Riemannian Surfaces Encode the Structure of Filament Bundles

Non-Euclidean geometry of twisted filament bundle packing

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Recommended with a commentary by Mark Bowick, Soft Matter Program, Syracuse University

The universe on the largest scales appear to be spatially flat to within 0.5% (see `http://map.gsfc.nasa.gov/universe/uni_shape.html`). The angles of geodesic triangles therefore add to 180° and geodesic circles of radius r have circumference $2\pi r$. Soft matter, on the other hand, is rife with systems that are spatially curved and topologically rich [1]. Examples include ordered states of particles that self-assemble at the interface between two distinct fluids (colloid-stabilized emulsions), multi-electron helium bubbles, viral capsids [2] and block copolymer vesicles. Crystalline colloidal arrays are particularly revealing because $3d$ images can be obtained by confocal microscopy. Many shapes are possible for colloidal crystals. Assembly on spherical droplets yields crystals on the the surface of as ball - the 2-sphere S^2 whilst assembly on capillary bridges yields crystals on the Delaunay constant mean curvature surfaces of revolution: the sphere, the cylinder, the catenoid, the nodoid and the unduloid [3]. Crystalline order on the 2-sphere has proven very rich [1]. The topology of the 2-sphere makes it impossible for the crystalline ground state to be a perfect triangular lattice: the sum of the departure of the coordination numbers of each particle from the triangular lattice value of 6 must be 6 times the Euler characteristic $\chi = 2$. Particles with coordination number c differing from 6, in a crystalline background of 6-fold coordinated particles, are topological defects called crystalline disclinations: they have strength $1/(6-c)$ or disclination charge $6-c$. The topological constraint noted above has many solutions: one can have any number of 6-fold coordinated particles together with a collection of defects such as 3 particles of coordination number 2 (glue two spherical triangles together to form a sphere), 4 particles of coordination number 3 (the tetrahedron or variants), 6 particles of coordination number 4 (take a close look at the spherical triangulation provided by the dark grid lines on a basketball) or 12 particles of coordination number 5. The latter solution is the most common as it utilizes the minimum defect charge (+1). Its dual Voronoi map contains 12 pentagons, as found on a standard soccer ball and in carbon fullerenes/bucky balls [4]. On a surface with the topology of a disk (one hole cut out of the 2-sphere) the Euler characteristic changes to 1 and the excess coordination number changes to 6. Crystalline arrays of air bubbles on the parabolical surface of a rotating soap film are one experimental realization. The simplest solution to the topological constraint in this case is 6 particles of coordination number 5 along with any number of 6s.

Bruss and Grason analyze the structure of a very different looking 3d system:

a bundle of filaments all with the same helical twist, a crucial structural motif in both macroscopic materials (cables) and synthetic and biological nanomaterials (fibrous proteins). What does this have to with order on curved surfaces? Imagine reconstructing the bundle as a collection of $2d$ slices as in a confocal scan. One could take horizontal slices but the filaments are better viewed along slices that minimize their separation. Since the filaments are helical and therefore tilted there is an optimal tilt angle for the slices that minimizes the spacing between neighboring filaments. The authors derive the tilt angle, the height difference between nearest neighbor filaments on an optimal slice and an elegant formula for the minimum spacing in terms of differences in the respective radial and azimuthal coordinates. This formula makes it clear that there is a natural curved surface associated with the filament packing problem. The original problem is thus mathematically mapped to a different packing problem on this associated curved surface. What surface arises? It has the shape of a silo or bullet - essentially a spherical cap that smoothly connects to a cylinder with radius that asymptotes to a constant (given by the inverse pitch of the helical twist of the individual fibers). The filament bundle problem turns out to be isomorphic to the problem of the densest packing of discs on the equivalent silo. This mapping is useful because one can then apply the machinery and intuition of optimal configurations on curved surfaces. In particular the spherical cap of the silo corresponds to the geometric structure of filaments near the core of the bundle. This connects to the crystalline structure of particles on disk-like topologies discussed above. Near the core of the bundle we expect filaments surrounded by fewer than 6 other filaments and we expect the total departure of the coordination number from 6 to also be 6.

Bruss and Grason check this with a deterministic packing simulation. They find bundles with an inner core of 2 4-fold coordinated filaments and 2 five-folded coordinated filaments, 1 4-fold coordinated filament and 5 6-fold coordinated filaments and a variety of structures with 6 five-folded coordinated filaments, differing in their exact configuration and symmetry. Far from the core all filaments are 6-fold coordinated and approximate a regular triangular lattice.

If one could design a capillary bridge with the shape of the bundle-equivalent silo and then adsorb colloidal particles on this surface which crystallize then one could compare the bundle geometry to the configuration of colloidal particles and the defect structure of the filament packing to the Delaunay triangulation of the colloidal crystal.

We see that two-dimensional geometry and topology continues to provide powerful tools in analyzing the physical structure of soft matter assemblies as beautifully illustrated in this paper. The cosmologists must be jealous. Soft matter assemblies are hardly ever flat and spatial curvature frequently leads to novel order.

References

[1] M. J. Bowick and L. Giomi, Adv. Phys. **58**, 449-563 (2009).

[2] D. L. D. Caspar and A. Klug, *Physical Principles in the Construction of Regular Viruses*, Cold Spring Harbor Symp. Quant. Biol. **27**, 1-24 (1962).

[3] W. T. M. Irvine, P. M. Chaikin and V. Vitelli, Nature **468**, 947 (2010).

[4] R. Smalley, *Great Balls of Carbon: The Story of Buckminsterfullerene*, The Sciences (March/April 1991).