Study of an Antiferromagnetic Sawtooth Chain
with Spin-1/2 and Spin-1 sites

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We study the low-energy properties of a sawtooth chain with spin-1’s at the bases of
the triangles and spin-1/2’s at the vertices of the triangles. The spins have Heisenberg
antiferromagnetic interactions between nearest neighbors, with a coupling $J_2$ between a
spin-1 and a spin-1/2, and a coupling $J_1 = 1$ between two spin-1’s. Analysis of the exact
diagonalization data for periodic chains containing up to $N = 12$ unit cells shows that the
ground state is a singlet for exchange couplings up to approximately $J_2 = 3.8$, whereas
for larger $J_2$, the system exhibits a ferrimagnetic ground state characterized by a net
ferromagnetic moment per unit cell of 1/2. In the region of small interactions $J_2$, the
mixed spin sawtooth chain maps on to an effective isotropic spin model representing two
weakly interacting and frustrated spin-1/2 Heisenberg chains composed of spin-1/2 sites
at odd and even vertices respectively. Finally, we study the phenomenon of a macroscopic
magnetization jump which occurs if a magnetic field is applied with a value close to the
saturation field for $J_2 = 2$.

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I. INTRODUCTION

There has been a great deal of interest in recent years in one-dimensional quantum spin systems with frustration\(^1\). The most common examples of such systems are those in which triangles of Heisenberg spins interact antiferromagnetically with each other. Some of the systems which have been studied analytically or numerically so far are the sawtooth spin-1/2 chain\(^2,3\), a chain of spin-1/2 triangles\(^4\), frustrated mixed spin ferrimagnetic chains\(^5\), and the spin-1/2 Kagome strip\(^6,7\).

Classically (i.e., in the limit in which the magnitudes of the spins \(S_i \to \infty\)), some of these frustrated systems have an enormous ground state degeneracy arising from local rotational degrees of freedom which cost no energy. Quantum mechanically, this degeneracy is often lifted due to tunneling between different classical ground states. However, one might still expect a remnant of the classical degeneracy in the form of a large number of low-energy excitations in the quantum system.

Recently, the ground state of the spin-1/2 sawtooth chain has been numerically studied as a function of the ratio \(J_2/J_1\), where \(J_1\) is the coupling between pairs of spins at the bases of the triangles, and \(J_2\) is the coupling between a spin at the base and a spin at the vertex of a triangle\(^8\). The system was found to be gapless for \(J_2/J_1 > 2.052\) and for \(J_2/J_1 < 0.65\). The low-energy excitations have the same dispersion for singlets and triplets. For \(J_2/J_1 = 1\), the system has some special properties. The ground state of an open chain has an exact degeneracy which increases linearly with the number of triangles\(^2\). This degeneracy arises from the existence of localized spin-1/2 kinks which do not cost any energy regardless of their position in the chain. There are also spin-1/2 antikinks which cost a finite energy. The lowest excitation in a chain with periodic boundary conditions is given by a kink-antikink pair which has a dispersionless gap; the pair may be either a singlet or triplet.

In this paper, we will carry out analytical and numerical studies of a mixed spin Heisenberg antiferromagnet on the sawtooth lattice shown in Fig. 1. (The arrows and angles (\(\theta\) shown in that figure refer to a canting state which will be discussed later). The sites at the vertices of the triangles have spin \(S_2\), and they are labeled \(1, 2, ..., N\). The sites at the bases of the triangles have spin \(S_1\), and they are labeled \(N + 1, N + 2, ..., 2N\). The number of triangles is therefore \(N\). The Hamiltonian governing the system is

\[
H = J_1 \sum_{i=N+1}^{2N} \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum_{i=1}^{N} \vec{S}_i \cdot \left[ \vec{S}_{i+N} + \vec{S}_{i+N+1} \right],
\]

where the couplings \(J_1, J_2\) are positive. It is convenient to set \(J_1 = 1\), and consider the properties of the system as a function of \(J_2\). We will impose periodic boundary conditions at the ends of the chain, so that the momentum is a good quantum number. (We will set Planck’s constant \(\hbar = 1\), and the nearest neighbor lattice spacings equal to 1).

The plan of our paper is as follows. In Sec. II, we will develop the spin wave theory (SWT) for this system\(^5\), taking the values of the spin \(S_1\) at the bases and the spin \(S_2\) at the vertices of the triangles to be very large, and \(S_1 > S_2\). If \(J_2 > 2S_1/S_2\), we find that the system is a ferrimagnet, with a magnetization per unit cell of \(S_1 - S_2\). If \(J_2 < 2S_1/S_2\), we find that there is an infinite number of classical ground states as mentioned above. For reasons explained below, we will consider the classical ground states which are coplanar; the number of even this restricted set of states grows exponentially with \(N\). We perform a linear SWT about these coplanar states, and find that the spin wave zero point energy does not break the classical degeneracy. Further, one of the spin wave modes turns out to have zero energy for all momenta. We will also see that SWT picks out two other values of \(J_2\), namely \(J_2 = 1\) and 2, as being special.

In Sec. III, we use the Lanczos algorithm to perform an exact diagonalization (ED) of finite systems to study the low-energy excitations and two-spin correlations in the ground state as a function of \(J_2\) for \(S_1 = 1\) and \(S_2 = 1/2\). We find that the system is a ferrimagnet for \(J_2 \gtrsim 3.8\) with a magnetization per unit cell of \(1/2\). We see that the transition to a collinear ferrimagnetic state takes place at a smaller value of \(J_2\) in the quantum case than in the classical case where the transition occurs at \(J_2 = 4\). This effect has
already been seen for other systems exhibiting transitions between collinear and non-collinear states (see, for example, Ref. 5), and it indicates a favoring of the collinear state by quantum fluctuations. There seems to be a first-order transition at \(J_2 \simeq 3.8\) with the total spin of the ground state changing rather abruptly at that value. For \(J_2 \lesssim 3.8\), the ground state is a singlet. We find that there are two other values, \(J_2 \simeq 1.9\) and 1.1, where the nature of the spin correlations changes significantly. Many of the correlations become very small or change sign at those two points. The structure factor seems to indicate crossovers at those points between ground states with different kinds of short-range correlations. In the region \(1.1 \lesssim J_2 \lesssim 1.9\), the canting spin configuration in Fig. 1 is consistent with the ED data representing the short-range spin-spin correlations, whereas for larger \(J_2\) up to the ferrimagnetic phase transition point, the commensurate spiral phase with a period of four lattice spacings seems to be in accord to the ED data for \(N = 12\). It is clear, however, that the periodic boundary conditions imposed on the chain prevent the appearance of the periodic structures with larger periods predicted by the classical analysis.

For \(J_2 \lesssim 1\), the correlations between the spin-1/2 sites show an unusual pattern. Namely, the spin-1/2 sites appear to decompose into two sublattices such that each sublattice has a substantial antiferromagnetic coupling within itself (with a strong frustration), but the coupling between the two sublattices is much weaker. We call this system the next-nearest-neighbor antiferromagnet (NNN-AFM). In Sec. IV, we use a perturbative expansion in \(J_2\) and an effective Hamiltonian description to provide some understanding of why this happens. This seems to be a remarkable property of the spin-1/2 - spin-1 sawtooth system.

In Sec. V, we will consider the particular case of \(J_2 = 2\) where we find that the system shows an interesting behavior if a magnetic field is applied with a strength which is close to the saturation value \(h_s\) (i.e., the value above which all the spins are aligned with the field). We will show that for \(J_2 = 2\), the system displays a macroscopic jump in the magnetization as the magnetic field crosses \(h_s\). This phenomenon is known to occur in some other strongly frustrated quantum spin systems.

**II. SPIN WAVE ANALYSIS**

To develop the SWT, we assume that the values of the spin \(S_1\) and \(S_2\) are much larger than 1. We will describe how to obtain the spin wave dispersion up to order \(S_i\). (This is called linear SWT because interactions between the spin waves do not appear at this order).

Since some of the classical ground states considered in this section have a coplanar configuration of the spins, it is convenient to use a technique for deriving the spin wave spectrum which can be applied to both collinear and coplanar configurations. For a coplanar configuration, let us assume that the spins lie in the \(z-x\) plane. Consider a particular spin of magnitude \(S\) which points at an angle \(\phi\) with respect to the \(\hat{z}\)-direction. Then we can write the Holstein-Primakoff representation for that spin as

\[
\begin{align*}
\cos \phi \ S_z + \sin \phi \ S_x &= S - a^\dagger a, \\
-\sin \phi \ S_z + \cos \phi \ S_x + iS_y &= \sqrt{2S} - a^\dagger a, \\
-\sin \phi \ S_z + \cos \phi \ S_x - iS_y &= a^\dagger \sqrt{2S} - a^\dagger a,
\end{align*}
\]

(2)

where \([a, a^\dagger] = 1\). We now introduce a coordinate and momentum

\[
q = \frac{a + a^\dagger}{\sqrt{2}}, \quad \text{and} \quad p = \frac{a - a^\dagger}{i\sqrt{2}},
\]

(3)

satisfying \([q, p] = i\). On expanding Eq. (2) up to quadratic order in \(a\) and \(a^\dagger\), we obtain

\[
S_z = \cos \phi \left[ S + \frac{1}{2} - \frac{1}{2} (p^2 + q^2) \right] - \sin \phi \sqrt{S} \ q,
\]

3
\[
S_x = \sin \phi [ S + \frac{1}{2} - \frac{1}{2} (p^2 + q^2) ] + \cos \phi \sqrt{S} q , \\
S_y = \sqrt{S} p .
\] (4)

We now consider a general Heisenberg Hamiltonian of the form

\[
H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j ,
\] (5)

where we count each bond \((ij)\) only once, and the spin at site \(i\) will be assumed to have a magnitude \(S_i\).

Consider a classical configuration in which the spin at site \(i\) lies in the \(z-x\) plane at an angle \(\phi_i\) with respect to the \(\hat{z}\)-axis. The condition for this configuration to be a ground state classically is that

\[
E_{cl}(\phi_i) = \sum_{ij} J_{ij} S_i S_j \cos(\phi_i - \phi_j) (6)
\]

should be a minimum with respect to each of the angles \(\phi_i\). We must therefore have

\[
\sum_{j} J_{ij} S_i S_j \sin(\phi_i - \phi_j) = 0 (7)
\]

for every value of \(i\). Using Eq. (4) and keeping terms up to order \(S_i\), we find that the spin wave Hamiltonian is given by

\[
H_{sw} = \sum_{ij} J_{ij} \left[ (S_i S_j + \frac{S_i}{2} + \frac{S_j}{2}) \cos(\phi_i - \phi_j) - \frac{1}{2} \cos(\phi_i - \phi_j) (S_j p_i^2 + S_j q_i^2 + S_i p_j^2 + S_i q_j^2) \right] + \sqrt{S_i S_j} \cos(\phi_i - \phi_j) q_i q_j + \sqrt{S_i S_j} p_i p_j .
\] (8)

The factor of \(S_i S_j+S_i/2+S_j/2\) in this expression appears on expanding a product like \((S_i+1/2)(S_j+1/2)\) coming from Eq. (4) and dropping the term of order 1.

We can obtain the spin wave spectrum from (8) as follows. The unit cell of our system is a triangle containing the two sites with spins \(S_1\) and \(S_2\) which lie on its left edge. Let us label the triangles by \(n\), where \(n = 1, 2, ..., N\), and let \(a = 1, 2\) denotes the spins \(S_1\) and \(S_2\) respectively; thus each site is labeled as \((a,n)\). [The mapping from the site labels used in Fig. 1 to the site labels \((a,n)\) being used here is as follows: \(n \rightarrow (2,n)\) if \(1 \leq n \leq N\), and \(n \rightarrow (1,n-N)\) if \(N+1 \leq n \leq 2N\).]

We define the Fourier transforms

\[
p_{a,k} = \frac{1}{\sqrt{N}} \sum_n p_{a,n} e^{-i kn} , \\
q_{a,k} = \frac{1}{\sqrt{N}} \sum_n q_{a,n} e^{-i kn} ,
\] (9)

where \(-\pi < k \leq \pi\). These operators satisfy the commutation relation \([q_{a,k}, p_{b,k'}] = i \delta_{a,b} \delta_{k,-k'}\). Let us now assume that the cosines appearing in Eq. (8) take the following simple forms: they are equal to \(\cos \alpha\) for every pair of neighboring spin-\(S_1\) sites, and equal to \(\cos \beta\) for every pair of neighboring spin-\(S_1\) - spin-\(S_2\) sites. [We will see below that this may happen even in situations where the angles \(\phi_{a,n}\) are themselves not the same in all the triangles]. Up to terms of order \(S_i\), the Hamiltonian in Eq. (1) takes the form
\[ H = E_{0,cl} + \sum_{ab} \sum_{k} \left[ p_{a,-k} M_{ab,k} p_{b,k} + q_{a,-k} N_{ab,k} q_{b,k} \right], \]
\[ E_{0,cl} = N \left[ (S_1^2 + S_1) \cos \alpha + 2J_2 (S_1 S_2 + \frac{S_1}{2} + \frac{S_2}{2}) \cos \beta \right], \]  
(10)

where \( E_{0,cl} \) is the classical ground state energy, and
\[ M_{ab,k} = \begin{pmatrix}
S_1 \cos k - S_1 \cos \alpha - J_2 S_2 \cos \beta & J_2 \sqrt{S_1 S_2} (1 + e^{-ik})/2 \\
J_2 \sqrt{S_1 S_2} (1 + e^{ik})/2 & -J_2 S_1 \cos \beta
\end{pmatrix}, \]
\[ N_{ab,k} = \begin{pmatrix}
S_1 \cos \alpha \cos k - S_1 \cos \alpha - J_2 S_2 \cos \beta & J_2 \sqrt{S_1 S_2} \cos \beta (1 + e^{-ik})/2 \\
J_2 \sqrt{S_1 S_2} \cos \beta (1 + e^{ik})/2 & -J_2 S_1 \cos \beta
\end{pmatrix}. \]  
(11)

Note that the 2 \times 2 matrices \( M_k \) and \( N_k \) satisfy \( M_{-k} = M_k^T \) and \( N_{-k} = N_k^T \). If we write \( p_{a,k} \) and \( q_{a,k} \) as the columns \( p_k \) and \( q_k \) respectively, then the classical Hamiltonian equations of motion take the form
\[ \frac{dq_k}{dt} = 2M_k p_k, \]
\[ \frac{dp_k}{dt} = -2N_k q_k. \]  
(12)

For each value of \( k \), the harmonic solutions of these equations have two possible frequencies \( \omega_k \) given by the eigenvalue equation
\[ \det (4M_k N_k - \omega^2_k I) = 0. \]  
(13)

The quantum mechanical energy levels are then given by \( (n_{a,k} + 1/2) \omega_{a,k} \), where \( n_{a,k} \) is the occupation number of the mode labeled as \((a, k)\), where \( a \) can take two different values. Note that the frequencies \( \omega_{a,k} \) are the same in all the coplanar configurations. Hence the zero point energy given by \( (1/2) \sum_{a,k} \omega_{a,k} \) does not break the classical degeneracy between the different configurations.

[The advantage of using the variables \( p \) and \( q \), instead of \( a \) and \( a^\dagger \), is the following. We never get cross-terms like \( p_i q_j \) in the Hamiltonian; hence it is straightforward to obtain the frequencies. On the other hand, if we use \( a \) and \( a^\dagger \), we get terms like \( a_i a_j \), which make it necessary to perform a Bogoliubov transformation to obtain the frequencies. It turns out, however, that in both cases we eventually have to diagonalize the same matrix (namely, \( D_k = 4M_k N_k \)) to obtain the frequencies.]

We can now obtain the spin wave dispersion for various values of \( J_2 \). For large values of \( J_2 \), the classical ground state is a collinear ferrimagnetic configuration in which the \( S_1 \) spins point in one direction, say, the \( \hat{z} \)-direction, and the \( S_2 \) spins point in the opposite direction; the total spin of the ground state is therefore equal to \( N(S_1 - S_2) \). Hence the cosines in Eq. (11) are given by \( \cos \alpha = 1 \) and \( \cos \beta = -1 \). The spin wave dispersions are then given by
\[ \omega_{\pm,k} = 2\sqrt{a_k^2 - c_k^2} \pm 2b_k, \]
\[ a_k = \frac{J_2}{2} (S_1 + S_2) - S_1 \sin^2 \left( \frac{k}{2} \right), \]
\[ b_k = \frac{J_2}{2} (S_1 - S_2) + S_1 \sin^2 \left( \frac{k}{2} \right), \]
\[ c_k = J_2 \sqrt{S_1 S_2} \cos \left( \frac{k}{2} \right). \]  
(14)
[We can show that the upper branch $\omega_{+1, n}$ corresponds to excitations with total spin one more than the ground state spin, while the lower branch $\omega_{-1, n}$ corresponds to excitations with total spin one less than the ground state spin]. These dispersions are shown in Fig. 2 for $J_2 = 5$, $S_1 = 1$ and $S_2 = 0.5$. At $k = 0$, we find that $\omega_{+0} = 2J_2(S_1 - S_2)$ and $\omega_{-0} = 0$. At $k = \pi$, $\omega_{+\pi} = 2J_2S_1$ while $\omega_{-\pi} = 2J_2S_2 - 4S_1$. When the ratio $J_2$ decreases to the value $2S_1/S_2$, the lower branch $\omega_{-1, n}$ vanishes for all values of $k$. This signals an instability to some other state for $J_2 < 2S_1/S_2$.

For later use, we note that up to order $S_i$, the ground state energy per unit cell in the ferrimagnetic phase is given by

$$ E_0 = E_{0,cl} + \frac{1}{2} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left[ \omega_{+1, n} + \omega_{-1, n} \right] = S_1^2 + S_1 - 2J_2 \left( S_1 S_2 + \frac{S_1}{2} + \frac{S_2}{2} \right) + \int_{0}^{\pi} \frac{dk}{2\pi} 4 \sqrt{a_k^2 - c_k^2}, \tag{15} $$

where $a_k$ and $c_k$ are given in Eq. (14).

For $J_2 < 2S_1/S_2$, the classical ground state is no longer a collinear state. To see this, note that the Hamiltonian in (1) can be written, up to a constant, as $H = (1/2) \sum_{n} W_n^2$, where

$$ W_n = J_2 \vec{S}_{2n} + \vec{S}_{1n} + \vec{S}_{1n+1} \tag{16} $$

Thus the classical ground state is one in which the vector $W_n$ has the minimum possible magnitude in each triangle $n$. For $J_2 < 2S_1/S_2$, we find that the lowest energy state in each triangle is one in which the magnitude of $W_n$ is zero; this is given by a configuration in which the spin-$S_2$ makes an angle of $\pi - \theta$ with both the spin-$S_1$’s, while the angle between the two spin-$S_1$’s is $2\theta$, where

$$ \theta = \cos^{-1} \left( \frac{J_2 S_2}{2S_1} \right) \tag{17} $$

(Fig. 1 shows a particularly simple example of such a configuration in which all the spin-$S_2$’s are aligned with each other; this is called the canted state). It is clear that there is an infinite number of such configurations even in a system with a finite number of triangles. This is because, in a triangle labeled $n$, we can continuously rotate the spins $S_{2n}$ and $S_{1n+1}$ around the spin $S_{1n}$ while maintaining the relative angles at the values given above. In many systems with such an enormous ground state degeneracy, it is known that the zero point energy in linear SWT breaks the degeneracy partially by selecting only the coplanar ground states; this is called the order-from-disorder phenomenon. Let us therefore consider only coplanar configurations, in which all the spins lie in the $z - x$ plane. Even with this restriction, there are about $2^N$ different configurations, because in triangle $n$, there are two possible directions of the spins $S_{2n}$ and $S_{1n+1}$ for a given direction of the spin $S_{1n}$.

Let us compute the spin wave dispersion in a coplanar configuration. The cosines in Eq. (11) are given by

$$ \cos \alpha = \cos(2\theta) = \frac{J_2^2 S_2^2}{2S_1^2} - 1, $$

$$ \cos \beta = - \cos \theta = - \frac{J_2 S_2}{2S_1} \tag{18} $$

We then find that $\det M_k = 0$ for all values of $k$. Eq. (13) then implies that one of the frequencies, say, $\omega_{-1, n} = 0$ for all $k$. We thus have a dispersionless zero mode. [This mode arises due to the invariance of the classical ground state energy under certain kinds of continuous rotations in each triangle as mentioned above. In the problem of the Heisenberg antiferromagnet on the Kagome lattice, it is known that]
interactions between spin waves, which appear when we go to higher orders in the $1/S$ expansion, remove
the degeneracy in the zero-mode branch, and produce a low-lying spin wave branch with an energy
scale proportional to $S^{2/3}$. We will restrict ourselves to linear SWT here, and will not consider such
corrections to the zero-mode branch).

Since $\omega_{-k,0} = 0$, the other frequency can be obtained from (13) as

$$
\omega_{+k}^2 = 4 \text{ tr } (M, N_k)
= 2J_2^2 S_2^2 (\cos k - J_2) (1 + \cos k) + 4S_1^2 \sin^2 k + J_2^4 S_2^2 .
$$

(19)

This dispersion is shown in Fig. 3 for $J_2 = 2$, $S_1 = 1$ and $S_2 = 0.5$. At $k = \pi$, we have $\omega_{+\pi} = J_2^2 S_2$,
while at $k = 0$, we have $\omega_{+0} = J_2 S_2 [2 - J_2]$. We thus see that the gap vanishes at $k = 0$ if $J_2 = 2$.

Up to order $S$, the ground state energy per unit cell in the coplanar phase is given by

$$
\frac{E_0}{N} = - S_1^2 - S_1 - \frac{J_2^2}{2} (S_2^2 + S_2) + \int_0^\pi \frac{dk}{2\pi} \omega_{+k} ,
$$

(20)

where $\omega_{+k}$ is given in Eq. (19). One can check that the expressions in (15) and (20) match at $J_2 = 2 S_1 / S_2$.

Let us now comment on a special feature of the value $J_2 = 2$. Within the set of $2^N$ classical coplanar
ground states, the total spin of the system can have a wide range of values depending on the exact
configuration of the spins. We can see this by noting that the total spin can be written as $S_{tot} = \sum_n \vec{V}_n$,
where

$$
\vec{V}_n \equiv \vec{S}_{2,n} + \frac{1}{2} (\vec{S}_{1,n} + \vec{S}_{1,n+1}) .
$$

(21)

In any of the classical ground states for $J_2 < 2 S_1 / S_2$, we find that the magnitude of this vector is given
by $|\vec{V}_n| = |S_2 + S_1 \cos \beta| = (S_2 / 2) [2 - J_2]$. Depending on how the vectors $\vec{V}_n$ in different triangles add up,
the total spin of the system can therefore range from 0 to $(N S_2 / 2) [2 - J_2]$. However, if $J_2 = 2$, we see
that $\vec{V}_n$ is proportional to $\vec{W}_n$ in (16); hence all the classical ground states have zero spin since we know
that each of the vectors $\vec{W}_n$ has zero magnitude. Quantum mechanically, we expect the exponentially
large classical degeneracy to be broken by tunneling; however we would still expect an unusually large
number of low-energy singlet excitations for $J_2 = 2$.

Another special value of $J_2$ is given by $J_2 = 1$. At this point, the Hamiltonian of a single triangle is
given by the square of the total spin $S_n = \vec{S}_{2,n} + \vec{S}_{1,n} + \vec{S}_{1,n+1}$. Thus the total spin of each triangle
vanishes in any of the classical ground states.

III. NUMERICAL RESULTS

We have used the Lanczos algorithm to study the ground state properties of the sawtooth chain with
$S_1 = 1$ and $S_2 = 1/2$ for even values of $N$ from 4 to 12 with periodic boundary conditions. To reduce
the sizes of the Hilbert spaces, we work in subspaces with a given value of the total component of the
spin $S_z$ and the momentum, since these operators commute with the Hamiltonian. If $S_z = 0$, we reduce
the Hilbert space further by working in subspaces in which the spin parity $P_s$ is equal to $\pm 1$; under the
transformation $P_s$, the values of the spins at all the sites are flipped from $S_{iz} \rightarrow -S_{iz}$. One can show
that the eigenvalue of $P_s$ is related to the total spin $S$ of the state by

$$
P_s = (-1)^{N(S_1 + S_2) - S} .
$$

(22)
Fig. 4 shows the ground state energy as a function of $J_2$ for $N = 8$. The solid line shows the numerical data, while the dashed line shows the spin wave results (obtained from (20) for $J_2 \leq 4$, and from (15) for $J_2 \geq 4$). (We do not present the data for $N = 12$ since the latter are almost indistinguishable from those presented in Fig. 4). In the inset, the solid lines show piecewise linear fits to the numerical data to the left and right of $J_2 = 3.8$, while the dotted lines show the continuations of the same two straight lines to the right and left of $J_2 = 3.8$ respectively. This shows a small discontinuity in the slope at $J_2 \simeq 3.8$; we find that $(1/N) dE_0/dJ_2$ is equal to -1.25 and -1.45 to the left and right respectively of $J_2 = 3.8$. (These numbers agree with the nearest neighbor spin-1/2 - spin-1 correlations discussed in Eq. (23) and Fig. 8 below).

For both $N = 8$ and $N = 12$, we find that the total spin of the ground state changes abruptly at $J_2 \simeq 3.8$. For $J_2 \gtrsim 3.8$, the ground state spin has the ferrimagnetic value of $N(S_1 - S_2) = N/2$. For $J_2 \lesssim 3.8$, the ground state is a singlet. The number 3.8 compares reasonably with the SWT value of $2S_1/S_2 = 4$, considering that SWT is only expected to be accurate for large values of $S_1$ and $S_2$. The total spin of the first excited state however shows a more complicated behavior as $J_2$ is varied; this is plotted in Fig. 5 for $N = 8$. For $J_2 \gtrsim 3.9$, the first excited state has a spin of 3 as expected from the spin wave calculations. For $J_2 \lesssim 2.9$, the first excited state is a singlet. For $2.9 \lesssim J_2 \lesssim 3.9$, the spin of the first excited state fluctuates considerably. The fluctuations near $J_2 \simeq 3.9$ may be due to the finite size of the system, and they may disappear in the thermodynamic limit.

For $J_2 \leq 3.8$ and $N = 8$, the energy gaps between the ground state and the first excited state (whose spin is shown in Fig. 5) and the first non-singlet state are plotted as functions of $J_2$ in Fig. 6; the two gaps are shown by stars and circles respectively. Although the gap to the first excited state fluctuates, we see that it is particularly small near $J_2 = 1$ and 2. These small gaps may represent either level crossings of the ground state (as discussed below) or genuine low-lying singlet excitations; it is difficult to distinguish between these two possibilities without going to much larger system sizes. (We note that low-lying singlet excitations are known to occur in the spin-1/2 Heisenberg antiferromagnet on a Kagome lattice which is a well known example of a highly frustrated system\textsuperscript{13}). For $0.5 \lesssim J_2 \lesssim 2.5$, we see that the gap to the first excited state (which is a singlet) is typically much smaller than the gap to the first non-singlet state. In fact, we find that in this range of $J_2$, there are several singlet excitations which lie below the first non-singlet excitation. For instance, for $N = 12$, we find four and eight singlet excitations lying below the first non-singlet excitation at $J_2 = 1$ and 2 respectively.

For $N = 12$, the ground state has the following properties. For $J_2 \lesssim 3.85$, the ground state is a singlet, and the parity symmetry in the subspace with $S_z = 0$ is given by $P_0 = 1$. However, the momentum $k$ of the ground state repeatedly changes between 0 and $\pi$. This is shown in Table 1. We observe that there are several crossings, particularly near $J_2 = 1.1$ and 1.9. Repeated level crossings like this in a finite sized system are often a sign of a spiral phase in the thermodynamic limit\textsuperscript{14}; we will discuss this possibility in more detail below.

| Range of $J_2$ | Ground state momentum |
|----------------|-----------------------|
| $0 < J_2 < 0.95$ | $\pi$ |
| $0.95 < J_2 < 1.05$ | 0 |
| $1.05 < J_2 < 1.26$ | $\pi$ |
| $1.26 < J_2 < 1.78$ | 0 |
| $1.78 < J_2 < 1.82$ | $\pi$ |
| $1.82 < J_2 < 1.99$ | 0 |
| $1.99 < J_2 < 3.75$ | $\pi$ |
| $3.75 < J_2 < 3.85$ | 0 |

Table 1. The momentum of the ground state for various values of $J_2$, for a chain with 12 triangles.
Next, we examine the two-spin correlations $< \vec{S}_i \cdot \vec{S}_j >$ in the ground state. These are of three types: spin-1/2 - spin-1/2, spin-1/2 - spin-1, and spin-1 - spin-1. These are shown in Figs. 7-9 for $N = 12$. (We have only shown six correlations in each case. All the other correlations are related to these by translation and reflection symmetries). The behaviors of all the correlations show large changes near three particular values of $J_2$, namely, 1.1, 1.9 and 3.8. For instance, many of the correlations approach zero or change sign near these three values.

It is particularly instructive to look at the nearest neighbor spin-1/2 - spin-1 correlation, i.e., $< \vec{S}_1 \cdot \vec{S}_{14} >$ in Fig. 8. By the Feynman-Hellmann theorem, this is related to the derivative with respect to $J_2$ of the ground state energy per triangle,

$$ \frac{1}{N} \frac{dE_0}{dJ_2} = 2 < \vec{S}_1 \cdot \vec{S}_{14} > , \quad (23) $$

where we have used the fact that all the nearest-neighbor spin-1/2 - spin-1 correlations are equal. We can see from Fig. 8 that (23) shows a jump at $J_2 \simeq 3.8$, which indicates a first-order transition (we know that the ground state spin changes abruptly at that point from $N/2$ to 0 without going through any of the intermediate values). The jump in the values of $< \vec{S}_1 \cdot \vec{S}_{14} >$ at $J_2 \simeq 3.8$ is consistent with the jump in the slope of the ground state energy in Fig. 4 as discussed above. At $J_2 \simeq 1.25$ and 1.75, (23) seems to show a change of slope but no jump. This could indicate either a second-order transition or a crossover at those points; it is difficult to distinguish between these two possibilities since a change of slope can also arise due to finite-size effects.

For small values of $J_2$, we observe that the spin-1 - spin-1 correlations in Fig. 9 decay rapidly with the separation $n$ between the two sites, and they also oscillate as $(-1)^n$. This is expected for small $J_2$ because the spin-1 chain is only weakly coupled to the spin-1/2’s: a pure spin-1 antiferromagnetic chain exhibits a Haldane gap and a finite correlation length of about six lattice spacings. The weak coupling also explains why the spin-1/2 - spin-1 correlations in Fig. 8 are small. However, the spin-1/2 - spin-1/2 correlations in Fig. 7 show an unexpected behavior for small $J_2$. We find that the spin-1/2’s on even and odd sites appear to decouple into two separate chains, with the correlation being very small between spins belonging to different chains; within each chain, the correlations have an antiferromagnetic character. In other words, $< \vec{S}_{2,i} \cdot \vec{S}_{2,j} >$ is small if $i - j$ is odd, and it oscillates as $(-1)^{(i-j)/2}$ if $i - j$ is even. We call this the next-nearest-neighbor antiferromagnet (NNN-AFM). In the next section, we will provide some understanding of this behavior.

To understand better the nature of the changes in the ground state, we looked at the structure factors for the spin-1 - spin-1 and spin-1/2 - spin-1/2 correlations. These are respectively defined as

$$ S^{11}(q) = \frac{1}{N} \sum_{i=1}^{N} < \vec{S}_{N+1} \cdot \vec{S}_{N+i} > \cos(qr_i) , $$

$$ S^{22}(q) = \frac{4}{N} \sum_{i=1}^{N} < \vec{S}_1 \cdot \vec{S}_i > \cos(qr_i) , \quad (24) $$

where we define

$$ r_i = i - 1 \quad \text{for} \quad 1 \leq i \leq \frac{N}{2} , $$

$$ = N + 1 - i \quad \text{for} \quad \frac{N}{2} + 1 \leq i \leq N , \quad (25) $$

to account for the periodic boundary conditions, and $q$ takes the values $2\pi n/N$, where $n = 0, 1, ..., N - 1$. We have included the factors of $1/S_1^2$ (equal to 1 and 4 for spin-1 and spin-1/2 respectively) on the right hand sides of Eq. (24) to make it easier to compare the magnitudes of $S^{11}(q)$ and $S^{22}(q)$. 


In Fig. 10, we show the values of $q$ where the two structure factors are maximum ($q_{max}$) as a function of $J_2$ for $N = 12$. For $0 < J_2 \lesssim 1$, $q_{max} = \pi/2$ for spin-1/2 and $\pi$ for spin-1. (The NNN-AFM behavior of the spin-1/2's discussed in the next section will explain why $q_{max} = \pi/2$ for spin-1/2 for small values of $J_2$). For $1.25 \lesssim J_2 \lesssim 1.75$, $q_{max} = 0$ for spin-1/2 and $\pi$ for spin-1; this suggests that the ground state is in a canted state with a period of two unit cells as shown in Fig. 1. For $1.9 \lesssim J_2 \lesssim 3.8$, $q_{max} = \pi/2$ for both spin-1/2 and spin-1; this suggests a spiral phase with a period of four unit cells. Finally, for $J_2 \gtrsim 3.8$, $q_{max}$ is equal to 0 for both spin-1/2 and spin-1; this is expected in the ferrimagnetic state.

It is possible that the period two and period four states which are suggested by the structure factor for $N = 12$ (the periodic boundary conditions only allow some limited periodicities for small systems) will turn into states with longer periods (which change more smoothly with $J_2$) if we go to larger system sizes. The repeated level crossings between $k = 0$ and $\pi$ shown in Table 1 also support this scenario.

Fig. 11 shows the values of $S_{\text{ii}}(q_{max})$ as a function of $J_2$. Once again, we see large fluctuations near $J_2 = 1.1, 1.9$ and 3.8. The structure factors are relatively large for both large (ferrimagnetic) and small values of $J_2$, and is smaller for intermediate values of $J_2$.

Finally, we examined the possibility of dimerization, namely, whether the ground state spontaneously breaks the invariance of the Hamiltonian under translation by one unit cell. [The unit cell of our system has half-odd-integer spin, and such systems are quite susceptible to dimerization in one dimension]. A simple way to study this question is to see if the spin-1/2 - spin-1/2 correlations between state 1 and its neighbors at sites 2 and N (i.e., $< \vec{S}_1 \cdot \vec{S}_2 >$ and $< \vec{S}_1 \cdot \vec{S}_N >$) are equal. The problem is that the energy eigenstates we have found are also eigenstates of momentum and are therefore translation invariant; hence the two correlations will be equal in such states. However, if dimerization does occur, we expect that the ground state (called |1$>$) will be almost degenerate with an excited state (called |2$>$)\textsuperscript{17}. Although each of these would be eigenstates of momentum and therefore translation invariant, the linear combinations $|2+> = (|1> + |2>)/\sqrt{2}$ and $|2-> = (|1> - |2>)/\sqrt{2}$ would not be translation invariant. Now, we see from Fig. 6 that the ground state is almost degenerate with the first excited state (and both are singlets) at two values of $J_2$, namely, 1 and 2. We therefore examine the two correlations mentioned above in the four states |1>, |2>, |2+> and |2-> at those two values of $J_2$. The results are shown in Table 2. We see that the states |2+> and |2-> do show an asymmetry in the two nearest neighbor correlations (and the values of the correlations are exchanged between the two states). However, the numerical values of all the correlations are quite small, so there is no clear evidence for dimerization.

| $J_2$ | State | $< \vec{S}_1 \cdot \vec{S}_2 >$ | $< \vec{S}_1 \cdot \vec{S}_N >$ |
|---|---|---|---|
| 1 | | -0.00562 | -0.00561 |
| 1 | | -0.07239 | -0.07240 |
| 1 | | -0.15152 | 0.07350 |
| 1 | | 0.07351 | -0.15151 |
| 2 | | 0.04198 | 0.04195 |
| 2 | | 0.06867 | 0.06871 |
| 2 | | 0.09063 | 0.02004 |
| 2 | | 0.02002 | 0.09062 |

Table 2. The correlations of a spin-1/2 with its two neighboring spin-1/2's in the ground state (|1$>$), first excited state (|2$>$), and the two linear combinations (|2+> and |2->) at $J_2 = 1$ and 2, for $N = 8$. 


IV. NEXT-NEAREST-NEIGHBOR ANTIFERROMAGNET NEAR $J_2 = 0$

In this section, we will study the system for small values of $J_2$ using perturbation theory and the idea of an effective Hamiltonian. (A more detailed discussion of the ideas in this section is given in Ref.\textsuperscript{18}). We write the Hamiltonian in Eq. (1) as the sum $H = H_0 + V$, where

$$H_0 = \sum_{i=N+1}^{2N} \vec{S}_i \cdot \vec{S}_{i+1},$$

$$V = J_2 \sum_{i=1}^{N} \vec{S}_i \cdot \left[ \vec{S}_{i+N} + \vec{S}_{i+N+1} \right]. \quad (26)$$

For $J_2 = 0$, we have an antiferromagnetic spin-1 chain with a coupling equal to 1, and $N$ decoupled spin-1/2’s. (Every state of the system will have a degeneracy of $2^N$ due to the decoupled spin-1/2’s). It is known that the ground state of a spin-1 chain is a singlet with an energy $E_0^1 = -\frac{1}{4}0148 N$, and it is separated by a gap of $\Delta E_{1-0} = 0.41050$ from the first excited state which is a triplet\textsuperscript{16}.

Let us denote the eigenstates of $H_0$ for the spin-1 chain by $|\psi_1^i\rangle$ with energy $E_{1,i}$, where $i=0$ denotes the ground state. The states of the spin-1/2 sites will be denoted by $|\psi_{1/2}^j\rangle$. The eigenstates of the full Hamiltonian $H$ can therefore be written as linear combinations of the form

$$|\psi_a\rangle = \sum_{i,j} c_{a,i,j} |\psi_1^i\rangle \otimes |\psi_{1/2}^j\rangle, \quad (27)$$

where the $c_{a,i,j}$ are appropriate coefficients.

We will now expand up to second order in the perturbation $V$ to find an effective Hamiltonian $H_{\text{eff}}$ which acts within the subspace of the $2^N$ ground states which are degenerate for $J_2 = 0$. The Hamiltonian $H_{\text{eff}}$ will only act on the spin-1/2’s. To first order in $V$, we have

$$H_{1,\text{eff}} = <\psi_0^1 | V | \psi_0^1 >. \quad (28)$$

Since $V$ involves both spin-1/2 and spin-1 operators, and the expectation value in (28) is being taken in a spin-1 state, we see that $H_{1,\text{eff}}$ will only involve spin-1/2 operators as desired. Now, the expectation value in (28) is equal to zero, because $V$ is linear in the spin-1 operators (which are not rotationally invariant), while $|\psi_0^1\rangle$ is a singlet and is therefore rotationally invariant.

We therefore have to go to second order in $V$. We then have

$$H_{2,\text{eff}} = \sum_{i\neq 0} \frac{<\psi_0^1 | V | \psi_i^1 > <\psi_i^1 | V | \psi_0^1 >}{E_i^1 - E_0^1}, \quad (29)$$

Clearly, this will be an operator which is of degree 2 or less in the spin-1/2 operators. Since the state $|\psi_0^1\rangle$, the sum over states $\sum_{i\neq 0} |\psi_i^1\rangle <\psi_i^1|/(E_0^1 - E_i^1)$ and $V$ are all invariant under rotations and translations, $H_{2,\text{eff}}$ must have the same invariances. The only operators which are of degree 2 or less in spin-1/2’s and are rotationally invariant are a constant and products of the form $\vec{S}_i \cdot \vec{S}_j$. Using translation invariance, we see that $H_{2,\text{eff}}$ must take the form

$$H_{2,\text{eff}} = Na + NJ_2^2 b + J_2^2 \sum_i [ c_1 \vec{S}_i \cdot \vec{S}_{i+1} + c_2 \vec{S}_i \cdot \vec{S}_{i+2} + c_3 \vec{S}_i \cdot \vec{S}_{i+3} + \cdots ] , \quad (30)$$

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where $a, b, c_1, c_2, \ldots$ are numbers which are independent of $J_2$, and appropriate periodic boundary conditions are assumed in the summations over $i$. For a periodic system with $N$ spin-1/2’s, the subscript $i$ of $c_i$ goes from 1 to $N/2$ (since $N$ is even), so a total of $2 + N/2$ numbers have to be determined. These numbers will of course depend on the system size; but since the ground state of a spin-1 chain has a finite correlation length, we would expect these numbers to converge quickly to some values as $N$ becomes large. (We will assume that $J_2$ is small enough so that terms of order $J_2^3$ and higher can be neglected in comparison with the terms of order $J_2^2$ which we are interested in).

A direct computation of the constants $a, b, c_i$ in Eq. (30) using the expression in (29) is difficult because we would need to accurately determine all the energy levels and eigenstates of a spin-1 chain as well as all the matrix elements appearing in that expression. We therefore assume the form in Eq. (30) (which we have so far found purely on grounds of symmetry), and numerically determine the constants as follows.

To determine the first number $a$ in (30), we set $J_2 = 0$ and numerically find the ground state energy which is equal to $Na$. Next, we turn on the $J_2$ couplings on the bonds connecting only two of the spin-1/2’s, say at sites 1 and $n + 1$, to the spin-1’s. In other words, we set four of the spin-1/2 - spin-1 couplings equal to $J_2$, and keep all the other spin-1/2 - spin-1 couplings equal to zero; let us call this truncated perturbation $V_1 + V_{n+1}$ (thus, $V = \sum_i V_i$). We ignore the $N - 2$ spin-1/2’s which are not coupled to the spin-1’s. The energy levels of the system consisting of the spin-1 chain and two spin-1/2’s will have four low-lying states (which would be degenerate with an energy of $Na$ if all the $J_2$’s had been set equal to zero). These four states are described by an effective Hamiltonian involving the two spin-1/2’s of the form

$$H_{ij,\text{eff}} = Na + J_2^2 \left( 2b + c_n \vec{S}_1 \cdot \vec{S}_{n+1} \right).$$

The important point is that the constants $b$ and $c_n$ in this expression have the same values as in Eq. (30) where all the $J_2$ couplings are turned on. The reason for this can be traced back to the expression in (29) which can be used for either the full perturbation $V$ or the truncated perturbation $V_1 + V_{n+1}$. A comparison between the two second order expressions shows that the constant $b$ arises from the product of a spin-1/2 operator at site 1 with itself (when we take the product of the two matrix elements in (29)); that is why it appears with a factor of $N$ in (30) and a factor of 2 in (31). On the other hand, the constant $c_n$ comes from a product of a spin-1/2 operator at site 1 with a spin-1/2 operator at site $n + 1$, and it comes with the same factor in (30) and (31).

We can numerically determine the constants $b$ and $c_n$ from the energies of the four low-lying states of the spin-1 chain plus two spin-1/2’s; three of these states will form a triplet with the same energy and one will form a singlet, so that there will be only two equations in two unknowns. We can then repeat the procedure and determine all the constants $c_i$ by successively coupling various pairs of spin-1/2’s to the spin-1 chain; in each case, we only have to look at the four low-lying energy levels to find $b$ and $c_i$. (The values of $b$ that we get in the different cases should of course be consistent with each other). This procedure will work provided that $J_2$ is small enough that the four-low lying energy levels lie far below the gap $\Delta E_1$ of the pure spin-1 chain, and the terms of third and higher orders are much smaller than those of second order. On the other hand, if we choose $J_2$ to be too small, the energy splittings of $J_2^2$ are very small, and the determination of the constants $b$ and $c_i$ will suffer from large numerical uncertainties. For our calculations with $N = 8$, we found that taking $J_2 = 0.1$ gives reasonably accurate and self-consistent results. We found the following values of the six numbers:

$$a = -1.41712, \quad b = -0.12665,$$

$$c_1 = 0.0183, \quad c_2 = 0.1291,$$

$$c_3 = -0.0108, \quad c_4 = 0.0942.$$  \hspace{1cm} (32)

We see that the value of $a$ found for $N = 8$ agrees quite well with the thermodynamic value ($N \to \infty$) of $-1.40148$ quoted earlier\textsuperscript{16}.

Looking at the values of $c_i$ in (32), we observe the curious pattern that $c_2$ is the largest number, followed by $c_4$; the numbers $c_1$ and $c_3$ are much smaller in comparison. Thus the spin-1/2’s governed by
the effective Hamiltonian in (30) seem to break up into two chains, one consisting of the odd numbered sites, and the other with the even numbered sites. Each of the chains has a nearest neighbor coupling of \( c_2 J_2^2 \) which is antiferromagnetic; we therefore call this the NNN-AFM. This explains the numerical result that the structure factor of the spin-1/2's is peaked at \( q = \pi/2 \) and that the next-nearest-neighbor correlation is the largest in magnitude (and has a negative sign) for small \( J_2 \).

Note, however, that the next-nearest-neighbor coupling in each chain (proportional to \( c_2 \)) is also antiferromagnetic and is not much smaller than the nearest neighbor coupling, so each of the spin-1/2 chains is strongly frustrated. For such a strong frustration, it is known that a spin-1/2 chain is disordered with a small correlation length of about two lattice spacings (this implies a correlation length of about four lattice spacings in the sawtooth system), and is also strongly dimerized. The small correlation length is supported by the correlation data for \( N = 12 \) and \( J_2 = 0.1 \); we find that the ratio of spin-1/2 - spin-1/2 correlations \(< \vec{S}_1 \cdot \vec{S}_3 > / < \vec{S}_1 \cdot \vec{S}_3 > \approx -0.411 \) while the ratio of spin-1 - spin-1 correlations \(< \vec{S}_{13} \cdot \vec{S}_{15} > / < \vec{S}_{13} \cdot \vec{S}_{14} > \approx -0.552 \). Thus the spin-1/2 correlations (within each chain) decay faster with increasing distance than the spin-1 correlations (which have a correlation length of six lattice spacings).

To examine the possibility of dimerization, we use a method similar to the one used at the end of Sec. III to look for dimerization at \( J_2 = 1 \) and 2. However, the present case is different for the following reasons. First, we are now considering a NNN-AFM, so we have to check if the spin-1/2 - spin-1/2 correlations between a site and its next-nearest-neighbors are equal. Secondly, we have to simultaneously look for dimerization in the two spin-1/2 chains which are almost decoupled from each other. If there is dimerization, we expect four low-lying states which are almost degenerate with each other. For \( N = 8 \), these four states will exhibit dimerization in the four quantities \(< \vec{S}_1 \cdot \vec{S}_3 > \), \(< \vec{S}_1 \cdot \vec{S}_7 > \), \(< \vec{S}_2 \cdot \vec{S}_4 > \), and \(< \vec{S}_2 \cdot \vec{S}_8 > \). For \( J_2 = 0.1 \), we find that there is a non-degenerate ground state \( |1 > \) and two degenerate excited states \(|2 > \) and \(|3 > \) which are separated from the ground state by a small gap of 0.000674. (The next excited state, \(|4 > \), is separated from the ground state by a gap of 0.001277; for simplicity, we will not include this state in the following computations). The states \(|2 > \), \(|3 > \), and \(|3 > \) are all translation invariant, and therefore cannot show dimerization. We therefore consider the four linear combinations, \(|2± > = (|1 ±|2 > )/√2 \) and \(|3± ± = (|1 ±|3 > )/√2 \) which are not translation invariant. We then compute the four correlations mentioned above in all the seven states; the results are shown in Table 3. We observe a substantial amount of dimerization in the states \(|2± > \) and \(|3± > \). If we define the dimerization in the two chains to be \( d_1 = < \vec{S}_1 \cdot \vec{S}_3 > - < \vec{S}_1 \cdot \vec{S}_7 > \), \( d_2 = < \vec{S}_2 \cdot \vec{S}_4 > - < \vec{S}_2 \cdot \vec{S}_8 > \),

\begin{equation}
\begin{array}{c|c|c|c|c}
\text{State} & < \vec{S}_1 \cdot \vec{S}_3 > & < \vec{S}_1 \cdot \vec{S}_7 > & < \vec{S}_2 \cdot \vec{S}_4 > & < \vec{S}_2 \cdot \vec{S}_8 > \\
|1 > & -0.49765 & -0.49765 & -0.49765 & -0.49765 \\
|2 > & -0.24630 & -0.24629 & -0.24630 & -0.24631 \\
|3 > & -0.24639 & -0.24638 & -0.24625 & -0.24624 \\
|2+ > & -0.06774 & -0.067620 & -0.067620 & -0.06775 \\
|2- > & -0.67621 & -0.06774 & -0.06775 & -0.67621 \\
|3+ > & -0.06781 & -0.67622 & -0.06765 & -0.67624 \\
|3- > & -0.67623 & -0.06781 & -0.67625 & -0.06765 \\
\end{array}
\end{equation}

Table 3. The correlations of the spin-1/2’s at sites 1 and 2 with their two next-nearest-neighboring spin-1/2’s in the ground state (\(|1 > \)), first excited states (\(|2 > \) and \(|3 > \)), and the four linear combinations
Hamiltonian is given by $|n\rangle$ absorbed in triangle $g_n$ in Eq. (1) and a magnetic field term given by $\text{state (above the ferromagnetic state)}$ is a superposition of three states: where we have assumed the same value of the gyromagnetic ratio $g$ at $\text{in which all the spins are aligned with the field.}$ Hence there will be a macroscopic magnetization jump $h \to 0$ at $\text{in which the spin-1/2's which leads to a non-trivial behavior for that subsystem.}$

V. MACROSCOPIC MAGNETIZATION JUMP AT $J_2 = 2$

In this section, we will discuss the phenomenon of a macroscopic magnetization jump which occurs in the sawtooth chain for arbitrary values of $S_1$ and $S_2$ if $J_2 = 2$. In general, this phenomenon can occur in highly frustrated quantum antiferromagnets in which one of the spin wave modes (above the fully polarized ferromagnetic state) is completely dispersionless. When a uniform magnetic field is applied to the system, the magnetization can show a macroscopic jump at the saturation field $h_s$ (defined as the minimum field for which all the spins are aligned in the ground state)\textsuperscript{9,10}. By macroscopic we mean that the magnetization per unit cell jumps by a finite amount $\Delta m$ at $h = h_s$. This occurs if, (i) there is a special kind of ferromagnetic one-magnon eigenstate of the Hamiltonian which is spatially localized (a few lattice spacings), (ii) this eigenstate has the lowest energy amongst all the one-magnon eigenstates, (iii) the energy of this one-magnon state is negative with respect to the fully aligned state if $h < h_s$, and (iv) there are no multi-magnon bound states with energy lower than the sum of the individual one-magnon states. If all these conditions are satisfied, then for a certain range of values of the magnetic field below $h_s$, the lowest energy state is one in which there is a macroscopic number of these magnons localized in disjoint regions of the lattice. Eventually, as the field $h$ is increased, the energy of these magnons will cross zero at $h = h_s$ and then turn positive; for $h > h_s$, therefore, the lowest energy state will be the one in which all the spins are aligned with the field. Hence there will be a macroscopic magnetization jump at $h_s$.

For the sawtooth chain with spins $S_1$ and $S_2$, we consider a Hamiltonian which is the sum of the one given in Eq. (1) and a magnetic field term given by

$$H_{mag} = -h \sum_{i=1}^{2N} S_{i,z},$$

where we have assumed the same value of the gyromagnetic ratio $g$ for spins $S_1$ and $S_2$, and we have absorbed $g$ in the definition of the magnetic field $h$. For this system with $J_2 = 2$, the special one-magnon state (above the ferromagnetic state) is a superposition of three states: $|2, n - 1 >$ in which the spin-$S_2$ in triangle $n - 1$ has $S_z = S_2 - 1$ (and all the other spins have the maximum possible values of $S_z$), $|1, n >$ in which the spin-$S_1$ in triangle $n$ has $S_z = S_1 - 1$, and $|2, n >$ in which the spin-$S_2$ in triangle $n$ has $S_z = S_2 - 1$. The particular superposition of these three states which is an eigenstate of the total Hamiltonian is given by

$$|\psi_n > = |2, n - 1 > + |2, n > - 2 \sqrt{\frac{S_2}{S_1}} |1, n > .$$

The energy of this state with respect to the fully aligned state is given by $E = h - 4(S_1 + S_2)$. (The total spin of this state is $N(S_1 + S_2) - 1$, since it has total $S_z = N(S_1 + S_2) - 1$ and is annihilated by total $S_z$.) If we look at all the one-magnon states (above the ferromagnetic state), we find that they have two branches with the dispersions $\omega_- = h - 4(S_1 + S_2)$ (which is independent of the momentum and is equal to the energy of the localized one-magnon state $|\psi_n >$), and $\omega_+ = h - 4S_1 \sin^2(k/2)$ which is greater than $\omega_-$ for all values of $k$. 

(|2± > and |3± >) at $J_2 = 0.1$, for $N = 8$. 

The occurrence of a NNN-AFM with strong frustration for small values of $J_2$ is one of the interesting features of the spin-1/2 - spin-1 sawtooth chain. Although the spin-1 chain is gapped and therefore plays no direct role at energy scales much smaller than $J_1 = 1$, it perturbatively induces an unusual kind of interaction between the spin-1/2’s which leads to a non-trivial behavior for that subsystem.
We thus see that the state $|\psi_n\rangle$ meets the conditions (i) and (ii) given above, and its energy is lower than that of the fully aligned state if $h < h_s$, where
\begin{equation}
    h_s = 4(S_1 + S_2) .
\end{equation}

We therefore identify $h_s$ as the saturation field, and we expect a macroscopic jump in the magnetization when $h$ crosses $h_s$

The magnitude of the magnetization jump can be found as follows. Since each of the special one-magnon states involves three sites, at most $N/2$ such states can exist in disconnected regions of a chain with $N$ triangles. The lowest energy of a state with $n$ magnons will be less than the energy of the fully aligned state by an amount equal to $n[h - 4(S_1 + S_2)]$ as long as $n \leq N/2$. Once the number of magnons exceeds $N/2$, some of them will be close enough to interact (repulsively) with each other, and we no longer expect the energy to vary linearly with the number of magnons. Hence, when the magnetic field is lowered slightly below $h_s$, we expect the magnetization to abruptly drop from the maximum possible value of $M_{\text{max}} = N(S_1 + S_2)$ to $M_{\text{max}} - N/2$. The magnetization jump is therefore given by $\Delta M = N/2$.

For general values of $S_1$ and $S_2$, we have not analytically checked condition (iv) that there are no multi-magnon bound states with energy lower than the sum of one-magnon bound states. However, this is numerically found to be true in many models due to the absence of attractive interactions between the magnons\cite{9,10}. This is also found to be true in our system with $S_1 = 1$ and $S_2 = 1/2$, as the data given below shows.

For $N = 12$, we numerically find that in the absence of a magnetic field, the lowest energy $E_0$ in subspaces with different values of the total $S_z$ is given by, $E_0(S_z = 18) = 36$, $E_0(S_z = 17) = 30$, $E_0(S_z = 16) = 24$, ..., $E_0(S_z = 12) = 0$, and $E_0(S_z = 11) = -5.167392$. Thus, when the magnetic field strength is lowered just below $h_s = 6$, the magnetization jumps abruptly from 18 to 12 in accordance with the arguments given above.

\section*{VI. DISCUSSION}

We have studied the ground state and low-energy properties of a spin-1/2 - spin-1 sawtooth chain using SWT and exact diagonalization of finite systems. Linear SWT shows that there are two phases (the ground state being ferrimagnetic in one phase and a singlet in the other phase) separated by the value of $J_2 = 4$. In addition, $J_2 = 2$ is special because all the classically degenerate states have total spin equal to zero at that point, and $J_1 = 1$ is special because the total spin in each triangle is zero in all the classical ground states.

The numerical studies indicate that there are four distinct regions. For $J_2 \gtrsim 3.8$, the ground state is ferrimagnetic, while for $J_2 \lesssim 3.8$, it is a singlet. The structure factors suggest that the ground state is in a spiral state with a period of four unit cells for $1.9 \lesssim J_2 \lesssim 3.8$, and in a canted state with a period of two unit cells for $1.1 \lesssim J_2 \lesssim 3.8$. Near $J_2 = 1$ and 2, the gap between the ground state and the first excited state is particularly small, and there are repeated level crossings, possibly indicating crossovers between ground states with different kinds of short-range correlations. (Numerical calculations on larger system sizes would be very useful for a complete understanding of the nature of the ground state for $1 \lesssim J_2 \lesssim 3.8$). Finally, the spin-1/2's form an interesting system called a NNN-AFM for $J_2 \lesssim 1$; the ground state of this system has a short correlation length and is strongly dimerized.
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1 C. Lhuillier and G. Misguich, in High magnetic fields, eds. C. Berthier, L. P. Lévy and G. Martinez, Lecture Notes in Physics 595 (Springer-Verlag, Berlin, 2001), pp. 161-190.
2 T. Nakamura and K. Kubo, Phys. Rev. B 53, 6393 (1996); D. Sen, B. S. Shastry, R. E. Walstedt, and R. Cava, Phys. Rev. B 53, 6401 (1996); K. Kubo, Phys. Rev. B 48, 10552 (1993).
3 S. A. Blundell and M. D. Nunez-Reguerio, Eur. Phys. J. B 31, 453 (2003).
4 C. Raghu, I. Rudra, S. Ramasesha, and D. Sen, Phys. Rev. B 62, 9484 (2000).
5 N. B. Ivanov, J. Richter, and U. Schollwöck, Phys. Rev. B 58, 14456 (1998); J. Richter, U. Schollwöck, and N. B. Ivanov, Physica 281 & 282, 845 (2000).
6 P. Azaria, C. Hooley, P. Lecheminant, C. Lhuillier, and A. M. Tsvelik, Phys. Rev. Lett. 81, 1694 (1998); S. K. Pati, and R. R. P. Singh, Phys. Rev. B 60, 7695 (1999).
7 Ch. Waldtmann, H. Kreutzmann, U. Schollwöck, K. Maisinger, and H.-U. Everts, Phys. Rev. B 62, 9472 (2000).
8 P. W. Anderson, Phys. Rev. 86, 694 (1952); R. Kubo, Phys. Rev. 87, 568 (1952).
9 J. Schunenburg, A. Honecker, J. Schnack, J. Richter, and H.-J. Schmidt, Phys. Rev. Lett. 88, 167207 (2002).
10 J. Schnack, H.-J. Schmidt, J. Richter and J. Schunenburg, Eur. Phys. J. B 24, 475 (2001).
11 B. Doucot and P. Simon, J. Phys. A 31, 5855 (1998).
12 A. Chubukov, Phys. Rev. Lett. 69, 832 (1992).
13 P. Lecheminant, B. Bernu, C. Lhuillier, L. Pierre, and P. Sindzingre, Phys. Rev. B 56, 2521 (1997); Ch. Waldtmann, H.-U. Everts, B. Bernu, P. Sindzingre, C. Lhuillier, P. Lecheminant, and L. Pierre, Eur. Phys. J. B 2, 501 (1998).
14 T. Tonegawa and I. Harada, J. Phys. Soc. Jpn. 56, 2153 (1987), and 58, 2902 (1989).
15 F. D. M. Haldane, Phys. Lett. 93A, 464 (1983); Phys. Rev. Lett. 50, 1153 (1983).
16 S. R. White and D. A. Huse, Phys. Rev. B 48, 3844 (1993).
17 M. Oshikawa, M. Yamanaka and I. Affleck, Phys. Rev. Lett. 78, 1984 (1997).
18 V. Ravi Chandra, M. S. project report, Indian Institute of Science (2003).
19 S. R. White and I. Affleck, Phys. Rev. B 54, 9862 (1996).
Figure Captions

1. Picture of a sawtooth chain with 8 triangles indicating the site labels for the spin-$S_2$’s at the vertices and the spin-$S_1$’s at the bases of the triangles, and the couplings $J_1$ and $J_2$. For the numerical studies, we take $S_1 = 1$ and $S_2 = 1/2$. The arrows and angles ($\theta$) indicate a canted state in which all the spin-$S_2$’s are aligned with each other.

2. Spin wave dispersions in the ferrimagnetic phase for $J_2 = 5$, $S_1 = 1$ and $S_2 = 0.5$.

3. Non-vanishing spin wave dispersion in the singlet phase for $J_2 = 2$, $S_1 = 1$ and $S_2 = 0.5$.

4. Ground state energy as a function of $J_2$. The solid line shows the numerical data from exact diagonalization for a chain with 8 triangles, while the dashed line shows the spin wave results. In the inset, the solid lines show piecewise linear fits to the numerical data to the left and right of $J_2 = 3.8$, while the dotted lines show the continuations of the same two straight lines to the right and left of $J_2 = 3.8$ respectively. This shows a small discontinuity in the slope at $J_2 \simeq 3.8$.

5. Total spin of the first excited state as a function of $J_2$ for a chain with 8 triangles.

6. Energy gaps between the ground state and the first excited state (lower curve) and the first non-singlet state (upper curve) as a function of $J_2$ for a chain with 8 triangles. The ground state is a singlet for the range of $J_2$ shown in the figure.

7. The spin-1/2 - spin-1/2 correlations as functions of $J_2$ for a chain with 12 triangles.

8. The spin-1/2 - spin-1 correlations as functions of $J_2$ for a chain with 12 triangles.

9. The spin-1 - spin-1 correlations as functions of $J_2$ for a chain with 12 triangles.

10. Values of $q$ where the structure factors $S^{11}(q)$ and $S^{22}(q)$ are maximum as functions of $J_2$ for a chain with 12 triangles.

11. The structure factors $S^{11}(q_{\text{max}})$ and $S^{22}(q_{\text{max}})$ as functions of $J_2$ for a chain with 12 triangles.
Fig. 1
Fig. 2
Fig. 3
Fig. 4
Fig. 5
Energy gaps to some excited states

First non-singlet state
First excited state

Fig. 6
Fig. 7
Fig. 9
Fig. 10

$\frac{q_{\text{max}}}{\pi}$ for spin 1/2

$\frac{q_{\text{max}}}{\pi}$ for spin 1
$S_{1}^{1}(q_{\text{max}})$ for spin 1

$S_{1/2}^{22}(q_{\text{max}})$ for spin $1/2$