Vector chiral states in low-dimensional quantum spin systems

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A class of exact spin ground states with nonzero averages of vector spin chirality, \( \langle S_i \times S_j \cdot \hat{z} \rangle \), is presented. It is obtained by applying non-uniform O(2) rotations of spin operators in the XY plane on the SU(2)-invariant Affleck-Kennedy-Lieb-Tasaki (AKLT) states and their parent Hamiltonians. Excitation energies of the new ground states are studied with the use of single-mode approximation in one dimension for \( S = 1 \). The excitation gap remains robust. Construction of chiral AKLT states is shown to be possible in higher dimensions. We also present a general idea to produce vector chirality-condensed ground states as non-uniform O(2) rotations of the non-chiral parent states. Dzyaloshinskii-Moriya interaction is shown to imply non-zero spin chirality.

PACS numbers: 75.10.Jm

Introduction: Vector spin chirality, defined as the projection onto the axis of rotation (here given by \( \hat{z} \)) of the average of the outer product of two adjacent spins, \( \kappa_{ij} = (\hat{k}_{ij}) \), measures the sense of rotation of the magnetic moments in a spiral magnet. Being even under time reversal and odd under the inversion of \( i \) and \( j \) sites, this chirality plays an important role in the recent study of spin-polarization coupling in multiferroic materials where the local dipole moment shares the same symmetry properties as \( \kappa_{ij} \) [1]. A linear coupling between the two order parameters is a generic phenomenon in spiral magnets.

In a quite different context, an interesting observation was made by Hikihara et al. for the \( S = 1 \) spin chain with both nearest (\( J_1 \)) and next-nearest (\( J_2 \)) neighbour interactions [2]. For \( J_2/J_1 \) larger than a critical ratio, the ground state was shown to possess long-range order in the chirality correlation function, \( \langle \hat{k}_{i+1,i}\hat{k}_{j+1,j} \rangle \), as \( |i - j| \rightarrow \infty \). Such a novel phase, in the context of multiferroicity, would result in a strong coupling to the local dipole moment even in the absence of magnetic order. A similar possibility of a non-magnetic, yet chirality-ordered phase was explored in the Ginzburg-Landau treatment of anisotropic spin models[3]. In both instances, the key is to reduce the symmetry of the Hamiltonian away from SU(2) and introduce frustration to suppress magnetic ordering.

In this paper, we discuss a simple route to produce the vector chiral ground state in low-dimensional spin systems. First we look to models of Heisenberg spin exchange together with the Dzyaloshinskii-Moriya (DM) interaction for each \( \langle ij \rangle \) bond is given by \( J_2 \sin \theta_{ij} \). One can implement a site-dependent unitary rotation of the spins, \( S_i^+ \rightarrow U_i S_i^+ U_i^\dagger \), with the angle \( \theta_i \), chosen to meet the condition \( e^{i(\theta_i - \theta_j)} = e^{i\theta_{ij}} \) [4]. A simple way to choose \( \theta_i \) is to start with \( \theta_1 = 0 \), then choose all successive angles as \( \theta_2 = \theta_{21} \), \( \theta_3 = \theta_{32} \), etc. according to \( \theta_i = \sum_{2 \leq j \leq i} \theta_{ij} \). Due to the periodic structure we need to require \( \theta_{N+1} = \theta_1 \), which equals the sum of all the bond angles \( \sum_{1 \leq i \leq N} \theta_{i,i-1} \), be an integer multiple of \( 2\pi \):

\[
\sum_{1 \leq i \leq N} \theta_{i,i-1} / 2\pi = n (= \text{integer}).
\]

Once this condition is met, it is always possible to “gauge away” the phase angles in the model given in Eq. (1) to reduce it to the XXZ Hamiltonian: \( U[\{\theta_i\}]H[\{\theta_i\}]U^\dagger[\{\theta_i\}] = H_{XXZ} \) where \( U[\{\theta_i\}] = \prod_i U_i \). The eigenstates of Eq. (1), \( \{\theta_{ij}\} \), have a one-to-one correspondence with those of the XXZ model, denoted \( |XXZ\rangle \), and given explicitly by \( |\{\theta_{ij}\}\rangle = U[\{\theta_{ij}\}]|XXZ\rangle \).

Symmetry consideration dictates that \( \langle S_i^+ S_j^- \rangle \) for the eigenstates of \( H_{XXZ} \) be equal to \( X_{ij} \), where \( X_{ij} \) is a real-valued number. It then follows that \( \langle S_i^+ S_j^- \rangle \) \( \langle S_i^- S_j^+ \rangle \) \( \langle S_i^z S_j^z \rangle \) for the eigenstates \( \{\theta_{ij}\} \). The imaginary part of this average is nothing but \( \langle S_i^x S_j^y \rangle \), which equals the sum of all the bond angles \( \sum_{1 \leq i \leq N} \theta_{i,i-1} \), be an integer multiple of \( 2\pi \):

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For \( S = 1/2 \), through Jordan-Wigner transformation, the Hamiltonian (1) is mapped to a model of spinless fermions coupled to the gauge flux \( \theta_{ij} \). While a persistent current will exist for general values of the flux \( \phi = \sum_i \theta_{i,i-1} \), the criteria given in Eq. (2) corresponds to having an integer multiple of the flux quantum threading the ring, for which we would expect vanishing fermion current. Here, however, one must note that the spin chirality maps onto \( i(f_i^+ f_{i+1} - f_{i+1}^+ f_i) \), whereas the gauge-invariant definition of the fermion current will be
The structure factor for the uniform chiral AKLT state
\[(\theta_i)\] = \((1/3)\langle S_i \cdot S_j \rangle_0 \cos \theta_{ij},
\]
\[(\theta_i)\] = \((1/3)\langle S_i^x S_j^y \rangle_0,
\]
\[(S_i \cdot S_j)_0 = 2\delta_{ij} + 4(1 - \delta_{ij})/(1 - 3)|i-j|.
\]
The identity, \[(\theta_i)\] = \((1/3)\langle S_i^x S_j^y \rangle_0\), is ensured by the global U(1) symmetry of the chiral Hamiltonian, Eq. (5). The exponential decay in the spin-spin correlation persists for chiral AKLT states. The ensuing SMA calculation, as well as the general argument for the invariance of the energy spectra given earlier, confirms that the excitation gap persists for non-zero chiral angles. The ground state is thus non-magnetic, gapped, and possesses non-zero chiral moments.

The structure factor for the uniform chiral AKLT state \([\theta]\), where \(\theta_{ij} = \theta \times (i - j)\), can be easily worked out. Denoting the structure factor in the AKLT state as
\[s(k) = \langle S_k^z S_k^y \rangle_0 = 2(1 - \cos k)/(5 + 3 \cos k), \quad \mathbf{r} \equiv -k,
\]
we have
\[\langle \theta | S_i^z (\mathbf{r}) S_j^z (\mathbf{r}) | \theta \rangle = [s(k + \theta) + s(k - \theta)]/2. \]
obtained. The excitation energies in the SMA are given
\[ E_x(k, \theta) = E_0(k, \theta) = \frac{f(k+\theta) + f(k-\theta)}{s(k+\theta) + s(k-\theta)} \]  
(8) using \( f(k) = (10/27)(1 - \cos k) \). The excitation spectra are displayed for \( \theta \) ranging from 0 to \( \pi \) in Fig. 1. The SMA energies for \( S^\alpha_k(\theta) \) and \( S^\alpha_{-k}(\theta) \) possess symmetry under \( k \leftrightarrow -k \), while those for \( S^+ \) and \( S^- \) will be given by \( f(k \pm \theta)/s(k \pm \theta) \), respectively, explicitly breaking the chiral symmetry. The SMA results are also in accord with the general argument that all the energy eigenstates remain in one-to-one correspondence through the rotation.

A string order parameter\(^8\) characterizes the inherent antiferromagnetic spin-spin correlation in the AKLT state better than the spin-spin correlation function itself, which has an exponential fall-off with the separation. The string order parameter in the chiral state is given by
\[ \langle \{ \theta_i \} | O_{ij}^{z(y)} | \{ \theta_i \} \rangle = -4/9 \cos \theta_{ij} \]  
(9) while the \( z \)-component of the string order is given by the usual one: \( O_{ij}^z = S^z_i \exp [i \pi \sum_{j<k<i} S^z_k S^z_j] \). The averages of the string operators for \( | \{ \theta_i \} \rangle \) is \( \langle \{ \theta_i \} | O_{ij}^{z(y)} | \{ \theta_i \} \rangle = -4/9 \). In particular for the uniform chiral phase, the factor \( \cos \theta_{ij} = \cos[\theta(i-j)] \) in the string order reflects the extra pitch angle \( \theta \) due to the helical spin structure introduced by the DM interaction.

**Higher-dimensional generalization:** Construction of chiral AKLT ground states and the associated parent Hamiltonians are possible in higher dimensions:

\[ | \chi \rangle = \prod_{\langle ij \rangle} (A_{ij}^{\dagger} | \theta_{ij} \rangle)^M | 0 \rangle \]  
(10)

Here \( M = 2S/z \) is determined by the value of the spin \( S \) and the lattice coordination number \( z \). Each \( \langle ij \rangle \) bond carries a bond angle \( \theta_{ij} \). With more bond variables than can be generated by the set of site angles, the gauge rotation argument of the one dimension does not readily apply in higher dimensions. An alternative proof is given as follows.

The projector to the angular momentum-\( J \) subspace\(^5, 7\) \( \mathcal{P}_{ij}^J[\theta_{ij}] \) in the AKLT Hamiltonian is constructed in terms of the bond spin operator \( J_{ij}^J = (S_i + S_j)^2 = 2S(S+1) + 2S_i S_j \). The replacement \( S^+_i S^-_j + S^+_j S^-_i \to e^{i \phi_{ij}} S^+_i S^-_j + e^{-i \phi_{ij}} S^-_i S^+_j \) in \( J_{ij}^J \) produces \( \mathcal{P}_{ij}^J[\theta_{ij}] \) in Eq. (10). To prove that \( | \chi \rangle \) is indeed the zero-energy ground state of \( H^X \) in Eq. (10), we will show that each projector \( \mathcal{P}_{ij}^J[\theta_{ij}] \) acting on \( | \chi \rangle \) produces zero.

First write

\[ \mathcal{P}_{ij}^J[\theta_{ij}] = V_j V_i \mathcal{P}_{ij}^J V_i^\dagger V_j^\dagger \]  
(11)

where \( V_i \) is the \( U(1) \) rotation \( V_i S^\pm_i V_i^\dagger = S^\pm_i e^{\mp i \phi_i} \). We can choose \( \phi_i \) and \( \phi_j \) freely as long as their difference is equal to \( \theta_{ij} \). Focusing on a given bond \( \langle ij \rangle \), the chiral ground state can be written out

\[ | \chi \rangle = \sum_{m_1+n_1, m_2+n_2} \cdots (a_i^\dagger)^{m_1} (b_i^\dagger)^{n_1} (e^{i \phi_{ij}} a_j^\dagger b_j^\dagger - e^{-i \phi_{ij}} a_j^\dagger b_j^\dagger)^M (a_j^\dagger)^{m_2} (b_j^\dagger)^{n_2} \cdots | 0 \rangle \]  
(12)
where the terms on the far left and far right stem from the product of $A_{pq}^\dagger[\theta_{pq}]$ with only one end of $\langle pq \rangle$ connected to either $i$ or $j$. The sum $m_i + n_i$ and $m_j + n_j$ are constrained to equal $2S - M$ in the terms above. Applying the projector $\mathcal{P}_{ij}^\dagger[\theta_{ij}]$ on $|\chi\rangle$ and using relation (11) we obtain

\[
\mathcal{P}_{ij}^\dagger[\theta_{ij}]|\chi\rangle = \sum_{m_i+n_i} \sum_{m_j+n_j} \cdots e^{i\psi(\phi_i, \phi_j)} V_i V_j \mathcal{P}_{ij}^\dagger \left[ (a_i^\dagger)^{m_i} (b_i^\dagger)^{n_i} (a_j^\dagger b_j^\dagger - a_j^\dagger b_j^\dagger)^M \right] \cdots |0\rangle.
\]

Here the phase $\psi(\phi_i, \phi_j) = (n_i - m_i)\phi_i + (n_j - m_j)\phi_j$ stems from the gauge transformation $V_i^\dagger V_i^\dagger \cdots V_j^\dagger$ applied on the terms shown in Eq. (12). The state shown inside the bracket $\cdots$ in Eq. (13) have an expansion in terms of states for which the total momentum $J_{ij} = S_i + S_j$ on the bond $\langle ij \rangle$ is less than or equal to $J_{max} = 2S - M$. Hence for projectors $\mathcal{P}_{ij}^\dagger[\theta_{ij}]$ with $J > 2S - M$, Eq. (13) is zero. Since the whole argument works for each bond $\langle ij \rangle$ we have proven that $H^N |\chi\rangle = 0$.

Although the proof holds for any bond angle configuration $\{\theta_{ij}\}$ and for any dimension of the lattice, the gauge transformation introduced in Eq. (11) is only a local one, without the possibility to define the global unitary operator constructed as the product of $V_i$’s. Hence, it is generally not correct to associate sin $\theta_{ij}$ with the local average of the chirality except when we can decompose the bond angle as the difference of the local angles, $\theta_{ij} = \theta_i - \theta_j$.

**Discussion:** In conclusion, we have identified a simple and straightforward way to produce ground states of spins carrying non-zero vector spin chirality. The key idea is to start with a spin Hamiltonian whose ground state is non-chiral, and introduce non-uniform phase twists of $S_i^+$ and $S_j^-$, but not of $S_i^z$. The difference of the twist angle for nearby sites $\theta_{ij} = \theta_i - \theta_j$ defines the degree of local vector chirality. The Dzyaloshinskii-Moriya interaction also emerges in a natural way, after implementing the non-uniform O(2) rotations on the Hamiltonian without the DM interaction. A simple argument shows that the ground state in the presence of the DM interaction will generally possess non-zero vector chiral moments.

The well-known AKLT ground states of spins can be generalized in this way, in both one and higher dimensions. The ground state correlation properties for one-dimensional chiral AKLT states, in particular, can be readily calculated as chiral rotations of the known correlations for the non-chiral AKLT state. The excitation energies for the uniformly chiral AKLT state is calculated within the SMA and possess the gap which does not close as the chiral angle is varied. We have in addition identified the string order parameter appropriate for the linear chiral AKLT chain. Since the states we constructed in this paper possess nonzero chiral moment, their long-range ordering follows automatically. Construction of a different kind of chiral state, without the chiral moment but only long-range order in its correlations[2], will be an interesting challenge for the future.

For the experiments, insulating systems having the DM interaction in addition to the Heisenberg superexchange, such as the parent compound La$_2$CuO$_4$[9], are the likely places to find ground states with non-zero vector spin chirality. While the lattice deformation responsible for the presence of DM interaction can be measured in the X-ray scattering, a direct, simultaneous measurement of the spin chirality $\kappa_{ij}$ in the same compound using the polarized neutron scattering[3] will highlight the correlation between the two phenomena involving the lattice and the spin.

H. J. H. was supported by the Korea Research Foundation through Grant No. KRF-2005-070-C00044. Insightful comments from Ki-Seok Kim are gratefully acknowledged.

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