General method for finding ground state manifold of classical Heisenberg model

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We investigate classical Heisenberg models with the translation symmetries of infinite crystals. We prove a spiral theorem, which states that under certain conditions there must exist spiral ground states, and propose a natural classification of all manageable models based on some “spectral properties,” which are directly related to their ground state manifolds. We demonstrate how the ground state manifold can be calculated analytically for all spectra with finite number of minima and some with extensive minima, and algorithmically for the others. We also extend the method to particular anisotropic interactions.

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Classical spin orders are the starting point of nearly every quantum mechanical treatment for the same subject. In the twentieth century, quantum spin wave theories were developed to analyze the low energy excitations of systems with ferromagnetic (F) and antiferromagnetic (AF) classical ground states \cite{1, 2}. By introducing local frames, one can extend such quantum fluctuation analysis to systems with non-collinear and non-coplanar classical spin orders (see e.g. \cite{3}).

This “quantum-classical” approach is suitable for large-$S$ systems such as rare earth materials, which have attracted special interests in the past decade due to their central role in quantum anomalies Hall effect \cite{4}. In this respect, non-coplanar classical spin orders are especially favored. In the opposite small-$S$ extreme, one either extrapolates the results of large-$S$ expansions, or in the case of spin-$\frac{1}{2}$'s takes classical spins as a mean-field approximation.

It is therefore of fundamental importance to understand classical spin orders. Among all existing methods, the most intuitive ones are probably what might be called the pairwise minimization method (see e.g. \cite{5}), and its generalized version the cluster method \cite{6}, where the energy is minimized locally, and the global compatibility is essentially left to chance. A different approach is to use weak constraints while minimizing the energy, and to check whether the strong constraints are met afterwards. This is the idea of the Luttinger-Tisza (LT) method \cite{7} and the generalized Luttinger-Tisza method \cite{8} (see also \cite{9} for a review). Additionally, there is a so called classical spin wave method (see e.g. \cite{10, 11}), in which the energy is minimized within a spiral or helical ansatz (see Fig. 1). The ansatz is partially justified by a spiral theorem proved using the LT methods \cite{9}. Superposition of spin waves is valid only in special cases.

We are concerned with a classical Heisenberg Hamiltonian with the following properties (will be referred to as the basic assumptions): (i) it has the translation symmetry of an infinite crystal, and (ii) all spins are real, unit 3-vectors. This Hamiltonian is rather general: we made no assumption about the crystal dimensionality, the Bravais lattice, the basis, or the pattern of interaction. It is also obvious that the difference in spin length can be absorbed into the coupling constants. We shall strive to find the \textit{entire exact} ground state manifold (GSM) of the Hamiltonian.

While in both the cluster method and the LT methods some of the constraints are first dropped and then restored, we shall take an approach in which full information is retained all the time. This turns out to be more straightforward conceptually, and practically it enables the determination of the entire GSM, which is crucial in numerous contexts. The formalism to be developed will suggest a natural classification of all manageable models (i.e. those in the realm of the spiral theorem) based on the correspondence between some simple spectral properties (to be explained) and the GSMs. Dictionaries from the spectral properties to GSMs could hence be compiled, so that understanding a classical Heisenberg model would become utterly trivial.

The spiral theorem to be proved is the following: for any classical Heisenberg model that satisfies the basic assumptions, if it has one spin per unit cell, or if it has multiple spins per unit cell and has some additional properties, then there is a spiral state in the GSM. The one-spin part has been proved previously in the LT framework \cite{9}, but to our knowledge no formal statement of the multi-spin part has ever existed.

\textit{One-spin case.}—Consider a classical Heisenberg system with a large number $N$ of single-spin unit cells. The

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{Schematic (a) spiral and (b) helical states.}
\end{figure}

\textit{FIG. 1:} Schematic (a) spiral and (b) helical states.
Hamiltonian can be written as
\[ H = \frac{1}{2} \sum_{\vec{q}} \sum_{\vec{n}} J_{\vec{q}} \vec{S}_{\vec{n}} \cdot \vec{S}_{\vec{n}+\vec{q}} = \frac{1}{2} \sum_{\vec{n}} \sum_{\vec{q}} J_{\vec{q}} \vec{S}_{\vec{n}} \cdot \vec{S}_{\vec{n}+\vec{q}}, \]  
where \( J_{\vec{q}} \) are the \( \vec{q} \)-dependent coupling constants, and real, unit 3-vectors \( \vec{S}_{\vec{n}} \) are the spins at Bravais lattice points \( \vec{n} \). We shall keep to the conventions of positive sign and factor \( \frac{1}{2} \). Passing to the Fourier space, we rewrite the energy per spin as
\[ \epsilon = \frac{1}{N} \sum_{\vec{k}} \frac{1}{2} \sum_{\vec{n}} J_{\vec{n}} e^{i \vec{k} \cdot \vec{n}}, \]  
where
\[ \epsilon_{\vec{k}} = \frac{1}{2} \sum_{\vec{n}} J_{\vec{n}} e^{i \vec{k} \cdot \vec{n}}, \]  
\[ \vec{S}_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{n}} \vec{S}_{\vec{n}} e^{-i \vec{k} \cdot \vec{n}}. \]  

Because Eq. (1) formally resembles a hopping Hamiltonian – in that case each component of \( \vec{S}_{\vec{n}} \) would have to be interpreted as an operator – it is appropriate to call \( \epsilon_{\vec{k}} \) the spectrum or the band structure of \( H \), and to perceive as the \( T \)-reversal symmetry the fact that \( J_{\vec{k}} \) are real. It follows from the \( T \)-reversal symmetry that \( \epsilon_{-\vec{k}} = \epsilon_{\vec{k}} \).

To find the GSM, we need to know exactly what \( \{ \vec{S}_{\vec{k}} \} \) are legitimate. A configuration \( \{ \vec{S}_{\vec{n}} \} \) is legitimate if and only if it is contained in
\[ \mathcal{D} = \{ \{ \vec{S}_{\vec{k}} \} | \vec{S}_{\vec{n}} \in \mathbb{R}^3, \vec{S}_{\vec{n}} \vec{S}_{\vec{n}} = 1 \}, \]  

It follows that the set of legitimate \( \{ \vec{S}_{\vec{k}} \} \) is
\[ \mathcal{I} = \{ \{ \vec{S}_{\vec{k}} \} | \vec{S}_{\vec{k}} \in \mathbb{C}^3, \vec{S}_{-\vec{k}} = \vec{S}_{\vec{k}}^{\dagger}, \sum_{\vec{k}} \vec{S}_{\vec{k}}^{\dagger} \vec{S}_{\vec{k}+\vec{p}} = N \delta_{\vec{p}}, \forall \vec{p} \}, \]  
where the summation over \( \vec{k} \) is taken in the Brillouin zone (BZ), and reciprocal translation vectors are implicitly added to wave vectors that lie outside the BZ. \( \mathcal{D} \) and \( \mathcal{I} \) are the domain and the image of the injective map Eq. (4), respectively. We are ready to prove the following theorem.

**Theorem 1** (Spiral theorem (one-spin case)). Every classical Heisenberg Hamiltonian with one spin per unit cell that satisfies the basic assumptions has a spiral state in its GSM.

**Proof.** It follows from the last condition in Eq. (6) that \( \sum_{\vec{k}} \frac{1}{N} \vec{S}_{\vec{k}}^{\dagger} \vec{S}_{\vec{k}} = 1 \), so if \( \vec{S}_{\vec{k}} \neq \vec{0} \) only at some global minima in the spectrum, then the resulting state must be a rigorous ground state. Suppose \( \vec{k}_1 \) is a global minimum. Since \( \epsilon_{-\vec{k}} = \epsilon_{\vec{k}}, \) so is \( -\vec{k}_1 \). One can verify that the specification \( \vec{S}_{\vec{k}_1} = \frac{\sqrt{N}}{2} (1, \pm i, 0) \) for inequivalent \( \pm \vec{k}_1 \), or \( \sqrt{N} (1, 0, 0)^T \) for equivalent \( \pm \vec{k}_1 \), and zero elsewhere, is allowable according to \( \mathcal{I} \). This corresponds to the configuration \( \vec{S}_{\vec{k}} = (\cos(\vec{k}_1 \cdot \vec{n}), -\sin(\vec{k}_1 \cdot \vec{n}), 0)^T \), or \((e^{i\vec{k}_1 \cdot \vec{n}}, 0, 0)^T\), respectively, which is a spiral state. \( \square \)

The absolutely lowest points in the spectrum (out of all bands, in the multi-spin case to come) will be called the “spectral minima.” Theorem 1 implies that the entire GSM can be found by discarding all \( \vec{S}_{\vec{k}} \) but those at the spectral minima, and plugging them into Eq. (6). It is also clear that there is a direct correspondence between the GSM and the spectral minimum distribution, which can hence be used to classify all one-spin models.

We shall now classify two-dimensional (D) systems and present their GSMs. Given any Bravais lattice, we can align the axes accordingly so that \( n_x, n_y \) are integers and that the BZ is \((-\pi, \pi) \times (-\pi, \pi)\). Let us restrict ourselves for now to the case of finite number of spectral minima. Due to the periodicity of \( \vec{k} \), some special distributions must be treated separately. Examples of them are given in Fig. 2 which is far from complete, of course; yet more complicated distributions appear less often. We summarize the GSMs for these special distributions along with the GSMs for some generic distributions in Table I [12]. The six entries in Table I represent systems with spiral ground states, F/AF ground states, frustrated ground states, spiral ground states, frustrated ground states, and (possibly alternating) helical ground states, respectively. With tables like this established, it would be really easy to read off the GSM of a model for each value of the parameters, and thereby sketch out its ground state phase diagram.

Let us apply our method to two classic problems. The first is the square lattice \( J_1 - J_2 \) model, where \( J_1 \) and \( J_2 \) are the nearest-neighbor (NN) and the next nearest-neighbor coupling constants, respectively. Its spectrum

![FIG. 2: Special spectral minimum distributions for 2D systems with one spin per unit cell. The boxes are the Brillouin zone (BZ), and reciprocal translation vectors are implicitly added to wave vectors that lie outside the BZ.](image-url)
is $\epsilon_\xi = J_1(\cos k_x + \cos k_y) + 2J_2 \cos k_x \cos k_y$. In regimes $J_1 < 0$, $J_2 < 0.5|J_1|$, $J_1 > 0$, $J_2 > 0.5|J_1|$, and $J_2 > 0.5|J_1|$, which fall under Figs. 2(a)(d)(l), the system is in $F$ phase, AF phase, and frustrated two-sublattice AF phase, respectively (see e.g. 10.13)). The second is the triangular lattice $J_1 - J_2$ model, where $J_1$, $J_2$ are again the coupling constants for NNs and next NNs, respectively. The spectrum is $\epsilon_\xi = J_1[\cos k_x + \cos k_y + \cos(k_x - k_y)] + J_2[\cos(k_x + k_y) + \cos(2k_x - k_y) + \cos(2k_y - k_x)]$ (for a particular alignment of the axes). In the regime $J_1 < 0$, $J_2 < J_1$, a single pair of minima appears at $\pm(\frac{\pi}{3}, -\frac{\pi}{3})$, resulting in the famous $\sqrt{3}$ phase (see e.g. 14). The remaining cases contain three pairs of minima, which are not covered in Table 1 but are solvable.

**Multi-spin case.**—Consider the following classical Heisenberg Hamiltonian of a system with $N$ unit cells and $m$ sublattices:

$$H = \frac{1}{2} \sum_{\vec{n}} \sum_{\alpha \neq \alpha'} \sum_{a,b=1}^{m} J_{\alpha\beta} S_{\alpha a} \cdot S_{\alpha'b} + \epsilon_{\alpha a}$$

$$= \frac{1}{2} \sum_{\vec{n}} \left[ \sum_{\alpha \neq \alpha'} \sum_{a,b=1}^{m} J_{\alpha\beta} S_{\alpha a} \cdot S_{\alpha'b} + \sum_{\alpha} \epsilon_{\alpha a} \right].$$

where $a$, $b = 1, 2, \ldots, m$ are the sublattice indices. In the momentum space, $H$, or more conveniently the energy per spin $\epsilon$, is partially diagonal, reading

$$\epsilon = \sum_{k,a,b} \frac{1}{Nm} S_{k a} \cdot h(k)_{ab} S_{k b},$$

with

$$S_{k a} = \frac{1}{\sqrt{N}} \sum_{\vec{n}} S_{\vec{n} a} e^{-i\vec{k} \cdot \vec{n}},$$

$$h(k)_{ab} \equiv \frac{1}{2} \sum_{\vec{n}} J_{\vec{n} a b} e^{i\vec{k} \cdot \vec{n}}.$$

We can further express $h(k)$ in terms of its eigenvalues $\epsilon_{\alpha a}$ and eigenvectors $\xi_{\alpha a}$, where $\alpha = 1, \ldots, m$, yielding

$$\epsilon = \sum_{k,a} \frac{1}{Nm} S_{k a} \epsilon_{\alpha a} = \sum_{k,a} \frac{1}{Nm} S_{k a} \xi_{\alpha a} \xi_{\alpha a}^*,$$

with

$$\xi_{\alpha a} \equiv \sum_{\vec{n}} S_{\vec{n} a} \xi_{\alpha a}.$$
Corollary 1. For a system with \( m \) spins per unit cell, if for each \( \mathbf{k} \), up to a gauge transformation (i.e. multiplying basis by phases), \( h(\mathbf{k})_{ab} \) only depends on \((a-b) \mod m\), then there exists a spiral ground state.

Corollary 2. For a system with two spins per unit cell, if \( h(\mathbf{k}) \) contain no \( \sigma_z \) for all \( \mathbf{k} \), or equivalently if \( H \) is invariant under an inversion that exchanges the two sub-lattices, then there exists a spiral ground state.

Corollary 3. For a system with three spins per unit cell, if \( h(\mathbf{k})_{11} = h(\mathbf{k})_{22} = h(\mathbf{k})_{33} \) and \( |h(\mathbf{k})_{12}| = |h(\mathbf{k})_{13}| \) for all \( \mathbf{k} \), then there exists a spiral ground state.

That \( h(\mathbf{k})_{ab} \) only depends on \((a-b) \mod m\) means that the sublattice degree of freedom has become an extra finite periodic dimension (think of nanotubes), and yet Corollaries 1-3 allow this to be achieved after gauge transformations. The condition in Theorem 2 is even weaker, as it only stipulates that \( \xi_{\pm} \) should take a particular form.

When the requirement in Theorem 2 is met, the GSM is determined by the spectral minimum distribution and the \( \xi_{\pm} \) thereof. We omit the similar classification here and simply point out some tractable classic models. First, Corollary 2 is applicable to the honeycomb \( J_1 - J_2 \) model (Fig. 3(a)) [3, 11]. Second, the \( h(\mathbf{k}) \) of the checkerboard \( J_1 - J_2 \) model (Fig. 3(b)) has no \( \sigma_z \) component along \( |k_x| = |k_y| \), which happens to include some of the spectral minima in all cases [13]. Finally, for the Kagome NN model (Fig. 3(c)), the conditions \( h(\mathbf{k})_{11} = h(\mathbf{k})_{22} = h(\mathbf{k})_{33} \) and \( |h(\mathbf{k})_{12}| = |h(\mathbf{k})_{13}| \) are satisfied only at \( \mathbf{k} = 0 \), which, luckily, is always a minimum [11, 17]. These models have extensive minimum distributions in some regimes, which are the topic of the following section.

Regarding robust non-coplanar spin orders, namely non-coplanar ground states that are not degenerate with any coplanar ones, we must search multi-spin models that do not fulfill the requirement in Theorem 2.

**Extensive spectral minima.**—Spectra with infinitely many minima are intimately connected with disorder, localization, frustration, etc., and in these contexts knowing the entire GSMs is a primary goal. In retrospect, we have determined GSMs by putting together the legitimacy conditions, which enforce unit spin length, and the energy minimization conditions, which rule out certain \( S_{\mathbf{k}}^\sigma \) or \( S_{\mathbf{k}_0}^\sigma \). The legitimacy conditions are decoupled in \( \bar{n} \) space and coupled in \( \bar{k} \) space, and previously we have sacrificed the decoupled form for the simplicity of the energy minimization conditions in \( \bar{k} \) space. In the case of extensive spectral minima, the latter conditions often remain simple in real space. It is hence no good idea to adhere to \( S_{\mathbf{k}}^\sigma \) or \( S_{\mathbf{k}_0}^\sigma \). (Nonetheless, passing to \( \bar{k} \) space is still an important intermediate step, because otherwise we cannot even determine the energy minimization conditions.)

To illustrate the point, consider the distributions in Fig. 4 for \( N_x \times N_y \) lattices with one spin per unit cell. For Fig. 4(a), in terms of \( \bar{S}_{\mathbf{k}}^\sigma \), the legitimacy conditions are simply Eq. (3), and energy minimization says nothing, so the GSM is given by Eq. (5). For Fig. 4(b), defining \( \bar{S}_{n_x \alpha, k_y} = \frac{1}{\sqrt{N_x}} \sum_{k_x} S_{\mathbf{k}}^\sigma e^{i k_x n_x} \), we derive the conditions \( \sum_{k_y} S_{n_x \alpha, k_y}^\sigma = N_y \delta_{p_x p_y} \), \( \bar{S}_{n_x \alpha, -k_y} = S_{n_x \alpha, k_y}^\sigma \) for legitimacy, and \( \bar{S}_{n_x \alpha, k_y} = 0 \), \( \forall k_y \neq \pm K_y \) for energy minimization, whence the GSM can be trivially computed. Now consider the less trivial situation Fig. 4(c), where the interaction is not purely local in any direction, even when restricted to the GSM. This distribution arises in, for instance, the spectrum \( \epsilon_{\mathbf{k}} = \cos k_x + \cos k_y + \frac{1}{2} \cos(k_x - k_y) + \cos(k_x + k_y) \). Energy minimization can be incorporated into the variables \( \bar{S}_{n_x, k_y = \pi} = \sum_{k_x} S_{n_x \alpha, k_y = \pi} e^{i k_x n_x} \), \( S_{k_a = \pi, n_y} = \frac{1}{\sqrt{N_y}} \sum_{k_y} \bar{S}_{k_a = \pi, k_y = \pi} e^{i k_y n_y} \), which are independent except that the two \( \bar{S}_{k_a = (\pi, \pi)}^\sigma \) must be identified. Plugging them into Eq. (12), we find that the GSM is given by [12],

\[
\begin{align*}
\mu_{n_x}, \nu_{n_y}, \bar{S}_{k_a = (\pi, \pi)}^\sigma & \in \mathbb{R}^3, \\
N_x |\mu_{n_x}|^2 + N_y |\nu_{n_y}|^2 & = N + |\bar{S}_{k_a = (\pi, \pi)}^\sigma|^2, \\
|\mu_{n_x}| & \text{ independent of } n_x, \quad |\nu_{n_y}| \text{ independent of } n_y, \\
\frac{1}{\sqrt{N}} \sum_{n} \mu_{n_x} \cdot \nu_{n_y} e^{-i p_x n} & = 0, \quad \forall p_x, p_y \neq 0, \\
\frac{1}{\sqrt{N_x}} \sum_{n_x} \mu_{n_x} = \frac{1}{\sqrt{N_y}} \sum_{n_y} \nu_{n_y} = \bar{S}_{k_a = (\pi, \pi)}^\sigma,
\end{align*}
\]
where \( \mu_{n_x} \equiv (-)^{n_x} \tilde{S}_{n_x,k_y=\pi} \) and \( \nu_{n_y} \equiv (-)^{n_y} \tilde{S}_{k_x=\pi,n_y} \), which is not just the sum of the two submanifolds developed from the edges \( L_1, L_2 \) individually. (We will obtain a simpler subset of the GSM if we extend the fourth line of Eq. (11) to all \( \vec{p} \not= \vec{0} \). In that case \( \mu_{n_x} \cdot \nu_{n_y} \) is independent of \( n_x, n_y \), and we can easily enumerate all the possible orientations of \( \mu_{n_x} \) and \( \nu_{n_y} \).)

In the multi-spin case, to preserve the simplicity of the energy minimization conditions, we undo the Fourier transform but not the unitary transformation by \( \xi_{\vec{k},a} \), thereby bringing in convolution structures, which can be handled numerically. Consider the minimum distributions in Fig. 4 for non-degenerate lowest band \( \alpha = 1 \), and assume the requirement in Theorem 2 is met. The GSM for Fig. 4(a) is given by \[ \tilde{S}_{n_x, \alpha = 1} = 1, \quad \tilde{S}_{n_y, \alpha = 1} \in \mathbb{R}^3, \] (15)

where

\[
(\tilde{S} \ast \xi)^{\dagger}_{\vec{n}, \alpha = 1} = \frac{1}{\sqrt{N}} \sum_{\vec{n}' \in \mathbb{Z}^3} \tilde{S}_{\vec{n}' \alpha} e^{i\vec{k} \cdot \vec{n}'}, \]

(16)

\[
\xi_{\vec{n}} \alpha = \frac{1}{\sqrt{N}} \sum_{\vec{k} \in \mathbb{R}^2} \xi_{\vec{k}, a} e^{i\vec{k} \cdot \vec{n}}, \]

(17)

\[
\tilde{S}_{\vec{n}} \alpha = \frac{1}{\sqrt{N}} \sum_{\vec{k} \in \mathbb{R}^2} \tilde{S}_{\vec{k}, a} e^{i\vec{k} \cdot \vec{n}}. \]

(18)

Note that we must take \( \tilde{S}_{\vec{n}, \alpha = 1} \), not \( (\tilde{S} \ast \xi)_{\vec{n}, \alpha = 1, \alpha} \), as independent variables in Eq. (15). Similarly, the GSM for Fig. 4(b) is given by \[ \tilde{S}_{n_x, k_y, \alpha = 1} = \frac{1}{\sqrt{N_z}} \sum_{n_x} \tilde{S}_{n_x, k_y, \alpha = 1}, \]

(19)

where

\[
(\tilde{S} \ast \xi)_{n_x, k_y, \alpha = 1} = \frac{1}{\sqrt{N_z}} \sum_{n_x} \tilde{S}_{n_x, k_y, \alpha = 1}, \]

(20)

\[
\xi_{n_x, k_y, \alpha} = \frac{1}{\sqrt{N_z}} \sum_{k_y} \xi_{k_y, a} e^{i\vec{k} \cdot \vec{n}}, \]

(21)

\[
\tilde{S}_{n_x, k_y, \alpha} = \frac{1}{\sqrt{N_z}} \sum_{k_y} \tilde{S}_{k_y, a} e^{i\vec{k} \cdot \vec{n}}. \]

(22)

As for Fig. 4(c), we get

\[
\tilde{S}_{n_x, n_y} = \frac{1}{\sqrt{N}} \sum_{\vec{n}} \tilde{S}_{n_x, n_y} e^{-i\vec{p} \cdot \vec{n}} = 0, \quad \forall p_x, p_y \not= 0, \]

\[
\frac{1}{\sqrt{N_z}} \sum_{n_x} (-)^{n_x} \tilde{S}_{n_x, k_y=\pi, \alpha = 1} = \tilde{S}_{k_y=\pi, \alpha = 1}, \]

\[
\frac{1}{\sqrt{N_y}} \sum_{n_y} (-)^{n_y} \tilde{S}_{k_x=\pi, n_y, \alpha = 1} = \tilde{S}_{k_x=\pi, n_y, \alpha = 1}, \]

(23)

FIG. 5: Examples of more complicated spectral minimum trajectories.

where

\[
\mu_{n_x, a} \equiv (-)^{n_x} (\tilde{S} \ast \xi)_{n_x, k_y=\pi, a = 1, \alpha}, \quad n_x \]

(24)

\[
\nu_{n_y, a} \equiv (-)^{n_y} (\tilde{S} \ast \xi)_{k_x=\pi, n_y, a = 1, \alpha}, \quad n_y \]

(25)

\[
(\tilde{S} \ast \xi)_{k_x, n_y, \alpha} = \frac{1}{\sqrt{N_y}} \sum_{n_y} \tilde{S}_{k_x, n_y, \alpha} e^{i\vec{k} \cdot \vec{n}}, \quad n_y \]

(26)

\[
\xi_{k_x, n_y, \alpha} = \frac{1}{\sqrt{N_y}} \sum_{k_x} \xi_{k_x, a} e^{i\vec{k} \cdot \vec{n}}, \quad n_y \]

(27)

\[
\tilde{S}_{k_x, n_y, \alpha} = \frac{1}{\sqrt{N_y}} \sum_{k_x} \tilde{S}_{k_x, a} e^{i\vec{k} \cdot \vec{n}}, \quad n_y \]

(28)

For even more complicated minimum distributions, the GSMs may be inferred from the sub-GSMs obtained numerically from finite meshes on the minimum trajectories or zones. For this purpose, prior analytical analysis is often labor-saving. Consider for instance the spectral minimum distribution in Fig. 5(a) for one-spin case, and suppose that in a ground state we have \( \tilde{S}_{\pm \vec{K}_1} = \vec{0} \). Then in light of the fourth entry in Table I which states that two generic pairs of minima interfere each other [12], we can convince ourselves that \( \tilde{S}_{\pm \vec{k}_1} = \vec{0} \), and by induction, \( \tilde{S}_{\pm \vec{K}_3, \vec{K}_5, \vec{K}_{2} \cdots} \), and eventually all \( \tilde{S}_{\vec{k}} \) on \( \pm \vec{L}_3 \) must vanish. It follows that if any point, not necessarily \( \vec{K}_1 \), on edge \( L_1 \) contributes to a ground state, then the entire \( L_1 \) does not. Analysis like this definitely simplifies the numerics. In the limit of infinite number of edges, that is when the trajectory becomes such a random curve \( C \) as the one in Fig. 5(b), no two pairs are compatible, and the GSM is simply

\[
\tilde{S}_{\vec{n}} = \rho \begin{pmatrix}
\cos(\vec{k}_j \cdot \vec{n}) \\
-\sin(\vec{k}_j \cdot \vec{n}) \\
0
\end{pmatrix}, \quad \rho \in SO_3, \quad \vec{k}_j \in C.
\]

(29)

We remark that the seemingly oversimplified situations exemplified by Fig. 4 and Fig. 5(b) actually cover a few familiar models. Fig. 4(a) is the case of the checkerboard model (see Fig. 3 same below) with \( J_1 \not= 0, J_2 = |J_1| \) [13], and the Kagome model with \( J_1 > 0 \) [16, 17]. Fig. 4(c) occurs in the square lattice \( J_1 - J_2 \) model with \( J_1 > 0, J_2 = \frac{1}{2} J_1 \) (see e.g. [10, 12]), and the checkerboard model with \( J_2 > |J_1| \) [15]. The square lattice
model with $J_1 < 0, J_2 = \frac{1}{2}|J_1|$ (see e.g. [10]), and the checkerboard model with $J_1 = 0, J_2 < 0$, have a similar distribution in which the minima lie on $k_x = 0$ and $k_y = 0$. Last but not least, Fig. 5(b) reflects the minimum distributions of the honeycomb model with $J_1 \neq 0$ and $0.17|J_1| < J_2 < 0.48|J_1|$, for which there is one loop, or $J_2 > 0.48|J_1|$, for which there are two loops (numbers are approximate) [3, 11].

Anisotropic interactions.—Consider XXZ Hamiltonians of the following form:

$$H = \frac{1}{2} \sum_{\vec{\eta}} \sum_{\vec{n}} J_{\vec{\eta} \vec{\eta}'} S^z_{\vec{n} \vec{\eta}} \Theta S^z_{\vec{n}+\vec{\eta}'}$$

(30)

or

$$H = \frac{1}{2} \sum_{\vec{n}} \sum_{\vec{\eta}} \sum_{a,b=1}^m J_{\vec{\eta} \vec{\eta}'} S^z_{\vec{n}a} \Theta S^z_{\vec{n}+\vec{\eta}b}$$

(31)

where $\Theta \equiv \text{diag}\{1,1,1+\theta\}$ is independent of $\vec{\eta}$, $a$, and $b$. Assume the requirement in Theorem 2 is met in the isotropic case. Then a positive $\theta$ simply contracts the GSM, whereas a negative $\theta$ may modify the ground states, which we do not plan to discuss. XY model is the XXZ model with $\theta = +\infty$ and can thus be put into our framework.

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Supplemental Material for “General method for finding ground state manifold of classical Heisenberg model”

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I. SELECTED EXAMPLES FROM TABLE I

A. Distribution with one generic pair of minima

Let $\pm \vec{k}_1$ be the spectral minima, and set $\vec{S}_{\pm \vec{k}_1} = x \pm iu$, where $x$ and $u$ are real, 3-component vectors. The second condition in Eq. (6) is automatically satisfied. The third condition stipulates

$$|x|^2 + |u|^2 = \frac{N}{2}, \quad \text{(S1)}$$

for $\vec{p} = \vec{0}$, and

$$|x|^2 - |u|^2 = 0, \quad x \cdot u = 0 \quad \text{(S2)}$$

for $\vec{p} = 2\vec{k}_1$ or $-2\vec{k}_1$. The solutions are apparently

$$\vec{S}_{\pm \vec{k}_1} = \rho \frac{\sqrt{N}}{2} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}, \quad \text{(S3)}$$

or in real space,

$$\vec{S}_{\vec{n}} = \rho \begin{pmatrix} \cos(\vec{k}_1 \cdot \vec{n}) \\ -\sin(\vec{k}_1 \cdot \vec{n}) \\ 0 \end{pmatrix}, \quad \text{(S4)}$$

where $\rho \in SO_3$ is an arbitrary rotation.

B. Distribution with two generic pairs of minima

Let $\pm \vec{k}_1$, $\pm \vec{k}_2$ be the spectral minima, and set $\vec{S}_{\pm \vec{k}_1} = x_1 \pm iu_1$, $\vec{S}_{\pm \vec{k}_2} = x_2 \pm iu_2$, where $x_1, u_1, x_2, u_2$ are real, 3-component vectors. Plugging these into the third condition in Eq. (6), we get

$$|x_1|^2 + |u_1|^2 + |x_2|^2 + |u_2|^2 = \frac{N}{2}, \quad \text{(S5)}$$

$$|x_1|^2 - |u_1|^2 = 0, \quad x_1 \cdot u_1 = 0 \quad \text{(S6)}$$

$$|x_2|^2 - |u_2|^2 = 0, \quad x_2 \cdot u_2 = 0 \quad \text{(S7)}$$

and

$$x_1 \cdot x_2 - u_1 \cdot u_2 = 0, \quad x_2 \cdot u_1 + x_1 \cdot u_2 = 0 \quad \text{(S8)}$$

$$x_1 \cdot x_2 + u_1 \cdot u_2 = 0, \quad x_2 \cdot u_1 - x_1 \cdot u_2 = 0 \quad \text{(S9)}$$

Eqs. (S5)-(S9) simplify to

$$|x_1| = |u_1|, \quad |x_2| = |u_2|, \quad \text{(S10)}$$

$$|x_1|^2 + |u_1|^2 + |x_2|^2 + |u_2|^2 = \frac{N}{2}, \quad \text{(S11)}$$

$$x_1, \quad u_1, \quad x_2, \quad u_2 \quad \text{are mutually orthogonal.} \quad \text{(S12)}$$

No four nontrivial, mutually orthogonal vectors can coexist in $\mathbb{R}^3$. Therefore, either $\vec{S}_{\pm \vec{k}_1}$ or $\vec{S}_{\pm \vec{k}_2}$ need to vanish. The ground state manifold (GSM) must be

$$\vec{S}_{\vec{n}} = \rho \begin{pmatrix} \cos(\vec{k}_j \cdot \vec{n}) \\ -\sin(\vec{k}_j \cdot \vec{n}) \\ 0 \end{pmatrix}, \quad \rho \in SO_3, \quad j = 1, 2. \quad \text{(S13)}$$

C. Distribution in Fig. 2(i)

Define $\vec{k}_1 \equiv (0,0)$ and $\vec{k}_2 \equiv (\pi,0)$. The second condition in Eq. (6) implies $\vec{S}_{\vec{k}_1}$ and $\vec{S}_{\vec{k}_2}$ are real. The third condition requires

$$|\vec{S}_{\vec{k}_1}|^2 + |\vec{S}_{\vec{k}_2}|^2 = N \quad \text{(S14)}$$

$$\vec{S}_{\vec{k}_1} \cdot \vec{S}_{\vec{k}_2} = 0 \quad \text{(S15)}$$

The solutions are

$$\vec{S}_{\vec{k}_1} = \rho \sqrt{N} \begin{pmatrix} \cos \gamma \\ 0 \\ 0 \end{pmatrix}, \quad \vec{S}_{\vec{k}_2} = \rho \sqrt{N} \begin{pmatrix} 0 \\ \sin \gamma \\ 0 \end{pmatrix}, \quad \text{(S16)}$$

where $\rho \in SO_3$ and $\gamma \in \mathbb{R}$, so the GSM is

$$\vec{S}_{\vec{n}} = \rho \begin{pmatrix} \cos \gamma \\ (-)^{n_z} \sin \gamma \\ 0 \end{pmatrix} \quad \text{(S17)}$$

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II. Extensive Spectral Minimum Distributions

A. Derivation of Eq. (14)

Define two families of new variables:

\[ \tilde{S}_{n,k} = \frac{1}{\sqrt{N_x}} \sum_{k_x} \vec{S}_{k} e^{i\vec{k}_x n_x}, \quad (S18) \]

\[ \tilde{S}_{k,n} = \frac{1}{\sqrt{N_y}} \sum_{k_y} \vec{S}_{k} e^{i\vec{k}_y n_y}. \quad (S19) \]

The energy minimization conditions can be stated as follows: \( \tilde{S}_{n,k_y} = 0, \forall k_y \neq \pi \), and \( \tilde{S}_{k,n_x} = 0, \forall k_x \neq \pi \). Now we want to express the conditions in Eq. (6) in terms of \( \tilde{S}_{n_x,k_y=\pi}, \tilde{S}_{k_x=\pi,n_y}, \) and \( \tilde{S}_{k=(\pi,\pi)}. \) The first two conditions go over into

\[ \tilde{S}_{n_x,k_y=\pi}, \tilde{S}_{k_x=\pi,n_y}, \tilde{S}_{k=(\pi,\pi)} \in \mathbb{R}^3, \quad (S20) \]

\[ \frac{1}{\sqrt{N_x}} \sum_{n_x} (-)^{n_x} \tilde{S}_{n_x,k_y=\pi} = \tilde{S}_{k=(\pi,\pi)} \quad (S21) \]

\[ \frac{1}{\sqrt{N_y}} \sum_{n_y} (-)^{n_y} \tilde{S}_{k_x=\pi,n_y} = \tilde{S}_{k=(\pi,\pi)} \quad (S22) \]

The third condition says, for \( \vec{p} = 0 \),

\[ N + |\tilde{S}_{k=(\pi,\pi)}|^2 \]

\[ = \sum_{k_x} \tilde{S}_{k_x=\pi,n_y} \tilde{S}_{k_x=\pi,k_y} + \sum_{l_y} \tilde{S}_{l_y=\pi,n_x} \tilde{S}_{l_y=\pi,k_x} \]

\[ = \sum_{n_x} \tilde{S}_{n_x,k_y=\pi} \tilde{S}_{n_x,k_y=\pi} + \sum_{n_y} \tilde{S}_{k_x=\pi,n_y} \tilde{S}_{k_x=\pi,n_y} \]

\[ = \sum_{n_x} |\tilde{S}_{n_x,k_y=\pi}|^2 + \sum_{n_y} |\tilde{S}_{k_x=\pi,n_y}|^2. \quad (S23) \]

For \( p_x \neq 0, p_y = 0 \), only \( L_1 \) contributes (see Fig. 4). Thus,

\[ 0 = \sum_{k_x} \tilde{S}_{k_x=\pi,n_y} \tilde{S}_{k_x=\pi,k_y=\pi} \]

\[ = \frac{1}{\sqrt{N_x}} \sum_{n_x} \sum_{n_y} \tilde{S}_{n_x,k_y=\pi} \tilde{S}_{n_x,k_y=\pi} e^{i(k_x+n_x) n_y} \]

\[ = \sum_{n_x} \tilde{S}_{n_x,k_y=\pi} \tilde{S}_{n_x,k_y=\pi} e^{-i p_x n_x}, \quad (S24) \]

which means that \( |\tilde{S}_{n_x,k_y=\pi}|^2 \) is independent of \( n_x \). Similarly, for \( p_x = 0, p_y \neq 0 \), we have

\[ 0 = \sum_{n_y} \tilde{S}_{k_x=\pi,n_y} \tilde{S}_{k_x=\pi,n_y} e^{-i p_y n_y}, \quad (S25) \]

which means that \( |\tilde{S}_{k_x=\pi,n_y}|^2 \) is independent of \( n_y \). Lastly, \( \vec{p} \) such that \( p_x \neq 0, p_y \neq 0 \) couples one point on \( L_2 \) to another point on \( L_2 \). Thus, we have

\[ 0 = \tilde{S}_{k_x=\pi-p_x,k_y=\pi} \tilde{S}_{k_x=\pi,k_y=\pi+p_y} \]

\[ = \frac{1}{\sqrt{N_x}} \sum_{n_x} \tilde{S}_{n_x,k_y=\pi} e^{i(k_x+n_x) n_y} \sum_{n_y} \tilde{S}_{k_x=\pi,n_y} e^{-i(k_x+n_x) n_y} \]

\[ = \frac{1}{\sqrt{N_x}} \sum_{n_x,n_y} (-)^{n_x+n_y} \tilde{S}_{n_x,k_y=\pi} \tilde{S}_{k_x=\pi,n_y} e^{-i\vec{p} \cdot \vec{n}}. \quad (S26) \]

In summary, the GSM is given by the following,

\[ \mu_{n_x}, \nu_{n_y}, \tilde{S}_{k=(\pi,p)} \in \mathbb{R}^3, \]

\[ N_x |\mu_{n_x}|^2 + N_y |\nu_{n_y}|^2 = N + |\tilde{S}_{k=(\pi,p)}|^2, \]

\[ |\mu_{n_x}| \text{ independent of } n_x, \quad |\nu_{n_y}| \text{ independent of } n_y, \]

\[ \frac{1}{\sqrt{N_x}} \sum_{n_x} \mu_{n_x} e^{-i\vec{p} \cdot \vec{n}} = 0, \quad \forall p_x, p_y \neq 0, \]

\[ \frac{1}{\sqrt{N_y}} \sum_{n_y} \nu_{n_y} = \frac{1}{\sqrt{N_x}} \sum_{n_x} \nu_{n_x} = \tilde{S}_{k=(\pi,\pi)}. \quad (S27) \]

where \( \mu_{n_x} \equiv (-)^{n_x} \tilde{S}_{n_x,k_y=\pi} \) and \( \nu_{n_y} \equiv (-)^{n_y} \tilde{S}_{k_x=\pi, n_y}. \)

B. Derivation of Eq. (15)

Define \( \tilde{S}_{\alpha} \equiv \frac{1}{\sqrt{N}} \sum_{k} \tilde{S}_{k \alpha} e^{i\vec{k} \cdot \vec{n}} \) and \( \xi_{\alpha} \equiv \frac{1}{\sqrt{N}} \sum_{k} \xi_{\alpha} e^{i\vec{k} \cdot \vec{n}} \). The energy minimization conditions are just \( \tilde{S}_{\alpha} = 0, \forall \alpha \neq 1 \). As for legitimacy, the first two conditions in Eq. (13) become

\[ \tilde{S}_{\alpha} \in \mathbb{R}^3. \quad (S28) \]

Fourier transforming the third condition, we find

\[ N = \frac{1}{N} \sum_{\vec{p}} \sum_{\alpha} \sum_{\alpha'} \sum_{\vec{n}} \tilde{S}_{\alpha}^* \tilde{S}_{\alpha'} \tilde{S}_{\alpha} \xi_{\alpha}^* \tilde{S}_{\alpha'} \xi_{\alpha'} - \tilde{S}_{\alpha} \xi_{\alpha} \tilde{S}_{\alpha'}^* \xi_{\alpha'} \]

\[ = \frac{1}{\sqrt{N}} \sum_{\vec{p}} \sum_{\alpha} \sum_{\alpha'} \sum_{\vec{n}} \tilde{S}_{\alpha}^* \tilde{S}_{\alpha'} \tilde{S}_{\alpha} \xi_{\alpha} \xi_{\alpha'}^* - \tilde{S}_{\alpha} \xi_{\alpha} \tilde{S}_{\alpha'}^* \xi_{\alpha'} \]

\[ = \left( \sum_{\vec{n}} \tilde{S}_{\alpha}^* \tilde{S}_{\alpha'} \xi_{\alpha'} - \tilde{S}_{\alpha} \xi_{\alpha} \right) \left( \sum_{\vec{n}} \tilde{S}_{\alpha} \xi_{\alpha}^* - \tilde{S}_{\alpha}^* \xi_{\alpha} \right), \quad (S29) \]

for all \( \vec{n} \). Combining Eqs. \( S28 \), \( S29 \) with the energy minimization conditions, we get

\[ (\tilde{S} \ast \xi)^{\dagger}_{\alpha=1, \alpha} (\tilde{S} \ast \xi)_{\alpha=1, \alpha} = 1, \quad \tilde{S}_{\alpha=1} \in \mathbb{R}^3, \quad (S30) \]

which will determine the GSM, where \( (\tilde{S} \ast \xi)_{\alpha} = \frac{1}{\sqrt{N}} \sum_{\vec{n}} \tilde{S}_{\alpha} \xi_{\alpha} \).
C. Derivation of Eq. (16)

Define \( \tilde{S}_{n_z,k_y,\alpha} = \frac{1}{\sqrt{N}} \sum_{k_y} S^-_{k_y,\alpha} e^{-ik_x n_z} \). The energy minimization conditions are \( \tilde{S}_{n_z,k_y,\alpha} = 0 \), \( \forall k_y \neq \pm K_y \) or \( \alpha \neq 1 \). The first two conditions in Eq. (13) go over into

\[
\tilde{S}_{n_z,-k_y,\alpha} = \tilde{S}_{n_z,k_y,\alpha}^*.
\] (S31)

Fourier transforming the third condition in Eq. (13) in the \( x \) direction, we get

\[
N \tilde{\delta}_{q_y} = \frac{1}{N_x} \sum_{p_x} \sum_{k_x} \sum_{\alpha^\prime,\alpha} \sum_{n_x,n_x'} \xi_{\alpha^\prime,\alpha}^* \tilde{S}_{n_x,k_y,\alpha'}^- \tilde{S}_{n_x,k_y+p_y,\alpha}^+ \times \frac{1}{\sqrt{N_x}} \sum_{k_x} \sum_{\alpha^\prime,\alpha} \sum_{n_x,n_x'} \xi_{\alpha^\prime,\alpha}^* \tilde{S}_{n_x,k_y,\alpha'}^- \tilde{S}_{n_x,k_y+p_y,\alpha}^+
\]

\[
\times \xi_{n_x',k_y+p_y,\alpha} e^{ik_x (n_x'-n_x)} e^{ip_y (n_y'-n_y)}
\]

\[
= \frac{1}{\sqrt{N_x}} \sum_{k_x} \sum_{\alpha^\prime,\alpha} \sum_{n_x,n_x'} \xi_{\alpha^\prime,\alpha}^* \tilde{S}_{n_x,k_y,\alpha'}^- \tilde{S}_{n_x,k_y+p_y,\alpha}^+
\]

\[
\times \xi_{n_x'-k_y+p_y,\alpha} e^{-ik_x (n_x'-n_x)} e^{-ip_y (n_y'-n_y)}
\]

\[
= \sum_{k_y} \left( \sum_{n_x} \tilde{S}_{n_x,k_y+p_y,\alpha} \xi_{n_x'} \tilde{S}_{n_x',k_y,\alpha'} \right) \left( \sum_{n_x} \tilde{S}_{n_x,k_y,\alpha'}^- \xi_{n_x} \tilde{S}_{n_x',k_y+p_y,\alpha}^+ \right),
\] (S32)

where \( \xi_{n_x,\alpha} = \frac{1}{\sqrt{N_x}} \sum_{k_x} \xi_{\alpha} e^{-ik_x n_x} \). Incorporating the energy minimization conditions into Eqs. \[ \[ \text{(S31)} \] \text{and} \[ \[ \text{(S32)} \] \], we get

\[
\sum_{k_y} (\tilde{S}^* \xi)_{n_z,k_y,\alpha=1} = N_y \tilde{\delta}_{q_y},
\]

\[
\tilde{S}_{n_z,-K_y,\alpha=1} = \tilde{S}_{n_z,K_y,\alpha=1},
\] (S33)

where \( (\tilde{S}^* \xi)_{n_z,k_y,\alpha} \equiv \frac{1}{\sqrt{N_x}} \sum_{n_x} \tilde{S}_{n_x,k_y,\alpha} \xi_{n_x} \).  

D. Derivation of Eq. (17)

Define

\[
\tilde{S}_{n_z,k_y,\alpha} = \frac{1}{\sqrt{N_x}} \sum_{k_y} S^-_{k_y,\alpha} e^{-ik_x n_z},
\] (S34)

\[
\tilde{S}_{k_x,n_y,\alpha} = \frac{1}{\sqrt{N_y}} \sum_{k_y} S^-_{k_y,\alpha} e^{-ik_y n_y},
\] (S35)

and

\[
\xi_{n_z,k_y,\alpha} = \frac{1}{\sqrt{N_x}} \sum_{n_y} \xi_{n_y} e^{-ik_y n_y},
\] (S36)

\[
\xi_{k_x,n_y,\alpha} = \frac{1}{\sqrt{N_y}} \sum_{k_y} \xi_{k_y} e^{-ik_y n_y},
\] (S37)

Energy minimization requires that \( \tilde{S}_{n_z,k_y,\alpha} = 0 \), \( \forall k_y \neq \pi \) or \( \alpha \neq 1 \), and that \( \tilde{S}_{k_x,n_y,\alpha} = 0 \), \( \forall k_x \neq \pi \) or \( \alpha \neq 1 \). Consistency implies

\[
\frac{1}{\sqrt{N_x}} \sum_{n_y} (-)^{n_z} S^-_{n_z,k_y=\pi,\alpha=1} = \tilde{S}^-_{k_y=(\pi,\alpha=1)} \] (S38)

\[
\frac{1}{\sqrt{N_y}} \sum_{n_y} (-)^{n_x} S^+_{k_x=n_y,\alpha=1} = \tilde{S}^+_{k_y=(\pi,\alpha=1)} \] (S39)

Again,

\[
\tilde{S}_{n_z,k_y=\pi,\alpha=1}, \tilde{S}_{k_x=n_y,\alpha=1}, \tilde{S}^-_{k_y=(\pi,\alpha=1)} \in \mathbb{R}^3. \] (S40)

Now we plug \( \tilde{S}_{n_z,k_y=\pi,\alpha=1}, \tilde{S}_{k_x=n_y,\alpha=1} \) into the last condition in Eq. (13). For \( \tilde{p} = 0 \), we have
which means

$$\frac{1}{\sqrt{N_x}} \sum_{n_x} \tilde{S}_{n_x,k_y=\pi-a}\xi_{n_x+n'_y,k_y=\pi-a} \equiv \sum_{n_y} \tilde{S}_{k_x,n'_y} \xi_{k_x+n'_y}$$

and

$$\sum_{n_y} \tilde{S}_{k_x,n'_y} \xi_{k_x+n'_y} \equiv \frac{1}{\sqrt{N_y}} \sum_{n_y} \tilde{S}_{k_x,n'_y} \xi_{k_x+n'_y}$$

where \((\tilde{S} \ast \xi)_{n_x,k_y=\pi-a}\) and \((\tilde{S} \ast \xi)_{k_x,n_y=\pi-a}\) and \((\tilde{S} \ast \xi)_{k_x,n_y=\pi-a}\) for \(p_x \neq 0, p_y = 0\), convolutions arise in a similar way:

$$0 = \sum_{k_z} \tilde{S}_{k_z,k_y=\pi-a} \tilde{S}_{k_z+k_x,k_y=\pi-a} \xi_{k_z+k_x,k_y=\pi-a} = \sum_{n_z} \tilde{S}_{n_z} \xi_{n_z}$$

$$= \frac{1}{N_x} \sum_{k_z} \sum_{n_z,n'_z} \tilde{S}_{n_z,k_y=\pi-a} \tilde{S}_{n_z,n'_z,k_y=\pi-a} \xi_{n_z,n'_z,k_y=\pi-a}$$

$$= \frac{1}{\sqrt{N}} \sum_{n_z} \tilde{S}_{n_z} \xi_{n_z} = 0, \forall p_x, p_y \neq 0.$$