The $S=\frac{1}{2}$ Heisenberg antiferromagnet on the triangular lattice: exact results and spin-wave theory for finite cells

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We study the ground state properties of the $S=\frac{1}{2}$ Heisenberg antiferromagnet (HAF) on the triangular lattice with nearest-neighbour ($J$) and next-nearest neighbour ($\alpha J$) couplings. Classically, this system is known to be ordered in a 120° Néel type state for values $-\infty < \alpha \leq 1/8$ of the ratio $\alpha$ of these couplings and in a collinear state for $1/8 < \alpha < 1$. The order parameter $M$ and the helicity $\chi$ of the 120° structure are obtained by numerical diagonalisation of finite periodic systems of up to $N = 30$ sites and by applying the spin-wave (SW) approximation to the same finite systems. We find a surprisingly good agreement between the exact and the SW results in the entire region $-\infty < \alpha < 1/8$. It appears that the SW theory is still valid for the simple triangular HAF ($\alpha = 0$) although the sublattice magnetisation $M$ is substantially reduced from its classical value by quantum fluctuations. Our numerical results for the order parameter $N$ of the collinear order support the previous conjecture of a first order transition between the 120° and the collinear order at $\alpha \simeq 1/8$.

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1 Introduction

Owing to the observation of quasi two dimensional antiferromagnetism in the undoped phase of high $T_c$ superconductors \cite{1}, the theory of two dimensional quantum antiferromagnetism has received much attention recently. The continuing discussion focuses on the question of whether or to which extent the classical picture of a Néel type ordered ground state remains valid in the presence of quantum fluctuations which are known to be particularly important in low dimensional systems. For the spin-1/2 isotropic Heisenberg antiferromagnet (HAF) with nearest neighbour interaction on a square lattice this question has been settled: the result of numerous quantum Monte Carlo (MC) simulations \cite{2} leave no doubt about the existence of Néel order in the ground state of the square lattice HAF. Moreover, by refined MC techniques \cite{3} it has been possible to determine the staggered magnetisation $M$ of this state with high accuracy. Quantum fluctuations are found to reduce $M$ to about 60% of its classical value, but surprisingly the relative difference between the most accurate numerical value $M = 0.3074(4)$ and the value obtained in first order spin-wave (SW) approximation $M_{1,SW} = 0.30340$ is only about 1%. Long range order is opposed not only by quantum fluctuations but also by frustration. For a spin-1/2 Heisenberg model, frustration is defined in the sense introduced by Toulouse \cite{4} for the z-z part of the coupling and, with respect to the x-x and y-y parts of the interaction, by the impossibility of using the Marshall Ansatz \cite{5} for the ground state wave function \cite{6}. The HAF on a triangular lattice (HAFT) which will be studied in this work is the prototypical example of a frustrated antiferromagnet. In early work, Anderson and Fazekas \cite{7} suggested that the combined effect of quantum fluctuations and of frustration would favour a disordered overall singlet state over an ordered Néel type ground state. The state proposed by Anderson and Fazekas consists of products of singlet pair states and is commonly referred to as a resonating valence bond (RVB) state. It has received much attention in the theory of high $T_c$ superconductivity. Numerous subsequent investigations have led to contradictory views of the ground state of the HAFT. The spin-wave analysis \cite{8,9} predicts that quantum fluctuations are insufficient to suppress the classical
Néel order. Certain variational calculations support this conclusion \cite{10}, others contradict it. In fact, an exotic RVB-type state which breaks time reversal invariance and parity has also been obtained by a variational method \cite{11}. Several attempts have been made to determine the nature of the ground state of the HAFT by extrapolating from results obtained by the exact numerical diagonalisation of the Hamiltonian of small periodic cells \cite{12, 13}. In all of these studies the results of the extrapolations have been interpreted as being indicatory of a disordered ground state or of a state that is close to the critical point of losing long range order. The analysis of a high-order perturbation expansion has lent support to this view \cite{14}. However, by extending the numerical studies of finite cells to include not only the ground state energy but the entire spectrum of the HAFT and by an appropriate interpretation of their results Bernu et. al. \cite{15} have very recently given convincing arguments in favour of a Néel ordered ground state of the HAFT. In view of the experience with spin-1/2 square lattice HAF, it might thus be hoped that the SW approximation also yields accurate results for the physical quantities of the HAFT. It is one of the purposes of this study to show that the results obtained by the exact numerical diagonalisation of small cells of the HAFT do indeed point towards the validity of the SW approximation.

With regard to this purpose it will prove useful to consider the HAFT with nearest (nn) and next nearest neighbour (nnn) interaction,

\begin{equation}
H = \sum_{nn} S_i S_j + \alpha \sum_{nnn} S_i S_j \tag{1.1}
\end{equation}

where $S_i$ denotes a spin-1/2 operator at the lattice site $R_i$. (We set the nn coupling equal to unity without loss of generality). As is seen in Fig. 1, the nnn interaction couples spin pairs within each of the three sublattices. Therefore, for sufficiently strong ferromagnetic nnn coupling, $-\alpha \gg 1$, the spins of each sublattice will order ferromagnetically, forming a macroscopic spin. In this situation, a SW expansion will certainly be applicable. Thus, the parameter region $-\alpha \gg 1$ of the model (1.1) provides a firm basis for a comparison of the SW approximation and of the exact numerical result.

The model (1.1) is also of considerable interest in its own right. In the classical approx-
imation one finds that its ground state changes discontinuously from the $120^\circ$ three sublattice state for $\alpha < \alpha_{cl} = 1/8$ to a four sublattice state for $\alpha_{cl} < \alpha < 1$ \cite{10}, Fig. 2. The four-sublattice state is degenerate with respect to the angle $\theta$, i.e. its energy is $E = -2(1 + \alpha)$ independent of $\theta$. As has been shown in Ref. \cite{10} quantum fluctuations select the state with $\theta = 0$ from the continuum of degenerate four sublattice states. We shall refer to this state, which is a two sublattice structure, as the collinear state. At $\alpha = 1$ the ground state structure changes again to become incommensurate for $\alpha > 1$. In the limit $\alpha \to \infty$, the three sublattices decouple so that a $120^\circ$ structure exists on each of them. The manifold of classical ground states of (1.1) that evolves as $\alpha$ increases from $-\infty$ to $\infty$ is concisely described by

$$S_i = \hat{e}_1 \cos QR_i + \hat{e}_2 \sin QR_i,$$

where $\hat{e}_1$ and $\hat{e}_2$ are an arbitrary pair of orthogonal unit vectors and where $Q = Q(\alpha)$ traces out the path in the Brillouin zone shown in Fig. 3.

The question of how the transition between the $120^\circ$ and the collinear state of the HAFT with $nn$ and $nnn$ couplings is affected by quantum fluctuations has attracted considerable interest \cite{10, 17, 18, 19}. If both types of long range order survive at the quantum level, the transition between them may be of first order, i.e. the order parameters of both states may remain finite at the transition point so that the symmetry breaking pattern changes discontinuously. Alternatively, one or both types of long range order could be suppressed in the vicinity of the classical transition point, and an intermediate ordered or disordered state could appear at the quantum level. Disregarding the first possibility, Baskaran conjectured that a time reversal and parity breaking chiral spin liquid state should evolve as the ground state of the model (1.1) when $\alpha$ exceeds a critical value \cite{17}. In a previous study \cite{18}, we could not confirm this conjecture. More recently, Chubukov and Jolicoeur \cite{19} investigated the collinear structure by a self-consistent SW approximation. These authors find that the stability region of the collinear structure extends to values of $\alpha < \alpha_{cl}$ and argue that the transition between the $120^\circ$ and the collinear structure should be of first order. It is the second purpose of this paper to provide and discuss further results concerning this
transition.

In section 2 we work out the second order SW expansion for physical properties of the HAFT pertaining to the 120° structure, and we show how finite size results are obtained within the SW approximation. Section 3 contains our numerical results for physical properties that characterise the ordered states of our model (1.1): the sublattice magnetisations, the helicity and the chirality. The emphasis is on a direct comparison of the exact numerical results with the predictions of the SW-theory for finite systems and on the discussion of the behaviour of the order parameters in the transition region between the 120° structure and the collinear structure. In section 4 we summarise our conclusions. Technical details are deferred to three appendices.

2 Spin-wave approximation

To order $1/S$, the spin-wave approximation for the model (1.1) has been discussed by Jolicœur et al [8] and a calculation of the $1/S^2$ corrections to the spin-wave spectrum of the collinear state has been performed by Chubukov and Jolicœur [19]. Furthermore, for $\alpha = 0$ the $1/S^2$ correction to the sublattice magnetisation has been obtained by Miyake [9]. Below we present the results of an extension of Miyake’s calculation to the range $-\infty \geq \alpha \geq 1/8$ where the 120° state is supposedly stable. With the objective of comparing the SW approximation with our numerical results we also include the first and second order results for the helicity of the 120° structure, and we discuss the finite size corrections to the sublattice magnetisation and the helicity.

The starting point of the SW expansion is the Hamiltonian

$$H = \sum_{nn} H_{ij} + \alpha \sum_{nmm} H_{ij} - B \sum_i \tilde{S}_i^z,$$

$$H_{ij} = \cos \theta_{ij} (\tilde{S}_i^x \tilde{S}_j^x + \tilde{S}_i^z \tilde{S}_j^z) + \sin \theta_{ij} (\tilde{S}_i^z \tilde{S}_j^x - \tilde{S}_i^x \tilde{S}_j^z) + \tilde{S}_i^y \tilde{S}_j^y$$ (2.1)

with $\theta_{ij} = \theta_j - \theta_i$,

which is obtained from (1.1) by rotating the local z-axis to the direction of the classical
sublattice magnetisation:

\[
S^x_i = \cos \theta_i \tilde{S}^x_i + \sin \theta_i \tilde{S}^z_i, \quad S^y_i = \tilde{S}^y_i, \quad S^z_i = \cos \theta_i \tilde{S}^z_i - \sin \theta_i \tilde{S}^x_i. \tag{2.2}
\]

For the 120° state \( \theta_i = 0, 2\pi/3, -2\pi/3 \), when \( i \) is a site of the sublattice A, B or C while \( \theta_i = 0, \pi \) on the sites of the two sublattice A or B of the collinear state. \( B \) represents a staggered magnetic field. From (2.1) the SW expansion is obtained by replacing the spin-operators \( \tilde{S}^\alpha_i \) by Holstein-Primakoff boson operators and by expanding with respect to \( 1/S \). In the case of the 120° state the result is

\[
H = S^2 (H_0 + H_1 + H_{3/2} + H_2), \tag{2.3}
\]

with

\[
H_0 = -\frac{3}{2} (1 + 2\alpha) N - \frac{B}{S} N, \tag{2.4a}
\]

\[
H_1 = -\frac{1}{S} \sum_{nn} \left\{ -\frac{1}{4} (a_i^+ a_j + h.c.) + \frac{3}{4} (a_i^+ a_j^+ + h.c.) - \frac{1}{2} (n_i + n_j) \right\}
+ \frac{B}{S} \sum_i n_i + \frac{\alpha}{S} \sum_{nn} \left\{ (a_i^+ a_j + h.c.) - (n_i + n_j) \right\}, \tag{2.4b}
\]

\[
H_{3/2} = -\sqrt{\frac{2}{3S}} \sum_{nn} \sin \theta_{ij} (n_i a_j + h.c.), \tag{2.4c}
\]

\[
H_2 = -\frac{1}{S^2} \sum_{nn} \left\{ \frac{1}{2} (n_i n_j) + \frac{1}{8} (n_i a_i a_j^+ + h.c.) - \frac{3}{8} (n_i a_i a_j + h.c.) \right\}
+ \frac{\alpha}{S^2} \sum_{nnn} \left\{ n_i n_j - (n_i a_i a_j^+ + h.c.) \right\}. \tag{2.4d}
\]

Diagonalisation of \( H_1 \) yields the SW frequency (we adopt the notation of Miyake [9] wherever possible):

\[
\omega(k, B) = 3S \nu(k, B)
= 3S \sqrt{\left(1 + \frac{B}{3S} - 2\alpha(k) - \gamma(k)\right) \left(1 + \frac{B}{3S} - 2\alpha(k) + 2\gamma(k)\right)}, \tag{2.5}
\]

where

\[
\alpha(k) = \alpha - \frac{\alpha}{3} \left( \cos(\sqrt{3}k_y) + \cos\left(\frac{3k_x}{2} + \frac{\sqrt{3}k_y}{2}\right) + \cos\left(\frac{3k_x}{2} - \frac{\sqrt{3}k_y}{2}\right) \right), \tag{2.6a}
\]

\[
\gamma(k) = \frac{1}{3} \left( \cos(k_x) + \cos\left(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2}\right) + \cos\left(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2}\right) \right). \tag{2.6b}
\]
For $\alpha < 1/8$, $\omega(k, 0) \equiv \omega(k)$ vanishes linearly in the centre of the Brillouin zone (BZ) and at opposite corners $k = \pm Q_1 = \pm (4\pi/3, 0)$. The zero modes are the three Goldstone modes of the symmetry broken state. The two modes at $\pm Q_1$, which are degenerate, correspond to an infinitesimal tilt of adjacent plaquettes of three spins around two orthogonal axes in the plane defined by the ideally ordered classical state. The third mode at $k = 0$ whose SW velocity is larger than that of the previous ones by a factor of $\sqrt{2}$ corresponds to an infinitesimal twist of adjacent plaquettes around an axis that is perpendicular to the plane defined by the $120^\circ$ state.

As $\alpha$ approaches the value $1/8$ from below, the SW frequency softens at $Q_2^{(1)}$, $Q_2^{(2)}$ and $Q_2^{(3)}$, Fig. 3, yielding new linear excitation branches at these points. Within this first order approximation, these new modes indicate the onset of collinear order at $\alpha = 1/8$. They are, however, unphysical since they are not Goldstone modes of the $120^\circ$ state.

In first order in $1/S$ the sublattice magnetisation is given by the expression

$$M_{1,SW} = S \left\{ 1 + \frac{1}{4S} \frac{1}{N} \sum_k (2 - A_1(k) - A_2(k)) \right\}, \quad (2.7)$$

where

$$A_1(k) = \frac{1 - 2\alpha(k) + 2\gamma(k)}{1 - 2\alpha(k) - \gamma(k)}, \quad A_2(k) = A_1(k)^{-1}.$$ 

To obtain the second order correction $M_{2,SW}$ we follow the method of Miyake and calculate the $1/S^2$ correction to the ground state energy

$$E_0^{(2)}(\alpha, B) = S^2 \langle H_2 \rangle_0 + S^2 \sum_{\{n_k\}} \frac{|\langle \{n_k\} | H_{3/2} | \{0\} \rangle|^2}{E(\{0\}) - E(\{n_k\})}, \quad (2.8)$$

where $\{n_k\}$ is an eigenstate of $H_1$ and $E(\{n_k\})$ is the corresponding energy

$$E(\{n_k\}) = \sum_k (n_k + 1/2) \omega(k). \quad (2.9)$$

The explicit expressions are given in the App. A. As in the case $\alpha = 0$ considered by Miyake, both contributions to $E_0^{(2)}(\alpha, B)$ contain singular parts proportional to $\sqrt{B}$ which, however, can be shown to cancel in the sum $(2.8)$. This feature has been utilised to control
the precision of the numerical computation of the integrals contributing to \( E_{0}^{(2)}(\alpha, B) \) and to extract the second order correction \( M_{2,SW} \) to the magnetisation from \( E_{0}^{(2)}(\alpha, B) \) in the small \( B \) limit,

\[
M_{2,SW} = - \frac{1}{N} \lim_{B \to 0} \frac{E_{0}^{(2)}(\alpha, B) - E_{0}^{(2)}(\alpha, 0)}{B}.
\] (2.10)

In Fig. 4a we show plots of \( M_{1,SW} \) and of the sum \( M_{1,SW} + M_{2,SW} \). A plot of \( M_{2,SW} \) is included in Fig. 8. Owing to the unphysical zeros which develop in \( \omega(k) \) at \( Q_{2}^{(1)}, Q_{2}^{(2)}, Q_{2}^{(3)} \) as \( \alpha \) approaches \( \alpha_{cl} \) the second order contribution \( M_{2,SW} \) diverges at \( \alpha = \alpha_{cl} \). However, \( M_{2,SW} \) enhances the sublattice magnetisation also for \( \alpha \approx 0.05 \) where the influence of the divergence is still small. Thus, it appears that the stability region of the 120° structure extends beyond \( \alpha_{cl} \) and hence overlaps with the stability region of the collinear structure. This corroborates the argument of Chubukov and Jolicoeur \[19\] according to which the transition between the two structures should be of first order.

In the classical 120° state an Ising-like variable can be attached to each triangular plaquette of the lattice \[21\]. It takes the values ±1 depending on whether the spins on the three sites of the plaquette turn clockwise or counterclockwise. For the quantum system the operator associated with this variable - we shall call it helicity - has been defined by

\[
\hat{\chi}_{\triangle} = \frac{2}{\sqrt{3}} (S_{i} \times S_{j} + S_{j} \times S_{k} + S_{k} \times S_{i}),
\] (2.11)

where \( i, j \) and \( k \) denote the sites of an elementary triangular plaquette in a clockwise sense. The normalisation has been chosen such that each component of \( \hat{\chi}_{\triangle} \) has eigenvalues +1, 0 and −1. Long range helicity order is measured by the expectation value \[22\]

\[
\chi^{y} = \frac{1}{N} \sum_{\triangle} \langle \hat{\chi}_{\triangle}^{y} \rangle,
\] (2.12)

where the sum extends over all upward pointing triangles of the lattice. Long range helicity order can exist in the absence of long range 120° order. In that case it is the signature of a spin nematic \[23\]. It must necessarily exist for a state that possesses long range 120° order. In the local reference frame (2.2) of the 120° state, \( S_{i} \times S_{j} \) takes the form

\[
(S_{i} \times S_{j}) \cdot \hat{e}_{y} = \sin \theta_{ij} (\tilde{S}_{i}^{z} \tilde{S}_{j}^{x} + \tilde{S}_{i}^{x} \tilde{S}_{j}^{z}) + \cos \theta_{ij} (\tilde{S}_{i}^{x} \tilde{S}_{j}^{z} - \tilde{S}_{i}^{z} \tilde{S}_{j}^{x}).
\] (2.13)
From this expression one immediately obtains the order parameter $\chi^y$ in first order SW approximation

$$\chi^y_{1,SW}(\alpha) = 3S^2 \left\{ 1 + \frac{1}{2S} \frac{1}{N} \sum_{\mathbf{k}} (2 - A_1(\mathbf{k}) - A_2(\mathbf{k}) - B_1(\mathbf{k})) \right\}$$

$$= 3S^2 \left\{ 1 + \frac{2}{S} (\mathcal{M}_{1,SW} - S) + \frac{1}{2S^3} \langle \tilde{S}_i^x \tilde{S}_j^x \rangle_{1,SW} \right\}, \quad (2.14)$$

where

$$B_1(\mathbf{k}) = \gamma(\mathbf{k}) A_1(\mathbf{k}). \quad (2.15)$$

A plot of $\chi_{1,SW}(\alpha)$ is contained in Fig. 4b. As is described in App. A, the second order correction $\chi_{2,SW}$ can be obtained by the same technique as has been applied in calculating $\mathcal{M}_{2,SW}$. A plot of $\chi_{2,SW}(\alpha)$ is included in Fig. 10. For $\alpha \lesssim -1$, the quantum fluctuations are seen to enhance $\chi^y$ slightly over the classical value. Quite generally, the quantum fluctuations are seen to be less effective in reducing the helicity $\chi^y$ than in reducing the magnetisation $\mathcal{M}$. This is not unexpected, since the long wavelength modes that twist the spin configuration around the axis perpendicular to the plane of the 120$^\circ$ structure are ineffective in reducing $\chi^y$.

As we have explained above we need to evaluate the SW expressions (2.7) and (2.14) for finite periodic systems. This requires modifications, since in (2.7) and (2.14) the members of the $\mathbf{k}$ sums that correspond to the zero modes $\mathbf{k} = 0$ and $\mathbf{k} = \pm Q_1$ are infinite. In his seminal work on quantum antiferromagnetism, Anderson [24] has pointed out that these infinities are unphysical, yet unavoidable consequences of the basic assumptions underlying the SW theory. In previous work on finite size effects [25] it has been shown that the leading size correction to $\mathcal{M}_{1,SW}(0, N)$ is obtained by omitting the infinite contributions $A_1(\mathbf{k} = 0)$ and $A_2(\mathbf{k} = \pm Q_1)$ from the sum in (2.7). As we show in App. B this omission yields an unphysical result in the limit of strong ferromagnetic $nnn$ coupling, $-\alpha/N \gg 1$,

$$\lim_{-\alpha/N \to \infty} \mathcal{M}_{1,SW}(\alpha, N) = S \left\{ 1 + \frac{1}{2S} \frac{3}{N} \right\} > S. \quad (2.16)$$
At the same time we find that the expression
\[
\mathcal{M}_{1,SW}(\alpha, N) = S \left\{ 1 + \frac{1}{4S} \frac{1}{N} \sum_{k \in BZ, k \neq 0, \pm Q_1} (2 - A_1(k) - A_2(k)) \right\},
\] (2.17)
in which not only the infinite parts of the zero mode contributions but also the finite parts have been neglected, yields the correct result
\[
\lim_{-\alpha/N \to \infty} \mathcal{M}_{1,SW}(\alpha, N) = S.
\] (2.18)
Furthermore, for finite \(\alpha\) the leading \(1/\sqrt{N}\) size correction remains unaffected by the neglect of the finite parts of the zero mode contributions. Thus, (2.17) qualifies as a finite size approximant for \(\mathcal{M}_{1,SW}\) in the entire region \(-\infty \leq \alpha \leq 1/8\) where the 120° structure is classically stable. Of course, for a specified finite periodic system of size \(N\) the sum (2.17) has to be extended over that discrete set of inequivalent \(k\)-vectors which represents the system in the \(k\) space. Plots of \(\mathcal{M}_{1,SW}(0, N)\) obtained in this way and of the asymptotics
\[
\mathcal{M}_{1,SW}(0, N) = \mathcal{M}_{1,SW}(0, \infty) + \frac{1.215}{\sqrt{N}},
\] (2.19)
are shown in Fig. 5. Obviously, for \(N \lesssim 10^2\) the subleading \(N^{-1}\) corrections preclude the use of the asymptotics (2.19) in an extrapolation to the bulk limit. Fig. 5 also contains a plot of
\[
\mathcal{M}_{1,SW}(0, N) = \mathcal{M}_{1,SW}(0, \infty) + \frac{1.215}{\sqrt{N}} - \frac{3}{2N},
\] (2.20)
in which the last term is the subleading correction that obtains in the limit \(-\alpha/N \gg 1\), App. B. Evidently, (2.20) provides a good approximation for \(\mathcal{M}_{1,SW}(0, N)\). The remaining fluctuations in the data points reflect the dependence of \(\mathcal{M}_{1,SW}(0, N)\) on the shape of the finite cells, i.e. on the specific set of \(k\) points to be used in (2.17).

By analogy with (2.17) we define the finite size approximants for the helicity by
\[
\chi_{1,SW}^\gamma(\alpha, N) = 3S^2 \left\{ 1 + \frac{1}{2S} \frac{1}{N} \sum_{k \in BZ, k \neq 0, \pm Q_1} (2 - A_1(k) - A_2(k) + B_1(k)) \right\}.
\] (2.21)
In principle, finite size values for the second order quantities $M_{2,SW}$ and $\chi_{2,SW}$ can also be obtained by omitting the contributions of the zero modes. However, in practice the results for $E_0^{(2)}(\alpha, B, N)$ turn out to depend irregularly on $\sqrt{B}$ so that the extrapolation (2.10) is not feasible.

3 Numerical results

Presently, exact results for the HAFT are available for system sizes up to $N = 36$ [13, 15]. Thus, in view of the results of the last section there is little use in attempting to extrapolate from such system sizes to the bulk properties of the HAFT. Clearly, however, one expects to find agreement between the exact results and finite size SW results of the previous section, at least in the region $-\alpha \gg 1$ where the SW approximation has a firm basis.

In the following subsections we shall discuss the order parameters $M$ and $N$ of the $120^\circ$ structure and of the collinear structure (subsections 3.1a and 3.1b). The helicity $\chi$ and the chirality $P$ will be studied in subsections 3.2 and 3.3. The numerical calculations include cells of sizes $N = 12, 18, 21, 24, 27$ and $30$ with periodic boundary conditions, Figs. 6a-f.

The translationally invariant $N = 21$ and $27$ cells are fully symmetric under the $C_{6v}$ symmetry group of the Hamiltonian but they do not accommodate the $2 \times 1$ cell of the order parameter of the collinear state. Since we are interested in obtaining both the order parameter of the $120^\circ$ state, whose unit cell is of size $\sqrt{3} \times \sqrt{3}$, and that of the collinear phase we include the $N = 18, 24$ and $30$ cells, which accommodate both unit cells but are not symmetric under all $C_{6v}$ operations. We diagonalise the Hamiltonian (1.1) for these finite systems by using the Lanczos algorithm. For $\alpha < 1/8$, the ground state of cells with an even number of sites are translationally invariant singlets, $S_{\text{tot}} = 0$, $Q = Q_0 = 0$, while the ground state of cells with an odd number sites are doublets, $S_{\text{tot}} = 1/2$, with wavevector $Q_1 = (4\pi/3, 0)$. At some value $\alpha > 1/8$ the ground state of the $N = 18$ and the $N = 30$ cells cross over to the wavevector $Q_2$, which is the Bragg vector of the collinear state. As has been discussed in [18] for the case $N = 21$, when $\alpha$ exceeds a critical value $\alpha_{qu}(N) > 1/8$ ($\alpha_{qu}(21) = 0.253$, $\alpha_{qu}(27) = 0.130$) the ground state of cells with odd $N$ cross
over to a wavevector $Q \neq Q_2$, since the periodicity of the collinear state is incompatible with the periodicity of these cells. We notice that the same type of behaviour already occurs at the classical level. For the $N = 21$ and the $N = 27$ cell the classical ground state jumps from $Q = Q_1$ to a $Q \neq Q_2$ at $\alpha_{cl}(21) = 0.173$ and $\alpha_{cl}(27) = 0.129$.

### 3.1 Sublattice magnetisation

#### 3.1a The 120° order

As a measure for the sublattice magnetisation $M$ of the 120° structure we calculate the structure function

$$S_N(Q_1) = \sum_{i,j} e^{iQ_1(r_i - r_j)} \langle S_i S_j \rangle_0$$

with $Q_1 = (4\pi/3, 0)$ (3.1)

from our numerically determined ground states. To find the connection between $S_N(Q_1)$ and the finite size approximants $\mathcal{M}(\alpha, N)$ for the sublattice magnetisation we consider the limit of large ferromagnetic $nnn$ coupling, $-\alpha \gg 1$. In this limit the spins of each of the sublattices A, B and C will align ferromagnetically forming macroscopic spins of magnitude

$S_A = S_B = S_C = N/6$. These macroscopic spins may fluctuate against each other so that the total spin $S_{tot} = |S_A + S_B + S_C|$ agrees with the values found in the numerical calculation, i.e. $S_{tot}(N) = 0$ for even $N$ and $S_{tot}(N) = 1/2$ for odd $N$. A simple calculation which is detailed in App. C yields

$$\lim_{\alpha \to -\infty} S_N(Q_1) = \begin{cases} \frac{1}{8} + \frac{3}{4N} & , \ N \text{ even}, \\ \frac{1}{8} + \frac{3}{4N} - \frac{3}{8N^2} & , \ N \text{ odd}. \end{cases}$$

(3.2)

Since

$$\lim_{\alpha \to -\infty} \mathcal{M}(\alpha, N) = \frac{3}{N} S_A = \frac{3}{N} S_B = \frac{3}{N} S_C = \frac{1}{2}$$

it follows from (3.2) that in the limit $\alpha \to -\infty$

$$\mathcal{M}^2(\alpha, N) = \begin{cases} 2 \left( \frac{S_N(Q_1)}{N^2} - \frac{3}{4N} \right) & , \ N \text{ even}, \\ 2 \left( \frac{S_N(Q_1)}{N^2} - \frac{3}{4N} + \frac{3}{8N^2} \right) & , \ N \text{ odd}. \end{cases}$$

(3.3)
Here, the factor of 2 reflects the fact that $S_N(Q_1)$ is the structure factor of only one of the two $120^\circ$ structures with wave vectors $\pm Q_1$ which are contained in the ground state with equal weight. The above considerations suggest that (3.3) still holds approximately for $-\alpha > 1$. The same argument also suggests that for $-\alpha > 1$ the numerically exact results $M(\alpha, N)$ should be well approximated by the finite size SW results $M_{SW}(\alpha, N)$. Plots of $M_{1,SW}^2(\alpha, N)$, i.e. of the first order SW result (2.17), and of $M^2(\alpha, N)$ as functions of $\alpha$ are shown in Figs. 7a-f. The difference

$$\Delta M(\alpha, N) = M(\alpha, N) - M_{1,SW}(\alpha, N)$$

(3.4)
is displayed in Fig. 8 together with the second order SW correction $M_{2,SW}$. Obviously, the asymmetric $N = 18$ cell yields exceptionally large values for $\Delta M$. Apart from this exception, the first order SW approximation is seen to approximate the exact results remarkably well even for small values of $|\alpha|$ where quantum fluctuations evidently lead to a considerable reduction of $M$ from its classical value. Notably, for negative values of $\alpha$ up to $\alpha \simeq -0.1$, the difference $\Delta M$ depends only weakly on the system size $N$. In this region, the second order correction $M_{2,SW}(\alpha)$ overestimates the difference between the first order SW approximation and the exact results. This is reminiscent of the SW expansion for the $S = 1/2$ square lattice HAF in which the third order correction is found to reduce the discrepancy between the exact results and the SW approximation by about 50% [24]. For $\alpha \to \alpha_{cl}$, $M_{2,SW}$ increases faster than $\Delta M$. It is tempting to attribute this discrepancy to the unphysical divergence of $M_{2,SW}(\alpha)$ at $\alpha_{cl}$. A selfconsistent SW treatment [19] which eliminates this divergence is certainly called for.

3.1b The collinear order

As in the case of the $120^\circ$ order we use the structure function $S_N(Q_2)$ at the Bragg vector $Q_2$ of the collinear structure as a measure for the order parameter $N$. If the collinear order of the ground states of the finite cells were perfect the same steps that led to the
relations \((3.3)\) would yield
\[
\mathcal{N}^2(N) = f \left( \frac{S_N(Q_2)}{N^2} - \frac{1}{N} \right).
\]
(3.5)

The factor \(f\) counts the number of inequivalent \(Q_2\) vectors in the BZ. Hence, we get \(f = 3\) for the \(C_{6v}\) symmetric \(N = 12\) cell, and \(f = 1\) for the \(N = 18, 24, 30\) cells which are not \(C_{6v}\) symmetric.

As in the previous subsection we assume that the relation \((3.3)\) still holds approximately when the ground state is not perfectly ordered. Figs. 7a,b,d and f show plots of \(\mathcal{N}^2(\alpha, N)\) for \(\alpha \geq 1/8\) obtained by employing the numerical values of \(S_N(Q_2)\) in \((3.3)\). The maxima of \(\mathcal{N}(\alpha, 18)\) and \(\mathcal{N}(\alpha, 24)\) are seen to be only slightly reduced from the saturation value \(\mathcal{N} = 1/2\). This lends support to our assumption about the validity of \((3.3)\). The stronger reduction of \(\mathcal{N}^2(\alpha, 12)\) and the small discontinuity in \(\mathcal{N}^2(\alpha, 12)\) at \(\alpha = 0.225\) can be attributed to certain peculiarities of the \(N = 12\) cell which will be discussed elsewhere [27].

In the transition region \(\alpha \simeq \alpha_{cl}\), the behaviour of \(\mathcal{N}(\alpha, N)\) is seen to differ qualitatively between the different system sizes. While \(\mathcal{N}(\alpha, 12)\) and \(\mathcal{N}(\alpha, 24)\) grow smoothly with \(\alpha\), \(\mathcal{N}(\alpha, 18)\) increases discontinuously at \(\alpha_{qu}(18) = 0.23\). This discontinuity is due to a crossover in the ground state of the \(N = 18\) system whose translational symmetry changes from \(Q = 0\) to \(Q = Q_2\) as \(\alpha\) increases through \(\alpha = \alpha_{qu}(18)\). In the classical picture ([1.2]), the wavevector \(Q_2\) characterises the periodicity of the collinear state so that for \(\alpha > \alpha_{qu}(18)\) the ground state of the \(N = 18\) system, \(|Q_2\rangle\), has the same periodicity as the classical state. For the \(N = 30\) system we observe the same type of crossover between ground states at \(\alpha_{qu}(30) = 0.2\). Because of limitations in computer memory we have not been able to calculate \(\mathcal{N}(30)\) for \(\alpha > \alpha_{qu}(30)\) where we would have had to work with a translationally noninvariant ground state \(|Q_2\rangle\). One can be sure, however, that the crossover between ground states will also result in a discontinuity in \(\mathcal{N}(30)\) at \(\alpha = \alpha_{qu}(30)\). The difference between the \(N = 12\) and \(N = 24\) systems, for which the ground state remains at \(Q = 0\) for all values of \(\alpha\), and the \(N = 18\) and \(N = 30\) systems is reminiscent of Marshall’s rule concerning the ground state of the square lattice HAF [3]: the ground state is translationally invariant, if the system size \(N\) is a multiple of 4;
otherwise, when $N$ is even but not a multiple of 4, it has the periodicity of the classical state.

As has been discussed in section 2 the SW theory suggests that the transition between the $120^\circ$ structure and the collinear structure is of first order. The discontinuities in the order parameter $\mathcal{N}$ of the $N = 18$ and $N = 30$ systems directly confirm this prediction. For the system sizes $N = 12$ and $N = 24$, the plots of $\mathcal{N}$ and $\mathcal{M}$ are seen to overlap in a finite interval around $\alpha = \alpha_{cl}$, Figs. 7a,d. While the overlap region decreases when the system size is doubled from $N = 12$ to $N = 24$, the slopes of $\mathcal{N}$ and $\mathcal{M}$ are seen to increase drastically at the transition points. These features agree with the behaviour of the order parameters of finite systems that exhibit a first order transition in the bulk limit. In summary, our numerical results support the view of a first order transition between the $120^\circ$ structure and the collinear structure of the HAFT.

### 3.2 Helicity

We wish to compare the SW results $\chi_\text{SW}^y(N)$ and the exact values of the helicity. Numerically we calculate

$$\left\langle \left( \frac{1}{N} \sum_\Delta \hat{\chi}_\Delta \right)^2 \right\rangle = 3 \left\langle \left( \frac{1}{N} \sum_\Delta \hat{\chi}_\Delta^k \right)^2 \right\rangle,$$

where $\hat{\chi}_\Delta$ has been defined in (2.11). The identity (3.6) holds because the ground states are invariant under rotations in spin space. To find the connection between $\chi_\text{SW}^y$ and $\left\langle (\sum_\Delta \hat{\chi}_\Delta)^2 \right\rangle$ we again consider the limit $\alpha \to -\infty$. Since the average $\left\langle (\sum_\Delta \hat{\chi}_\Delta)^2 \right\rangle$ contains four spin correlations an exact analytical evaluation is not possible in the limit. By a mean field approximation we find

$$\lim_{\alpha \to -\infty} \left\langle \left( \frac{1}{N} \sum_\Delta \hat{\chi}_\Delta \right)^2 \right\rangle_{mf} = 95^4 + \frac{a_{mf}}{N} + O(N^{-2}),$$

(3.7)
with \( a_{mf} = \frac{31}{4} \) for \( S = \frac{1}{2} \). If \( \chi^y_{1,SW}(\alpha, N) \), \( \text{(2.14)} \), is evaluated for finite \( N \) one finds that the \( S^{-1} \) corrections vanish in the limit \( \alpha \to -\infty \) so that from \( \text{(2.14)} \) and \( \text{(3.7)} \)

\[
\lim_{\alpha \to -\infty} [\chi^y_{1,SW}(\alpha, N)]^2 = \lim_{\alpha \to -\infty} \left\langle \left( \frac{1}{N} \sum_\Delta \hat{\chi}_\Delta \right)^2 \right\rangle_{mf} - \frac{a_{mf}}{N} + O(N^{-2}) = 9S^4. \quad (3.8)
\]

Instead of working with the approximate finite size correction \( a_{mf} \) we fit our exact results in the limit \( \alpha \to -\infty \) by a second order polynomial in \( N^{-1} \),

\[
\lim_{\alpha \to -\infty} \left\langle \left( \frac{1}{N} \sum_\Delta \hat{\chi}_\Delta \right)^2 \right\rangle_0 = 9S^4 + \frac{a}{N} + \frac{b}{N^2}. \quad (3.9)
\]

The fit is done separately for even \( N \) (\( N = 18, 24 \)) and odd \( N \) (\( N = 21, 27 \)). We find

\[
a_{\text{even}} = 7.63, \quad b_{\text{even}} = 20.02; \quad a_{\text{odd}} = 7.81, \quad b_{\text{odd}} = 5.75. \quad (3.10)
\]

Obviously, \( a_{mf} = 7.75 \) is a good approximation for the leading finite size correction. That the finite size corrections of the helicity are large in comparison with the corresponding corrections of the sublattice magnetisation \( \text{(3.3)} \) is not surprising since each of the plaquettes in \( \langle (\sum_\Delta \hat{\chi}_\Delta)^2 \rangle_0 \) overlaps with six neighbouring plaquettes. In Figs. 9a-d we show plots of the numerical results

\[
\chi^2(\alpha, N) = \left\langle \left( \frac{1}{N} \sum_\Delta \hat{\chi}_\Delta \right)^2 \right\rangle_0 - \frac{a}{N} - \frac{b}{N^2} \quad (3.11)
\]

and of the SW approximations \( \chi^2_{1,SW}(\alpha, N) \). As is seen in Fig. 10, where we plot the difference \( \Delta \chi(N) = \chi(N) - \chi_{1,SW}(N) \) between the first order SW results and the exact values for the helicity, the agreement is not as good as in the case of the sublattice magnetisation. The difference \( \Delta \chi(N) \) deviates appreciably from the second order SW approximation shown in Fig. 10 even for the large \( C_{6v} \) symmetric cells \( N = 21 \) and \( N = 27 \). Nevertheless, the enhancement of the helicity over the classical value, Figs. 9a-d, in the region \(-\infty < \alpha < -0.2\), which must be attributed to quantum fluctuations, is exhibited by both \( \chi(N) \) and \( \chi_{1,SW}(N) \) in a similar fashion. Furthermore, the decrease of \( \chi(N) \) and \( \chi_{1,SW}(N) \) to zero as \( \alpha \) approaches \( \alpha_{cl} \) which is concomitant to the decrease of the sublattice magnetisation \( \mathcal{M} \) indicates clearly that the helicity is just another measure for the 120° long range spin order of the HAFT and has no independent significance as in the case of a spin nematic.
3.3 Chirality

As we have discussed in the introduction, a RVB state which breaks time reversal and parity invariance has been proposed as the ground state of the HAFT [18]. Chiral symmetry breaking, i.e. a nonvanishing expectation value of the operator $S_i(S_j \times S_k)$ defined on an elementary triangular plaquette with sites $i, j, k$, is known to be the signature of such a state [28]. According to Baskaran [17] chiral symmetry breaking should only occur when the nnn coupling $\alpha$ exceeds a critical value.

In Fig. 11 we plot the expectation value

$$P_{\pm} = \frac{1}{N^2} \langle C_{\pm}^+ C_{\pm} \rangle,$$

where $C_{\pm}$ are the uniform and staggered chiralities

$$C_+ = \frac{2}{\sqrt{3}} \sum_{\Delta \nabla} \left( S_i(S_j \times S_k) + S_j(S_l \times S_k) \right),$$

$$C_- = \sqrt{2} \sum_{\Delta \nabla} \left( S_i(S_j \times S_k) - S_j(S_l \times S_k) \right).$$

Here, $i, j, k$ and $l$ denote the sites of a four-spin plaquette as depicted in Fig. 12, and the sums extend over the set of such plaquettes which covers the lattice. The normalisation in (3.13a,b) is chosen such that the maximum modulus of the eigenvalues is unity in both cases. Contrary to Baskaran’s conjecture and in agreement with the picture of the ground state as it has emerged so far no significant increase with $\alpha$ of either $P_+$ or $P_-$ is observed.

4 Summary and Conclusion

In this work two important tools for investigating the ground state structure of quantum antiferromagnets, spin-wave theory and numerical diagonalisation of small periodic systems, have been applied to the HAFT with $nn$ and $nnn$ interactions. Our spin wave calculations extend previous work [3] on the 120° structure of the model in various ways. The extension of the SW-expansion of the sublattice magnetisation $M$ to order $S^{-2}$ appears to corroborate the previous conjecture [19] that the transition between the 120° order
and the collinear order of the HAFT is of first order. With the aim of comparing the SW results with the exact numerical results we develop finite size approximants for the former. By the example of the first order SW approximation for the sublattice magnetisation we demonstrate that the subleading \(1/N\) size corrections must not be neglected for system sizes \(N \lesssim 10^2\). Moreover, irregular corrections which reflect the dependence of the finite size results on the shapes of the systems are seen to be relevant for smaller sizes \(N \lesssim 36\). These results of the SW approximation indicate that extrapolations from system size \(N \lesssim 36\) which exclusively rely on the leading \(1/\sqrt{N}\) size dependence are unwarranted. Therefore, in the discussion of our exact numerical results we do not attempt to extrapolate to the bulk limit. Rather, we compare directly the finite size data obtained by the SW approximation with the corresponding exact data.

In our numerical investigation we calculate quantities which are suited to characterise the \(120^\circ\) order and the collinear order of the ground state of the HAFT, namely, the order parameter \(M\) and the helicity \(\chi_y\) of the \(120^\circ\) structure and the order parameter \(N\) of the collinear structure. To check whether there is an indication for unconventional order we also calculate the chirality \(P\). Incommensurate structures which evolve in the classical picture for \(\alpha > 1\) are outside the scope of the present study since we work with finite periodic systems.

For strong ferromagnetic \(nnn\) coupling, \(\alpha \ll -1\), one expects to find agreement between the exact results \(M(\alpha, N)\) and the first order SW approximation \(M_{1,SW}(\alpha, N)\) on physical grounds. Surprisingly, however, we find that \(M_{1,SW}(\alpha, N)\) approximates \(M(\alpha, N)\) very well also for small values of \(|\alpha|\) where \(M(\alpha, N)\) is substantially reduced from its classical value by quantum effects. This suggests that the SW approximation remains valid even for small positive values of \(\alpha\) where the frustration already present in the triangular antiferromagnet is further enhanced by the \(nnn\) coupling. It appears that frustration is not as detrimental to long range order in spin-1/2 quantum antiferromagnets as has been thought \[7, 13, 29\]. The comparison of the first order SW approximation for the helicity \(\chi\) with the exact values supports this conclusion: \(\chi\) is tied to the sublattice magnetisation just as it should be for an ordered \(120^\circ\) structure.
The behaviour of the order parameter $\mathcal{N}(\alpha, N)$ of the collinear structure is found to differ between the $N = 12$ and $N = 24$ systems on the one hand and the $N = 18$ and $N = 30$ systems on the other. While $\mathcal{N}(\alpha, 12)$ and $\mathcal{N}(\alpha, 24)$ increase smoothly as $\alpha$ increases through the classical transition point between the $120^\circ$ order and the collinear order, $\mathcal{N}(\alpha, 18)$ and $\mathcal{N}(\alpha, 30)$ increase discontinuously at $\alpha_{qu}(18) = 0.23$ and $\alpha_{qu}(30) = 0.2$ where $\mathcal{M}(\alpha, 18)$ and $\mathcal{M}(\alpha, 30)$ are still finite. These discontinuities are related to a crossover from a translationally invariant ground state for $\alpha < \alpha_{qu}$ to a ground state that has the periodicity of the collinear structure for $\alpha > \alpha_{qu}$. Thus, for the system sizes $N = 18$ and 30 one recovers the classical picture of a first order transition between the $120^\circ$ order and the collinear order. In the cases $N = 12$ and 24 the ground states remain translationally invariant for all values of $\alpha$. For these system sizes, the dependence of $\mathcal{M}(\alpha, N)$ and $\mathcal{N}(\alpha, N)$ on $\alpha$ and $N$ agrees with the finite size behaviour of the order parameters of a system that undergoes a first order transition between the ordered states characterised by $\mathcal{M}$ and $\mathcal{N}$ in the bulk limit. In summary, our exact results support the conjecture [19] of a first order transition between $120^\circ$ order and collinear order. In agreement with this we see no significant enhancement of the chirality in the transition region.

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Appendix A: Second order spin wave approximation

A straightforward evaluation of the expectation values in (2.8) yields the following expressions:

\[
\frac{\langle H_2 \rangle_0}{N} = -\frac{3}{32S^2} F(b) + \frac{3}{16S^2} \alpha G(b), \quad b \equiv \frac{B}{3S}
\]  

(A.1)

where

\[
F(b) = \left( 2 - 2J_1 + \frac{1}{N} \sum_k (b - 2\alpha(k)) (A_1(k, B) + A_2(k, B)) \right)^2 
+ B_1^2 + 4B_1B_2 - 2B_2^2 - (B_1 + 2B_2)(A_1 - A_2), \]

\[
G(b) = (A_1 + A_2 - 2 - C_1 - C_2)^2 + (C_1 - C_2)(C_1 - C_2 - A_1 + A_2).
\]

and

\[
J_1 = \frac{1}{N} \sum_k \nu(k, B),
\]

with \(\nu(k, B)\) as defined in (2.8). \(A_i, B_i\) and \(C_i\) denote the sums

\[
A_i = \frac{1}{N} \sum_k A_i(k), \\
B_i = \frac{1}{N} \sum_k \gamma(k) A_i(k), \\
C_i = \frac{1}{N} \sum_k \left( 1 - \frac{\alpha(k)}{\alpha} \right) A_i(k), \quad i = 1, 2
\]

where

\[
A_1(k) = [A_2(k)]^{-1} = \sqrt{\frac{1 + b - 2\alpha(k) + 2\gamma(k)}{1 + b - 2\alpha(k) - \gamma(k)}},
\]

with \(\alpha(k)\) and \(\gamma(k)\) as defined in (2.6a,b).

Similarly,

\[
\sum_{\{n_k\}} \frac{\langle \{n_k\} | H_{3/2} | \{n_k\} \rangle}{E(\{0\}) - E(\{n_k\})} = -\frac{3}{16S^2} \frac{1}{N^2} \sum_{k,p} \frac{l^2(k, p)}{\nu(k) + \nu(p) + \nu(k + p)}. \quad (A.2)
\]

19
where

\[ I^2(k, p) = A_1(k)A_1(p)A_1(k + p) \{ \beta(k)(1 - A_2(p)A_2(k + p)) + \beta(p)(1 - A_2(k)A_2(k + p)) - \beta(k + p)(1 - A_2(k)A_2(p)) \}^2, \]

with

\[ \beta(k) = -\frac{1}{3} \left[ \sin(k_x) - \sin\left(\frac{1}{2}k_x - \frac{\sqrt{3}}{2}k_y\right) - \sin\left(\frac{1}{2}k_x + \frac{\sqrt{3}}{2}k_y\right) \right]. \]

Miyake’s result [9] is reproduced by setting \( \alpha = 0 \) in these expressions.

To obtain the second order correction \( \chi^y_{2,SW} \) to the helicity we follow the same procedure as in the determination of \( \mathcal{M}_{2,SW} \). We replace the Zeeman term in (2.1) by the term

\[ -h \sum_{\Delta} \chi^y_{\Delta}, \]

which couples the helicity to a fictitious source field \( h \) so that

\[ \chi^y = -\frac{1}{N} \frac{\partial}{\partial h} E_0(\alpha, h) \bigg|_{h \to 0}, \]

where \( E_0(\alpha, h) \) is the \( h \)-dependent ground state energy of the system. The second order term in the expansion of \( E_0(\alpha, h) \) with respect to \( S^{-1} \) has the same structure as \( E_0(\alpha, B) \), (2.8), i.e. it consists of two additive contributions that contain singular parts proportional to \( \sqrt{h} \) which cancel in the sum. Thus, the limit

\[ \chi^y_{2,SW} = -\frac{1}{N} \lim_{h \to 0} \frac{E_0^{(2)}(\alpha, h) - E_0^{(2)}(\alpha, 0)}{h} \]

can be performed numerically in exactly the same way as in (2.10).

**Appendix B: \( \mathcal{M}_{1,SW} \) in the limit \( -\alpha/N \to \infty \)**

From (2.6a,b) it follows that for \( k \neq 0, \pm Q_1 \)

\[ |\alpha(k)| \geq 3\pi^2 \frac{|\alpha|}{N}. \]  

(B.1)
and hence, in the limit $|\alpha|/N \gg 1$,

$$|\alpha(k)| \gg 1 > |\gamma(k)|,$$  \hspace{1cm} (B.2)

so that $A_{1,2}(k)$ can be expanded in this limit:

$$A_{1,2}(k) = 1 \mp \frac{1 + 2\gamma(k)}{2\alpha(k)} \pm \frac{1 - \gamma(k)}{2\alpha(k)} + O(N^2/\alpha^2).$$  \hspace{1cm} (B.3)

Using this expansion in (2.17) one finds the physically correct result

$$\mathcal{M}_{1,SW}(\alpha, N) = S + O(N^2/\alpha^2).$$  \hspace{1cm} (B.4)

By contrast, the expression

$$\mathcal{M}_{1,SW}(\alpha, N) = S \left\{ 1 + \frac{1}{4S} \left( 2 - \frac{1}{N} \sum_{k \in \mathbb{BZ}, k \neq 0} A_1(k) - \frac{1}{N} \sum_{k \in \mathbb{BZ}, k \neq \pm Q_i} A_2(k) \right) \right\},$$  \hspace{1cm} (B.5)

which derives from (2.7) if one neglects only the infinite contributions of the zero modes, yields the unphysical result

$$\mathcal{M}_{1,SW}(\alpha, N) = S \left\{ 1 + \frac{1}{4S} \frac{6}{N} + O(N^2/\alpha^2) \right\}.$$  \hspace{1cm} (B.6)

Obviously, the finite size correction $-3/(2N)$ which is accounted for in (2.17) is important for systems sizes $N \leq 36$ for which exact numerical results are available.

**Appendix C: Connection between the structure function and the order parameter**

To evaluate $S_N(Q_1)$ in the limit $-\alpha \gg 1$ we start from the expression

$$S_N(Q_1) = 3 \left\langle \left( \sum_{i,j \in \mathcal{A}} - \sum_{i \in \mathcal{A}, j \in \mathcal{B}} \right) S_i S_j \right\rangle_0$$  \hspace{1cm} (C.1)

which follows from (3.1) by taking the equivalence of the three sublattices into account. Since the spins of one sublattice are ferromagnetic aligned for $-\alpha \gg 1$ we have

$$\lim_{\alpha \to -\infty} \langle S_i S_j \rangle = S^2 \quad \text{for} \quad i, j \in \mathcal{A}, \; i \neq j.$$  \hspace{1cm} (C.2)
However,

$$\lim_{\alpha \to -\infty} \langle S_i S_j \rangle = S^2 c \quad \text{for} \quad i \epsilon A, j \epsilon B,$$

(C.3)

where \( c \) can differ from the value \( \cos(2\pi/3) = -1/2 \), since the spins of different sublattices may fluctuate against each other. \( c \) is fixed by the condition that the ground state of systems of size \( N \) must be a singlet or a doublet depending on whether \( N \) is even or odd:

$$\lim_{\alpha \to -\infty} S_{\text{tot}}(N) = \lim_{\alpha \to -\infty} \langle (\sum_i S_i)^2 \rangle$$

$$= \frac{N^2}{12} \left( 1 + 2c + \frac{6}{N} \right) = \begin{cases} 
0, & N \text{ even}, \\
\frac{3}{4}, & N \text{ odd}.
\end{cases}$$

(C.4)

Hence,

$$c = \begin{cases} 
-\frac{1}{2} - \frac{3}{N}, & N \text{ even}, \\
-\frac{1}{2} - \frac{3}{N} + \frac{9}{2N^2}, & N \text{ odd}.
\end{cases}$$

(C.5)

Using (C.2), (C.3) and (C.5) we find from (C.1) the expressions (3.3) of the main text for \( S_N(Q_1) \).
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Figure Captions

**Fig.1** Classical ground state configuration in the regime $\alpha < 1/8$. Bold lines: $nn$ bonds; dashed bold line: $nnn$ bond

**Fig.2** Classical ground state configuration in the regime $1/8 < \alpha < 1$. The state is degenerate with respect to the angle $\theta$.

**Fig.3** The Brillouin zone of the triangular lattice. The arrows indicate the path which the Bragg vector $Q$ of the ground state configuration takes when $\alpha$ increases: $Q = Q_1$ for $-\infty < \alpha \leq 1/8$; $Q = Q_2$ for $1/8 < \alpha \leq 1$; for $1 < \alpha < \infty$ $Q$ moves continuously from $Q_2$ towards the corner of the $\sqrt{3} \times \sqrt{3}$ Brillouin zone.

**Fig.4 a,b** First and second order spin wave results: (a) the sublattice magnetisation $M$ as a function of $\alpha$; (b) the helicity $\chi^y$ as a function of $\alpha$.

**Fig.5** Size dependence of the first order spin wave approximation for $M$ at $\alpha = 0$. $\circ$: $M_{1,SW}(\alpha = 0, N)$; full line: leading size correction to $M_{1,SW}(0, \infty)$; dashed line: leading and subleading correction to $M_{1,SW}(0, \infty)$

**Fig.6 a-f** Finite systems studied in this work. For the $N = 18, 24$ and $30$ cells which are not $C_{6v}$ symmetric, the triangular lattice has been distorted such that the outer contours of the cells take the shape of regular hexagons. The degree of distortion illustrates the deviation from the $C_{6v}$ symmetry.
Fig. 7 a-f  The square of the order parameters $\mathcal{M}$ and $\mathcal{N}$ of the 120° structure and of the collinear structure as a function of $\alpha$ for various system sizes. $\mathcal{M}_{1,SW}$ is obtained from eq. (2.17). The insets in (a) and (d) show an enlargement of the transition region.

Fig. 8  The difference $\Delta \mathcal{M}(\alpha, N) = \mathcal{M}(\alpha, N) - \mathcal{M}_{1,SW}(\alpha, N)$ and the second order spin wave correction $\mathcal{M}_{2,SW}(\alpha)$ as functions of $\alpha$.

Fig. 9 a-d  The square of the helicity $\chi^y$ of the 120° structure as a function of $\alpha$ for various system sizes. $\chi_{1,SW}$ is obtained from eq. (2.21).

Fig. 10  The difference $\Delta \chi(\alpha, N) = \chi(\alpha, N) - \chi_{1,SW}(\alpha, N)$ and the second order spin wave correction $\chi_{2,SW}(\alpha)$ as functions of $\alpha$.

Fig. 11  The chiralities $P_\pm(\alpha, N)$ as functions of $\alpha$.

Fig. 12  A plaquette of four spins on which the uniform and staggered chiral operators are defined.