mathbf{r}$ and $\mathbf{m}_l$, the transformation is given by following unitary transformation:

$$\mathcal{U} = \exp\left\{ i \sum_l \theta_l \mathbf{n}_l \cdot \mathbf{S}_l \right\} \tag{37}$$

which rotates any vector operator associated with site l by an angle θ_l around $\mathbf{n}_l$, bringing it to the reference direction $\mathbf{r}$. The ground state of the classical limit of the transformed Hamiltonian $\mathcal{U}^{-1}\mathcal{H}\mathcal{U}$ will then be the ferromagnetic state.

The perturbation away from the classical ground state, which is now a ferromagnetic state, is performed on the transformed Hamiltonian by using boson operators through the usual Holstein–Primakoff transformation

$$S_l^z = S - a_l^+ a_l \tag{38}$$

$$S_l^+ = S_l^x + iS_l^y = (2S)^{1/2}\left(1 - \frac{a_l^+ a_l}{2S}\right)^{1/2} a_l \tag{39}$$

$$S_l^- = S_l^x - iS_l^y = (2S)^{1/2} a_l^+ \left(1 - \frac{a_l^+ a_l}{2S}\right)^{1/2} \tag{40}$$

For the range of values of p and Δ given by (4) and (6), the classical modulated structures are of helical type, so that $\mathbf{m}_l$ will lie in a certain plane independently of l. Choosing this plane to be the yz plane and the reference direction along the z direction, that is, $\mathbf{r} = (0, 0, 1)$, we have

$$\mathbf{m}_l = (0, \sin\theta_l, \cos\theta_l) \tag{41}$$

and $\mathbf{n}_l = (1, 0, 0)$. The unitary transformation is then given by

$$\mathcal{U} = \exp\left\{ i \sum_l \theta_l S_l^x \right\} \tag{42}$$

and rotates the spin operator $\mathbf{S}_l$ by an angle θ_l around the x axis, that is,

$$\mathcal{U}^{-1} S_l^x \mathcal{U} = S_l^x \tag{43}$$

$$\mathcal{U}^{-1} S_l^y \mathcal{U} = S_l^y \cos\theta_l - S_l^z \sin\theta_l \tag{44}$$

$$\mathcal{U}^{-1} S_l^z \mathcal{U} = S_l^y \sin\theta_l + S_l^z \cos\theta_l \tag{45}$$

The transformed Hamiltonian $\mathscr{H}' = \mathscr{U}^{-1}\mathscr{H}\mathscr{U}$ will be

$$\mathscr{H}' = -\sum_l \{\Delta S_l^x S_{l+1}^x + f_l^{yy} S_l^y S_{l+1}^y + f_l^{zz} S_l^z S_{l+1}^z + f_l^{yz} S_l^y S_{l+1}^z + f_l^{zy} S_l^z S_l^y\}$$
$$+ p \sum_l \{\Delta S_l^x S_{l+1}^x + g_l^{yy} S_l^y S_{l+2}^y + g_l^{zz} S_l^z S_{l+2}^z$$
$$+ g_l^{yz} S_l^y S_{l+2}^z + g_l^{zy} S_l^z S_{l+2}^y\} \tag{46}$$

where the coefficients $f_l^{\alpha\beta}$ and $g_l^{\alpha\beta}$ are given by

$$f_l^{yy} = \Delta \cos\theta_l \cos\theta_{l+1} + \sin\theta_l \sin\theta_{l+1} \tag{47}$$
$$f_l^{zz} = \Delta \sin\theta_l \sin\theta_{l+1} + \cos\theta_l \cos\theta_{l+1} \tag{48}$$
$$f_l^{yz} = -\Delta \cos\theta_l \sin\theta_{l+1} + \sin\theta_l \cos\theta_{l+1} \tag{49}$$
$$f_l^{zy} = -\Delta \sin\theta_l \cos\theta_{l+1} + \cos\theta_l \sin\theta_{l+1} \tag{50}$$

and

$$g_l^{yy} = \Delta \cos\theta_l \cos\theta_{l+2} + \sin\theta_l \sin\theta_{l+2} \tag{51}$$
$$g_l^{zz} = \Delta \sin\theta_l \sin\theta_{l+2} + \cos\theta_l \cos\theta_{l+2} \tag{52}$$
$$g_l^{yz} = -\Delta \cos\theta_l \sin\theta_{l+2} + \sin\theta_l \cos\theta_{l+2} \tag{53}$$
$$g_l^{zy} = -\Delta \sin\theta_l \cos\theta_{l+2} + \cos\theta_l \sin\theta_{l+2} \tag{54}$$

Using the Holstein–Primakoff transformation and expanding to order S^{-1}, we obtain the following expression for $\mathscr{H}'$ up to quadratic terms in boson operators a_l and a_l^+:

$$\mathscr{H}' = \sum_l \{A_l(a_l a_{l+1}^+ + a_l^+ a_{l+1}) + B_l(a_l a_{l+1} + a_l^+ a_{l+1}^+)$$
$$+ C_l(a_l a_{l+2}^+ + a_l^+ a_{l+2}) + D_l(a_l a_{l+2} + a_l^+ a_{l+2}^+)$$
$$+ F_l a_l^+ a_l\} + E \tag{55}$$

where the coefficients A_l, B_l, C_l, D_l and F_l are given by

$$A_l = -\frac{S}{2}(\Delta + f_l^{yy}) \tag{56}$$

$$B_l = -\frac{S}{2}(\Delta - f_l^{yy}) \tag{57}$$

$$C_l = p\frac{S}{2}(\Delta + g_l^{yy}) \tag{58}$$

$$D_l = p\frac{S}{2}(\Delta - g_l^{yy}) \tag{59}$$

and

$$F_l = S(f_l^{zz} + f_{l-1}^{zz} - pg_l^{zz} - pg_{l-2}^{zz}) \tag{60}$$

and $E = S^2 \mathcal{H}_{cl}(\{\mathbf{m}_l\})$ is the classical ground-state energy, given by

$$E = S^2 \sum_{l=1}^{N} \{ -\Delta \sin\theta_l \sin\theta_{l+1} - \cos\theta_l \cos\theta_{l+1} + p\Delta \sin\theta_l \sin\theta_{l+2} + p \cos\theta_l \cos\theta_{l+2} \} \tag{61}$$

Defining the Fourier-transformed operators

$$a_k = \frac{1}{\sqrt{N}} \sum_l e^{ikl} a_l \tag{62}$$

and

$$a_k^+ = \frac{1}{\sqrt{N}} \sum_l e^{-ikl} a_l^+ \tag{63}$$

we find that the Hamiltonian in momentum space is

$$\mathcal{H}' = \sum_{kk'} \{ A_{kk'} a_k^+ a_{k'} + \tfrac{1}{2} B_{kk'} a_k a_{k'} + \tfrac{1}{2} B_{kk'}^* a_k^+ a_{k'}^+ \} + E \tag{64}$$

where $A_{kk'}$ and $B_{kk'}$ are given by

$$A_{kk'} = \frac{1}{N} \sum_l \{ (e^{ik} + e^{-ik'}) A_l + (e^{2ik} + e^{-2ik'}) C_l + F_l \} e^{i(k-k')l} \tag{65}$$

and

$$B_{kk'} = \frac{1}{N} \sum_l \{ (e^{-ik} + e^{-ik'}) B_l + (e^{-2ik} + e^{-2ik'}) D_l \} e^{-i(k+k')l} \tag{66}$$

Diagonalization of the Hamiltonian (64) yields the spin-wave dispersion relation. This is obtained in two cases: (a) $\Delta = 1$ (isotropic case), and (b) $p = 1/2$.

3.1. The Case $\Delta = 1$

In this case the classical helical structure has a constant pitch, that is, the angle between successive magnetizations is a constant. Writing $\theta_l = l\theta$, we find that the minimum of $\mathcal{H}_{cl}(\{\mathbf{m}_l\})$ gives

$$\cos\theta = \frac{1}{4p} \tag{67}$$

if $p > 1/4$ and $\theta = 0$ if $p \leqslant 1/4$. The coefficients in expressions (46) and (55) are then all independent of l and we get $f_l^{yy} = f_l^{zz} = \cos\theta$ and $f_l^{zy} = -f_l^{yz} = \sin\theta$ and

$$A_l = -\frac{S}{2}(1 + \cos\theta) \tag{68}$$

$$B_l = -\frac{S}{2}(1 - \cos\theta) \tag{69}$$

$$C_l = p\frac{S}{2}(1 + \cos 2\theta) \tag{70}$$

$$D_l = p\frac{S}{2}(1 - \cos 2\theta) \tag{71}$$

$$F_l = 2S(\cos\theta - p\cos 2\theta) \tag{72}$$

The classical ground-state energy E is given by

$$E = NS^2\left(-p - \frac{1}{8p}\right) \tag{73}$$

if $p > 1/4$ and

$$E = NS^2(-1 + p) \tag{74}$$

if $p \leqslant 1/4$.

The coefficients $A_{kk'}$ and $B_{kk'}$ reduce to $A_{kk'} = A_k\delta_{kk'}$ and $B_{kk'} = B_k\delta_{k,-k'}$, where

$$A_k = S\{-(1 + \cos\theta)\cos k + p(1 + \cos 2\theta)\cos 2k + 2\cos\theta - 2p\cos 2\theta\} \tag{75}$$

and

$$B_k = S\{-(1 - \cos\theta)\cos k + p(1 - \cos 2\theta)\cos 2k\} \tag{76}$$

so that the Hamiltonian in momentum space will be

$$\mathcal{H}' = \sum_k \{A_k a_k^+ a_k + \tfrac{1}{2}B_k(a_k a_{-k} + a_k^+ a_{-k}^+)\} + E \tag{77}$$

Using a Bogoliubov transformation

$$\alpha_k = a_k \cosh\phi_k + a_{-k}^+ \sinh\phi_k \tag{78}$$

and choosing ϕ_k so that the coefficients of the off-diagonal terms $\alpha_k^+ \alpha_{-k}^+$ and $\alpha_k \alpha_{-k}$ vanish, we get the following Hamiltonian:

$$\mathscr{H}' = \sum_k \{\varepsilon_k \alpha_k^+ \alpha_k + \tfrac{1}{2}(\varepsilon_k - A_k)\} + E \tag{79}$$

where the spin-wave dispersion relation is given by

$$\varepsilon_k = (A_k^2 - B_k^2)^{1/2} \tag{80}$$

When $p \leqslant 1/4$ (the case in which the quantum ground state was rigorously shown to be ferromagnetic) we get the following expression for ε_k:

$$\varepsilon_k = 2S(1 - \cos k - p + p \cos 2k) \tag{81}$$

which gives, for small k,

$$\varepsilon_k = S(1 - 4p)\, k^2 \tag{82}$$

if $p < 1/4$, as expected, and

$$\varepsilon_k = \frac{S}{4} k^4 \tag{83}$$

if $p = 1/4$.

When $p > 1/4$, the spin-wave spectrum ε_k vanishes for $k = 0$ and also for $k = \theta$, with a linear dispersion relation

$$\varepsilon_k = c\,|k|, \qquad k \to 0 \tag{84}$$

and

$$\varepsilon_k = c\,|k - \theta|, \qquad k \to \theta \tag{85}$$

The spin-wave velocity c is the same for both cases and is given by

$$c = \frac{S}{4p}(4p - 1)^{3/2}(4p + 1)^{1/2} \tag{86}$$

Figure 1 shows the dispersion relation ε_k versus k for the case of $p = 1/2$ and $\Delta = 1$. Notice that in this case ε_k vanishes at $k = 0$ and $k = \pi/3$.

The spin-wave representation can be used to calculate the reduction of the magnetization due to quantum fluctuations:

$$m_z \equiv \frac{1}{N}\left\langle \sum_l S_l^z \right\rangle = S - \frac{1}{N}\left\langle \sum_k a_k^+ a_k \right\rangle = S - \frac{1}{N}\sum_k \frac{1}{2}\left(1 - \frac{A_k}{\varepsilon_k}\right) \tag{87}$$

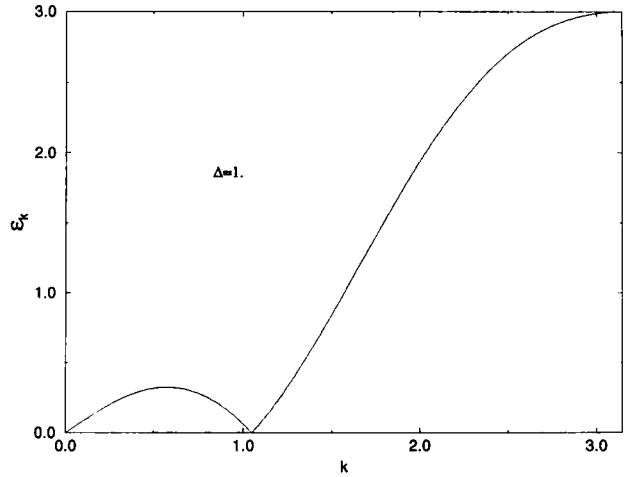

Fig. 1. Dispersion relation ε_k versus k for the case $p = 1/2$ and $\Delta = 1$. Notice that ε_k vanishes linearly at $k = 0$ and $k = \pi/3$.

In the limit $N \to \infty$, we get

$$m_z = S - \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{2} \left(1 - \frac{A_k}{\varepsilon_k} \right) dk \tag{88}$$

When $p > 1/4$, the integral diverges due to the linear dispersion relation given by Eq. (84) and the fact that A_k is a nonzero constant for $k = 0$. This indicates that the (classical) helical structure is destabilized by quantum fluctuations, no matter how large S is.

3.2. The Case $p = 1/2$

Here we consider the case $p = 1/2$ and $0 < \Delta < 1$. In this case the classical ground state corresponds to a modulated structure with a rotational number equal to 1/6. The angles θ_l have the following properties: $\theta_{l+6} = \theta_l$. Choosing

$$\begin{aligned} \theta_1 &= \theta & \theta_4 &= \pi + \theta \\ \theta_2 &= \pi - \theta & \theta_5 &= 2\pi - \theta \\ \theta_3 &= \pi & \theta_6 &= 0 \end{aligned} \tag{89}$$

we find that the minimum of the classical Hamiltonian gives a unique value for $\cos\theta$, namely

$$\cos\theta = \frac{1}{1+\Delta} \tag{90}$$

In the isotropic case (Section 3.1) there is a continuous family of degenerate ground states due to full rotation symmetry. In the present anisotropic case, in contrast, the only symmetry is rotation around the z axis which does not generate any other distinct eigenstates.

We find that the coefficients A_l, B_l, C_l, and D_l do not depend on l and are given by

$$A_l = -2D_l = -\frac{S}{2}\left(\Delta + \frac{\Delta}{1+\Delta}\right) \tag{91}$$

$$B_l = -2C_l = -\frac{S}{2}\left(\Delta - \frac{\Delta}{1+\Delta}\right) \tag{92}$$

We find also that the coefficient F_l has the property $F_{l+3} = F_l$ so that it is necessary to know, for instance, only F_{-1}, F_0, and F_1. They are

$$F_0 = 3S\frac{1}{1+\Delta} \tag{93}$$

and

$$F_{-1} = F_1 = \frac{3S}{2}\Delta \tag{94}$$

The classical ground-state energy E is given by

$$E = -NS^2\frac{1}{2}\left(\Delta + \frac{1}{1+\Delta}\right) \tag{95}$$

The coefficients $A_{kk'}$ and $B_{kk'}$ reduce to

$$A_{kk'} = F\delta_{k,k'-2\pi/3} + A_k\delta_{k,k'} + F\delta_{k,k'+2\pi/3} \tag{96}$$

and

$$B_{kk'} = B_k\delta_{k,-k'} \tag{97}$$

where

$$A_k = S\left\{\Delta + \frac{1}{1+\Delta} - \left(\Delta + \frac{\Delta}{1+\Delta}\right)\cos k + \frac{1}{2}\left(\Delta - \frac{\Delta}{1+\Delta}\right)\cos 2k\right\} \quad (98)$$

$$F = S\left(\frac{1}{1+\Delta} - \frac{\Delta}{2}\right) \quad (99)$$

$$B_k = S\left\{-\left(\Delta - \frac{\Delta}{1+\Delta}\right)\cos k + \frac{1}{2}\left(\Delta + \frac{\Delta}{1+\Delta}\right)\cos 2k\right\} \quad (100)$$

so that the Hamiltonian in momentum space is

$$\mathscr{H}' = \sum_k \{A_k a_k^+ a_k + F(a_k^+ a_{k+2\pi/3} + a_k^+ a_{k-2\pi/3}) + \tfrac{1}{2}B_k(a_k a_{-k} + a_k^+ a_{-k}^+)\} + E \quad (101)$$

We write the Hamiltonian in the form

$$\mathscr{H}' = \tfrac{1}{6}\sum_k \mathbf{\Phi}_k^+ \mathbf{H}_k \mathbf{\Phi}_k - \tfrac{1}{2}\sum_k A_k + E \quad (102)$$

where $\mathbf{\Phi}_k$ is the column matrix consisting of the operators

$$a_k \qquad a_{k+2\pi/3} \qquad a_{k-2\pi/3} \qquad a_{-k}^+ \qquad a_{-k-2\pi/3}^+ \qquad a_{-k+2\pi/3}^+ \quad (103)$$

the row matrix $\mathbf{\Phi}_k^+$ is its transposed Hermitian adjoint, and $\mathbf{H}_k$ is the c-number Hermitian 6×6 matrix given by

$$\mathbf{H}_k = \begin{pmatrix} \mathbf{Q}_k & \mathbf{R}_k \\ \mathbf{R}_k & \mathbf{Q}_k \end{pmatrix} \quad (104)$$

where 3×3 matrices $\mathbf{Q}_k$ and $\mathbf{R}_k$ are defined by

$$\mathbf{Q}_k = \begin{pmatrix} A_k & F & F \\ F & A_{k+2\pi/3} & F \\ F & F & A_{k-2\pi/3} \end{pmatrix} \quad (105)$$

and

$$\mathbf{R}_k = \begin{pmatrix} B_k & 0 & 0 \\ 0 & B_{k+2\pi/3} & 0 \\ 0 & 0 & B_{k-2\pi/3} \end{pmatrix} \quad (106)$$

Next, we prove that the eigenvalues ε_k of the quadratic form $\mathbf{\Phi}_k^+ \mathbf{H}_k \mathbf{\Phi}_k$ are the square roots of the eigenvalues of the matrix $(\mathbf{Q}_k - \mathbf{R}_k)(\mathbf{Q}_k + \mathbf{R}_k)$.

Let us defined the matrix $\mathbf{G}$ by

$$\mathbf{G} = [\mathbf{\Phi}_k, \mathbf{\Phi}_k^+] \equiv \mathbf{\Phi}_k (\mathbf{\Phi}_k^*)^T - (\mathbf{\Phi}_k^* \mathbf{\Phi}_k^T)^T \tag{107}$$

where $\mathbf{\Phi}_k^*$ is the column matrix of the Hermitian adjoint operators, and the superscript T stands for transpose. The matrix $\mathbf{G}$ is diagonal and its elements are actually c-numbers. It is given by

$$\mathbf{G} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} \tag{108}$$

where $\mathbf{I}$ is the 3×3 identity matrix. Suppose now that $\mathbf{T}_k$ is a linear transformation that diagonalizes the quadratic form in boson operators $\mathbf{\Phi}_k^+ \mathbf{H}_k \mathbf{\Phi}_k$. That is, $\mathbf{T}_k$ is a square matrix such that $\mathbf{\Phi}_k^+ \mathbf{H}_k \mathbf{\Phi}_k = \mathbf{\Psi}_k^+ \mathbf{D}_k \mathbf{\Psi}_k$, where $\mathbf{\Psi}_k = \mathbf{T}_k \mathbf{\Phi}_k$ and $\mathbf{D}_k = \mathbf{T}_k^+ \mathbf{H}_k \mathbf{T}_k$ is the diagonal eigenvalue matrix. Notice that $\mathbf{T}_k$ is not, in general, a unitary matrix. According to White *et al.*,[21] the diagonal eigenvalues of $\mathbf{D}_k$ are the same as the eigenvalues of the matrix

$$\mathbf{G}\mathbf{H}_k = \begin{pmatrix} \mathbf{Q}_k & \mathbf{R}_k \\ -\mathbf{R}_k & -\mathbf{Q}_k \end{pmatrix} \tag{109}$$

Consider next the unitary matrix $\mathbf{U}$ defined by

$$\mathbf{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{I} & \mathbf{I} \\ -\mathbf{I} & \mathbf{I} \end{pmatrix} \tag{110}$$

Hence

$$\mathbf{M}_k \equiv \mathbf{U}^T (\mathbf{G}\mathbf{H}_k) \mathbf{U} = \begin{pmatrix} \mathbf{0} & \mathbf{Q}_k + \mathbf{R}_k \\ \mathbf{Q}_k - \mathbf{R}_k & \mathbf{0} \end{pmatrix} \tag{111}$$

will have the same eigenvalues of $\mathbf{D}_k$. But

$$\mathbf{M}_k^2 = \begin{pmatrix} (\mathbf{Q}_k + \mathbf{R}_k)(\mathbf{Q}_k - \mathbf{R}_k) & \mathbf{0} \\ \mathbf{0} & (\mathbf{Q}_k - \mathbf{R}_k)(\mathbf{Q}_k + \mathbf{R}_k) \end{pmatrix} \tag{112}$$

and the proof is finished. Notice that the 3×3 matrices $(\mathbf{Q}_k + \mathbf{R}_k)(\mathbf{Q}_k - \mathbf{R}_k)$ and $(\mathbf{Q}_k - \mathbf{R}_k)(\mathbf{Q}_k + \mathbf{R}_k)$ have the same eigenvalues, which we denote by λ_k.

The resulting dispersion relation $\varepsilon_k = \sqrt{\lambda_k}$ exhibits forbidden zones (gaps) in the excitation spectrum at $k = \pi/3$ and at $k = 2\pi/3$. When $\Delta \to 1$,

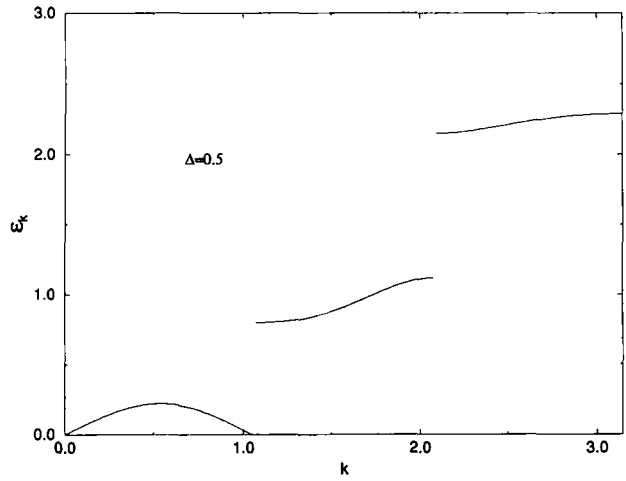

Fig. 2. Dispersion relation ε_k versus k for the case $p = 1/2$ and $\Delta = 1/2$. There are forbidden zones (gaps) in the spectrum at $k = \pi/3$ and $k = 2\pi/3$.

the two gaps at $k = \pi/3$ and at $k = 2\pi/3$ vanish as $\sim(1-\Delta)^{1/2}$ and $\sim(1-\Delta)$, respectively. Figure 2 shows the dispersion relation ε_k versus k for the case $p = 1/2$ and $\Delta = 1/2$. In this case there are gaps at $k = \pi/3$ and $k = 2\pi/3$.

We considered in this section only *one* of the ground states with period six, which we refer to as case 1. Consider the other high-symmetry case with $\theta_{l+3} = \pi + \theta_l$ defined by

$$\begin{aligned} \theta_1 &= -\theta^* & \theta_4 &= \pi - \theta^* \\ \theta_2 &= \theta^* & \theta_5 &= \pi + \theta^* \\ \theta_3 &= \pi/2 & \theta_6 &= 3\pi/2 \end{aligned} \tag{113}$$

which we refer to as case 2. The minimum of the classical Hamiltonian gives $\sin\theta^* = \Delta/(1+\Delta)$ and the classical energy E coincides with that of case 1. Moreover, the Hamiltonian in momentum space will be the one given by Eq. (101) with A_k and B_k the same as in case 1. The only distinct coefficient is F, which is now given by $F = S[\Delta/(1+\Delta) - 1/2]$.

In both cases the diagonalized Hamiltonian can be written in a form identical to (79), valid for the isotropic case, namely

$$\mathcal{H}' = \sum_k \varepsilon_k \alpha_k^+ \alpha_k + \tfrac{1}{2}\sum_k (\varepsilon_k - A_k) + E \tag{114}$$

Table I. Spin-Wave Corrections to the Classical Ground-State Energy for Cases 1 ($\Delta E_Q^{(1)}$) and 2 ($\Delta E_Q^{(2)}$) Corresponding to the Configurations Given by Eqs. (89) and (113), Respectively, for $p = 1/2$

Δ	$\Delta E_Q^{(1)}/S$	$\Delta E_Q^{(2)}/S$
0	0	0
0.2	−0.010	−0.004
0.4	−0.024	−0.015
0.6	−0.040	−0.032
0.8	−0.060	−0.054
1	−0.090	−0.090

where E is the classical energy and α_k are the new boson operators, so that the energy E_Q of the quantum ground state is given by

$$E_Q = \tfrac{1}{2}\sum_k (\varepsilon_k - A_k) + E \tag{115}$$

This formula allows us to calculate the quantum correction $\Delta E_Q = E_Q - E$ without the knowledge of the eigenvectors. Table I shows the values of $\Delta E_Q^{(1)}$ and $\Delta E_Q^{(2)}$ for the cases 1 and 2, respectively. It is clear that case 1 has lower energy, except in the cases $\Delta = 0$ and $\Delta = 1$, where they agree. Hence, case 1 is selected by the quantum fluctuations.

4. THE HUSE–ELSER VARIATIONAL WAVE FUNCTION

Huse and Elser[16] proposed a very elegant variaional wave function for the ground state of spin-1/2 Heisenberg antiferromagnets on bipartite lattices. One of the most interesting features of their approach is the reduction of a quantum problem, namely finding a variational ground state, to a numerical simulation of a long-range Ising model using standard Monte Carlo techniques. In order to understand our adaptation of their method it is convenient to review briefly their work.

The Huse and Elser variational wave function (HEVWF) has the form

$$|0\rangle = \sum_\alpha e^{R/2}\,|\alpha\rangle \tag{116}$$

where $\tilde{H}$ is an operator which contains the variational parameters and is not necessarily Hermitian; the $\{|\alpha\rangle\}$ are eigenstates of $\tilde{H}$

$$\tilde{H}|\alpha\rangle = \lambda_\alpha |\alpha\rangle \tag{117}$$

and form a complete set of orthonormal basis functions. The expectation value of an operator $\mathcal{O}$, for instance, the Hamiltonian $\mathcal{H}$, in the ground state (116) is given by

$$\frac{\langle 0|\,\mathcal{O}\,|0\rangle}{\langle 0\,|\,0\rangle} = \frac{\sum_{\alpha\beta} e^{\lambda_\alpha^*/2}\,\mathcal{O}_{\alpha\beta} e^{\lambda_\beta/2}}{\sum_\alpha e^{\mathrm{Re}\,\lambda_\alpha}} = \frac{\sum_\alpha e^{\mathrm{Re}\,\lambda_\alpha} \sum_\beta \mathcal{O}_{\alpha\beta} e^{(\lambda_\beta-\lambda_\alpha)/2}}{\sum_\alpha e^{\mathrm{Re}\,\lambda_\alpha}} \tag{118}$$

where $\mathrm{Re}\,\lambda_\alpha$ stands for the real part of λ_α. Equation (118) shows that, using the wave function (116), we end up evaluating the expectation value of

$$\sum_\beta \mathcal{O}_{\alpha\beta} \exp\{\tfrac{1}{2}(\lambda_\beta - \lambda_\alpha)\} \tag{119}$$

in an ensemble where configuration α occurs with probability proportional to $\exp\{\mathrm{Re}\,\lambda_\alpha\}$. Clearly, $\exp\{\mathrm{Re}\,\lambda_\alpha\}$ plays the role of a Boltzmann factor and this kind of average can be calculated using Monte Carlo methods.

Note that the exact ground state can be written as in Eq. (116). However, when it is not known, choosing a good $\tilde{H}$ is not trivial. For spin-1/2 Heisenberg antiferromagnets on bipartite lattices the essential ingredient seems to be a phase discovered by Marshall.[22] He showed that, if one chooses a basis of eigenfunctions $\{|\alpha\rangle\}$ of the operators $S^z = \sum_l S_l^z$, the ground state can be written as

$$|0\rangle = \sum_\alpha (-1)^{n_\alpha} a_\alpha |\alpha\rangle \tag{120}$$

where n_α is the number of spins pointing down on one sublattice in configuration α and the coefficients a_α are all real and positive. Huse and Elser incorporated the Marshall phase $(-1)^{n_\alpha} = \exp\{i\pi n_\alpha\}$ in their wave function choosing the $\{|\alpha\rangle\}$ as eigenstates of S^z and

$$\tfrac{1}{2}\,\mathrm{Im}\,\tilde{H} = \pi \sum_{i\in B} (\tfrac{1}{2} - S_i^z) \tag{121}$$

where the sum is over spins on sublattice B. Quantum corrections were introduced by taking the real part of $\tilde{H}$ as

$$\mathrm{Re}\,\tilde{H} = \sum_{ij} K_{ij} S_i^z S_j^z \tag{122}$$

with $K_{ij}=K_1$ if $|i-j|=1$ and $K_{ij}=K_2/|i-j|^{\sigma}$ if $|i-j|>1$. The parameters K_1, K_2, and σ are variational. For the two-dimensional spin-1/2 Heisenberg antiferromagnet on a square lattice the HEVWF, with $K_1=2.6$, $K_2=1.9$, and $\sigma=0.7$, gives a variational ground-state energy per link equal to -0.3319, which is less than 1% above the series estimate.[23]

The phase $(-1)^{n_\alpha}$ has a simple physical interpretation, as first pointed out by Thouless[24] and emphasized in ref. 16. Observe that

$$\sum_{\alpha} e^{(1/2)i\,\mathrm{Im}\,\tilde{H}}|\alpha\rangle=\prod_{i\in A}(|\uparrow\rangle_i+|\downarrow\rangle_i)\prod_{i\in B}(|\uparrow\rangle_i-|\downarrow\rangle_i) \tag{123}$$

Recalling that $|\uparrow\rangle_i\pm|\downarrow\rangle_i$ are eigenstates of S_i^x with eigenvalues $\pm 1/2$, it is clear that the imaginary part of $\tilde{H}$ gives the classical Néel ground state with spins on sublattice A (B) pointing in the positive (negative) x direction. We believe, although we could not prove it, that the best choice for Im $\tilde{H}$ for any spin system gives the classical ground state. We used this Ansatz to construct our variational wave function.

In order to keep our notation as in ref. 16 and 22, which use a basis of eigenstates of S^z, we rotate our coordinate axes so that the spin chain lies in the z direction. The Hamiltonian becomes

$$\begin{aligned}\mathscr{H}=&-\sum_{i=1}^{N}\{S_i^xS_{i+1}^x+\Delta(S_i^yS_{i+1}^y+S_i^zS_{i+1}^z)\}\\&+p\sum_{i=1}^{N}\{S_i^xS_{i+2}^x+\Delta(S_i^yS_{i+2}^y+S_i^zS_{i+2}^z)\}\end{aligned} \tag{124}$$

For the isotropic case ($\Delta=1$) nothing changes. However, in the Ising case ($\Delta=0$) the spins now point in the x direction.

To determine the variational parameters, we have to calculate the expectation value of $\tilde{H}$ in eigenstates of S^z generated by a Monte Carlo simulation. Thus, it is convenient to rewrite S^x and S^y in terms of raising and lowering spin operators, $S^{\pm}=S^x\pm iS^y$, respectively,

$$\begin{aligned}\mathscr{H}=&\sum_i\{\tfrac{1}{4}(1+\Delta)D_{i,i+1}+\tfrac{1}{4}(1-\Delta)E_{i,i+1}+\Delta Z_{i,i+1}\}\\&-p\sum_i\{\tfrac{1}{4}(1+\Delta)D_{i,i+2}+\tfrac{1}{4}(1-\Delta)E_{i,i+2}+\Delta Z_{i,i+2}\}\\&+\tfrac{1}{4}N(1-p)\Delta\end{aligned} \tag{125}$$

and

$$D_{ij}=S_i^+S_j^-+S_i^-S_j^+,\quad E_{ij}=S_i^+S_j^++S_i^-S_j^-,\quad Z_{ij}=S_i^zS_j^z-\tfrac{1}{4} \tag{126}$$

There is strong evidence in the isotropic case ($\Delta = 1$; see Section 2) that the ground state of Hamiltonian (125) is a singlet. In this way we can restrict ourselves to the subspace of configurations with $S^z = 0$. This restriction is implemented in our Monte Carlo simulation using a generalized Kawasaki dynamics where any pair of antiparallel spins can be exchanged in order to produce a new state. For the anisotropic case ($\Delta \neq 1$) we sample the configuration space using the heat-bath Metropolis algorithm.

For the classical isotropic system ($\Delta = 1$) the lowest energy has helicoidal ordering. The spins lie in the xy plane and as one moves from one site to the next on the chain along the z axis, the spins rotate by a fixed angle φ_p. To find φ_p we replace the operators $\mathbf{S}_i$ in Eq. (124) by classical spins with components

$$S_i^x = \cos\varphi, \qquad S_i^y = \sin\varphi, \qquad S_i^z = 0 \tag{127}$$

and minimize $\mathscr{H}$ with respect to φ. In this way we obtain

$$\varphi_p = \arccos\left(\frac{1}{4p}\right) \tag{128}$$

and a classical energy given by $E_{cl} = -(p + 1/8p)/4$. As discussed above, $\operatorname{Im} \tilde{H}/2$ should produce this classical configuration. To implement the spin rotation we choose

$$\operatorname{Im} \tfrac{1}{2}\tilde{H} = -\sum_{l=0}^{N-1} \varphi_l S_l^z \tag{129}$$

where $\varphi_l = l\varphi_p$ and we take the real part of $\tilde{H}$ the same as in the HEVWF; see Eq. (122).

We define the following notation: L stands for the chain size, *NEQ* is the number of Monte Carlo steps used to reach equilibrium, *NSTEP* is the number of Monte Carlo steps used to calculate the energy after equilibrating the system, and *NRUN* is the number of independent runs, starting from different initial conditions, used to estimate the errors. We used periodic boundary conditions in all simulations.

We summarize the results of our simulation of the isotropic model in Table II and Fig. 3. Several comments are in order. In order to avoid commensurability problems, that is, changes in rotation angle between the first and last spins larger than φ_p, the chain size is a multiple of the spatial period of the helix. The values of p were chosen so that this period is not too large. For fixed values of K_1, K_2, and σ the statistical errors in the energy are usually very small; they are typically of the order of 10^{-5}. However, there is another error source which reduces our precision. It is

Table II. Ground-State Energy E of the Helical Phase for Some Values of p^a

L	K_1	K_2	σ	φ_p	p	E
440	0.9	1.0	0.01	$\pi/11$	0.2605	−0.1852
320	3.6	4.0	0.07	$\pi/8$	0.2705	−0.1835
360	1.9	2.4	0.10	$\pi/6$	0.2886	−0.1821
300	5.1	6.0	0.09	$\pi/5$	0.3090	−0.1820
320	10.0	11.4	0.08	$\pi/4$	0.3535	−0.1866
360	19.6	22.3	0.10	$\pi/3$	0.5000	−0.2242

[a] The rotation angle φ_p is related to p through $\cos\varphi_p = 1/4p$. The quantities K_1, K_2, and σ are variational parameters. For all lattice sizes $NEQ = 5000$, $NSTEP = 5000$, and $NRUN = 16$.

associated with the determination of the best values of K_1, K_2, and σ. There are many combinations of K_1, K_2, and σ which give essentially the same value for the energy. This probably reflects the fact that these parameters are not independent. A more careful estimate would put the uncertainty in the energy equal to about 0.0001. But we believe that the error is not much larger that this value. It is also worth mentioning that finite-size effects are negligible. Reducing the lattice size by a factor 10 changes the energy by less than 0.4% in the worst case.

The state where all spins point in the same direction is the eigenstate of Hamiltonian (124) associated with the ferromagnetic phase. Its energy, for $\Delta = 1$, is given by

$$\frac{E_F}{N} = \frac{1}{4}(p-1) \tag{130}$$

For $p < 1/4$ the ferromagnetic phase has lower energy than the helicoidal. For $p > 1/4$ the situation is reversed. Thus, the transition between the two phases occurs at $p = 1/4$, in agreement with the results of Section 2. These results are illustrated in Fig. 3, where we have also plotted the asymptotic behavior for $p \to \infty$. In this limit the term multiplied by p in Hamiltonian (124) is dominant and the system behaves as two noninteracting isotropic Heisenberg chains. In this case the ground-state energy is given by the Bethe Ansatz and the equation of the dotted straight line in Fig. 3 is given by

$$E = 2\varepsilon p \tag{131}$$

where $\varepsilon = -0.22157$ is the energy per site of one chain.

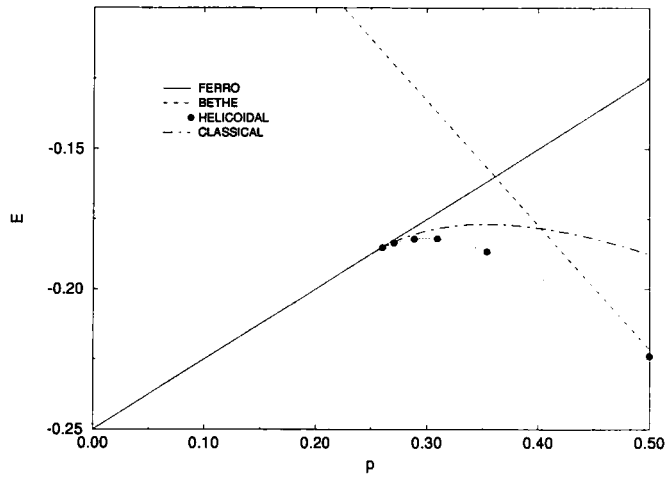

Fig. 3. Ground-state property of the helical phase for some values of p (filled circles). The dotted line is drawn only to guide the eye. The solid line gives the energy of the ferromagnetic phase. The dashed line is the asymptotic behavior of the model in the limit $p \to \infty$ and is given by the Bethe Ansatz.

The results shown in Table II for $p > 1/4$ were obtained using Kawasaki dynamics, which kept the system in the $M = 0$ sector. The same simulations were performed by using the heat-bath algorithm, which allows the system to sample all M sectors. The results obtained were the same within the errors. Thus, the agreement between the two algorithms for $p > 1/4$ gives strong evidence that the ground state belongs to the $M = 0$ sector for $\Delta = 1$. This is in contrast to the case $p < 1/4$, where the ground state is ferromagnetic and the Kawasaki algorithm, which keeps the system

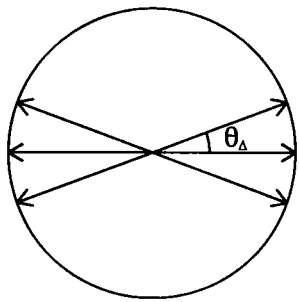

Fig. 4. Rotation of the classical spins in the $\langle 6 \rangle$ phase when $0 \leqslant \Delta < 1$.

in the $M=0$ sector, gives a poor energy bound. In this case, only the heat-bath algorithm gives a good ground-state energy.

We have also investigated numerically the $\langle 6 \rangle$ phase in the anisotropic case. When $\Delta = 1$ (isotropic case), the rotation angle $\varphi_p = \pi/3$. As Δ decreases to zero (Ising case) the spatial period remains equal to six lattice units, but the rotation angle is not uniform as we move along the chain; see Fig. 4. The angle θ_Δ in Fig. 4 can be obtained replacing the operators $\mathbf{S}_l$ in Hamiltonian (124) by classical spins in the xy plane, that is, $S_l^x = \cos\theta_l$ and $S_l^y = \sin\theta_l$, where

$$\begin{aligned} \theta_{6k} &= 0 & \theta_{6k+3} &= \pi \\ \theta_{6k+1} &= \theta & \theta_{6k+4} &= \pi + \theta \\ \theta_{6k+2} &= \pi - \theta & \theta_{6k+5} &= 2\pi - \theta \end{aligned} \tag{132}$$

where $0 \leqslant k < N/6$, and minimizing the energy with respect to θ. Due to the factorization of the p dependence in the energy, the angle θ_Δ does not depend on p,

$$\theta_\Delta = \arccos\left(\frac{1}{1+\Delta}\right) \tag{133}$$

For this value of θ the classical energy is

$$\frac{E_{cl}}{N} = -\frac{1}{12}(1+p)\left(\Delta + \frac{1}{1+\Delta}\right) \tag{134}$$

We implemented the nonuniform rotation choosing φ_l in Eq. (129) in such a way that the spins point in the direction of the classical vectors given by (132) with $\theta = \theta_\Delta$.

In Table III we fix $p = 1/2$ and present the ground-state energy of the $\langle 6 \rangle$ phase for several values of Δ. For comparison we also give the classical energy E_{cl}; see Eq. (130). Except for $\Delta = 0$, the quantum corrections introduced by the real part of $\tilde{H}$ lower the energy. For $\Delta = 0$, the classical wave function, obtained with $\mathrm{Re}\,\tilde{H} = 0$, gives the lowest energy and the behavior of the chain is of the Ising type. Apparently the crossover between the Ising and the helical behavior occurs at $\Delta = 0$. Even for $\Delta = 0.1$ it is not difficult to obtain a variational wave function which gives an energy less than the classical one.

Since $\mathrm{Re}\,\tilde{H}$ and $\mathrm{Im}\,\tilde{H}$, which depends only on θ_Δ, are both independent of p, the variational wave function for the $\langle 6 \rangle$ phase is p independent. Examining Eq. (125), we note that we can determine $\langle 0 | \mathscr{H} | 0 \rangle / \langle 0 \mid 0 \rangle$ by

Table III. Phase Boundaries[a]

K_1	K_2	σ	Δ	$V_1(\Delta)$	$V_2(\Delta)$	p_{F6}	p_{62}
0.0	0.0	—	0.00	−0.0833	0.0833	0.500	0.500
0.1	3.3	2.5	0.25	−0.0846	0.1009	0.471	0.567
0.4	3.8	1.6	0.50	−0.0888	0.1400	0.413	0.807
6.0	8.6	0.3	0.75	−0.0952	0.1886	0.353	1.550
19.6	22.3	0.1	1.00	−0.1102	0.2281	0.292	5.032

[a] For each value of the anisotropy Δ we give the corresponding values of p on the boundaries between the ferromagnetic phase and the $\langle 6 \rangle$ phase (p_{F6}) and between the $\langle 6 \rangle$ phase and the $\langle 2 \rangle$ phase (p_{62}). The quantities $V_1(\Delta)$ and $V_2(\Delta)$ are given by Eq. (135), and K_1, K_2, and σ are variational parameters. For all Δ, $L = 360$, $NEQ = 5000$, $NSTEP = 5000$, and $NRUN = 16$.

first calculating separately the expectation values of the terms with interactions between nearest neighbors and next nearest neighbors and introducing the p dependence later. Thus

$$\frac{\langle 0 | \mathscr{H} | 0 \rangle}{\langle 0 | 0 \rangle} = V_1(\Delta) - pV_2(\Delta) \tag{135}$$

where

$$V_\alpha = -\left(\frac{1+\Delta}{4}\right) \sum_i \frac{\langle 0 | D_{i,i+\alpha} | 0 \rangle}{\langle 0 | 0 \rangle} - \left(\frac{1-\Delta}{4}\right) \sum_i \frac{\langle 0 | E_{i,i+\alpha} | 0 \rangle}{\langle 0 | 0 \rangle}$$
$$- \Delta \sum_i \frac{\langle 0 | Z_{i,i+\alpha} | 0 \rangle}{\langle 0 | 0 \rangle} - N\frac{\Delta}{4} \tag{136}$$

with $\alpha = 1, 2$.

In this way, for each value of Δ we obtain the energy of the $\langle 6 \rangle$ phase for all p. Equating Eq. (135) with Eq. (130), which gives the exact energy of the ferromagnetic phase, we can determine the boundary between these two phases. In Fig. 5 this boundary is represented by the solid line. The dotted line in the same figure represents the maximum possible extension of the $\langle 6 \rangle$ phase. It was found in the following way. For $\Delta = 0$, the vector

$$|++--\cdots\rangle = |+\rangle\,|+\rangle\,|-\rangle\,|-\rangle\cdots \tag{137}$$

where $|+\rangle$ and $|-\rangle$ are eigenstates of S_i^x, is the eigenstate of Hamiltonian (124) associated with the $\langle 2 \rangle$ phase. For $\Delta > 0$, the vector (137) is no

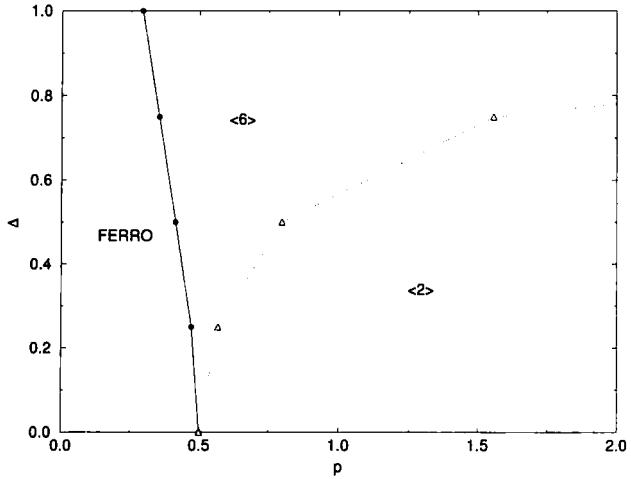

Fig. 5. Phase boundaries. The coordinates of circles (Δ, p_{F6}) and triangles (Δ, p_{62}) are given in Table III. The lines are drawn only to guide the eye.

longer an eigenstate of (124). However, we can show that there are values of p for which the energy

$$\frac{\langle ++--\cdots|\,\mathcal{H}\,|++--\cdots\rangle}{\langle ++--\cdots\,|\,++--\cdots\rangle} = -\frac{1}{4}Np \tag{138}$$

is less than the energy of the $\langle 6\rangle$ phase, given by Eq. (135). This suggests, in analogy with the classical case, that the $\langle 6\rangle$ phase does not extend itself indefinitely to the right of the diagram in Fig. 5. The values of $V_\alpha(\Delta)$, with $\alpha = 1, 2$, for some values of Δ and the coordinates of the points in Fig. 5 are given in Table III.

Thus, numerical simulations for the isotropic chain ($\Delta = 1$) are in agreement with the results of Section 2, where it was shown that, at $p = 1/4$, the system undergoes a transition from a ferromagnetic to a helicoidal type phase. In addition, simulations of the anisotropic chain ($0 \leqslant \Delta < 1$) suggest the existence of a very rich phase structure where the quantum analogs of the classical modulated phases occupy well-defined regions of the phase diagram.

It should be emphasized that Fig. 5 is not really a *ground-state* phase diagram, but only part of the (conjectured) phase diagram, since other phases were not examined. There may be other commensurate, incommensurate, and/or disordered phases in the real phase diagram.

5. CONCLUSION

We have shown that Monte Carlo results, obtained using the Huse–Elser variatonal wave function with a phase which gives the classical ground state, are in good agreement with other methods. For antiferromagnets on a bipartite lattices this *classical phase* is an exact result. We believe, although we could not prove it, that this classical phase is an essential ingredient of the exact ground-state wave function of any quantum spin system. But even if it is only an approximate property, it can be used to classify the quantum phases. In this way it is possible to draw phase diagrams similar to the ones found in classical theories.

In spite of the various results presented in this paper, much remains to be done. One of the open problems is to complete the phase diagram, i.e., the conjectured line to the right of the point $p = 1/2$. Another question is the interesting conjecture that the gaps found in Section 3 are (quantum) boundaries of other stable ground states, analogous to the commensurate phases of other models (e.g., ref. 13). Is there a "devil's staircase" of such gaps? Of course, these problems, fascinating as they are, must be considered with due caution. Indeed, one expects that fractal structures disappear upon quantization. For instance, the strange attractor in the Kaplan–Yorke map[25] (see also ref. 9) disappears when the map is quantized due to the delocalization of the individual branches of the attractor by quantum interference effects.[26] However, it is not clear what replaces the fractal structures in the quantum version of these systems, and we hope that the present study will stimulate interest in such problems.

Finally, the existence of a critical size of the clusters in the Bader–Schilling method and which is achieved for a small, almost minimal, number of spins is very surprising. This feature has also been found to be present in a one-dimensional model of ferromagnetic domains.[27] It is intriguing to determine whether it holds in higher dimensions.

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