The view of TK-SVM on the phase hierarchy in the classical kagome Heisenberg antiferromagnet

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Abstract
We illustrate how the tensorial kernel support vector machine (TK-SVM) can probe the hidden multipolar orders and emergent local constraint in the classical kagome Heisenberg antiferromagnet. We show that TK-SVM learns the finite-temperature phase diagram in an unsupervised way. Moreover, in virtue of its strong interpretability, it identifies the tensorial quadrupolar and octupolar orders, which define a biaxial $D_{3h}$ spin nematic, and the local constraint that underlies the selection of coplanar states. We then discuss the disorder hierarchy of the phases, which can be inferred from both the analytical order parameters and an SVM bias parameter. For completeness we mention that the machine also picks up the leading $\sqrt{3} \times \sqrt{3}$ correlations in the dipolar channel at very low temperature, which are however weak compared to the quadrupolar and octupolar orders. Our work shows how TK-SVM can facilitate and speed up the analysis of classical frustrated magnets.

Keywords: machine learning, TK-SVM, multipolar order, classical spin liquid

(Some figures may appear in colour only in the online journal)

1. Introduction

The kagome Heisenberg antiferromagnet (KHAMF) is one of the most characteristic many-body systems where a simple Hamiltonian hosts strikingly rich physics. A kagome lattice is built from corner-shared triangular plaquettes, as illustrated in figure 1. By placing Heisenberg spins on each lattice site and coupling the nearest-neighboring spins, one defines a kagome Heisenberg model, $H = J \sum_{ij} S_i S_j$. When the interaction is antiferromagnetic, $J > 0$, the system is highly geometrically frustrated and fails to find a unique ground state [1]. Such frustration has played a crucial role in the search for spin liquids and other exotic states of matter [2].

In the most general formulation of the problem one takes the interplay between geometric frustration, quantum fluctuations, and thermal fluctuations into account. However, it turns out that the thermodynamics of the classical KHAMF is already quite rewarding. In reference [3], Chalker et al realized that there exists a hidden quadrupolar order parameterized by a rank-2 tensorial order parameter. The emergence of this order is driven by an order-by-disorder phenomenon [4, 5], where coplanar states are entropically selected at low temperatures owing to the presence of soft modes [3]. Shortly afterwards, Reimers and Berlinsky [6] carried out a thorough investigation of excitations of the soft modes and the correlations of degenerate magnetic states. In spite of limited computational resources the authors showed, by classical Monte
Carlo simulations, convincing signatures that the quadrupolar order indeed appears to be (quasi-)long ranged. At around the same time, Huse and Rutenberg [7] and Ritchey et al [8] proposed that the physics in the selected plane might be effectively described by three-state Potts-like degrees of freedom, and the latter paper also discussed the associated topological defects which can support a generalized Berezinskii–Kosterlitz–Thouless (BKT) transition [9–11]. This is highly non-trivial, because the BKT transition is not realized in a typical two dimensional Heisenberg magnet as the fundamental group $\pi_1(SO(3)/SO(2)) = 0$ is trivial [12, 13]. It, however, becomes possible with the effective Potts-like degrees of freedom, where the fundamental group is $\pi_1(O(3)/D_{ab}) = D_3$ which gives rise to gapped topological defects [13], where $D_{ab} (D_3)$ denotes the (binary) dihedral group. Although these results firmly evidenced that there is further structure in the selected coplanar states, it was only much later that Zhitomirsky pointed out that the structure is described by another hidden order, a rank-3 octupolar order [14, 15]. This author also showed that such order coexists with pinch points, which are usually seen in classical spin liquids such as spin ice [16, 17]. While the quadrupolar and octupolar orders are firmly established, they do not exhaust the rich hierarchy of phases in the classical KHAFM; specifically, the possibility of dipolar order is debated in the literature. Already in reference [7], the authors argued that fluctuations around the extensively degenerate KHAFM ground states interact in a non-linear way and will lead to unequally weighted Potts states. As a consequence, there may exist a critical point for a long-range antiferromagnetic $\sqrt{3} \times \sqrt{3}$ order in the $T \to 0$ limit. This scenario was further developed by Henley with a self-consistent effective Hamiltonian approach [18]. A recent Monte Carlo simulation, equipped with an ingenious cluster update, by Chern and Moessner also suggests that the $\sqrt{3} \times \sqrt{3}$ magnetization retains a finite, though remarkably small, value in the thermodynamical limit as $T \to 0$ [19].

Whereas establishing the $T \to 0$ magnetic order is very difficult because of the lack of a controlled theory [18] and efficient algorithms to simulate large system sizes from first principles at extremely low temperature [19, 20], a major challenge in understanding the hidden multipolar orders in the classical KHAFM is rooted in the complexity of those high-rank tensorial order parameters. It is therefore interesting to ask whether machine learning (ML), which is designed to analyze complex patterns, can assist in the analysis of such problems. This also concerns ML techniques as practical tools for physics. Although these techniques have proven useful for classifying phases and detecting phase transitions [21–27], representing quantum wave functions [28–33], designing algorithms [34–37], and predicting properties of materials [38–41] (see references [42–44] for recent reviews), the number of applications to intricate issues remains limited.

In the present paper, we apply our recently developed tensorial kernel support vector machine (TK-SVM) [45–47], which is an unsupervised and interpretable approach, to the classical KHAFM. We show that our machine readily picks up the hidden quadrupolar and octupolar orders and gives their tensorial order parameters in analytical form while its only inputs are real-space spin configurations. It identifies the ground-state constraint (GSC) and different temperature scales in the KHAFM. In addition, the machine also recognizes that the magnetic correlation of classical KHAFM at low-temperature is dominated by a $\sqrt{3} \times \sqrt{3}$ structure.

The manuscript is organized as follows. In section 2, we review the method of TK-SVM. In section 3, the finite-temperature phase diagram of KHAFM is discussed. Section 4 is devoted to the multipolar order parameters and GSC. Section 5 discusses magnetic correlations. We conclude in section 6.

## 2. Tensorial-kernel support vector machine

The TK-SVM is a numerical method to detect general symmetry-breaking orders [45, 46] and emergent local constraints [47, 48] in the problem of phase classifications; see also reference [49]. It inherits from support vector machines [50, 51], a well-known and successful classifying technique in machine learning, the property that it is interpretable: the decision function, which is the optimal classifier between two sets of data with a distinct property, can be shown to learn the square of order parameters when a quadratic kernel is used [21, 45, 46]. In TK-SVM the order parameter (or local constraint) can be any local tensor of a possibly high rank [45, 46].

Furthermore, the decision function also contains an offset known as the bias. Specifically for phase classification, the bias is sensitive to the presence of phase transitions or crossovers [46, 47]. It can be analyzed prior to and independent of the determination of the order parameters and allows one to perform an unsupervised graph partitioning of the phase diagram.

The main advantages of our approach are that the user does not need to devise suitable order parameters, which are typically very hard to construct for exotic states of matter, and that one gets near certainty about all phases with learned order parameters without supervision, resulting in enormous speedups for the analysis of an (unknown) phase
diagram. Below we explain the most important concepts of TK-SVM.

2.1. TK-SVM decision function

The TK-SVM finds the optimal decision function

\[ d(x) = \sum_{\mu} C_{\mu} \phi_\mu(x) - \rho, \]

in classifying two sets of data with a distinct property (e.g., a different order parameter or local constraint) in the sense of determining a maximal margin between the sets.

Here, \( x \) denotes a real-space configuration of \( N \) spins, which serves as the training data,

\[ x = \{ S_{ai} | a = x, y, z; i = 1, 2, \ldots, N \}. \]

The power of SVMs lies in the usage of appropriate kernel methods. Samples are mapped by some transformation \( \phi \) onto a featurespace where only the inner product of the transformed data needs to be known. The conditions on \( \phi \) are very mild. Often, a linear separation in feature space is possible; hence, a highly non-linear separation in real space can be uniform or not in case one wants to have a higher density of spatial points for example, magnetic orders are defined as rank-1 tensors, and quadrupolar orders correspond to rank-1 tensors. Emergent local constraints, such as ground-state constraints for spin liquids, show up as relations between local tensors. The dimension of the \( \phi \)-space is \( 3r^n \). However, as it contains a massive amount of redundant information, the actual complexity in the SVM optimization problem is linearly determined by the number of independent components, given by \( 3r^n(n-1)! \). While this can still be a big number, a bottleneck is only encountered in extreme situations when dealing with very large clusters at high ranks. In real applications, a TK-SVM can handle, for example, a cluster of several hundreds spins at rank-2 without a problem, which is only necessary when a quadrupolar order or a spin-liquid constraint has such a vast ‘unit cell’. In the case of rank \( n = 1 \), which detects magnetic orders, the size of a feasible cluster can be even greater.

Coefficient matrices, \( C_{\mu} \), will be constructed by support vectors,

\[ C_{\mu} = \sum_{k} \lambda_k \phi_\mu(x^{(k)}) \phi_\mu(x^{(k)}), \]

where \( \lambda_k \) is the Lagrangian multiplier related to the \( k \)th sample \( x^{(k)} \) and is solved in the underlying SVM optimization problem. The coefficient matrices can be viewed as encoders of order parameters, from which analytical expressions of the detected orders and constraints are extracted. As we investigated in reference [45] by comparing results using \( N_s = 10^3 \) to \( 10^4 \) samples, a few hundred samples can already give coefficient matrices of decent quality; more samples reduce statistical errors. The complexity of the underlying SVM optimization problem generally scales as \( O(N_s^2) \) to \( O(N_s^3) \) [55]. However, the computational cost for carrying out the machine learning is in general small compared to that of generating the training data.

The parameter \( \rho \) is called the bias. In a binary classification over two sample sets \( A \) and \( B \), its behavior can be summarized as follows [47]

\[ \rho(A | B) \begin{cases} \gg 1 & A, B \text{ in the same phase}, \\ \ll -1 & A \text{ in the disordered phase}, \\ \approx 1 & \text{ in different phases}. \end{cases} \]

Therefore, the \( \rho \) parameter can act as an indicator of phase transitions and crossovers. Its magnitude indicates the absence or presence of a phase transition or crossover,

\[ |\rho_{AB}| \begin{cases} \gg 1 & A, B \text{ in the same phase}, \\ \approx 1 & A, B \text{ in different phases}. \end{cases} \]

The sign of \( \rho \) further reveals which sample set originates from the (dis-)ordered side, namely, the orientation of the transition or crossover. The last case in equation (5) corresponds to situations where \( A \) and \( B \) have characteristics that can not straightforwardly be compared; hence, a relative disorderedness may not be well defined.

2.2. Graph partitioning

The use of graph partitioning in TK-SVM maximally exploits the reduced criterion equation (6) for \( \rho \). Consider a spin model involving a set of physical parameters such as interactions and temperature, whose phase diagram we seek to learn. We collect spin configurations from distinct parameter points in the physical parameter space. The distribution of the points can be uniform or not in case one wants to have a higher density of points in the regions of special interests. We then perform SVM multi-classification over the collected data. For \( M \) sets of samples, one multi-classification produces \( M(M-1)/2 \) decision functions; each is responsible for a binary classification between two sample sets [56].

The graph is constructed by viewing those parameter points as vertices and assigning an edge to each pair of them, while the edge weights are determined by the value of \( \rho \) in the corresponding decision function, leading to a graph of \( M \) vertices and \( M(M-1)/2 \) edges.

The graph may be partitioned by different means. A simple yet efficient approach is Fiedler’s theory of spectral clustering [57, 58]. According to Fiedler’s theory, the graph can be
Figure 2. Graphs corresponding to the multiclassification along four different TK-SVM setups [two cluster choices (a kagome unit cell and a single spin) combined with the two ranks, \( n = 2 \) and \( n = 3 \)]. Each vertex represents a different temperature \( T/J \). Edges connecting the vertices are weighted by the bias parameter \( \rho \) in the decision function equation (1); see section 2.2 for details. In order to facilitate the graphical representation of the one-dimensional parameter space, a random second coordinate is introduced, which offsets the temperatures vertically and which hence avoids overlaps of edges. The clustering of the vertices is described by the respective Fiedler vector in figure 3.

3. The phase diagram learned by TK-SVM

In order to learn the phase diagram of the classical KHAFM in an unsupervised way, we start the analysis with the graph partitioning. For this purpose, we collect spin configurations ranging from high to extremely low temperatures: we choose 85 logarithmically equidistant temperatures between \( T/J = 10^3 \) and \( 10^{-5} \), and store 1000 independent configurations at each
temperature. The samples are obtained by classical Monte Carlo simulations utilizing parallel tempering and heat-bath updates for a lattice consisting of 3072 spins ($32 \times 32$) at various temperatures. The samples are obtained by classical Monte Carlo simulations utilizing parallel tempering and heat-bath updates for a lattice consisting of 3072 spins ($32 \times 32$) at various temperatures. The curve corresponding to the triangle cluster at rank-2 realizes the high-temperature phase at $T = 0.004 J$. The dashed lines indicate the boundaries of the three regimes: I, hidden nematic; II, cooperative paramagnet; III, trivial paramagnet. The interval between $T/J = 0.4$ and 10 is a crossover region where the ground-state constraint develops.

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Partitioning these graphs leads to four different Fiedler vectors, depicted in figure 3. Clearly, the temperature axis is divided into three regions: a rank-2 quantity constructed from the spin cluster [see also panel (c) in figure 2] discriminates around a temperature $T/J \approx 1$ a high-temperature region (region III) from the rest. Both the single-spin and the triangle cluster (cf. panels (b) and (d) in figure 2) define a rank-3 quantity which distinguishes the very low temperatures (region I, $T/J \leq 0.004$) from the intermediate temperature region II. The result of the single-spin cluster at rank-2 (cf. panel (a) in figure 2) is in line with the results the rank-3 ones. The discrimination of these regions reproduces in fact the finite-temperature phase diagram of the kagome Heisenberg model [3, 15]—even before we visit the nature of those phases.

4. Analytical order parameters

Having learned the topology of the KHAFM phase diagram, we now interpret the nature of each phase by their order parameters and possible local constraints. This will be done by extracting the analytical order parameters from the $C_{\mu\nu}$ matrices. In order to reduce the statistical errors on $C_{\mu\nu}$, we pool the data according to the phase diagram of figure 3. In addition, we introduce 25 000 fictitious configurations generated at $T = +\infty$ which represent completely disordered states. This sets up a reduced multi-classification problem among four classes: regime I (28 000 samples), regime II (21 000 samples), regime III (21 000 samples), and regime $T_{\infty}$. Consequently, we obtain six $C_{\mu\nu}(A|B)$ for each rank and cluster, with $A, B \in \{I, II, III, T_{\infty}\}$ [49].

Not surprisingly, the high-temperature regime III is not distinct from the $T_{\infty}$ regime; the associated coefficient matrices are noise-like. Hence, only the two low-temperature regimes need further interpretation.

4.1. Ground-state constraint

We first discuss the emergent local constraint in the two low-temperature phases, which drives the system to coplanar order and is manifest using the triangular cluster at rank-2. The term ‘emergent’ in the current case is intended to distinguish from the trivial constraint of spin normalization $|\bm{\rho}| = 1$. The discrimination of these regions reproduces in fact the finite-temperature phase diagram of the kagome Heisenberg model [3, 15]—even before we visit the nature of those phases.
Figure 4. The coefficient matrix $C_{\mu\nu}^{(II)}|T_\infty|$ learned from a rank-2 TK-SVM on a three-spin triangular cluster. The dotted lines demarcate $9 \times 9$ blocks corresponding to identical spin indices $(\alpha, \beta)$, $(\alpha', \beta')$ while the contents of each $9 \times 9$ block is enumerated in a similar way by component indices $(a, b), (a', b')$. On-site blocks $(\alpha = \beta, \alpha' = \beta')$ are seen to be empty, while ‘cross’ and ‘bond’ blocks exhibit a non-vanishing $\delta_{a\alpha b\beta}$ pattern with relative weights of $-1$ and $0.446 = -\gamma$, respectively. See also tables 1 and 2.

Substituting $C_{ab\alpha'\beta'}^{\alpha\beta}$ into the decision function equation (1), one obtains

$$d(\{S_i\}) \sim \sum_{\alpha, \beta} \sum_{a, b} C_{ab\alpha'\beta'}^{\alpha\beta} \left\langle S_a^\alpha S_b^\beta \right\rangle \left\langle S_{a'}^\alpha S_{b'}^\beta \right\rangle$$

$$= \left( \gamma \left( \sum_a S_a^\alpha \right)^2 + \gamma \sum_\alpha \left\langle \|S^\alpha\|^2 \right\rangle \right)^2$$

$$- \left( \sum_\alpha \left\langle \|S^\alpha\|^2 \right\rangle \right)^2$$

$$= 9 \left[ \gamma^2 \left( \Gamma - \frac{1}{\gamma} \right)^2 - 1 \right], \quad (9)$$

where $\Gamma$ is a normalized constraint order parameter whose meaning will become transparent in the forthcoming discussion.

$$\Gamma = 1 - \frac{1}{3} \left\langle \sum_\alpha \|S^\alpha\|^2 \right\rangle_{cl}. \quad (10)$$

As seen in figure 4 and table 1, the only non-vanishing quadratic correlation in $C_{\mu\nu}(II|T_\infty)$ is

$$Q_{x^2+y^2+z^2}^{x^2+y^2+z^2} = S_x^2 S_y^2 + S_y^2 S_z^2 + S_z^2 S_x^2. \quad (11)$$

$\gamma$ is then determined by

$$Q_{x^2+y^2+z^2}^{x^2+y^2+z^2} / Q_{x^2+y^2+z^2}^{x^2+y^2+z^2} \sim -0.446$$

for regime II.

The value of $\gamma$ in fact appears to be temperature-dependent and converges to $-\frac{1}{2}$ in regime I. This can be understood from the constraint order parameter, equation (10). As the squared sum in $\Gamma$ comprises three on-site $(\alpha = \beta)$ and six bond $(\alpha \neq \beta)$ correlations, and that their ratio is $\gamma$, the fulfillment of $\gamma = -\frac{1}{2}$ is equivalent to the relation

$$\left\langle \|S^{(1)} + S^{(2)} + S^{(3)}\|^2 \right\rangle_{cl} = 0. \quad (12)$$

Since $\|\ldots\|^2$ is semi-positive definite, this in turn means a local constraint at each triangular plaquette,

$$S^{(1)} + S^{(2)} + S^{(3)} = 0. \quad (13)$$

Namely, $\gamma = -\frac{1}{2}$, or equivalently $\Gamma = 1$, expresses the ground-state constraint of the KHAFM (the spins of every triangle lie in a plane), while the deviation of $\gamma \sim -0.446$ in the higher-temperature regime II reflects thermal fluctuations of the constraint.

### 4.2. Hidden nematic order

We proceed by examining the order parameter of regime I. Given the Fiedler vectors in figure 3, it is evident that the $C_{\mu\nu}$ matrices learned with the single-spin cluster are able to distinguish regime I from the high-temperature phases. We now look at the corresponding coefficient matrices, and will afterwards revisit this issue with the three-spin triangular cluster.

The patterns of $C_{\mu\nu}(II|T_\infty)$ using the single-spin cluster are shown in figure 5, where it is a $9 \times 9$ matrix for rank-2 and $27 \times 27$ matrix for rank-3.

The rank-2 pattern, shown in figure 5(a), has the following analytic expression,

$$\frac{3}{4} \delta_{ab} \delta_{b'a'} + \frac{3}{4} \delta_{a'b} \delta_{ab'} - \frac{1}{2} \delta_{a'b} \delta_{bb'}. \quad (14)$$

Substituting this into the decision function equation (1), we obtain

$$d(x) \sim \frac{3}{2} \sum_{ab} \left( \langle S_a S_b \rangle - \frac{1}{3} \delta_{ab} \right)^2$$

$$= \frac{3}{2} \text{Tr}[Q_{ab} Q_{ba}], \quad (15)$$

where

$$Q_{ab} = \langle S_a S_b \rangle - \frac{1}{3} \delta_{ab}. \quad (16)$$

is the famous uniaxial nematic tensor [59]. This shows that a rank-2 $C_{\mu\nu}(II|T_\infty)$ using a single-spin cluster probes the hidden quadrupolar order in the KHAFM [3, 15].

The rank-3 pattern figure 5(b) is interpreted in the same way. It can be expressed as

$$\delta_{a'b'} \delta_{bb'} \delta_{cc'} = \frac{1}{5} \left( \delta_{a'b'} \delta_{bc} \delta_{bb'} + \delta_{a'b'} \delta_{bb'} \delta_{cc'} + \delta_{a'b'} \delta_{bb'} \delta_{cc'} \right), \quad (17)$$

leading to a rank-3 tensor

$$T_{abc} = S_a S_b S_c - \frac{1}{5} S_a \delta_{bc} - \frac{1}{5} S_b \delta_{ac} - \frac{1}{5} S_c \delta_{ab}, \quad (18)$$

which is precisely the octupolar order parameter [60].
**Table 1.** The weights of quadrupolar ordering components, $p_i(Q_i)$, extracted from the corresponding coefficient matrices. These weights are calculated through a least-squares fit based on all blocks in the full coefficient matrix of each of the site-site (‘on-site’), site-bond (‘cross’), and bond-bond (‘bond’) types. The ratios between these weights for the three block types are given in table 2.

| $T_\infty$ | $\|\|/\|\|$ | $\|\|/\|\|$ | $\|\|/\|\|$ | $\|\|/\|\|$ | $\|\|/\|\|$ | $\|\|/\|\|$ | $\|\|/\|\|$ |
|------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| On-site    | $-0.487$        | $1.460$         | $0.731$         | $0.732$         | $0.733$         | $0.727$         | $0.735$         |
| Cross      | $0.081$         | $-0.730$        | $-0.366$        | $-0.366$        | $-0.367$        | $-0.363$        | $-0.367$        |
| Bond       | $0.038$         | $0.365$         | $0.183$         | $0.183$         | $0.183$         | $0.182$         | $0.184$         |

We are left with the consideration of the three-spin cluster. Although it is not quite visible from the Fiedler vector in figure 3, TK-SVM with a triangular cluster at rank-2 does in fact discriminate between regime I and II, but the distinction is blurred by the constraint, equation (10), which appears as the primary order parameter: the triangular rank-2 curve in figure 3 varies in the low-temperature regions, but the gradient is much more modest than the profound change seen when the constraint emerges.

Figure 6 shows the $C_{\mu\nu}(\|\|)$ obtained from a three-spin cluster at rank-2, which displays a richer structure than the $C_{\mu\nu}(T_\infty)$ shown in figure 4. Following a similar analysis, it gives rise to another quadrupolar tensor,

$$O_{\text{quad}} = \left\langle \frac{1}{3} \sum \alpha S^0 \otimes S^\alpha - \left( \frac{1}{3} \sum \alpha S^\alpha \right)^{\otimes 2} \otimes 3 \right\rangle_{\text{cl}}. \quad (19)$$

The first term is equivalent to the single-spin nematic tensor equation (16), while the second term expresses the constraint, equation (13). In other words, the triangular cluster at rank-2 simultaneously detects the hidden quadrupolar order and the ground-state constraint.

In figure 7, we show the block structure of the rank-3 $C_{\mu\nu}(T_\infty)$ using the triangular cluster. The full matrix has a dimensionality of 729 × 729, which is composed of 27 × 27 blocks. Each block exhibits the same pattern as that in figure 5(b) for the single-spin cluster, but is further multiplied with a weight. Its analytic expression displays a new octupolar tensor,

$$O_{\text{oct}} = \left\langle \frac{1}{5} \left[ \sum \alpha (S^\alpha)^{\otimes 3} + \sum\sum\sum\sum (S^\alpha)^{\otimes 3} \right] \right\rangle_{\text{cl}}. \quad (20)$$

The first term of $O_{\text{oct}}$ reproduces the single-spin order parameter equation (18). The second term represents the ground-state constraint equation (13) and will become a constant term, 0^{[3]}, when $\Gamma$ saturates to $\Gamma = 1$, which is the case in regime I. The second term is a rank-3 tensor defined by the three spins in a triangular plaquette. It serves as an alternative characterization of the octupolar order and is equivalent to the single-spin form. This also explains the agreement of the two rank-3 Fiedler vectors in figure 3.

**4.3. Phase hierarchy**

Let us put the learned order parameters and constraints together and infer a single coherent physical picture. Regime III is a trivial paramagnet (PM) which is equivalent to the infinite temperature state. Regime II is an instance of a cooperative paramagnet (CPM), which may also be referred to as a classical spin liquid and is characterized by an emergent...
Figure 5. Coefficient matrices for regime I learned from a single-spin cluster at rank-2 and 3. They represent the quadrupolar (equation (16)) and octupolar (equation (18)) tensor order parameters, respectively. They also appear to be the motifs for the blocks shown in figures 6 and 7 obtained with a triangular cluster.

Accordingly, the temperature scales in the phase diagram figure 3 can be understood from a hierarchy of disorderedness,

\[
O(3) \rightarrow O(3) \rightarrow D_{3h}. \tag{21}
\]

In the high-temperature PM phase, spins can freely fluctuate. In the intermediate CPM phase, although the system still preserves the \(O(3)\) symmetry of the KHAFM Hamiltonian, fluctuations of spins become correlated. Then the BSN order emerges from a constrained subset of the phase space.

This phase hierarchy is also reflected by the bias parameters in the four different multi-classification setups, which are shown in table 3. Following the bias criterion of equation (5), regime I (BSN) has the least disorder since \(\rho(I\mid I, II, III) \lesssim -1\) in all instances. The \(\rho(I\mid II)\) learned with the triangular cluster at rank-2 acquired a value noticeably smaller than \(-1\), since the constraint equation (13) is satisfied in both phases (\(\Gamma \sim 1\)). However, its sign remains revealing that regime II is more disordered. Regime III (PM) is the most disordered...
as $\rho(I, II, III) \leq -1$ in all cases, with one exception as the single-spin cluster cannot represent the three-spin constraint equation (13).

5. Magnetic correlations

We now examine the magnetic correlations in the low-temperature regime, $T = 10^{-3}J$, of the classical KHAFM, learned by rank-1 TK-SVM.

We first consider a cluster containing $3 \times 3$ kagome unit cells, i.e. 27 spins (see figure 8), for a system defined on a lattice of linear size $L = 36$. The resulting $C_{\mu\nu}$ matrix is shown in figure 9. It has dimension $81 \times 81$ and can be divided into small $3 \times 3$ blocks. The structure of those blocks evinces in which way the correlation between two spins is defined. Because the small $3 \times 3$ blocks have only entries on the diagonal, the correlation is simply captured by the usual inner product $S_\mu S_\nu \delta_{\mu\nu}$. (In general, the contraction can be more complicated even for magnetic orders). The change of color between the blocks indicates an antiferromagnetic arrangement of the spins: The blue blocks correspond to positive correlations, and their locations precisely reflect a $\sqrt{3} \times \sqrt{3}$ structure.

Next, in figure 10, we show the result using a cluster of $12 \times 12$ kagome unit cells (432 spins). Owing to the large dimensionality of the $C_{\mu\nu}$ matrix, $\dim C_{\mu\nu} = 1296^2$, only the block structure is plotted, where each of its pixels corresponds to a $3 \times 3$ block in figure 9. In the presence of long-range order for an order parameter that can be defined on a small cluster, $C_{\mu\nu}$ learnt for a large cluster should display the same structure as for that small cluster. However, the pattern of figure 10 does not repeat that of figure 9: it fades rather fast, indicating that the linear correlation between two spins is not robustly established at longer distances. (Note that $C_{\mu\nu}$ does not directly measure the strength of spin–spin correlations. Instead, it probes the form of the correlations and order parameters. See equations (14) and (15) for a concrete example.)

Therefore, consistent with observations in the literature [6, 7, 15, 19, 20], our machine detects that the antiferromagnetic $\sqrt{3} \times \sqrt{3}$ structure is the dominant type of correlation in the dipolar channel of the classical KHAFM at low temperature. However, to establish the $T \to 0$ critical point, a systematic analysis of temperature and finite-size effect is needed.
of the \( \nu \)-SVM formulation [61], the LIBSVM library [62, 63], and the ALPScore library [64].

### Open source

The TK-SVM library has been made openly available with documentation and examples [65].

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