Symmetry breaking on icosahedral lattices of dipoles

Simon Čopar
Department of Physics, Faculty of Mathematics and Physics,
University of Ljubljana, Ljubljana, Slovenia

Anže Božič
Department of Theoretical Physics, Jožef Stefan Institute, Ljubljana, Slovenia
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Abstract
Symmetry is one of the key properties of spherical assemblies in biological and complex matter, and examples include viral capsids, virus-like particles, and nanocontainers designed for various purposes. Anisotropic interactions between building blocks of these assemblies, such as dipole-dipole interaction, can induce symmetry breaking, aid self-assembly, and affect the stability of the structures. We investigate a system of long-range interacting dipole arrangements on a sphere, focusing specifically on their symmetry properties. We find ground states of dipoles positioned on Caspar-Klug icosahedrally symmetric spherical lattices in relation to different symmetry constraints. We analyze the stability of highly symmetric metastable states, their symmetry breaking into subsymmetries of the icosahedral symmetry group, and present a phase diagram of symmetries with respect to lattice parameters. Furthermore, we show how the symmetry of any dipole configuration can be analyzed using vector spherical harmonics. The observed relationship between positional order and dipole-induced symmetry breaking hints at ways of fine-tuning the structure of spherical assemblies and their design.

* simon.copar@fmf.uni-lj.si
I. INTRODUCTION

Particle assemblies in complex matter are often spherical in shape, at least in the first approximation; examples include liquid droplets, hard and soft colloidal particles, micelles, vesicles, some cells, and viral capsids [1]-[6]. What is more, virus-like particles (VLPs) and spherical nanocontainers are ideal to be designed as drug carriers, molecular storage containers, and nanoreactors, and a large amount of research has been invested into understanding the properties of their assembly [7]-[11]. In many cases, interactions between the elementary building blocks of spherical assemblies result in structures with high symmetry. For instance, a large number of viruses and VLPs have icosahedrally symmetric structure [12], where the constituent proteins lie in equivalent or quasi-equivalent neighbourhoods [13]. Their positions are usually described well by the Caspar-Klug (CK) lattice construction [14, 15], which also enables a classification of virus particles by their triangulation number [16]. Recently, more general models that either look at the maxima of symmetrized spherical harmonics [17, 18] or construct quasicrystalline tilings [19, 20] have been proposed, and these can explain the structure of anomalous lattices which cannot be described within the CK model.

Not only is symmetry an important geometric property of these structures, it also governs their self-assembly, stability, crystallization and dissolution—for instance, phenomenological Landau models based on symmetry arguments give predictions of density distributions and symmetry-breaking transitions in capsids [21, 22].

Spherical assemblies can also be better understood by considering the interactions between their building blocks and how these interactions contribute to the free energy functional. At close distances, hard-core repulsion usually dominates, frequently modeled by the Lennard-Jones potential or simple sterical exclusion [23, 24]. The assembly is often further directed by anisotropic weak interactions such as hydrogen-bonding, van der Waals, π-π stacking, dipole-dipole, and metal coordination [25]. In the assembled state, the positional order is then mostly fixed, giving rise to the CK model and related constructions. If the particles are electrostatically charged, these interactions have to be taken into account as well, as they can play a significant role both during the assembly and for the stability of the resulting structure [13, 26]. This is usually done through multipole expansion, modeling the charge distribution as a superposition of point charges, dipoles, quadrupoles, and less frequently also higher multipole contributions [27, 28]. The simplest example of an anisotropic
interaction which goes beyond the monopole moment is the unscreened interaction between point dipoles, which can often play an important role in particle assemblies [29, 32], and is known to affect their thermal fluctuations and stability, as was demonstrated on the example of crystalline membranes [33].

In the Euclidean plane, dipoles can arrange themselves into a number of different states—including an antiferromagnetic state, a periodic tiling of closed vortex lines, or a macrovortex state—strongly depending on the lattice on which they are positioned [29, 34–36]. On a sphere, translational periodicity is ill-defined and a suitable spherical equivalent of the lattices must be considered, leading to novel phenomena specific to the sphere. It was recently shown that if no additional restrictions are imposed, dipoles arrange themselves into a polar vortex state if their positional order on the sphere resembles a triangular grid [37] (given by, e.g., lattices that result as solutions to the Thomson problem [38]). However, in spherical structures such as viruses and VLPs with icosahedral symmetry, the positional order of their building blocks differs from triangular close packing due to the different interactions involved in their assembly. Their building blocks impose additional symmetries on the final assembled structure, and if these building blocks carry in-plane electrostatic polarization, they will orient themselves differently compared to unrestricted dipole systems, and so the symmetry has to be explicitly taken into account.

In this work, we utilize the CK lattice construction to obtain positional order of (electrostatic) point dipoles and calculate the ground states of the dipole-dipole interaction. We focus on determining the orientational order of dipoles restricted to icosahedral symmetry and its subgroups. This allows us to investigate the electrostatic energy cost of keeping the dipoles in an icosahedrally symmetric orientation and the energy landscape of states with lower symmetries, reached by allowing symmetry breaking into selected subgroups of the icosahedral group. We show that the symmetry of the ground state depends on the positions of the dipoles within the fundamental domain of the lattice, and ranges anywhere from full icosahedral symmetry to completely asymmetric structures. Imposing a symmetry higher than the one of the ground state naturally enforces a state with a higher electrostatic energy, which in most cases remains metastable when the symmetry restriction is lifted. We calculate symmetry phase diagrams with respect to the underlying lattices and perform stability analysis for selected lattices. With this, we show that by choosing a correct lattice, dipole pair interactions can be utilized to induce a desired rotational symmetry of the final
FIG. 1. Construction of a Caspar-Klug lattice where \((n, m)\) determines the triangulation number on the icosahedron, \(T = n^2 + nm + m^2\), and \((u, v)\) determines the placement of the dipole positions (marked in blue) within the fundamental domain (marked by the shaded deltoid in the unit triangle). Reflecting the deltoid across its diagonal produces a mirror image of the same states, so we restrict our analysis to lattice positions in the lower right triangle (dashed half of the deltoid).

structure, suggesting a mechanism for fine-tuning self-assembly of spherical structures.

II. THEORETICAL BACKGROUND

Having \(N\) dipoles \(p_i\) positioned on the sphere at positions \(r_i\), we can state our problem in terms of the minimization of electrostatic potential energy, defined as the sum of dipole-
dipole interaction energies over all pairs of dipoles:

\[ V = \sum_{i>j} V_{ij} = \sum_{i>j} \frac{3(\hat{p}_i \cdot \hat{r}_{ij})(\hat{p}_j \cdot \hat{r}_{ij}) - \hat{p}_i \cdot \hat{p}_j}{||\hat{r}_{ij}||^3}; \]  

\( \hat{r}_{ij} = \hat{r}_i - \hat{r}_j \) are distances between dipoles, and unit vectors are denoted by a hat. We restrict the dipoles to lie tangentially to the sphere, which has previously been shown to be the preferred solution for dipoles on a sphere in absence of an external field (see Ref. [37] for the case without symmetry constraints). We parameterize the dipoles relative to the local coordinate frame in the form \( \hat{p}_i = \hat{e}_x \cos \phi_i + \hat{e}_y \sin \phi_i \), allowing the problem to be restated in the matrix form inspired by Luttinger and Tisza [39]

\[ V = x^t M x, \quad x = \{ \cos \phi_1, \sin \phi_1, \cos \phi_2, \ldots \}. \]  

Here, \( M \) is a constant matrix that depends only on the lattice geometry and the choice of the local coordinate frames at each lattice point.

Dipole positions are fixed to a chosen Caspar-Klug (CK) lattice, which maps a triangular Euclidean tiling onto an icosahedron (see Fig. 1), with position vectors normalized to project them to the unit sphere. The positions are determined by the CK parameters \((n, m)\) and the coordinates of the dipoles within the fundamental domain, parametrized by \((u, v)\), where \( u \) and \( v \) correspond to unit vectors pointing from one vertex of the unit triangle to the other two. The number of lattice positions on a CK lattice, \( N = 60T \), is given by its triangulation number \( T = n^2 + nm + m^2 \). Unless stated differently, we limit our analysis to lattices with \((n, m) = (1, 0)\), which places \( N = 60 \) dipoles onto the sphere.

Before minimization, we apply symmetry restrictions, equating angles that correspond to the equivalent lattice points. The form in Eq. 2 is symmetry-reduced by adding together the corresponding rows and columns of matrix \( M \), resulting in a smaller matrix. The minimization was performed by recursive application of gradient descent \( x \mapsto x - \gamma M x \) followed by renormalization of dipole vectors. The results were verified by comparison with Quasi-Newton method from Wolfram Mathematica [40]. Minimization was performed several hundred times to obtain both the ground state as well as the higher energy states with high certainty.
FIG. 2. Symmetry-restricted lowest energy states for truncated icosahedron and small rhombicosidodecahedron (lattices A and B, respectively). On lattice A, the ground state has tetrahedral symmetry. Ground states with lower symmetries are also present, and all of them, including the general higher energy local minima without symmetries, show closed loops of dipoles arranged head-to-tail. Found local minima with higher energies are shown in gray, and they indicate that the icosahedral state remains metastable as long as the dihedral symmetry persists. The inset shows the symmetry breakings in which the previously lowest energy state becomes unstable and is no longer a minimum. On lattice B, the ground state has full icosahedral symmetry and consists of 5-dipole loops around the symmetry axes. Dipoles are shown in the hemispherical azimuthal equidistant projection, and the symmetry axes are denoted by blue (5-fold), green (3-fold) and red (2-fold) markers.

III. RESULTS AND DISCUSSION

Placing a single dipole in the fundamental domain of a CK lattice with \((n, m) = (1, 0)\) produces a tiling with 60 dipoles, 5 around each of the 12 icosahedron vertices. We can consider any combination of the dipole coordinates \((u, v)\) that falls into the fundamental domain, but three of them—which we will denote as lattices A, B, and C—are special, as they lead to polyhedra with equal distances between the dipoles (Archimedean polyhedra). Lattice A with \((u, v) = (1/3, 0)\) corresponds to a truncated icosahedron (a football), a spherical analog of the hexagonal tiling. Lattice B, \(u = v = (3 - \sqrt{3})/6,\) corresponds to
a small rhombicosidodecahedron, a spherical analog of the rhombitrihexagonal tiling, and lattice C, \((u, v) = (2/7, 1/7)\), corresponds to the snub dodecahedron, analogous to snub hexagonal tiling, and is also observed in viral capsids [18]. Lattice C has a mirror image with \((u, v) = (1/7, 2/7)\).

The structure and the behaviour of the assemblies do not depend only on the ground state; metastable states are often important, for example, if they are kinetically more accessible or if additional interactions or external stimuli can trigger symmetry-breaking transitions between local energy minima. Figure 2 shows the energy spectrum of dipoles on lattice A, together with some of the dipole orientations, shown on a single hemisphere unless the distinction between the hemispheres is relevant to the discussion. The icosahedral \(I\) ground state at \(V_A^I = -1917.13\) has a straightforward structure: it consists of closed loops of 5 tail-chasing dipoles around each icosahedron vertex. The lowest energy state \(V_A^T = -1946.67\) possesses tetrahedral \(T\) symmetry in which pairs of adjacent dipole loops merge into larger peanut-shaped loops. Two other symmetries have a unique lowest energy state: in \(D_3\) symmetry, a state at \(V_{D3}^A = -1927.02\) is based on a 6-dipole central loop and antiparallel neighboring dipole orientations, and in \(C_5\) symmetry, the state with \(V_{C5}^A = -1930.61\) takes a form of antiparallel concentric loops with additional kinks on the opposite hemisphere. Importantly, none of these structures resemble the macrovortex state ubiquitously observed in dipoles arranged on Thomson lattices [37]. There are also many local minima with higher electrostatic energies for each symmetry restriction. A generic ground state without symmetry consists of loops of dipoles meandering across the surface, as shown in one example in Fig. 2.

The icosahedral structure remains metastable as long as the 2-fold axis orthogonal to the main symmetry axis is present in the lower symmetry, such as in the tetrahedral and dihedral symmetries; otherwise it cascades into a lower energy state. In fact, most symmetry-restricted solutions remain local minima when symmetry is broken, except in a few selected symmetry breakings: aforementioned transitions from \(I\) to a group without dihedral symmetry axis, and from \(C_5\) or \(D_5\) if the 5-fold symmetry axis is removed. Symmetry breakings that destabilize the local minimum are shown in the inset of Fig. 2.

On lattice \(B\), the icosahedrally symmetric state is a global energy minimum, so any symmetry breaking has no effect. The ground state consists again of 5-dipole loops around the icosahedron vertices (see Fig. 2). Lattice \(C\) tells a different story (Fig. 3): The ground
FIG. 3. Symmetry-restricted lowest energy states for snub dodecahedron (lattice C). The ground state has a $C_5$ symmetry. Dihedral symmetry forces a reversal of dipole circulation across the equator, while uniaxial rotational symmetry allows macrovortex states with much lower energies (best seen from the side view of $C_5$ and $C_3$ structures). The insets show that the lowest energy states of $T$ and $D_5$ structures are unstable with respect to certain symmetry breakings, while in the rest of the cases the lowest energy states remain local energy minima. The visualization follows the style from Fig. 2.

state in this case has a $C_5$ symmetry, and has a macrovortex structure across the entire hemisphere, similar to the ground states of dipoles on Thomson lattices (cf. Ref. [37]). This is expected, as a large part of the snub lattice consists of adjacent triangles, similar to those on closely packed spherical lattices. The structure with $C_3$ symmetry is similar, but has more distorted dipole loops, and $C_2$ structure is also close to a macrovortex. The corresponding dihedral structures $D_5$, $D_3$, and $D_2$ have similar circumpolar structures, but the dihedral axes enforce antiparallel cycles on opposite hemispheres, leading to significantly higher energies. The only structures that decay upon symmetry breaking are the $T$ and $D_5$ structures, as shown in the inset of Fig. 3.
The differences between configurations with different symmetries manifest themselves in their vector spherical harmonic expansion \([41, 42]\). As the dipoles are restricted to lie tangent to the sphere, we can expand their configurations on any lattice over the orthonormal set of tangent basis vectors consisting of gradient (electric-type) \( \nu_{\text{g}}^{\ell m} = \sqrt{\ell(\ell + 1)} \hat{r} \nabla Y_{\ell m} \) and curl (magnetic-type) \( \nu_{\text{c}}^{\ell m} = \sqrt{\ell(\ell + 1)} \hat{\epsilon} \times \nabla Y_{\ell m} \) vector spherical harmonics (for details, see Refs. \([41]\) and \([42]\)). This allows us to write the vector analog of the spherical structure factor in the form:

\[
S_{\ell}^{\text{g,c}} = \frac{1}{N} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell + 1} \left| \sum_{i=1}^{N} \mathbf{p}_i \cdot \nu_{\ell m}^{\text{g,c}} \right|^2.
\]  

(3)

This definition is analogous to the definition of the spherical structure factor for the standard (scalar) multipole expansion, and is trivially related to multipole magnitudes \([43, 44]\).

Symmetries of different dipole configurations result in the restriction of the allowed spherical wave number \( \ell \): for the icosahedral symmetry, only the values of \( \ell = 6i + 10j (+15) \) are permitted \([27]\); for tetrahedral symmetry, \( \ell = 4i + 6j (+3) \) (only excluding \( \ell = 1, 2, \) and 5); \( D_5 \) symmetry forbids \( \ell = 1 \) and \( \ell = 3 \) and \( D_{2,3} \) forbid \( \ell = 1 \). Figure 4 shows the spectra of the vector spherical structure factor for dipoles on lattice \( C \) with four different symmetries, also shown in Fig. 3. We can see that they indeed observe the \( \ell \) selection rules pertaining to each individual symmetry. Large components of the curl harmonics \( S_{\ell}^{\text{c}} \) describe vortices (closed dipole loops) of different sizes, with \( \ell = 1 \) describing a macrovortex around a single axis, such as those seen in the solutions of \( C_3 \) and \( C_5 \) symmetries (the latter also being the ground state on lattice \( C \)). Gradient terms \( S_{\ell}^{\text{g}} \) describe alignment that resembles potential flow, and are less prominent because closed dipole loops are favored. This analysis also shows that an approach using vector spherical harmonics is suitable for the analysis of empirical and simulation data.

Despite lattices A, B, and C being Archimedean polyhedra and thus all having constant nearest neighbour distances, their ground state symmetries and transitions between them are very different. The question arises of how different lattices are related and how the ground states and transitions look for general \((u, v)\) coordinates. We performed a ground state calculation for 3104 different dipole positions \((u, v)\) in the fundamental domain, and summarized the results in the symmetry phase diagram in Fig. 5. We observe a very complex phase diagram that is based on the competition of different phenomena. In the left corner of the fundamental domain, the dominant interaction is among 5 dipoles around the
FIG. 4. Curl and gradient vector spherical harmonic spectra $S_c^\ell$ and $S_g^\ell$ for dipoles on lattice $C$ and with $I$, $T$, $D_5$, and $C_5$ symmetries, shown with respect to the spherical wave vector $\ell$ (orbital angular momentum number). Top histograms (red) show the contributions of curl vector harmonics, and the bottom histograms (blue) show the contribution of gradient vector harmonics. Depending on the symmetry of the structure, certain $\ell$ are forbidden and the corresponding coefficients are zero. The right side of the Figure shows the dipole arrangements in 3D, where dipoles equivalent under symmetry operations have the same color. Vertical axis in these plots is one of the symmetry axes of the system (3-fold for the tetrahedral structure and 5-fold for the rest). The ground state with $C_5$ symmetry is a macrovortex state, which is reflected in a large nonzero curl component $S_c^\ell$ at $\ell = 1$. 

\[10\]
FIG. 5. Phase diagram of ground state symmetries with respect to the position \((u, v)\) of the dipole in the fundamental domain. Top views of selected structures are shown in insets. The structures in the left part of the diagram are very similar to the icosahedral one, with barely noticeable symmetry breaking. The bottom right side of the diagram features parallel coupling of neighboring dipoles. Note the asymmetric states at the right edge, where symmetry is broken by buckling and reversal of direction of some of the dipole pairs. Isolated points of different symmetries present throughout the diagram can be attributed to numerical artefacts. Lattices \(A\), \(B\), and \(C\), corresponding to the Archimedean solids shown in previous figures, are marked with crosses.

Icosahedron vertices. These ground states consist of dipole loops which resemble those seen in \(I\) structures, but their senses of rotation may alternate in different ways, giving rise not only to structures with \(I\) symmetry (black markers in Fig. 5), but also to \(C_2\) and \(C_5\) symmetries (structures shown as insets), and even to \(D_3\) symmetry in a very small portion of the phase diagram. In the top right corner of the fundamental domain, the proximity of 3 dipoles dominates the interactions. This stabilizes \(T\) symmetry, and to a lesser extent, lower 3-fold symmetries. The lower right portion of the phase diagram puts dipoles into close pairs centered around the edges of the icosahedra. These pairs tend to align and act as a single dipole, which, due to the polar nature of the dipoles, breaks all the 2-fold sym-
metry axes a structure could have, so the main symmetries observed are \( C_3 \) and \( C_5 \). The middle of the phase diagram corresponds to states with balanced interactions between the closest neighbours, similar to lattice \( C \) that is representative of this region. These lattices are locally triangular and feature macrovortex-like states.

Between these regimes, we observe a complex interplay of symmetries caused by competition between interactions that favour different structures. A large region of the phase diagram has no symmetries at all, and a snapshot corresponding to its right edge shows why: the resulting structure is similar to the \( C_5 \) structure with aligned dipoles, but some of the pairs are reversed and the pairs of dipoles are just far enough apart to allow “buckling” instead of acting as a single dipole. Other disordered structures are observed at the transition from tetrahedral to 5-fold parts of the phase diagram. The energy landscapes of the observed configurations have many local minima, and even after many repetitions, the lowest one is not always found. In the parts of the phase diagram where energies of states with different symmetries are close together, this leads to isolated points with incorrectly determined ground state symmetry.

Electrostatic energy of these systems is dominated by the closest neighbors due to the divergent nature of the dipole-dipole interaction. In Fig. 6, we show the total energy of the ground state configuration with respect to the lattice parameters \((u, v)\), as well as the energy difference between the highest symmetry \((I)\) state and the ground state. We see that \( C_5 \) symmetry offers an incremental improvement over the \( I \) structures on an angle bisector extending from the left corner of the fundamental domain, and the same holds true for the \( T \) symmetry extending from the upper corner of the domain, related to the \( C_3 \) symmetry axis. Conversely, the part of the phase diagram corresponding to dipole pairing offers significant improvement over the \( I \) structure due to the very strong binding of an aligned dipole pair. The electrostatic energy is lowest by absolute value, \( |V|_{\text{min}} = 1425.7 \), when the dipoles are farthest apart, which is very close to the lattice \( C \). However, this is still higher than closely packed spherical lattices, such as the Thomson lattice, whose energy is \( |V|_{\text{Th}} = 1378.0 \) for the same number of particles \( N = 60 \).

The results presented thus far were obtained on a CK lattice with \( T = 1 \), consisting of \( N = 60 \) dipoles. In Fig. 7 we present a symmetry phase diagram equivalent to the one in Fig. 5 for a larger lattice with CK parameters \( n = m = 1 \). This lattice has a triangulation number \( T = 3 \) and thus contains \( N = 180 \) dipoles. It features local hexagonal regions in
FIG. 6.  Electrostatic interaction energy in the ground state $V$ (lower right triangle) and difference between energies in the icosahedral and ground states $\Delta V$ (upper left triangle). Note that the largest differences occur in the corner corresponding to the dipole pairing $(u, v) = (1/2, 0)$, while the other two corners are compatible with $I$ symmetry, and the $C_5$ and $T$ regions only extend out as minor improvements in energy. In the energy plot, the position and coordinates of the absolute electrostatic energy maximum (minimum by absolute value, $|V| = 1425.7$) are marked; it is located very close to the lattice $C$ coordinates $(2/7, 1/7)$. For comparison, 60 dipoles placed on the lattice derived from the Thomson problem have the energy $|V| = 1378.0$.

In addition to 12 pentagons of the icosahedron vertices. The main observation on the $T = 3$ lattice is that, in general, states with higher symmetries are preferred—icosahedral symmetry dominates almost the entire left portion of the phase diagram; similarly, more tetrahedral structures are observed in its upper right part. We observe no asymmetric ground states,
and the region of $C_2$ symmetry is shrunk to a small patch in the middle of the diagram, with structures that can be described as longer strings of head-to-tail arranged dipoles. It is noteworthy that the “fundamental domain” of CK lattices with larger triangulation numbers $T > 1$ is no longer the fundamental domain of the icosahedral symmetry group. Because of the 5-fold lattice defects, the lattice sites are similar, but not equivalent. Not only do the dipoles have slightly different environments, but, more importantly, the dipoles around a hexagonal face can arrange in an alternating fashion while the pentagonal dipoles do not have that option. The “almost symmetry” between lattice sites is most apparent in the left and upper corner of the diagram, where trimers and pentamers behave almost as independent entities, as seen in Fig. 7.

We can also expand the dipole configurations on a $T = 3$ lattice in terms of vector spherical harmonics $\nu^k_{lm}$ and $\nu^c_{lm}$, where we again observe that different symmetries give rise to spectra of selected wave vectors $\ell$ only. What is more, since 180 dipoles are positioned on a $T = 3$ lattice, the spectra do not always peak at the lowest allowed $\ell$ (as was the case for $T = 1$ lattice containing 60 dipoles, shown in Fig. 4). One can, for instance, observe spectra of icosahedrally symmetric lattices with peaks either at $\ell = 6$, similar to a $T = 1$ lattice, or at $\ell = 10$—in this way, vector spherical harmonic expansion can be used also to distinguish between different types of dipole order which otherwise possesses the same symmetry. For general $T$, the dominant $\ell$ scales inversely with the distance between nearest neighbors and is proportional to $\sqrt{T}$. For the same reason, for $(u, v)$ closer to the edge of the fundamental domain, higher spatial frequencies (higher $\ell$) will be present compared to the Archimedean lattices A, B, and C. High curl coefficient at $\ell = 1$, equivalent to the angular velocity parameter introduced in Ref. [37], is expected to signify the macrovortex state at any triangulation number.

The macrovortex state—the main type of ordering in Euclidean space and on Thomson problem-derived lattices on the sphere—is in general not energetically preferred on CK lattices, as they have a honeycomb-like structure instead of a closely-packed triangular one. The fundamental difference between CK lattices (honeycomb-like) and closely-packed lattices (triangular-like) are the 6- and 5-fold lattice vacancies that accommodate microvortex states—local dipole loops with no net dipole moment. With growing lattice size, ever larger parts of the lattice resemble the Euclidean honeycomb lattice and thus the effect of 5-fold lattice defects and long-range interactions through the bulk of the sphere become less and
FIG. 7. Phase diagram of ground state symmetries for a $(1,1)$, $T = 3$ CK lattice with $N = 180$ dipoles on the sphere. The rough division of the phase diagram is similar to the $(1,0)$ lattice (Fig. 5), but with a much larger region of stability of icosahedral structures, and without any asymmetric ground states. Note that the lowest symmetry, $C_2$, is also restricted to only a very small portion of the phase diagram. More numerical artifacts are present due to a larger number of local minima that make identification of the true ground state difficult.

less pronounced. This in turn leads to degeneracy, as loops with zero lowest order multipole moments interact very weakly across large distances over the sphere. With a further increase in triangulation numbers, we thus expect the limiting regimes to persist: 3-dipole microvortices (supporting $I$ or $T$ symmetries) in the top right part of the phase diagram, 5-fold microvortices in the left part of the phase diagram, dipole pairings with $C_{3,5}$ symmetries, and most likely, macrovortex-like states in the middle of the fundamental domain, where triangular patches can be found on the lattice.

IV. CONCLUSIONS

We have shown that dipole-dipole interactions produce very diverse results when the dipoles are positioned on the surface of a sphere. In contrast to the Euclidean case, where lattices possess only translational symmetries, spherical lattices reflect the rich structure of the point symmetry groups in three dimensions. By starting with the highest symmetry—
the icosahedrally symmetric CK positional order—we have demonstrated that dipole pair interactions can conspire to stabilize any point symmetry, although dihedral symmetry is less favored. Fixed-position dipole order alone can therefore be used to control the symmetry of the resulting structures, and if the interaction can be varied—for example with screening or by shifting the position of the dipoles—symmetry-changing transitions are possible. The symmetry phase diagrams also show how controlling the positions of the dipoles within the fundamental unit of the lattice can regulate the resulting symmetry of the structure and its stability. A drawback of this mechanism is the multitude of metastable states, which decreases the likelihood of finding the true ground state, although in potential experimental realizations, favored kinetic pathways could improve their reproducibility.

The general properties observed in our simplified model are expected to hold even for more complicated and modified cases—for positional lattices with different symmetries, such as octahedral or tetrahedral, and for dipole positions displaced radially from a perfect sphere, which is expected to be the case in biological systems where the structures themselves are polyhedral. Here, vector spherical harmonics present a natural way of analyzing such configurations and determining their symmetries. In a manner similar to the one presented in this work it is also worth exploring other pair interactions, such as the quadrupole-quadrupole interaction, which pertains to physical building blocks with head-tail symmetry and thus without polar order. Finally, the question of the ground state symmetry of ideal multipoles is also interesting from a purely mathematical perspective, just like the Thomson problem, which still inspires new discoveries even a century after its conception.

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[1] C. P. Royall, W. C. Poon, and E. R. Weeks, Soft Matter 9, 17 (2013).
[2] E. S. Popko, Divided spheres: Geodesics and the orderly subdivision of the sphere (CRC press, 2012).
[3] S. A. Kim, K.-J. Jeong, A. Yethiraj, and M. K. Mahanthappa, Proc. Natl. Acad. Sci. USA **114**, 4072 (2017).

[4] L. Athanasopoulou and P. Ziherl, Soft Matter **13**, 1463 (2017).

[5] T. Baker, N. Olson, and S. Fuller, Microbiol. Mol. Biol. Rev. **63**, 862 (1999).

[6] R. Zandi, B. Dragnea, A. Travesset, and R. Podgornik, Phys. Rep. (2020).

[7] C. Chen, M.-C. Daniel, Z. T. Quinkert, M. De, B. Stein, V. D. Bowman, P. R. Chipman, V. M. Rotello, C. C. Kao, and B. Dragnea, Nano Lett. **6**, 611 (2006).

[8] J. K. Pokorski and N. F. Steinmetz, Mol. Pharm. **8**, 29 (2011).

[9] M. Truffi, L. Fiandra, L. Sorrentino, M. Monieri, F. Corsi, and S. Mazzucchelli, Pharmacol. Res. **107**, 57 (2016).

[10] R. Savić, L. Luo, A. Eisenberg, and D. Maysinger, Science **300**, 615 (2003).

[11] S. B. Timmermans and J. C. van Hest, Curr. Op. Colloid Interface Sci. **35**, 26 (2018).

[12] R. Zandi, D. Reguera, R. F. Bruinsma, W. M. Gelbart, and J. Rudnick, Proc. Natl. Acad. Sci. USA **101**, 15556 (2004).

[13] A. ለበሔ, A. Lošdorfer Božić, and R. Podgornik, Phys. Chem. Chem. Phys. **14**, 3746 (2012).

[14] R. F. Bruinsma and W. S. Klug, Annu. Rev. Condens. Matter Phys. **6**, 245 (2015).

[15] S. B. Rochal, O. V. Konevtsova, and V. L. Lorman, Nanoscale **9**, 12449 (2017).

[16] M. Carrillo-Tripp, C. M. Shepherd, I. A. Borelli, S. Venkataraman, G. Lander, P. Natarajan, J. E. Johnson, C. L. Brooks III, and V. S. Reddy, Nucleic Acids Res. **37**, D436 (2009).

[17] V. Lorman and S. Rochal, Phys. Rev. Lett. **98**, 185502 (2007).

[18] S. B. Rochal, O. V. Konevtsova, A. E. Myasnikova, and V. L. Lorman, Nanoscale **8**, 16976 (2016).

[19] R. Twarock, J. Theor. Biol. **226**, 477 (2004).

[20] O. Konevtsova, V. Lorman, and S. Rochal, Phys. Solid State **57**, 810 (2015).

[21] V. L. Lorman and S. B. Rochal, Phys. Rev. B **77**, 1 (2008).

[22] S. Dharmavaram, F. Xie, W. Klug, J. Rudnick, and R. Bruinsma, Phys. Rev. E **95**, 862 (2017).

[23] A. Scala, T. Voigtmann, and C. De Michele, J. Chem. Phys. **126**, 134109 (2007).

[24] A. F. Tillack, L. E. Johnson, B. E. Eichinger, and B. H. Robinson, J. Chem. Theory Comput. **12**, 4362 (2016).

[25] R. A. Bilbeisi, J.-C. Olsen, L. J. Charbonnière, and A. Trabolsi, Inorganica Chim. Acta **417**,
[26] D. A. Walker, C. E. Wilmer, B. Kowalczyk, K. J. Bishop, and B. A. Grzybowski, Nano Lett. 10, 2275 (2010).

[27] A. Lošdorfer Božič and R. Podgornik, J. Chem. Phys. 138, 074902 (2013).

[28] A. Lošdorfer Božič and R. Podgornik, Biophys. J. 113, 1454 (2017).

[29] A. Baskin, W.-Y. Lo, and P. Král, ACS Nano 6, 6083 (2012).

[30] M. A. Gharbi, M. Cavallaro Jr, G. Wu, D. A. Beller, R. D. Kamien, S. Yang, and K. J. Stebe, Liq. Cryst. 40, 1619 (2013).

[31] D. Morphew and D. Chakrabarti, Curr. Op. Colloid Interface Sci. 30, 70 (2017).

[32] D. Morphew and D. Chakrabarti, Nanoscale 10, 13875 (2018).

[33] A. Mauri and M. I. Katsnelson, Ann. Phys. 412, 168016 (2020).

[34] P. Belobrov, V. Voevodin, and V. Ignatchenko, Zh. Eksp. Teor. Fiz. 88, 889 (1985).

[35] J. Brankov and D. Danchev, Physica A 144, 128 (1987).

[36] G. O. Zimmerman, A. K. Ibrahim, and F. Y. Wu, Phys. Rev. B 37, 2059 (1988).

[37] A. Gnidovec and S. Čopar, “Orientational ordering of point dipoles on a sphere,” (2019), arXiv:1912.04327 [cond-mat.soft].

[38] D. J. Wales and S. Ulker, Phys. Rev. B 74, 212101 (2006).

[39] J. M. Luttinger and L. Tisza, Phys. Rev. 70, 954 (1946).

[40] Wolfram Research, Inc., “Mathematica, Version 12.0,” (2019).

[41] K. S. Thorne, Rev. Mod. Phys. 52, 299 (1980).

[42] B. Carrascal, G. Estevez, P. Lee, and V. Lorenzo, Eur. J. Phys. 12, 184 (1991).

[43] A. Lošdorfer Božič and S. Čopar, Phys. Rev. E 99, 032601 (2019).

[44] S. Franzini, L. Reatto, and D. Pini, Soft Matter 14, 8724 (2018).