Quantum spin model with frustration on the union jack lattice


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A quantum spin model with frustration, the Heisenberg antiferromagnet on the union jack lattice, is analyzed using spin-wave theory. For small values of the frustrating coupling \( \alpha \), the system is Néel ordered as usual, while for large \( \alpha \) the frustration is found to induce a canted phase. The possibility of an intermediate spin-liquid phase is discussed.

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I. INTRODUCTION

Frustrated lattice spin models in two dimensions have attracted much discussion in recent years. They exhibit new and interesting phase structures and phase transitions; in particular, they may develop “spin-liquid” states, without long-range order.\(^1\) It is also believed that frustrating interactions may play a role in the high-temperature superconducting cuprate materials. Primary examples are the anisotropic triangular lattice Heisenberg antiferromagnet [Fig. 1(a)], the square lattice \( J_1-J_2 \) model [Fig. 1(b)], and the Shastry-Sutherland model [Fig. 1(c)]. In this paper we discuss another member of this group, the Heisenberg antiferromagnet on the union jack lattice [Fig. 1(d)], which is another frustrated lattice model and might be expected to display some interesting properties.

The spin-1/2 \( J_1-J_2 \) model on the square lattice\(^2\) involves antiferromagnetic Heisenberg spin interactions with coupling \( J_1 \) between nearest neighbors and coupling \( J_2 \) between diagonal next-nearest neighbors, as illustrated in Fig. 1(b). The union jack lattice model has \( J_1 \) interactions on only half the diagonal bonds, in the pattern shown in Fig. 1(d), so that the lattice consists of two different site types \( A \) and \( B \) and the unit cell is \( 2 \times 2 \) sites. Both models will exhibit quantum phase transitions as the coupling ratio \( \alpha = J_2/J_1 \) is varied.

In the \( J_1-J_2 \) model at small \( \alpha \), the \( J_1 \) coupling is dominant and produces antiferromagnetic Néel ordering of the spins. At large \( \alpha \), the \( J_2 \) interaction is dominant and produces antiferromagnetic ordering on the two diagonal sublattices, and then the effect of the \( J_1 \) interaction is to align the two sublattices to form a columnar ordered state as illustrated in Fig. 2, an example of the “order-by-disorder” phenomenon. Numerical investigations\(^3\)\(-\)\(^{10,13}\) have shown that the boundaries of these two phases lie at \( \alpha = 0.38 \) and \( \alpha = 0.60 \), respectively.

The nature of the intermediate phase or phases remains controversial. Monte Carlo simulations are hampered by the “minus sign” problem, exact diagonalizations are limited to small lattices, and series expansions are based on some particular ordered reference state and are only valid within a single phase. It is generally believed that the intermediate phase is gapped and shows no long-range magnetic order. Field-theory approaches\(^5,6\) and dimer series expansions\(^5,7,9\) seem to indicate a columnar dimerized state in the intermediate region, with spontaneous breaking of translational symmetry, as illustrated in Fig. 2. Capriotti and co-workers, on the other hand, have suggested a homogeneous spin-liquid plaquette resonant valence bond (RVB) state\(^10,11\) and have found that exact diagonalization up to \( 6 \times 6 \) sites shows no strong evidence of dimerization.\(^12\) Another Monte Carlo study has suggested a columnar dimer state with plaquette-type modulation.\(^13\) Sushkov et al.\(^9\) have even suggested that there may be three different phases in the intermediate region: reading from left to right, a Néel state with columnar dimerization, a columnar dimerized spin liquid, and a columnar dimerized spin liquid with plaquette-type modulation.

Several discussions have centered on the Lieb-Schulz-Mattis theorem in higher dimensions,\(^14\)\(-\)\(^{16}\) which shows that for a spin system with half-integer spin per unit cell, there is an excitation energy gap behaving like \( 1/L \), where \( L \) is the linear size of the system. Takano et al.\(^17\) have argued that a uniform RVB state without gapless singlet excitations is excluded by the theorem and that the true ground state is a plaquette state with spontaneously broken translation invariance and fourfold degeneracy. Later arguments\(^11,16,18\) have refuted this, however, and shown that the theorem may be satisfied if the translation symmetry remains unbroken, but the ground state has a fourfold “topological” degeneracy instead, as in a simple dimer model.

![Fig. 1. Lattice spin models with frustration. Solid lines represent nearest-neighbor antiferromagnetic interactions \( J_1 \); dashed lines represent next-nearest-neighbor interactions \( J_2 \). Case: (a) anisotropic triangular lattice, (b) \( J_1-J_2 \) model, (c) Shastry-Sutherland model, and (d) union jack lattice model.](image-url)
The Hamiltonian for the union jack lattice model is

\[ H = J_1 \sum_{(NN)} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{A:\langle NNN \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1) \]

where the \( J_1 \) and \( J_2 \) interactions connect sites as shown in Fig. 1(d). A classical variational analysis shows that for \( \alpha = J_2/J_1 < 0.5 \), the ground state is the Néel state, as in the \( J_1-J_2 \) model. For \( \alpha > 0.5 \), the ground state is the canted ferrimagnetic state shown in Fig. 3, where the spins on the \( A \) sublattice are canted at an angle \( \theta \) to those on the \( B \) sublattice and \( 2\theta \) to their neighbors on the \( A \) sublattice. The energy of this state is

\[ E_0 = N S^2 \left[ \alpha \cos 2\theta - 2 \cos \theta \right], \quad (2) \]

where we have set \( J_1 = 1 \), \( S \) is the total spin per site, and \( N \) is the number of sites. This energy is minimized when

\[ \sin \theta(2\alpha \cos \theta - 1) = 0. \quad (3) \]

For \( \alpha < 0.5 \), the lowest energy corresponds to \( \sin \theta = 0 \)—i.e., the simple Néel state. For \( \alpha > 0.5 \), the lowest-energy solution is

\[ \cos \theta = \frac{1}{2\alpha}, \quad (4) \]

corresponding to the canted state. In the limit \( \alpha \to \infty \), the angle \( \theta \to \pi/2 \): the spins on the \( A \) sublattice are Néel ordered, as expected, and the spins on the \( A \) and \( B \) sublattices are at right angles to each other.

In the canted phase, there is a net magnetization per site in the \( z \) direction,

\[ M_z = \frac{S}{2} \left( 1 - \cos \theta \right) = \frac{S}{2} \left( 1 - \frac{1}{2\alpha} \right), \quad (5) \]

and a staggered magnetization per site in the \( z \) direction,

\[ M_z = \frac{S}{2} \left( 1 + \cos \theta \right) = \frac{S}{2} \left( 1 + \frac{1}{2\alpha} \right). \quad (6) \]

There is also a staggered magnetization on the \( A \) sublattice in the \( x \) direction, which we shall not discuss further.

The model thus demonstrates a new mechanism for causing ferrimagnetism. Ferrimagnetism usually arises when the individual ionic spins are different on different sublattices. Here the spins have the same magnitude on each sublattice and the interactions are antiferromagnetic, but the frustration between them produces a nonzero overall magnetic moment.

In the neighborhood of the transition point \( \alpha_c = 0.5 \), we find for the ground-state energy per bond \( \epsilon_0 = E_0/2N \) in zero magnetic field:

\[ \epsilon_0 \sim -\frac{3S^2}{4}, \quad \alpha \to \alpha_c, \quad (7) \]

\[ \frac{d\epsilon_0}{d\alpha} \sim \frac{S^2}{2}, \quad \alpha \to \alpha_c, \quad (8) \]

\[ \frac{d^2\epsilon_0}{d\alpha^2} \sim \left\{ \begin{array}{ll} 0, \quad \alpha \to \alpha_c^-, \\ -4S^2, \quad \alpha \to \alpha_c^+. \end{array} \right. \quad (9) \]

while for the net magnetization in the \( z \) direction,

\[ M_z \sim S(\alpha - \alpha_c), \quad \alpha \to \alpha_c. \quad (10) \]

Thus the transition is not quite the simple first-order transition found classically for other frustrated models. There is no “latent heat”—i.e., no discontinuity in \( d\epsilon_0/d\alpha \)—although there is a finite discontinuity in the second derivative. The magnetization \( M_z \) vanishes linearly at \( \alpha_c \), and the energy gap is zero on both sides of the transition, corresponding to spontaneous breaking of the spin rotation symmetry. Translation symmetry on the lattice is also broken on both sides of the transition. The question then arises whether quantum fluctuations will change the character of the transition.

In the remainder of this paper, we shall discuss how this picture is modified when one goes beyond the classical analysis to a spin-wave treatment. In Sec. II we shall present a modified spin-wave treatment of the Néel phase to second order, and in Sec. III we shall give a spin-wave treatment of the canted phase to first order. The results are discussed in Sec. IV. Our conclusions are summarized in Sec. V.

II. SPIN-WAVE THEORY FOR THE NÉEL PHASE

A. Formulation

A review of spin-wave approaches to the \( J_1-J_2 \) model has been given by Gochev.\(^19\) Chandra and Doucot\(^2\) gave the first conventional spin-wave treatment. The results of this approach were found to become unstable as the frustration \( \alpha \)
increases, due to strong interactions between the spin-wave bosons. The interactions involve a quadratic term

$$\hat{H}_2 = \sum_k \mathcal{O}_k (\alpha_k \beta_k + \alpha_k^\dagger \beta_k^\dagger),$$  \hspace{1cm} (11)$$

which is comparable with the zeroth-order Hamiltonian for $S=1$ and $\alpha \approx 1$. Thus one needs to go to a modified treatment in which this quadratic term is absent: this requirement turns out to be equivalent to Takahashi’s modified spin-wave theory.\(^\text{23}\) A very similar treatment can be applied to the union jack lattice model. We will follow Gochev’s notation\(^\text{19}\) as far as possible.

Let us rewrite the Hamiltonian (1), adding in a staggered magnetic field $h$:

$$H = \sum_{\langle lm \rangle} \mathbf{S}_l \cdot \mathbf{S}_m + \alpha \sum_{\langle l,l+1 \rangle} \mathbf{S}_{l+1} \cdot \mathbf{S}_l + h \left( \sum_l \mathbf{S}_l^z - \sum_m \mathbf{S}_m^z \right),$$  \hspace{1cm} (12)$$

where we have divided the lattice into even ($A$) and odd ($B$) sublattices, denoted by indices $l$ and $m$, respectively, and set $J_1 = 1$.

Introduce creation and annihilation operators for the “spin deviation” on the two sublattices by means of a Dyson-Maleev transformation,

$$S_l^z = -a_l^\dagger a_l,$$
$$S_l^x = (2S)^{1/2} a_l - (2S)^{-1/2} a_l^\dagger a_l,$$
$$S_l^y = (2S)^{1/2} a_l^\dagger,$$
$$S_m^z = b_m^\dagger b_m - S,$$
$$S_m^x = (2S)^{1/2} b_m^\dagger - (2S)^{-1/2} b_m^\dagger b_m^\dagger b_m,$$
$$S_m^y = (2S)^{1/2} b_m^\dagger,$$

and then perform a Fourier transform

$$a_k = \frac{2}{N} \sum_l e^{ikl} a_l,$$
$$b_k = \frac{2}{N} \sum_m e^{-ikm} b_m,$$  \hspace{1cm} (13)$$

to give the Hamiltonian in the form

$$H = -2SN \left( 1 - \frac{\alpha}{2} - \frac{h}{2S} \right) + 4S \left( 1 - \frac{\alpha}{2} - \frac{h}{4S} \right) \sum_k a_k^\dagger a_k$$
\[+ \left( \frac{1}{4} - \frac{h}{4S} \right) \sum_k b_k^\dagger b_k + \sum_k \left( \gamma_k (a_k b_k + a_k^\dagger b_k^\dagger) + \alpha \eta_k a_k^\dagger a_k \right) \]
\[- \frac{4}{N} \sum_{\delta \in \{1,2,3,4\}} \delta_k \gamma_{\delta-4} a_{\delta-4}^\dagger b_{\delta-4} + \gamma_4 a_{\delta-4}^\dagger a_{\delta-4} b_{\delta-4}^\dagger + \gamma_4 a_{\delta-4}^\dagger a_{\delta-4} b_{\delta-4}^\dagger \]
\[+ \gamma_4 a_{\delta-4}^\dagger b_{\delta-4}^\dagger \]
\[+ \frac{4\alpha}{N} \sum_{\delta \in \{1,2,3,4\}} \delta_k \gamma_{\delta-4} a_{\delta-4}^\dagger a_{\delta-4} b_{\delta-4}^\dagger a_{\delta-4} b_{\delta-4}^\dagger \]
\[\times \left( \eta_{\delta-4} - \frac{1}{2} (\eta_1 + \eta_2) \right), \hspace{1cm} (15)\]$$

where we have used the shorthand notation $1 \cdots 4$ for momenta $k_1 \cdots k_4$, $\gamma_k, \eta_k$ are the structure factors for the full lattice and the $A$ sublattice, respectively,

$$\gamma_k = \cos \frac{k_x}{2} \cos \frac{k_y}{2},$$
$$\eta_k = \frac{1}{2} (\cos k_x + \cos k_y),$$  \hspace{1cm} (16)$$

if we set the spacing of each sublattice equal to 1, and $k_x, k_y$ are the components of momentum along the diagonal axes of the two sublattices.

The Hamiltonian can now be diagonalized up to second order by a Bogoliubov transformation:

$$a_k = u_k a_k^\dagger - v_k b_k^\dagger, \hspace{0.5cm} b_k = u_k b_k^\dagger - v_k a_k^\dagger,$$  \hspace{1cm} (17)$$

where

$$u_k^2 - v_k^2 = 1.$$  \hspace{1cm} (18)$$

After normal ordering the transformed Hamiltonian, the condition that off-diagonal quadratic terms vanish turns out to be

$$Q_k = 4S \left[ \gamma_k (u_k^2 + v_k^2) - 2u_k v_k \left( 1 - \frac{h}{4S} - \frac{\alpha}{2} \right) (1 - \eta_k) \right]$$
\[+ 4(R_1 - R_2) \left[ \gamma_k (u_k^2 + v_k^2) - 2u_k v_k \right] - 4\alpha u_k v_k (R_2 - R_1) \]
\[\times (1 - \eta_k) = 0, \hspace{1cm} (19)\]$$

where the lattice sums $R_i$ are

$$R_1 = \frac{2}{N} \sum_k \gamma_k u_k v_k, \hspace{0.5cm} R_2 = \frac{2}{N} \sum_k v_k^2, \hspace{0.5cm} R_3 = \frac{2}{N} \sum_k \eta_k v_k^2.$$  \hspace{1cm} (20)$$

A solution to Eq. (19) can easily be found (for $h \ll 0$):

$$u_k = \left[ 1 + \frac{\epsilon_k}{2\epsilon_k} \right]^{1/2}, \hspace{0.5cm} v_k = \text{sgn}(\epsilon_k) \left[ 1 - \frac{\epsilon_k}{2\epsilon_k} \right]^{1/2}, \hspace{1cm} (21)$$

$$\epsilon_k = \left( 1 - \frac{\gamma_k^2}{f_k} \right)^{1/2},$$
$$f_k = 1 - h\sigma - \rho \frac{\alpha}{2} (1 - \eta_k),$$  \hspace{1cm} (22)$$

where

$$\sigma = \frac{1}{4(S + R_1 - R_2)}.$$
\[ \rho = \frac{S + R_3 - R_2}{S + R_1 - R_2} \]  

(23)

(the parameter \( \rho \) is Gochev’s \( \tilde{\alpha} \)). Then one merely has to find self-consistent solutions for the two parameters \( \sigma \) and \( \rho \), given by Eqs. (23).

We can now write the Hamiltonian as

\[ H_{DM} = W_0 + H_0 + V_{DM}. \]  

(24)

The constant term is

\[
W_0 = 2N\epsilon_0 = 2N \left[ -(S + R_1 - R_2)^2 + \frac{\alpha}{2}(S + R_3 - R_2)^2 \right] + \frac{\hbar}{2}(S - R_2)
\]  

(25)

(note that there is a misprint in Gochev \( ^{19} \) at this point). The quadratic part \( H_0 \) is diagonal,

\[
H_0 = \sum_k \left( E^\alpha_k \alpha_k \alpha_k + E^\beta_k \beta_k \beta_k \right),
\]  

(26)

where the \( \alpha \) and \( \beta \) bosons have different spin-wave energies in this case,

\[
E^\alpha_k = 4S \left[ u_k^2 \left( 1 - \alpha (1 - \eta_k) - \frac{\hbar}{4S} \right) + v_k^2 \left( 1 - \frac{\hbar}{4S} \right) - 2u_k v_k \eta_k \right] + 4(R_1 - R_2)(u_k^2 + v_k^2 - 2u_k v_k \eta_k) + 4\alpha u_k^2
\]
\[
\times (R_2 - R_3)(1 - \eta_k),
\]  

(27)

and \( E^\beta_k \) is a similar expression with \( u_k \) and \( v_k \) interchanged.

The normal-ordered quartic interaction operator \( V_{DM} \) is

\[
V_{DM} = -\frac{2}{N} \sum_{N \neq 1234} \delta_{1,2,3,4} \left( \Phi^{(1)} \right)_1 \alpha_1 \alpha_2 \beta_3 \beta_4 + \Phi^{(2)} \alpha_1 \alpha_2 \beta_3 \beta_4
\]
\[
-2 \Phi^{(3)} \alpha_1 \alpha_2 \beta_3 \alpha_2 - 2 \Phi^{(4)} \alpha_1 \alpha_2 \beta_3 \beta_4 - 2 \Phi^{(5)} \beta_2 \beta_3 \beta_4 \alpha_1
\]
\[
-2 \Phi^{(6)} \alpha_1 \alpha_2 \beta_3 \beta_4 + 2 \Phi^{(7)} \beta_1 \beta_2 \beta_3 \beta_4 + 2 \Phi^{(8)} \alpha_1 \alpha_2 \beta_3 \beta_4
\]
\[
+ 4 \Phi^{(9)} \alpha_1 \alpha_2 \beta_3 \beta_4.
\]  

(28)

Explicit expressions for the vertex functions \( \Phi^{(i)}(1234) \) of the Néel phase are given in Appendix A.

### B. Higher-order corrections

To order 1 in a \( 1/S \) expansion, the ground-state energy per bond is \( \epsilon_0 \), as given by Eq. (25). The staggered magnetization per site is

\[ M_s = \frac{1}{2} \frac{\partial \epsilon_0}{\partial \sigma} \bigg|_{\sigma=0} = S - R_2, \]  

(29)

and the spin-wave energy is that given by Eq. (27).

We can now use perturbation theory to calculate the next-order \( 1/S \) corrections to these results. The leading correction to the ground-state energy corresponds to Fig. 4(a) and is given by

\[ \frac{\Delta \epsilon_0}{2N} = \left( \frac{2}{N} \right)^2 \sum_{N \neq 1234} \delta_{1,2,3,4} \Phi^{(1)}(1234) \Phi^{(2)}(3412), \]  

(30)

while the corrections to the spin-wave energies \( \epsilon^\alpha_k \) and \( \epsilon^\beta_k \) [Fig. 4(b)] are

\[ \Delta \epsilon^\alpha_k = -8 \left( \frac{2}{N} \right)^2 \sum_{N \neq 1234} \delta_{1,2,3,4} \Phi^{(6)}(1k23) \Phi^{(7)}(1k32), \]  

\[ \Delta \epsilon^\beta_k = -8 \left( \frac{2}{N} \right)^2 \sum_{N \neq 1234} \delta_{1,2,3,4} \Phi^{(10)}(1k23) \Phi^{(11)}(k321), \]  

\[ \Delta \epsilon^\alpha_k = \frac{1}{N^2} \sum_{l m} S^l - \frac{1}{N^2} \sum_{l m} S^l \phi_0 \]  

(32)

\[ \langle \phi_0 | S - R_2 - V'_M | \phi_0 \rangle, \]  

(33)

where

\[ V'_M = \sum_k (u_k^2 + v_k^2)(\alpha_k \alpha_k + \beta_k \beta_k), \]  

(34)

\[ V''_M = \sum_k 2u_k v_k (\alpha_k \beta_k + \alpha_k \beta_k). \]  

(35)

Hence the leading corrections to \( M_s \) of \( O(1/S) \) correspond to the diagrams shown in Fig. 5 and are given by
and the z axes on the sublattices $A_1$ and $A_2$ are canted at angle $\theta$ to the downwards direction as shown, where $\theta$ is a parameter to be determined. The y axes are taken to lie perpendicular to the paper in each case. In terms of spin components, we then have

$$H = \sum_{B,n,\mu} \left[ -(S_{B,n}^z S_{A,n+\mu}^z + S_{B,n}^z S_{A,n+\mu}^\dagger) \cos \theta + \eta_{n,\mu}(S_{B,n}^z S_{A,n+\mu}^\dagger - S_{B,n}^z S_{A,n+\mu}^\dagger) \sin \theta + S_{B,n}^z S_{A,n+\mu}^\dagger + \alpha \sum_{A_1,n,\mu'} \left[ (S_{A_1,n}^z S_{A_2,n+\mu'}^\dagger) \cos 2\theta + (S_{A_1,n}^z S_{A_2,n+\mu'}^\dagger) \sin 2\theta + h_1 S_{B,n}^z + h_2 \sum_{A,n} S_{A,n}^z \right] \right]$$

(40)

where the direction vectors are $\{\mu\} = \pm \mathbf{i}, \pm \mathbf{j}$, $\{\mu'\} = \pm (\mathbf{i} \pm \mathbf{j})$ and the phase factor $\eta_{n,\mu} = \pm (-1)^n$ for $\mu$ equals $\pm \mathbf{i}$ or $\pm \mathbf{j}$, respectively.

Now we introduce boson creation and annihilation operators for the spin deviation on the two sublattices by means of the Dyson-Maleev transformation,

$$S_{A,m}^z = S - \hat{a}_m^\dagger \hat{a}_m,$$

$$S_{A,m}^+ = (2S)^{1/2} \hat{a}_m,$$

$$S_{B,n}^- = (2S)^{1/2} \hat{b}_n^\dagger - (2S)^{-1/2} \hat{a}_m^\dagger \hat{a}_m \hat{b}_n,$$

$$S_{B,n}^+ = (2S)^{1/2} \hat{b}_n.$$

(41)

and perform a Fourier transform

$$\hat{a}_k = \left( \frac{2}{N} \right)^{1/2} \sum_{n} e^{ikn} \hat{a}_n,$$

$$b_k = \left( \frac{2}{N} \right)^{1/2} \sum_{m} e^{ikm} \hat{b}_m,$$

(42)

to obtain

$$H = -N S^2 \left( 2 \cos \theta - \alpha \cos 2\theta - \frac{(h_1 + h_2)}{2S} \right) + 2(N S^3)^{1/2} \left( \frac{2 \cos \theta - \frac{h_1}{2S}}{\frac{h_2}{2S}} \right) \sum_{k} b_k^\dagger b_k$$

$$+ \left( 2 \cos \theta - \alpha \cos 2\theta - \frac{h_1}{2S} \right) \sum_{k} \hat{a}_k^\dagger \hat{a}_k$$

$$- (1 + \cos \theta) \sum_{k} \gamma_k (b_k a_{-k}^\dagger + b_k^\dagger a_{-k}) + (1 - \cos \theta)$$

$$\sum_{k} \gamma_k (b_k a_{k}^\dagger + b_k^\dagger a_k) + \frac{\alpha}{2} \sum_{k} \eta_k [2(1 + \cos \theta) a_k^\dagger a_k$$

III. SPIN-WAVE THEORY FOR THE CANTED PHASE

In this section we shall present a modified spin-wave treatment of the canted phase. The formalism turns out to be somewhat more complicated in this case, and we shall only keep terms down to $O(S)$ in the energy. We write the Hamiltonian as

$$H = \sum_{(nn)} S_n^z \cdot S_{n+1} + \alpha \sum_{A,(nn)} S_n^z \cdot S_{n+1} + h_1 \sum_{B} S_n^+ + h_2 \sum_{A} S_n^z,$$

(39)

quantizing the spins with respect to the configuration shown in Fig. 3, so that the z axis on the B sublattice points upwards.
to order $S$, where, as usual,

$$\gamma_k = \frac{1}{4} \sum_\mu e^{i k \mu}, \quad \eta_k = \frac{1}{4} \sum_\mu' e^{i k \mu'}.$$  

(44)

The term of order $S^2$ is simply the classical energy of this configuration, Eq. (2). The term of order $S^{3/2}$, proportional to $(a_{x, \pi} + a_{y, \pi})^4$, would indicate that we have not chosen the optimum reference state and should be set to zero: this gives a condition on the angle $\theta$ identical to the classical condition, Eq. (3). At higher orders, this condition would give a “renormalized” value for the angle $\theta$.

The term of order $S$ is quadratic in fermion operators and can be diagonalized by a Bogoliubov transformation. In the sector involving momenta $(\pm k)$, the quadratic part of the Hamiltonian is

$$H_k = 2S \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} a_k & b_k \\ b_k^\dagger & a_k^\dagger \end{pmatrix} + N_k,$$  

(45)

where to leading order the matrix $H_k$ has elements $h_{ij}$ given by

$$h_{11} = h_{44} = 2(\cos \theta - \alpha \cos 2\theta) + \alpha(1 + \cos 2\theta) \gamma_k - \frac{h_2}{2S},$$  

(46)

$$h_{22} = h_{33} = 2 \cos \theta - \frac{h_1}{2S},$$  

(47)

$$h_{12} = h_{21} = h_{34} = h_{43} = - (1 + \cos \theta) \gamma_k,$$  

(48)

$$h_{13} = h_{31} = h_{24} = h_{42} = (1 - \cos \theta) \gamma_k,$$  

(49)

$$h_{23} = h_{32} = 0,$$  

(50)

$$h_{14} = h_{41} = - \alpha (1 - \cos 2 \theta) \gamma_k.$$  

(51)

Note that the matrix $H_k$ is symmetric about both diagonals. The normal-ordering correction to $O(S)$ is

$$N_k = - h_{11} - h_{22}.$$  

(52)

Thus the procedure here involves a $4 \times 4$ matrix diagonalization, rather than $2 \times 2$. We want a transformation which preserves commutation relations and the symmetries of the problem; i.e., we need to find a symplectic transformation

$$\begin{pmatrix} a_k \\ b_k^\dagger \end{pmatrix} = S_k \begin{pmatrix} a_k \\ b_k \\ b_k^\dagger \end{pmatrix},$$  

(53)

where the elements $s_{ij} \in S_k$ obey

$$\sum_j s_{ij} (-1)^{j+1} = (-1)^{i+1},$$  

$$\sum_j s_{ij} s_{kj} (-1)^{j+1} = 0,$$  

$$s_{ij} = s_{i+1,j},$$  

(54)

Then,

$$\hat{H}_k' = S^T \hat{H}_k S.$$  

(55)

There are initially 16 unknown parameters, corresponding to the elements of the transformation matrix $S_k$. The conditions (54) turn out to eliminate 12 of these, leaving only 4 independent parameters; these 4 parameters are determined by the condition that $\hat{H}_k'$ should be diagonal—i.e.,

$$h_{12}' = h_{13}' = h_{14}' = h_{23}' = 0.$$  

(56)

We have determined the solution to this problem numerically. In its diagonalized form, the Hamiltonian now reads

$$H_k = 2S \left[ \alpha_k a_k^\dagger a_k + \beta_k^\dagger \beta_k + \alpha_k a_k + \beta_k^\dagger \beta_k \right] + N'_k,$$  

(57)

where

$$N'_k = h_{11}' + h_{22}' - h_{11} - h_{22}.$$  

(58)

Hence one can easily obtain numerical results for the ground-state energy and single-particle dispersion relations. The staggered magnetization in the $z$ direction is given by

$$M_z = \frac{1}{N} \left\langle \psi_0 \sum_B S_B^z + \cos \theta \sum_A S_A^z + \sin \theta \left( \sum_{A_2} S_{A_2}^z \right) - \sum_{A_1} S_{A_1}^z \right\rangle \psi_0,$$  

(59)

and the net magnetization in the $z$ direction:

$$M_z = \frac{1}{N} \left\langle \psi_0 \sum_B S_B^z - \cos \theta \sum_A S_A^z - \sin \theta \left( \sum_{A_2} S_{A_2}^z \right) \right\rangle \psi_0,$$  

(60)

IV. NUMERICAL RESULTS

Numerical results for the model have been obtained using the finite-lattice method. The momentum sums were carried out for a fixed sublattice size $L = \sqrt{N/2}$, using discrete values for the momenta $k_x$ and $k_y$—e.g.,

$$024407-6$$
TABLE I. Ground-state energy per bond as a function of $\alpha$. Linear spin-wave theory: $\epsilon_0^{(1)}$. Modified second-order spin-wave theory: $\epsilon_0^{(2)}$, with higher-order corrections $\epsilon_0^{(3)}$.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$\epsilon_0^{(1)}$</th>
<th>$\epsilon_0^{(2)}$</th>
<th>$\epsilon_0^{(3)}$</th>
<th>$\epsilon_0^{(1)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>-0.32897</td>
<td>-0.33521</td>
<td>-0.33503</td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>-0.31778</td>
<td>-0.32523</td>
<td>-0.32496</td>
<td></td>
</tr>
<tr>
<td>0.2</td>
<td>-0.30666</td>
<td>-0.31543</td>
<td>-0.31509</td>
<td></td>
</tr>
<tr>
<td>0.3</td>
<td>-0.29561</td>
<td>-0.30586</td>
<td>-0.30543</td>
<td></td>
</tr>
<tr>
<td>0.4</td>
<td>-0.28465</td>
<td>-0.29652</td>
<td>-0.29602</td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>-0.27377</td>
<td>-0.28746</td>
<td>-0.28691</td>
<td>-0.27377</td>
</tr>
<tr>
<td>0.6</td>
<td>-0.26300</td>
<td>-0.27870</td>
<td>-0.27817</td>
<td>-0.25465</td>
</tr>
<tr>
<td>0.7</td>
<td>-0.25233</td>
<td>-0.27028</td>
<td>-0.26990</td>
<td>-0.24458</td>
</tr>
<tr>
<td>0.8</td>
<td>-0.24180</td>
<td>-0.26224</td>
<td>-0.26224</td>
<td>-0.24050</td>
</tr>
<tr>
<td>0.9</td>
<td>-0.23141</td>
<td>-0.25462</td>
<td></td>
<td>-0.24058</td>
</tr>
<tr>
<td>1.0</td>
<td>-0.22119</td>
<td>-0.24746</td>
<td></td>
<td>-0.24367</td>
</tr>
</tbody>
</table>

where we take half-integer values corresponding to antiperiodic boundary conditions to avoid any integrable singularities at $k=0$. Results were obtained for $L=8,9,\ldots,12$, and a fit in powers of $1/L$ was made to extrapolate to the bulk limit $L\rightarrow\infty$. The finite-size corrections for the ground-state energy per bond scale asymptotically like $1/L^2$ and those for the magnetization like $1/L$. The resulting bulk estimates are shown in Tables I and II. The values at $\alpha=0$ agree with those obtained by Gochev for the pure Heisenberg case.

Figure 6 shows the behavior of the ground-state energy resulting from the classical calculation and linear spin-wave theory for both the Néel phase and the canted phase and the modified treatment with corrections for the Néel phase. In linear spin-wave theory, the Néel and canted results coincide

$$k_i = \frac{2\pi (i-1/2)}{L}, \quad i = 1, \ldots, L,$$ (61)

at $\alpha=0.5$, as they must do since $\theta=0$ there. Somewhat surprisingly, however, the Néel energy remains the lower of the two beyond that point, until the two curves cross once more at $\alpha=0.84$. In other words, the transition between the Néel and canted phases is pushed out to $\alpha=0.84$ in linear spin-wave theory and is clearly first order. The modified treatment to second order lowers the energy a little further, while the higher-order corrections are virtually negligible and indistinguishable in the diagram.

Figure 7 shows the magnetizations $M_s$ and $M_z$ as functions of the coupling $\alpha$. In linear spin-wave theory, the staggered magnetization $M_s$ in the Néel phase is reduced by quantum fluctuations, as expected, but the effective coupling is only half that in the $J_1-J_2$ model, and so $M_s$ remains substantial at $\alpha=0.5$. In the modified second-order treatment it is lowered somewhat further, while the higher-order corrections are small and positive for low $\alpha$, and turn negative beyond $\alpha=0.7$. The staggered magnetization in the canted phase is also reduced by quantum fluctuations, although the effect is reduced at large $\alpha$.

Figure 8 illustrates the spin-wave dispersion of the $\alpha$ and $\beta$ bosons in the Néel phase as given by the second-order theory. It can be seen that the dispersion curve for the $\beta$
bosons remains virtually unchanged at all \( \alpha \). That for the \( \alpha \) bosons, however, develops an instability at \( k=(\pi,\pi) \) and the energy gap is predicted to vanish when \( \alpha \) gets too large, signaling a transition. The instability occurs at \( \alpha=1.0 \) in linear spin-wave theory and \( \alpha=0.645 \) in the modified second-order theory.

Figure 9 shows similar plots from the linear theory in the canted phase. The energy gap for the \( \beta \) bosons remains zero at all couplings, with linear dispersion near the origin, but as soon as we move away from \( \alpha=0.5 \) (i.e., \( \theta=0 \)) an energy gap opens up for the \( \alpha \) bosons, with quadratic dispersion near the origin. Now the ground state in this system has ferromagnetic order in one direction and antiferromagnetic order in another, as shown in Fig. 3, corresponding to a spontaneous symmetry breaking pattern SU(2) → 1 (or \( Z_2 \)). According to the general counting of Goldstone modes in nonrelativistic systems\(^{26}\) and with previous discussions of Goldstone modes in canted phases,\(^{27–29}\) such a system should possess one linear and one quadratic Goldstone mode: in other words, the quadratic mode should be gapless also. In general, according to Nielsen and Chadha,\(^{26}\) each linear Goldstone mode is counted once and each quadratic Goldstone mode is counted twice, the total number of “bosons” so obtained is equal to or greater than the number of symmetry generators that are spontaneously broken. It seems that the spin-wave expansion in this case breaks the symmetry of the model in such a way as to give the quadratic mode an unphysical energy gap. A more sophisticated approach is needed to avoid this problem.

V. CONCLUSIONS

The union jack lattice model is another example of a spin-1/2 Heisenberg antiferromagnet with frustration. A classical variational analysis predicts a transition at \( \alpha=0.5 \) between the Néel phase at small \( \alpha \) and a canted ferrimagnetic phase at large \( \alpha \). Thus the system exhibits a new phenomenon: namely, ferrimagnetism induced by frustration.

In linear spin-wave theory, the transition is pushed out to \( \alpha_c=0.84 \). This makes the model potentially much more interesting, because it is very likely that the Néel magnetization will vanish at or before that point. This is not evident in our spin-wave results (Fig. 7), where the Néel magnetization remains substantial at \( \alpha=0.8 \), but the spin-wave results become unreliable near the transition region, as was shown in the case of the \( J_1-J_2 \) model. In that model, numerical studies\(^{3,5,7–10,13}\) show that the Néel magnetization vanishes at about \( \alpha_c=0.38 \). The frustration in the union jack lattice model is only half as strong, as seen by a glance at Fig. 1 or from linear spin-wave theory, and so we conjecture that the magnetization will vanish at about \( \alpha_c=0.76 \) in this model. A plausible scenario, then, is that a second-order Néel transition might occur at \( \alpha_c=0.76 \), possibly followed by an intermediate spin-liquid phase as in the \( J_1-J_2 \) model, and then a first-order transition to the canted phase at somewhat larger \( \alpha \). Numerical experiments would be necessary to ascertain if this is indeed the case.

ACKNOWLEDGMENTS

We would like to thank Professor J. Oitmaa, Professor O. Sushkov, and Dr. G. Misguich for very useful discussions and advice. This work forms part of a research project supported by a grant from the Australian Research Council.

APPENDIX

The vertex functions \( \Phi^{(i)} \), \( i=1,\ldots,9 \), are

\[
\Phi^{(1)}(1234) = \gamma(4-1)u_1v_2v_3u_4 + \gamma(4-2)u_1v_2v_3u_4 + \gamma(3-1)u_1u_2v_3v_4 + \gamma(3-2)u_1v_2u_3v_4 - \gamma(4-2)u_1u_2v_3v_4 - \gamma(3-1)u_1u_2v_3v_4
\]
QUANTUM SPIN MODEL WITH FRUSTRATION ON THE...

\[ -\gamma(3)v_1v_2v_3u_4 - \gamma(4)u_1v_2v_3v_4 - \alpha Q u_1u_2v_3v_4, \]

\( (A1) \)

\( \Phi^{(2)}(1234) = \gamma(4 - 2)v_1u_2v_3u_4 + \gamma(3 - 2)v_1u_2v_3u_4 + \gamma(4 - 1)u_1v_2v_3u_4 + \gamma(3 - 1)u_2v_3u_4 + \gamma(3)u_1v_2v_3u_4 + \gamma(2)v_1v_2v_3u_4 \]

\[ + \gamma(3 - 2)v_1u_2v_3u_4 + \gamma(4 - 1)u_1v_2v_3u_4 + \gamma(3)u_1u_2v_3u_4 - \alpha Q u_1u_2v_3u_4, \]

\( (A2) \)

\( \Phi^{(3)}(1234) = \gamma(4 - 1)v_1u_2v_3u_4 + \gamma(3 - 1)v_1u_2v_3u_4 + \gamma(4 - 2)v_1u_2v_3u_4 + \gamma(3)u_1u_2v_3u_4 - \alpha Q u_1u_2v_3u_4, \]

\( (A3) \)

\( \Phi^{(4)}(1234) = \gamma(4 - 1)v_1u_2v_3u_4 + \gamma(3 - 1)v_1u_2v_3u_4 + \gamma(4 - 2)v_1u_2v_3u_4 - \alpha Q u_1u_2v_3u_4, \]

\( (A4) \)

\( \Phi^{(5)}(1234) = \gamma(4 - 1)v_1u_2v_3u_4 + \gamma(3 - 2)v_1u_2v_3u_4 + \gamma(3)u_1u_2v_3u_4 - \alpha Q u_1u_2v_3u_4, \]

\( (A5) \)

\[ \Phi^{(6)}(1234) = \gamma(4 - 1)u_1u_2u_3v_4 + \gamma(3 - 2)v_1v_2v_3u_4 + \gamma(3 - 1)v_1v_2v_3u_4 + \gamma(3)u_1v_2v_3u_4 + \gamma(2)v_1v_2v_3u_4 \]

\[ + \gamma(3 - 2)v_1u_2v_3u_4 + \gamma(4 - 1)u_1v_2v_3u_4 + \gamma(3)u_1u_2v_3u_4 - \alpha Q u_1u_2v_3u_4, \]

\( (A6) \)

\( \Phi^{(7)}(1234) = \gamma(4 - 2)v_1u_2v_3u_4 + \gamma(3 - 2)v_1u_2v_3u_4 + \gamma(3)u_1u_2v_3u_4 - \alpha Q u_1u_2v_3u_4, \]

\( (A7) \)

\( \Phi^{(8)}(1234) = \gamma(4 - 2)v_1u_2v_3u_4 + \gamma(3 - 1)v_1u_2v_3u_4 + \gamma(3)u_1u_2v_3u_4 - \alpha Q u_1u_2v_3u_4, \]

\( (A8) \)

\( \Phi^{(9)}(1234) = \gamma(4 - 2)v_1u_2v_3u_4 + \gamma(3 - 2)v_1u_2v_3u_4 + \gamma(3)u_1u_2v_3u_4 - \alpha Q u_1u_2v_3u_4, \]

\( (A9) \)

where

\[ Q = \eta(3 - 2) + \eta(4 - 2) - \eta(3) - \eta(4). \]

\( (A10) \)

2494 (1989).


