Continuous ground-state degeneracy of classical dipoles on regular lattices

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Dipolar interactions are crucial in the modeling of many complex magnetic systems, such as the pyrochlores and artificial spin systems. Remarkably, many classical dipolar coupled spin systems exhibit a continuous ground-state degeneracy, which is unexpected as the Hamiltonian does not possess a continuous symmetry. In this paper, we explain, how such a finite point-symmetry leads to a continuous ground-state degeneracy of specific classical dipolar-coupled systems. This work, therefore, provides new insight into the theory of classical dipolar-coupled spin-systems and opens the way to understand more complex dipolar coupled systems.

I. INTRODUCTION

In the early 20th century, adiabatic demagnetization associated with the magnetocaloric effect1 was exploited to reach temperatures below 1 K, in particular in the paramagnetic salt.2 The magnetic order limits the coldest temperatures achievable with this method,3 which called for a better understanding of the ordered states in such systems. The difficult problem of the ground-state determination in dipolar-coupled spin-systems was, however, not successfully tackled until the pioneering work of Luttinger and Tisza4 (LT), who introduced a theory to determine the ground state of translationally invariant systems. While the construction scheme provided by LT can be extended beyond dipolar-coupled systems,5 its original purpose was to find the ground-state configuration of classical dipoles such as those in the paramagnetic salts. The ground-state configuration was found to be strongly dependent on the geometry of the lattice, and it is even sample-shape dependent for ferromagnetic alignment of the spins.6 The LT-construction scheme does not apply to all lattices, it enables the determination of the ground-state configuration of common systems, such as the dipolar-coupled spins placed on the square lattice.7

Remarkably, dipolar-coupled spin systems exhibit a continuous ground-state degeneracy in many different geometries.8–11 The origin of this degeneracy is still not fully understood, although it has become clear that the degeneracy is not protected by symmetry so that even small perturbations, such as temperature or disorder, lift the degeneracy entirely through an order-by-disorder transition.12,13

In recent years, the interest in dipolar systems has increased due to experimental work on the pyrochlore spinices.16,17, leading to theoretical studies on systems with similar spin arrangements.18–20 Furthermore, the desire to better understand the physics governing the spinices provided the motivation to explore correlated magnetic behavior in artificial spin systems with nanomagnetic moments taking on the role of the spins.21,22 Such artificial spin systems are, in contrast to the pyrochlores, neither restricted in lattice geometry nor the single particle magnetic anisotropy. Therefore, even though initial investigations focused on Ising degrees of freedom,23–26 there has since been an increased interest in nanomagnets with continuous degrees of freedom.27,28

The theory for the artificial spin systems with continuous degrees of freedom discussed in Ref.25–28 has been discussed in previous works.11,12 However, the field lacks a generalization that is free from assuming a specific lattice. In this paper, we provide a more general approach via a detailed symmetry discussion, which gives a framework to determine the ground-state degeneracy for some generic lattices. This leads to a guide for the determination of whether a particular classical dipolar system has a continuous ground-state degeneracy. We provide the essence of this discussion in the flow diagram shown in Fig. 1

The remainder of this paper is structured as follows: In Section II, the model of classical dipolar spins is introduced through the Hamiltonian with an emphasis on symmetries. After a brief review of the LT-method in Section III A, we extend this method in Section III B using the representation theory for the point-symmetry group of the lattice to calculate the ground-state degeneracy. We then illustrate the method on several examples in Section IV. Finally, we summarize our results in Section V where we give an outlook on how the method presented here can be generalized to include the order-by-disorder transitions commonly found in dipolar-coupled systems.
FIG. 1. (color online) This flow diagram summarizes the findings of this article. Applying this scheme to a generic classical dipolar-coupled spin system, the LT-method is extended by an additional classification based on the point symmetry $P$, which determines the nature of ground-state degeneracy.

II. MODEL & SYMMETRIES

Here, we introduce the classical model of dipolar-coupled spins with the Hamiltonian

$$H = \frac{D}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_{ij}|^3} \left[ \mathbf{S}_i \cdot \mathbf{S}_j - 3 \left( \mathbf{S}_i \cdot \mathbf{r}_{ij} \right) \left( \mathbf{S}_j \cdot \mathbf{r}_{ij} \right) \right], \quad (1)$$

where $D$ is the dipolar interaction strength, defined for $|\mathbf{S}_i| = 1$. The vector $\mathbf{r}_{ij}$ is the difference vector between the positions of the sites $i$ and $j$ on a regular lattice. Finally, $\mathbf{r}_{ij}$ is the normalization of $\mathbf{r}_{ij}$ to unit length.

A classical spin $\mathbf{S}_i$ is typically described by a vector on the unit sphere, i.e., a Heisenberg spin. However, additional anisotropies can lower the effective degree of freedom of the spins. For example, in artificial spin ice, shape anisotropy can give rise to Ising-like behavior or XY-like behavior, and magnetocrystalline anisotropy can lead to clock-model-like behavior. For the remainder of the article, we will focus on spins with XY or Heisenberg behavior, as we want to determine when continuous ground-state degeneracies arise.

Regardless of whether the spin is Heisenberg or XY, the dipolar Hamiltonian (1) is geometrically frustrated. Namely, the first term $\mathbf{S}_i \cdot \mathbf{S}_j$ is minimized for antiparallel spin alignment, whereas the second term $-3(\mathbf{S}_i \cdot \mathbf{r}_{ij})(\mathbf{S}_j \cdot \mathbf{r}_{ij})$ is minimized for parallel alignment if the spins can align along their bond. As a consequence, in a system with dipolar interactions given by Eq. (1), the alignment of spins follows the “head-to-tail” rule, i.e., spins align parallel if they can align along their bond, and antiparallel if the spins are orthogonal to the bond. Moreover, the dipolar interaction is long-range, with its strength decaying as $r^{-3}$. Thus, at low dimensions ($d = 1, 2$), the Hamiltonian can be safely truncated, whereas, at higher dimensions ($d \geq 3$), the energy is super-extensive, i.e., the energy-density grows with the system size. Hence, boundary effects become crucial and thus sample-shape dependent corrections are expected.

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The symmetry group of the Hamiltonian Eq. (1) is the group $\mathbb{Z}_2 \times T \times P$. In this group, the time-reversal symmetry follows directly from the invariance of Eq. (1) under $\hat{V}, \hat{S}_i \rightarrow -\hat{S}_i$. The translational invariance $T$ is explicitly given by the mapping

$$\langle \mathbf{r}_i, \mathbf{S}_i \rangle \overset{T}{\rightarrow} \langle \mathbf{r}_i - \mathbf{t}, \mathbf{S}_i \rangle = \langle \mathbf{r}_i - \mathbf{t}, \mathbf{S}_i \rangle. \quad (2)$$

Since only relative coordinates appear in the dipolar Hamiltonian in Eq. (1), a shift of the system by a vector $\mathbf{t}$ is irrelevant whenever $\mathbf{t}$ is a lattice vector. Finally, the point-symmetry group $P$ is inherited by the underlying lattice. If we denote the vector representation of $P$ in the $d$-dimensional vector space with $V$, where $d$ is the dimension of a spin (and the dimension of the lattice), then a vector $\mathbf{v} \in \mathbb{R}^d$ transforms under the action of $g \in P$ according to $V(g)\mathbf{v}$, such that the Hamiltonian (1) stays invariant under

$$\langle \mathbf{r}_i, \mathbf{S}_i \rangle \overset{P}{\rightarrow} V(g)\langle \mathbf{r}_i, \mathbf{S}_i \rangle. \quad (3)$$

Here, $V$ acts on both the lattice and the spin simultaneously. This simultaneous action of $P$ on both vectors $\mathbf{r}_i$ and $\mathbf{S}_i$ is required by the second term in the Hamiltonian (1), which tightly connects real-space and spin-space. We discuss specific examples of complete symmetry groups in Section IV.

Formally, the model incorporates two different dimensions, the real-space lattice dimension $d_{\text{lattice}}$ and the spin-space dimension $d_{\text{spin}}$. The two spaces are coupled as a result of the dipolar interaction described by the Hamiltonian given by Eq. (1). Hence, it is useful to introduce a working dimension $d$, which is the dimension
of the space in which both the spins and the lattice can be embedded. For some simple situations, it can be sufficient to work in the smaller of the two spaces. This can be seen, for example, for in-plane XY spins on the cubic lattice. Here, the XY anisotropy reduces the point symmetry group of the system to the point symmetry group of the square lattice. Therefore, the problem of XY spins on a cubic lattice reduces to the problem of XY spins on the square lattice. Therefore, the problem of XY spins can be embedded. For some simple situations, it can be sufficient to work in the smaller of the two spaces. This can be seen, for example, for in-plane XY spins on the cubic lattice. Here, the XY anisotropy reduces the point symmetry group of the system to the point symmetry group of the square lattice. Therefore, the problem of XY spins on a cubic lattice reduces to the problem of XY spins on square-lattice layers.

III. GROUND STATES

In this section, we use the symmetries of the dipolar Hamiltonian to explain the origin of the ground-state degeneracy. For this purpose, we first summarize the LT-method and subsequently extend the LT-method by using the representation theory for the point-symmetry group to determine the nature of the ground-state degeneracy.

A. Luttinger-Tisza construction

The LT-method is based on an ansatz for the magnetic unit cell that stays invariant under lattice symmetries (\(\mathcal{T}\) and \(\mathcal{P}\)) and subsequent minimization of the dipolar energy associated with the magnetic unit cell. If the LT-method can successfully be applied to the system, then a suitable magnetic unit cell leads to the exact ground-state of the system. When unphysical solutions appear, then the LT-method fails. We will discuss the issue of unphysical solutions towards the end of this section after introducing the LT-method for finding the ground-state of spin systems.

For a general dipolar-coupled spin system, one starts by making an ansatz for the magnetic unit cell that respects the point-symmetry group of the lattice. Subsequently, the \(N\) spins in the magnetic unit cell are collected into one vector \(\vec{S} = (\vec{S}_1, \vec{S}_2, \ldots, \vec{S}_N)\) as illustrated in Fig. 2. Since the Hamiltonian in Eq. (1) is quadratic, the effective Hamiltonian for the magnetic unit cell can be written in terms of \(\vec{S}\) as \(\mathcal{H} = -\vec{S}^\dagger \mathcal{H} \vec{S}\), where \(\mathcal{H} \vec{S}\) is the induced dipolar field of the configuration \(\vec{S}\). This finite-dimensional diagonalization problem is further simplified by taking into account the translational invariance \(\mathcal{T}\) of the Hamiltonian: Using the representation theory for the translational invariance in the magnetic unit cell gives a symmetry-guided basis for \(\vec{S}\), the so-called basic arrays. This basis is constructed using the irreducible representations of \(\mathcal{T}\) in the magnetic unit cell, which correspond to the discrete Fourier states. Therefore, typical basic arrays are, for example, the ferromagnetic configuration \(\vec{S}_{\text{ferro}, x} = (\vec{e}_x, \vec{e}_x, \ldots)\) or the antiferromagnetic configuration \(\vec{S}_{\text{afm}, x} = (\vec{e}_x, -\vec{e}_x, \ldots)\). These symmetry-guided configurations are mutually orthogonal by construction and, because of the translational invariance, the different sectors such as the ferromagnetic sector (ferro) or the antiferromagnetic sector (afm) are not mixed. This leads to a further simplification of the ground state, since \(\mathcal{H} = \oplus_i \mathcal{H}_i\), i.e., \(\mathcal{H}\) is block-diagonal. Each of the blocks \(\mathcal{H}_i\) describes the coupling between basic arrays of one type of ordering (for example one block describes the coupling between the ferromagnetic configurations \(\vec{S}_{\text{ferro}, x}, \vec{S}_{\text{ferro}, y}, \ldots\)). Hence, each of the blocks is \(d\)-dimensional. Therefore, with the LT-method, we find

\[
\mathcal{H} = \begin{pmatrix}
\mathcal{H}_{\text{ferro}} & 0 & \cdots \\
0 & \mathcal{H}_{\text{afm}} & \cdots \\
\vdots & \vdots & \ddots
\end{pmatrix},
\]

which significantly simplifies the problem, since only a small number of explicit lattice summations have to be carried out.

However, the LT-method only guarantees the “weak condition” \(\vec{S}^2 = \sum_i N \vec{S}_i^2 = N\), and can therefore give unphysical solutions where the “strong condition” \(|\vec{S}_i| = 1\) is violated. If an unphysical lowest-energy configuration \(\vec{S}\) is identified by this method, then the method fails to provide the ground state. For such systems, one can either introduce Lagrange-multiplier or resort to numerical methods or Lagrange-multipliers render the problem non-linear, numerical methods typically find non-orthogonal states as ground-state configurations. When the method fails, it is not clear if the system possesses a continuous degeneracy or a discrete degeneracy. Nevertheless, as seen from the table, the LT-method works for many important systems. We show in the next section that, for these systems, \(\mathcal{P}\) uniquely defines the type and dimension of the degeneracy.
TABLE I. Overview of previous studies of dipolar-coupled coupled spins planted at the sites of various lattices and whether the ground state can be constructed by the LT-method.

| Lattice          | Is LT? |
|------------------|--------|
| chain lattice    | Yes    |
| rectangular lattice | Yes    |
| square lattice   | Yes    |
| honeycomb lattice | Yes    |
| kagome lattice   | No     |
| cubic lattice    | Yes    |
| “fcc-kagome” lattice | No     |

B. Continuous ground-state degeneracy

The point-symmetry group $\mathcal{P}$ determines the type of degeneracy in the following way: Since $\mathcal{P}$ is a symmetry of the Hamiltonian, as described in Eq. (3), it is therefore also a symmetry of $\mathcal{H}$. Hence, symmetry-group operations have to commute with $\mathcal{H}$, formally expressed as $[R(g), \mathcal{H}] = R(g)\mathcal{H} - \mathcal{H}R(g) = 0$ for all $g \in \mathcal{P}$, where $R$ is a representation of $\mathcal{P}$. The representation $R$ can be found considering that each block matrix $H_i$ has dimension $d$, since given one spin (for example $S_i$), the others are derived from the index $i \in \{\text{ferro, afm, . . .}\}$. Therefore the representation of $\mathcal{P}$ acting on the subspace for $H_i$ is $V$, the vector representation of $\mathcal{P}$. Hence, the representation for the entire matrix $\mathcal{H}$ is given by $R = \oplus_N V$.

The symmetry condition on one block matrix is $[V(g), H_i] = 0$ for all $g \in \mathcal{P}$, such that if $V$ is irreducible, then the first lemma of Schur implies $H_i = h_i \mathbf{1}$. Therefore, there are $d$ mutually orthogonal configurations $S_1, \ldots, S_d$, all having the same energy. Hence, any superposition $\sum_i \alpha_i S_i$, with the normalization constraint $\sum_i |\alpha_i|^2 = 1$, yields the same energy as the basis states since the Hamiltonian from Eq. (1) is quadratic in $S_i$. The normalization constraint itself is the equation of a $(d - 1)$-sphere. Hence, the ground-state manifold is described by a $(d - 1)$-dimensional sphere.

For the case that $V$ is reducible, the block matrices $H_i$ decompose into smaller block matrices. The explicit summation over the lattice identifies the smaller block matrix with dimension $d_b$, which is lowest in energy. Then the ground-state manifold is described by the reduced $(d_b - 1)$-dimensional sphere. If $d_b = 1$, the 0-sphere is found, which is equivalent to $\mathbb{Z}_2$ and therefore only a discrete degeneracy is found and not a continuous degeneracy that is found for systems where $d_b > 1$.

To conclude, the use of representation theory, not only for the translational invariance but also for the point-symmetry group leads to a more generic treatment than that implemented by Luttinger and Tisza. Even though Luttinger and Tisza used the point-symmetry group to simplify their problem, their approach did not exploit the representation theory for the point-symmetry group. In contrast, the extension presented here uses representation theory for both the translational invariance and the point-symmetry group, so that continuous ground-state degeneracies appear naturally. Furthermore, the continuous degeneracy is not accidental, as it does not require a fine-tuning of parameters, but instead follows from symmetry. Thus, the degeneracy is not guaranteed by a continuous symmetry of the Hamiltonian, but it rather follows from the finite point-symmetry group.

IV. EXAMPLES

As the concepts presented in Section II are rather abstract, we want to illustrate them with some examples. Namely, we consider the dipolar-coupled XY spins on the square lattice, and Heisenberg spins on the cubic lattice and the tetragonally distorted cubic lattice.

A. XY spins on the square lattice

Here we determine the ground-state of dipolar-coupled XY spins on the square lattice, as this example has already been well studied. The point-symmetry group of this system is given by $\mathbb{Z}_2 \times \mathbb{T}_{sq} \times C_4v$, where $\mathbb{Z}_2$ is the time-reversal symmetry and $C_4v$ is a point-symmetry group of the square lattice. The translational invariance $\mathbb{T}_{sq}$ can be parameterized via vectors $\vec{t} = x\hat{e}_x + y\hat{e}_y$, with $x, y \in \mathbb{Z}$ and $\hat{e}_x, \hat{e}_y$ being the unit vectors along the $x$-axis and the $y$-axis, respectively. Therefore, $\mathbb{T}_{sq}$ is isomorphic to $\mathbb{Z} \times \mathbb{Z}$.

In the next step, the LT-method is applied to a two-by-two magnetic unit cell, so that $\vec{S} = (S_1, S_2, S_3, S_4)$. Since $C_4$ is a symmetry of the system, it is sufficient to only consider basic arrays with spins parallel or antiparallel to $\hat{e}_y$. The LT-method then suggests a suitable basis based on the translational invariance $\mathbb{T}_{sq}$, which is, however, broken by the two-by-two magnetic unit cell. Hence, the basic arrays correspond to (discrete) Fourier components that arise due to the reduced translational invariance. Since the translational invariance is reduced by a factor of two in every direction, the basic arrays are formed by the square root of unity in every direction. The resulting basic arrays are depicted in Fig. 3, with the Fourier vector that characterizes the elements in the caption of the figures. By explicit calculation, it can be observed that the configuration depicted in Fig. 3c is the basic array with the lowest energy.

Finally, we need to validate if $V$ is irreducible (for details how this is done, see for example Ref. [11]). The reduction is carried out in Table I, where we indeed observe that $V$ is irreducible over $C_4v$. Hence, we know that the basic array aligned along $\hat{e}_x$ corresponding to Fig. 3c has the same energy. Hence, we have found a continuous ground-state degeneracy described by the 1-sphere, which is depicted in Fig. 4, in agreement with previous studies.
The four basic arrays for the two-by-two magnetic unit cell on the square lattice, which are aligned along the y-axis. Below each figure the Fourier vector is indicated, which generates the basic array. The lattice summations associated with the dipolar Hamiltonian reveal that the configuration shown in (c) has the lowest energy.

To provide a higher dimensional example, we consider dipolar-coupled Heisenberg spins on the cubic lattice with lattice constants \( a = b = c \). Here, the symmetry of the system is given by \( Z_2 \times T_{cu} \times O_h \), where \( Z_2 \) is time reversal, \( O_h \) is the point symmetry group of the cubic lattice and \( T_{cu} \cong Z \times Z \times Z \) parametrizes the translational invariance with vectors \( \mathbf{t} = x\hat{e}_x + y\hat{e}_y + z\hat{e}_z \). Then, the LT-method requires the evaluation of \( 2^3 = 8 \) lattice summations analogous to the ones for the square lattice. This calculation shows that the striped configuration depicted in Fig. 4 has the lowest energy of all basic arrays. Finally, we reduce \( V \) in \( O_h \) in Table III which results in \( V = T_{1u} \), so that the vector representation is once more irreducible. This yields a continuous ground-state degeneracy corresponding to the 2-sphere, again in accordance with previous studies. This reference also provides a graphical representation of this ground-state manifold in their Fig. 1.

If the cubic lattice has a tetragonal distortion, i.e., one lattice constant (e.g. \( c \)) is different from the other two \((a = b)\), then the three-dimensional block matrix describing the ground state of the undistorted cubic lattice \( H_{\text{striped}} \) reduces to two block matrices of dimensions 1 and 2, respectively. To determine which block matrix is lower in energy, one can consider the two cases \( c < a = b \) and \( c > a = b \). If \( c > a \), the system behaves as weakly interacting layers, that follow the symmetry constraints given by a square lattice. As a consequence, the two-dimensional representation is lower in energy, which yields a continuously degenerate ground-state whose manifold resembles the unit circle. This is
analogous to the manifold found for XY spins on a square lattice. If \( c < a \), the system consists of weakly interacting chains of spins, whose low-energy sector is described by the one-dimensional block. Therefore, no continuous degeneracy emerges. Both cases are in agreement with previous literature.\(^{11}\)

V. CONCLUDING REMARKS

In this work, the origin of the continuous ground-state degeneracy in classical dipolar-coupled systems was traced back to general properties of the underlying lattice. Using representation theory for the point-symmetry group, a generic rule for the degeneracy of Luttinger-Tisza ground states was determined. In doing so, previously known results \(^{31}\) could be recovered. We showed that the ground-state degeneracy crucially depends on the vector representation \( V \) of the point-symmetry group. If the representation \( V \) is irreducible, then a continuous ground-state manifold is found. In contrast, if \( V \) is reducible, a reduced dimension of the degenerate manifold or the absence of a continuous degeneracy altogether is expected.

However, as the degeneracy only arises in the ground-state discussion and is not protected by a symmetry of the Hamiltonian, it is not expected to persist after introducing excitations. We expect, in analogy to Ref.\(^{12}\), that the inclusion of fluctuations in the form of positional disorder or thermal fluctuations restores the finite symmetry of the Hamiltonian through an order-by-disorder transition.\(^{13-15,24}\) Similarly, higher-order multipoles, especially relevant for artificial spin ice systems, have been found to affect the ground-state degeneracy.\(^{22,23}\) However, to answer how excitations and disorder affect the ground-state degeneracy, fluctuations on top of a generic system would need to be considered. While this is outside of the scope of this work, a symmetry-guided discussion of the fluctuations seems feasible.

Finally, we only considered systems where the LT-method was applicable. While this method is valid for many interesting systems,\(^{31,12}\) there exist interesting systems where the LT-method does not apply. One example is given by the system of dipolar-coupled Heisenberg spins on the “fcc-kagome lattice”, where a continuous ground-state degeneracy is found.\(^{13}\) However, the ground-state manifold found in this paper is not equivalent to a sphere and their basis states are not orthogonal, so that it is clear that the LT-method does not apply. While such phenomena lie outside the work presented here, it seems feasible to perform a symmetry-guided discussion of non-LT systems, and we hope that this work serves as an inspiration to extend the symmetry discussion to all such systems.

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